The 19th International Conference on Radiation Effects in Insulators

2nd – 7th July 2017, Versailles, France

REI-19

VERSAILLES 2017

Book of abstracts

ORGANIZERS

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REI in 2017 is the 19th international conference dedicated to research relating to radiation effects in insulators and non-metallic materials. In 2017, discover REI in Versailles, a city which was shaped by French History and in particular under the period of King Louis XIV, at only 20 km from Paris.

Since its first edition held in 1981 in Arco, Italy, REI has been the international forum held every two years to present and discuss the latest achievements in the field of insulating materials modification through different kinds of radiation source (ions, electrons, neutrons...). The REI conference is one of the most prominent and long running conference series in the field of radiation effects in materials.

REI-19 is organized by several laboratories all members of the new Université Paris-Saclay:

(i) the CSNSM, a joint research unit of Université Paris-Sud and CNRS (IN2P3),
(ii) the SRMP(DEN/DMN), SCCME and INSTN at CEA Saclay,
(iii) and the LSI lab, a joint research unit of CEA(DRF/IRAMIS)-CNRS-Polytechnic School.

We greatly acknowledge the support of our sponsors. REI-19 is organized in cooperation with the International Atomic Energy Agency.

Welcome in Versailles!

Gaël Sattonnay, Chair, on behalf of the organizing committee.

Local committee:

Chair: Gaël Sattonnay (CSNSM, Univ Paris Sud)

Co-chairs:

- Aurélie Gentils (CSNSM, CNRS)
- Lionel Thomé (CSNSM, CNRS)
- Jean-Paul Crocombette (SRMP, CEA)
- Nadège Ollier (LSI, CEA, Ecole Polytechnique)

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- Emilie Bonnardel (CSNSM, CNRS), *REI-19 financial manager*
- Cyril Bachelet (CSNSM, CNRS)
- Cédric Baumier (CSNSM, CNRS)
- Aurélien Debelle (CSNSM, Univ Paris-Sud)
- Frédérico Garrido (CSNSM, Univ Paris-Sud)
- Stéphanie Jublot-Leclerc (CSNSM, CNRS)
- Olivier Plantevin (CSNSM, Univ Paris-Sud)
- Alain Chartier (SCCME, CEA)
- Gaëlle Guttierez (SRMP, CEA)
- Stéphanie Pellegrino (INSTN, SRMP, CEA)
- Pierre-Eugène Coulon (LSI, CEA, Ecole Polytechnique)
- Giancarlo Rizza (LSI, CEA, Ecole Polytechnique)

Students:

- Anaïs Alleysson, CSNSM, 1st year internship
- Jean-Noël Brottier, CSNSM, Master 1 internship
- Suheyla Bilgen, LAL-CSNSM, PhD student
- Olga Emelianova, CSNSM, PhD student
- Driffa Guerfa, CSNSM, Master 1 internship
- Harsh Gupta, IIT-CSNSM, PhD student
- Yara Haddad, CSNSM, PhD student
- Xin Jin, CSNSM, Master 2 internship
- Mohamed Mahfoudhi, LSI, PhD student
- Samrit Mainali, CSNSM, Master 2 internship
- Martin Owusu-Mensah, CSNSM, PhD student

Program committee:

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- A. Gentils (CSNSM, CNRS, France)
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- O. Plantevin (CSNSM, Univ Paris-Sud, France)
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- P.-E. Coulon (LSI, CEA, Ecole Polytechnique, France)
- G. Rizza (LSI, CEA, Ecole Polytechnique, France)
- I. Swainson (IAEA)

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Financial support (1/3)

P2IO
http://www.labex-p2io.fr

P2IO is one of the 100 laboratories of excellence (Labex) approved by the French Government in March 2011 within the framework of future investments funded by the large governmental loan, officially called "Grand Emprunt" of 2010. P2IO defines itself as the network of all laboratories in Paris region involved in physics of the infinitely small to the infinitely large and study of conditions for the appearance of life. P2IO acts like as such networks, in a direct way, by funding a number of actions, and more indirectly, by promoting better cooperation between its members and providing a contact point for external partnerships, including those from the Saclay's Plateau.

Faculté des Sciences, Université Paris-Sud
http://www.sciences.u-psud.fr/en/the_faculty.html

The Faculty of Sciences of the Université Paris-Sud, located on the Orsay campus, welcomes over 13,000 students and 2,100 PhD students, and has a staff of 1,700 professors and researchers and 1,800 administrative and technical workers. Its numerous academic buildings and 41 research laboratories are located on an exceptional 200-acre woodland site containing many rare species of flora. Education and research programs cover the fields of biology, chemistry, electronics, computer sciences, mechanics, mathematics, physics, earth sciences and physical education.

MINOS
http://www.materials.cea.fr/en/Phocea/Vie_des_labos/Ast/ast_groupe.php?id_groupe=109

As the French leader for research on materials for nuclear applications, CEA launched the MINOS project (Materials Innovation for Nuclear Optimized Systems) in 2011. This centre of excellence for nuclear materials was created by the Nuclear Energy Division (DEN) to promote, strengthen, and optimize research programs on materials used for nuclear power reactors and activities for the back end of the fuel cycle. It brings together all of the skills and means of DEN division dedicated to nuclear materials.

Financial support (2/3)

DIM OxyMORE
http://www.dim-oxymore.fr

Le "Réseau d'excellence francilien sur les Matériaux oxydes - OxyMORE " a été créé le 18 Novembre 2011 dans le cadre des 16 Domaines d'Intérêt Majeur (DIM) décidés par le Conseil Régional d'Ile-de-France. Il vise à permettre des partenariats multidisciplinaires originaux entre des équipes de recherche à forte visibilité nationale et internationale en Physique et Chimie du solide, sciences de l'Univers et de l'Environnement, sciences de l'Ingénieur, sciences du Patrimoine.

Polytech Paris-Sud
http://www.u-psud.fr/en/university/schools/school-of-engineering.html

Polytech Paris-Sud is a selective School of Engineering. Over 650 students enrol at the Paris-Sud University School of Engineering every year. One of the distinctive characteristics of Polytech engineers is that throughout their training they are in close contact with the world of research, thus gaining cutting-edge knowledge in high technology fields (electronics and embedded systems, electrical engineering, computer engineering, materials engineering and photonics), together with the communication, language, and management skills every engineer needs. In addition to the conventional curriculum, in which students start their studies after completing an initial two-year course, Paris-Sud Polytech also offers sandwich degrees. Students holding a Master of Engineering degree can either then choose to pursue a PhD, or enter their career field

NEC
http://www.pelletron.com

NEC employees pride themselves on making a wide variety of Pelletron accelerator systems to meet customers' needs. To date we have manufactured over 230 Pelletron systems with sales in over 50 countries throughout the world. These systems produce ion beams of essentially all stable nuclei with energies ranging from a few keV to hundreds of MeV. The Pelletron is the world's only commercially available accelerator that incorporates an all metal and ceramic acceleration tube with no organic material in the vacuum volume.

Financial support (3/3)

Labex PALM
https://www.labex-palm.fr

PALM (Physics: Atoms, Light, Matter) is a laboratory of excellence of the Paris-Saclay campus scientific community. It was created by the Fondation for Scientific Cooperation of the Paris-Saclay campus.
PALM is supported by the great French research and University training institutions (CNRS, Université Paris-Sud, Ecole Polytechnique, CEA, Institut d'Optique Graduate School, Onera, ENSTA, ENS Cachan, Ecole Centrale and Synchrotron Soleil). PALM gathers more than 700 permanent physicists (researchers, university lecturers and researchers, engineers...) working on a broad set of subjects in fundamental and applied physics.

Ecole Polytechnique
https://www.polytechnique.edu

École Polytechnique is a leading French institute which combines top-level research, academics, and innovation at the cutting-edge of science and technology. Its curriculum promotes a culture of excellence with a strong emphasis on science, anchored in humanist traditions. The school produces socially responsible professionals who excel in leading complex and innovative projects which address current and future challenges facing our society.
The École Polytechnique Research Center combines the most fundamental aspects of research with the pursuit of progress in the most applied main fields in order to meet future scientific, technological and societal challenges.

Venue

In 2017, discover REI conference in Versailles, a city which was shaped by French History and in particular under the period of King Louis XIV, at only 20 km from Paris.

Versailles is worldly famous for the "Château de Versailles" which is the symbol of French power and force during the 17th and 18th centuries. Gardens "à la française", "Galerie des Glaces" show majesty and luxury which were part of the empire at that time. Touristic information can be found on the Versailles tourist office web site.

The conference sessions will be held in the amphitheater Bertin and Fermat building of Université Versailles Saint-Quentin (USVQ), which is a member of Université Paris-Saclay, located at a walking distance of the Château de Versailles (bus are also available in the city). The address of the campus is 45 avenue des Etats Unis, 78000 Versailles.

Versailles is connected to Paris centre by several train lines (see Access information and maps). Touristic information in Paris can be found on the Paris tourist office web site.

Excursion

The excursion on Wednesday afternoon at Versailles will include the four following tours (up to 6:00 pm):

- **Guided tour of the Salle du Jeu de Paume (45 min):** This gymnasium built for the court of Louis XIV is famous for the oath pronounced by a group of deputies of the "Etats Généraux", June 20, 1789. This was the founding act of democracy. The hall now houses a museum on the characters and revolutionary events that took place in Versailles.
- **Guided tour of the Saint-Louis district (45min):** Built on the site of the former "parc aux cerfs" of Louis XIII, the Saint-Louis district is today one of the historical centers of the city of Versailles. Developed in checkerboard around its magnificent cathedral, it is also remarkable for its "squares", formed of small barracks with mansard roofs, typical in the eighteenth century.
- **Guided tour of the Grand Apartments of the Palace of Versailles (1h15):** Discover the apartments of the King, in which sumptuous gold and marble harmonize. Measuring 73 meters long, 10.5 meters wide and 12.3 meters high, **the Hall of Mirrors** with its 17 windows and 357 mirrors will leave you stunned. It is the absolute symbol of the French monarchy and shows the incredible skill of the craftsmen and painters who made it unique in the world.
- **Guided tour of the French gardens of the Palace of Versailles (1h):** Designed by André Le Nôtre for Louis XIV, the gardens of the Versailles became the model of the regular garden "à la française". Their well-designed layout, characterized by their symmetry and their great perspective, is reinforced by the multitude of sculptures that make it one of the richest and prestigious open-air museums of the world.

Welcome reception & conference dinner

The welcome reception will take place on Sunday evening (5 pm - 9 pm) at the *Potager du Roi*. A banquet is organized in Versailles at the *Hotel de France* venue on Thursday 6th July evening.

Useful information

Wireless Internet will be available at the venue. You will need to login in order to access this service. The access details will be given upon your arrival.

Lunches will be served in the CROUS building close to the venue. Various restaurants for diner are located in Versailles city centre.

Guidelines for presentations

Oral presentations

- Invited talks are 30 minutes, including 6 minutes for discussion. Oral contributions have a duration of 20 minutes, including 4 minutes for discussion. **All speakers are urged to respect these time limits.**
- Speakers should identify themselves to the chairperson of the session before the start of the session.
- A Windows-based computer will be available, , with the following software installed (Powerpoint 2016 MSO 16.0.4266.1001, and Acrobat Reader DC 2017.009.2044). Special requests (e.g. regarding movie clips) should be discussed with the organizers well before the start of the conference. Speakers can also use their own laptop but should check the compatibility with the available beamer well in advance of the session in which they are scheduled. A standard VGA connection to the LCD projector will be available. If needed, speakers are requested to bring adapting connectors (e.g. for Apple laptops).
- Presenters who will make use of the conference computer are requested to upload and check their presentation well before the session starts. Please bring your presentation on a USB memory stick.

Poster presentations

- Poster boards are formatted for posters having a DIN A0 format (1189 mm x 841 mm) in **portrait orientation**. The available poster boards do not allow affixing posters in landscape orientation. Posters are attached to the poster boards using clamps at the top (provided by the conference organizers).
- Poster presenters are asked to mount their posters not later than the morning of their respective poster session and they are requested to take away the poster after the end of the poster session (before Wednesday midday for Tuesday's poster session, and before Friday midday for Thursday's poster session).
- Poster presenters are requested to be available near their posters during the full duration of the poster session.

Proceedings

Along the tradition of the conference, the proceedings of REI 2017 will be published as a Special Issue of the journal *"Nuclear Instruments and Methods B: Beam Interactions with Materials and Atoms"* .
Invited talks as well as oral and poster contributions will be included in the conference proceedings. Before being accepted for publication, all submitted manuscripts will be peer reviewed according to international standards. All fully registered regular participants will receive a complimentary printed copy of the full REI 2017 Proceedings. **Submission deadline is Friday 21st July 2017**.

Guidelines:

- The entire submission process occurs via the Elsevier-NIMB website. Authors should select the section "SI: NIMB_REI 2017" when they reach the "Section" step in the submission process. Note: The special issue site will be open by June 9th.
- Specific guidelines for preparing an REI 2017 paper are summarized in the "REI-2017-AUTHOR'S GUIDE". In particular, this document includes a front page to be (mandatorily) added to your manuscript. Latex users should upload a pdf version of the cover page separately.
- Authors should aim at a paper filling at least three published pages (extended abstracts are not accepted).
- All manuscripts submitted to the REI 2017 proceedings will be subject to the same high standard peer review as regular submissions to NIMB. It should be full and independent papers.
- The published work should be original and not published (or under consideration) anywhere else.
- The manuscript must be approved by all coauthors, all of whom have materially participated in the research and/or article preparation.
- Only contributions that were effectively presented at the conference by one of the authors can be considered.

International school

An international school, coordinated by Aurélien Debelle (CSNSM, Univ Paris-Sud, France), will take place before the REI-19 conference on June 30th and July 1st, 2017.

This REI-19 International School, principally dedicated to young researchers (PhD students, post-docs, junior assistant researchers…), focuses on **techniques for the characterization of irradiated materials**.

Courses will mainly deal with experimental techniques, but computational methods will be presented as well; furthermore, the coupling between experimental and computational works will be highlighted. The basic physical principles of the techniques will be explained, and actual applications for irradiated materials will be addressed. An introductory lecture on ion/solid interactions will be given. The program of the school is given hereafter.

The lectures will be held in the FERMAT building of the Université Versailles-Saint Quentin, Versailles, France.

Friday, June, 30th

8:30 am - 9:00 am Registration - Welcome

9:00 am - 12:30 pm **Ion/solid interactions**
F. Garrido, CSNSM, Univ. Paris-Sud, France

2:00 pm - 4:15 pm **XRD techniques**
A. Boulle, SPCTS, Univ. Limoges, France

4:30 pm - 6:45 pm **IBA techniques**
A. Redondo-Cubero, Auton. Univ. of Madrid, Spain

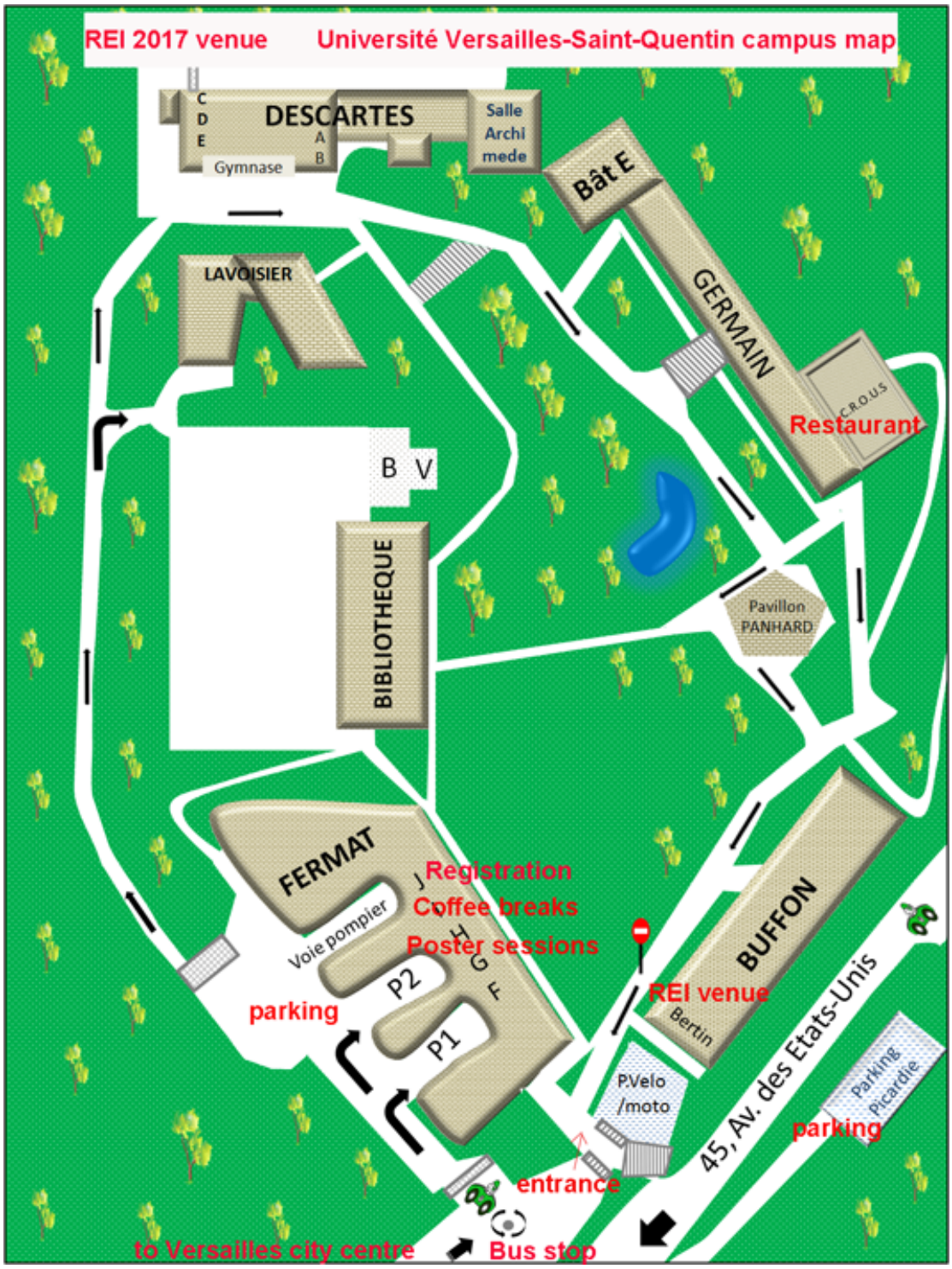
Saturday, July, 1st

9:00 am - 12:30 pm **Computational methods**
B. Uberuaga, Los Alamos National Laboratory, USA

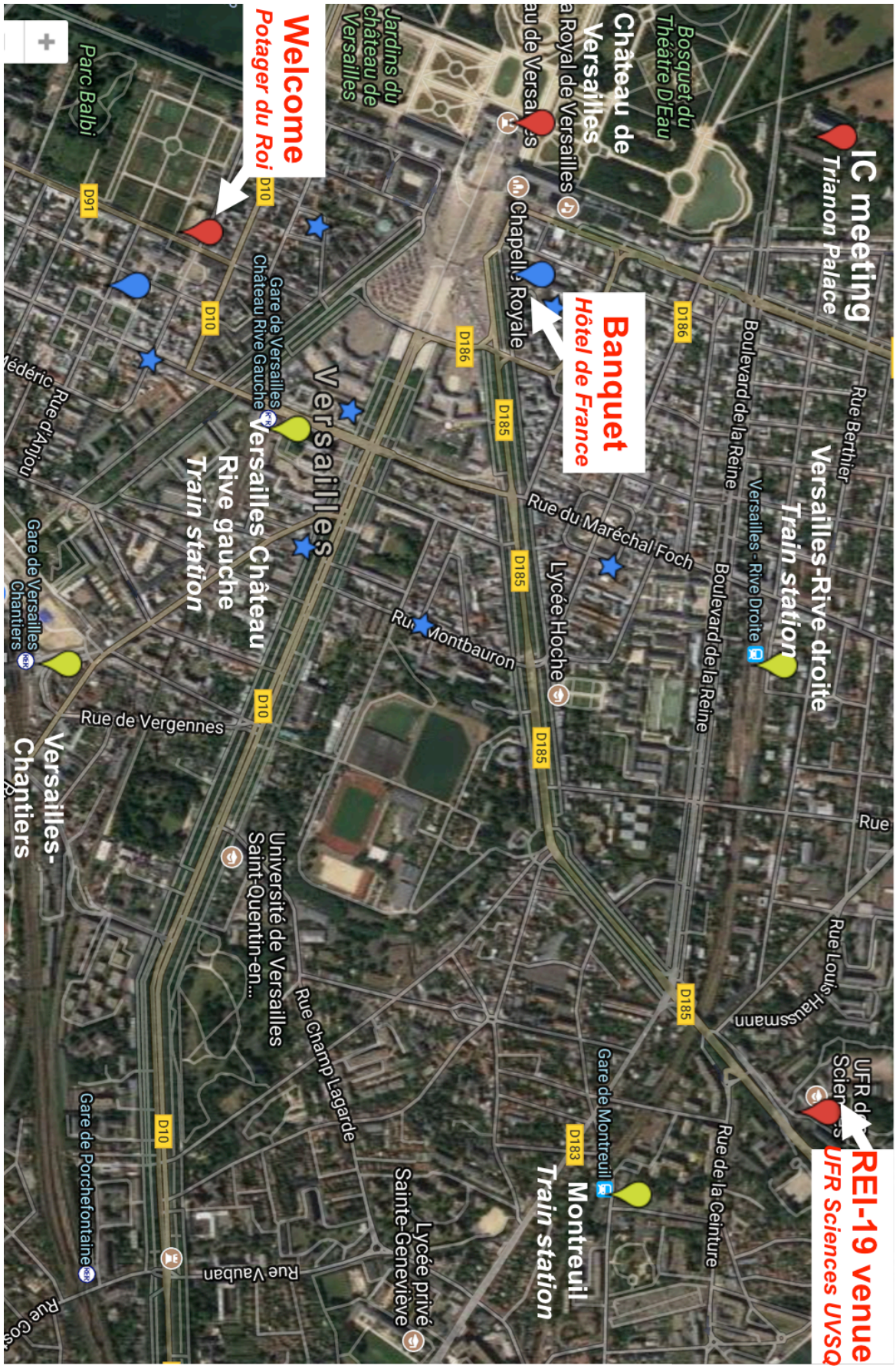
2:00 pm - 4:15 pm **Optical spectroscopy techniques**
T. Cesca, Univ. of Padova, Italy

4:30 pm - 6:45 pm **TEM and spectroscopy techniques**
Ph. Edmondson, Oak Ridge National Laboratory, USA

Location of the venue (UVSQ, Versailles)



Versailles city centre



REI-19 conference's detailed programme

Monday, July 3, 2017

TIME	EVENT
8:00 am - 9:00 am	Registration - Registration
9:00 am - 9:30 am	Opening - Opening
9:30 am - 10:40 am	Session I (Bertin amphitheater)
09:30 - 10:00	› Damage accumulation studies in irradiated oxides: current status and new perspectives - *Jacek Jagielski, Institute of Electronic Materials Technology, National Centre for Nuclear Research*
10:00 - 10:20	› Dislocation-Driven Amorphization of α-Alumina by Swift Heavy Ions? - *Siegfried Klaumünzer, GSI Helmholtzzentrum für Schwerionenforschung GmbH*
10:20 - 10:40	› Using Machine Learning to Identify Factors That Govern Amorphization of Irradiated Pyrochlores - *Blas Uberuaga, Los Alamos National Laboratory*
10:40 am - 11:00 am	Coffee break (Fermat building)
11:00 am - 12:30 pm	Session II (Bertin amphitheater)
11:00 - 11:30	› Synthesis of Metastable Oxide Phases by Dense Electronic Excitation - *Cameron Tracy, Department of Geological Sciences, Stanford University*
11:30 - 11:50	› Influence of composition on phase transformations induced by high and low energy ion irradiations in rare earth sesquioxides - *Suheyla Bilgen, Centre de Sciences Nucléaires et de Sciences de la Matière*
11:50 - 12:10	› Radiation-induced amophization and Polygonization of Uranium Silicides by Ion beam Irradiation - *Jie Lian, Rensselaer Polytechnic Institute*
12:10 - 12:30	› Small Angle X-ray Scattering and X-ray Absorption Spectroscopy Investigations of Ion Tracks in MgAl2O4 - *Satoru Yoshioka, Kyushu University*
12:30 pm - 1:30 pm	Lunch (CROUS restaurant)
1:30 pm - 3:00 pm	Session III (Bertin amphitheater)
13:30 - 14:00	› Swift Heavy Ion shaping of oxide-structures at (sub)-micrometer scales - *Wolfgang Bolse, Institute for Semiconductor Optics and Functional Interfaces, Stuttgart University*
14:00 - 14:20	› Molecular Dynamics study of hillock formation under grazing angle SHI irradiation: - *Henrique Vazquez Muiños, University of Helsinki*
14:20 - 14:40	› Damage in LiTaO3 induced by high energy heavy ion irradiation: from nuclear to electronic damage - *José Olivares, Instituto de Óptica, Consejo Superior de Investigaciones Científicas, Centro de Micro-Análisis de Materiales, Universidad Autonoma de Madrid*
14:40 - 15:00	› Role of atomic-level defects and electronic energy loss on amorphization in LiNbO3 single crystals - *Neila Sellami, Materials Science and Technology Division, Oak Ridge National Laboratory*
3:00 pm - 3:30 pm	Coffee break (Fermat building)
3:30 pm - 5:20 pm	Session IV (Bertin amphitheater)
15:30 - 16:00	› Recent Developments on Nanostructures Fabricated by Ion-Track Technology for Photoelectrochemical Applications - *Maria Eugenia Toimil Molares, GSI Helmholtz Center for Heavy Ion Research*
16:00 - 16:20	› The effect of local structure in the ion beam modification of PECVD and LPCVD silicon nitride: ion track formation and nanoparticle synthesis - *Pablo Mota-Santiago, Department of Electronic Materials Engineering, Research School of Physics and Engineering, The Australian National University*
16:20 - 16:40	› Tailoring through ion implantation of the near-field coupling of Er3+ emitters with plasmonic and pre-plasmonic nanostructures - *Tiziana Cesca, University of Padova*
16:40 - 17:00	› Formation of three-dimensional interconnected network of nanowires by ion beam irradiation - *SATYANARAYAN DHAL, School of Basic Sciences, IIT Bhubaneswar - Shyamal Chatterjee, School of Basic Sciences, IIT Bhubaneswar*
17:00 - 17:20	› Tuning ferromagnetic semiconductors by ion irradiation - *Shengqiang Zhou, Helmholtz-Zentrum Dresden Rossendorf [Allemagne]*
6:30 pm - 9:00 pm	IC meeting - International Committee Meeting

Tuesday, July 4, 2017

TIME	EVENT
9:00 am - 10:30 am	Session V (Bertin amphitheater)
09:00 - 09:30	› Latent tracks and surface hillocks in high resolution: A study of simple oxides - *Jacques O'Connell, Centre for High Resolution Transmission Electron Microscopy, Nelson Mandela Metropolitan University*
09:30 - 09:50	› Investigating Radiation Effects in Materials by Neutron Total Scattering - *Maik Lang, Department of Nuclear Engineering, University of Tennessee*
09:50 - 10:10	› Response of pre-damaged strontium titanate to electronic energy loss - *William Weber, Oak Ridge National Laboratory, The University of Tennessee*
10:10 - 10:30	› Ion irradiation induced absorption band in the transparent UV range of AlN: real synergetic effect between electronic excitations and nuclear collisions - *Mamour Sall, Centre de recherche sur les Ions, les MAtériaux et la Photonique*
10:30 am - 12:30 pm	Poster session A (Fermat building)
12:30 pm - 1:30 pm	Lunch (CROUS restaurant)
1:30 pm - 3:20 pm	Session VI (Bertin amphitheater)
13:30 - 14:00	› Competition between annealing and damage in carbon nanostructures by swift heavy ions - *Ambuj Tripathi, Inter University Accelerator Centre*
14:00 - 14:20	› Investigation of 2D-hBN and graphene after swift heavy ion irradiation - *Lara Bröckers, University of Duisburg-Essen [Duisburg]*
14:20 - 14:40	› Track-associated radiation damage in Y-Ti-O nanoparticles in ODS alloys - *Vladimir Skuratov, Dubna State University, National Research Nuclear University, Flerov Laboratory for Nuclear Reactions, Joint Institute for Nuclear Research*
14:40 - 15:00	› Conical etched ion tracks charaterised by small angle x-ray scattering - *Andrea Hadley, Department of Electronic Materials Engineering, Research School of Physics and Engineering, The Australian National University*
15:00 - 15:20	› Effect of an initial lattice state on the kinetics of Al2O3 excitation in tracks of swift heavy ions - *Alexander Volkov, National Research Nuclear Institute MEPhI, National University of Science & Technology MISIS, National Research Centre 'Kurchatov Institute', Joint Institute for Nuclear Research, P. N. Lebedev Physical Institute*
3:20 pm - 3:50 pm	Coffee break (Fermat building)
3:50 pm - 5:40 pm	Session VII
15:50 - 16:20	› Radiation Effects and Quantum Well Intermixing in InGaN/GaN Multi Quantum Wells - *Katharina Lorenz, Instituto Superior Técnico*
16:20 - 16:40	› Swift Heavy Ion Track Dynamics in Gallium Nitride - *Miguel Sequeira, Instituto Superior Técnico - Technical University of Lisbon*
16:40 - 17:00	› Quantum dot synthesis by ion beam mixing in Si-SiO2 heterostructures and nanopillars - *Flyura Djurabekova, University of Helsinki*
17:00 - 17:20	› Radiation hardness of Kr+ ion implanted BaWO4 at room temperature - *Elke Wendler, Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik*
17:20 - 17:40	› Cathodoluminescence analysis of damage build-up in irradiated spinel mono- and polycrystals - *Iwona Jozwik, Institute of Electronic Materials Technology*

Wednesday, July 5, 2017

TIME	EVENT
9:00 am - 10:30 am	Session VIII (Bertin amphitheater)
09:00 - 09:30	› Time-of-Flight Secondary Neutral & Ion Mass Spectrometry Using Swift Heavy Ions - *Andreas Wucher, Fakultät für Physik, Universität Duisburg-Essen*
09:30 - 09:50	› Thermal effects in ion irradiated Ti2AlC and Ti3SiC2 - *Shaoshuai Liu, State Key Laboratory of Nuclear Physics and Technology, Peking University, China*
09:50 - 10:10	› Radiation tolerance of Yttria stabilized Zirconia against SHI irradiation: Effect of grain size and temperature - *Parswajit Kalita, Department of Physics, Indian Institute of Technology Delhi*
10:10 - 10:30	› Microstructure of Si3N4 and AlN Irradiated with Swift Heavy Ions at 80-1000 K - *Arno Janse van Vuuren, Centre for HRTEM*
10:30 am - 10:50 am	Coffee break (Fermat building)
10:50 am - 12:30 pm	Session IX (Bertin amphitheater)
10:50 - 11:10	› Raman scattering spectroscopy and irradiation damage in actinide oxides : From post-irradiation to in situ measurements - *Patrick Simon, CEMHTI CNRS Université Orléans*
11:10 - 11:30	› Formation mechanisms of the high burnup structure in the spent nuclear fuel – in situ experimental simulation with ion beams in urania - *yara haddad, Centre de Sciences Nucléaires et de Sciences de la Matière*
11:30 - 11:50	› Mo migration in UO2 under swift heavy ion irradiation - *Lola Sarrasin, Institut de Physique Nucléaire de Lyon*
11:50 - 12:10	› Anomalous kinetics of diffusion-controlled F center annealing in neutron irradiated sapphire - *Eugene Kotomin, Max-Planck-Institute for solid state research*
12:10 pm - 1:10 pm	Lunch (CROUS restaurant)
1:10 pm - 6:30 pm	Excursion

Thursday, July 6, 2017

TIME	EVENT
9:00 am - 10:30 am	Session X (Bertin amphitheater)
09:00 - 09:30	› Fluoropolymer-based nanostructured membranes created by swift-heavy-ion irradiation and their energy and environmental applications - *Tetsuya YAMAKI, Takasaki Advanced Radiation Research Institute, National Institutes for Quantum and Radiological Science and Technology*
09:30 - 09:50	› In situ SAXS investigation of ion track nano-pore etching in polymer membranes - *Patrick Kluth, Australian National University*
09:50 - 10:10	› On the radiolytic efficiency of high-energy ions in ultrathin polymer films - *Ricardo Papaleo, Pontificia Universidade Católica do Rio Grande do Sul*
10:10 - 10:30	› Study of writing laser polarization dependence of femtosecond laser induced circular optical properties in silica glass - *Jing TIAN, Institut de Chimie Moléculaire et des Matériaux d'Orsay*
10:30 am - 10:50 am	Coffee break (Fermat building)
10:50 am - 12:20 pm	Session XI (Bertin amphitheater)
10:50 - 11:20	› Ion irradiation of nanomaterials and optical waveguides for photonic applications - *Feng Chen, Shandong University*
11:20 - 11:40	› Fabrication by ion implantation and optical characterization of single-photon emitters in nanodiamonds - *Jacopo Forneris, Università degli studi di Torino, Istituto Nazionale di Fisica Nucleare, Sezione di Torino*
11:40 - 12:00	› Magnetic properties and microstructure of metal nanoparticles in oxides induced by energetic ion irradiation - *Kengo Fukuda, Department of Materials Science, Osaka Prefecture University, Sakai, Osaka 599-8531*
12:00 - 12:20	› Understanding the ion-induced elongation of silver nanoparticles embedded in silica - *Alejandro Prada, Instituto de Fusión Nuclear, Universidad Politécnica de Madrid*
12:20 pm - 1:30 pm	Lunch (CROUS restaurant)
1:30 pm - 3:40 pm	Session XII (Bertin amphitheater)
13:30 - 14:00	› Ab initio simulations of tritium release from Li2TiO3 - *Samuel Murphy, Lancaster University*
14:00 - 14:20	› Microstructural evolution of graphite under irradiation: large scale molecular dynamics simulations - *Laurent Van Brutzel, Den-Service de la Corrosion et du Comportement des Matériaux dans leur Environnement*
14:20 - 14:40	› Atomistic simulation of radiation damage at interfaces in glass/crystal composites - *Paul Fossati, Imperial College London*
14:40 - 15:00	› Monitoring the surface density kinetics of silica irradiated with swift heavy ions by means of in situ reflectance measurements - *Pablo Díaz Núñez, Instituto de Fusión Nuclear, Universidad Politécnica de Madrid*
15:00 - 15:20	› Confocal-micro-luminescence characterization of femtosecond laser irradiated silica and borosilicate glasses - *Antonino Alessi, LAboratoire Hubert Curien*
15:20 - 15:40	› Rare earth ions environment modification by Electron and femtosecond Laser irradiation in phosphate glasses - *Mohamed Mahfoudhi, Laboratoires des Solides Irradiés (LSI)*
3:40 pm - 4:00 pm	Coffee break (Fermat building)
3:40 pm - 5:40 pm	Poster session B
7:00 pm - 11:00 pm	Banquet

Friday, July 7, 2017

TIME	EVENT
9:00 am - 10:30 am	Session XIII (Bertin amphitheater)
09:00 - 09:30	› Upconversion luminescence processes in rare earth doped fluorides and transparent oxyfluoride ceramics - *A. I. Popov, Institute of Solid State Physics, University of Latvia*
09:30 - 09:50	› Is there any evidence of amorphous to amorphous phase transformation due to radiation in oxide glasses? - *Sylvain Peuget, CEA - Marcoule*
09:50 - 10:10	› Comparison between the optical properties of defects induced by 2.5 MeV electrons and by neutrons in crystalline and amorphous SiO2. - *Linards Skuja, Institute of Solid State Physics, University of Latvia*
10:10 - 10:30	› Velocity correlated emission of nanocrystalline clusters in keV surface sputtering by a large polyatomic projectile - *eli kolodney, Schulich Faculty of Chemistry, Technion–Israel Institute of Technology,*
10:30 am - 10:50 am	Coffee break (Fermat building)
10:50 am - 12:20 pm	Session XIV (Bertin amphitheater)
10:50 - 11:20	› In situ Raman spectroscopy in hot cell of nuclear materials / comparison with ion beam irradiations - *Sandrine MIRO, DEN/DE2D/SEVT/LMPA*
11:20 - 11:40	› Radiation defect dynamics studied by pulsed ion beams - *Sergei Kucheyev, Lawrence Livermore National Laboratory*
11:40 - 12:00	› Optical detection of spin-dependent recombination for electron and hole defects induced by ionizing radiation in the wide-gap materials - *Pavel Baranov, Ioffe Institute*
12:00 - 12:20	› CREATION AND ANNEALING OF STRUCTURAL DEFECTS IN PARTICLE IRRADIATED MgAl2O4 SINGLE CRYSTALS AND CERAMICS - *Aleksandr LUSHCHIK, Institute of Physics, University of Tartu*
12:20 pm - 1:00 pm	Closing of the REI-19 conference (Bertin amphitheater)
12:45 pm - 2:00 pm	Lunch (CROUS restaurant)

Abstracts

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Session I

Damage accumulation studies in irradiated oxides: current status and new perspectives

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A complete description of the damage accumulation process in irradiated solids is one of the key issues of nuclear engineering. The development of predictive models of the behavior of materials in nuclear installations requires detailed understanding of the mechanisms leading to structural transformations and, consequently, changes in their functional properties. In general damage accumulation analysis involves three main aspects: (i) identification of the kind of defects at various stages of the damaging process, (ii) quantitative measurement of the damage level and (iii) modelling of the damage accumulation process.
Various experimental and simulation tools may be used for damage accumulation studies. The method of choice for the analysis of defect structure is Transmission Electron Microscopy (TEM), whereas for quantitative analysis of the damage level Rutherford Backscattering/Channeling (RBS/C) method is mainly used.

Numerous studies performed in the past allowed to collect a solid database describing the evolution of defects upon irradiation and to build models (mainly phenomenological) of damage accumulation. The current status of the results collected for irradiated oxides will be reviewed in the first part of the presentation.

A critical review of the currently available information points to the missing elements in damage accumulation approach. Among them the need to: (i) find a technique providing a quantitative assessment of the damage level in polycrystals, and (ii) close a gap between atomistic simulations (essentially made by using Molecular Dynamics) and experimental results, appears as the most urgent tasks. The preliminary results of already commenced attempts to answer these needs using luminescence techniques and new approach to MD simulations will be presented in the second part of the talk.

The last part of the presentation will be devoted to the proposition of a more complete approach in the analysis of damage accumulation in irradiated oxides combining several experimental techniques (RBS/C, TEM, XRD) with molecular dynamic simulations and phenomenological modelling.

*Speaker

Dislocation-Driven Amorphization of α-Alumina by Swift Heavy Ions?

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Several publications report on the amorphization of alumina under swift heavy ion exposure at high fluences where multiple track overlap occurs. However, important details on the amorphization process are still unknown. In this contribution, new insights will be reported by using tilted ion beam incidence in combination with in situ x-ray diffraction revealing a new defect relaxation channel.

The irradiation of polycrystalline alumina samples was performed with 940-MeV-Au ions at room temperature. At normal beam incidence (

theta = 0) the irradiation led to a build-up of an in-plane stress of about -4.5 GPa. No non-equilibrium alumina phases were found. In contrast, irradiations of alumina single crystals ((11$\underline{2}$0)-orientation) with the same ions under a tilt angle of

theta = 45∘ transformed the samples into a state of well-aligned nanocrystallites at fluences below 5×10ˆ12 Au/cm2. With ongoing irradiation, the nanocrystallites exhibited rotations. There are several rotation axes so that the original alignment was eventually lost. The x-ray diffraction linewidth continuously increased without a tendency to saturation. Obviously, there is a continuous decrease of the grain sizes. At a fluence of 2×10ˆ13 Au/cm2, the average grain diameter was about 10 nm.

The experimental results provide clear evidence that the generation of dislocations, their motion and agglomeration to dislocation walls (= unrelaxed grain boundaries) play a fundamental role in the destruction of the long-range crystalline order of alumina. A more quantitative analysis corroborates this statement. However, whether perfect amorphization or simply a nanocrystalline state with extremely small crystallites (diameter of the order of 1 nm) is finally attained cannot be answered by conventional x-ray diffraction and needs further investigations.

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Using Machine Learning to Identify Factors That Govern Amorphization of Irradiated Pyrochlores

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Understanding the factors that dictate radiation tolerance in complex materials provides new avenues for the design of radiation-resistant materials for future applications. However, identifying those factors can be challenging, particularly because the response of a material to irradiation can be a complex convolution of multiple factors. Here, using machine learning approaches informed by density functional theory calculations, we examine the factors that dictate amorphization resistance in pyrochlores, taken here to be characterized by the experimentally-measured critical amorphization temperature. For a broad family of pyrochlores, simple ionic properties such as ionic radius and electronegativity correlate with the observed critical amorphization temperatures. However, when considering just the titanate pyrochlores, the energetics of disordering and amorphization best predict the experimental behavior. We propose that the energy gap between the disordered and amorphous structures is a critical factor dictating the amorphization resistance of pyrochlores. We discuss why static properties such as these energies correlate with inherently kinetic phenomena such as the critical amorphization temperature.

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Session II

Influence of composition on phase transformations induced by high and low energy ion irradiations in rare earth sesquioxides

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Rare-earth oxides (RE2O3) possess remarkable physico-chemical properties that are interesting for technological applications. These compounds find use in diverse applications, as high-dielectrics, nanoparticles for biomedical imaging, materials for ultrafast lasers, neutron absorbers in nuclear fuels and scintillators for the detection of ionizing radiation. RE2O3 compounds exist in three main polymorphic forms (cubic, monoclinic, hexagonal) depending on the nature of RE. Some of their properties depend on the crystalline phase : for instance, the europium photoluminescence in Eu2O3 is different between cubic and monoclinic phase. Radiation-damage created by low or high energy heavy ions were investigated in order to compare the effects of both nuclear collisions and electronic excitations in rare earth oxides Ln2O3 (with Ln=Eu, Gd, Dy, Ho, Er, Yb). These compounds were irradiated: (i) with 4-MeV Au ions (ballistic regime) at JANNUS (Orsay); (ii) with swift heavy ions (94-MeV Pb, 96-MeV Xe and 1 GeV-Xe ions, electronic excitation regime) at GANIL (Caen). X-ray diffraction, with in situ measurements, Raman Spectroscopy and Transmission Electron Microscopy were implemented to determine the modifications induced by irradiation. Moreover, the influence of composition on the damage-build up in these compounds in both energy ranges (electronic excitation versus ballistic nuclear collisions) was also determined. X-ray diffraction and Raman Spectroscopy data show that heavy ion irradiation of all rare earth sesquioxides leads to a cubic-to-monoclinic transformation, except for Yb2O3. For this latter, no transformation is observed for low energy ion irradiations. For high energy ion irradiations, results show that the structural changes are strongly dependent on the sample composition. The irradiation induces a cubic to monoclinic transition. However, for Yb2O3, Ho2O3 and Er2O3, an intermediate transformation from C to an X-type phase was observed before the formation of the final B-type structure. Kinetics of these modifications was

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found to depend strongly on composition. As the atomic number of the lanthanide cation in Ln2O3 compounds increases (and its ionic radius decreases), these oxides become more resistant to an irradiation-induced transformation.

Radiation-induced amophization and Polygonization of Uranium Silicides by Ion beam Irradiation

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Uranium silicide combining with advanced cladding is considered as a leading form of accident tolerant fuels for light water reactors due to its excellent thermal conductivity and higher fissile element density. Ion beam irradiation-induced amorphization was previously reported for U3Si2 with a low critical temperature of 250 oC. However, limited data is available on the radiation response of U3Si2 under relevant reactor temperatures. In this work, U3Si2 was irradiated by intensive ion beam of 300 keV Xe+ and U3Si5 was irradiated by 1 MeV Kr2+ and 150 keV Kr+, respectively, at 350 ∘C close to the operation temperature of light water reactors. The microstructure evolution upon intensive ion beam irradiations is characterized by in-situ transmission electron microscopy. U3Si5 is sensitive to radiation-induced amorphization at room temperature with a low critical amorphization dose (less than 0.6 dpa). When irradiated by 1 MeV Kr2+ at 350 oC, U3Si5 is highly resistant against amorphization even up to a very high dose of 60 dpa. Radiation-induced polygonization and grain subdivision occur in U3Si2 irradiated by 300 keV Xe at 350 oC. The polygonization begins at a low dose _˜0.8 dpa and continues above 48 dpa. The radiation-induced polygonization leads to the formation of high density of nanoparticles which experience grain coarsening with increased radiation dose up to _˜20 nm. High density nano-sized Xe bubbles form in Xe-irradiated U3Si2 and a radiation-induced bubble coaelescence is also identified. Due to its high susceptibility to oxidation, uranium silicide nanoparticles upon grain subdivision are oxidized during in-situ TEM irradiation, eventually leading to the formation of UO2 nanocrystals stable up to 80 dpa. These results indicated that at relevant reactor operation conditions, uranium silicide as the leading candidate of ATFs is stable against radiation–induced amorphization, but likely experiences grain subdivision and possible a rim structure, similar to oxide fuels.

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Synthesis of Metastable Oxide Phases by Dense Electronic Excitation

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Phase transformations are conventionally induced in oxides by doping or by exposure to high temperatures or pressures. However, many potentially useful metastable phases do not occur in equilibrium pressure-temperature-composition space, such that far-from-equilibrium processing conditions are necessary to access them. Irradiation with swift heavy ions or ultrafast lasers induces dense electronic excitation in oxide materials, modifying interatomic forces and making accessible transformation pathways not achievable through conventional processing techniques. This presentation covers several examples of metastable phase synthesis by irradiation in the electronic excitation regime. When irradiated with swift heavy ions, bixbyite-structured lanthanide sesquioxides transform to either monoclinic high-temperature polymorphs or a highly disordered cubic phase that has not previously been stabilized to ambient conditions [1,2]. The structure of the latter metastable phase yields exceptionally high ionic conductivity. Irradiation of the same materials with an ultrafast laser can induce formation of the monoclinic phase, even for compounds with heavy lanthanide cations, for which this phase is not a stable polymorph [3]. Irradiation of actinide dioxides with swift heavy ions extends the stability range of the dense, high-pressure cotunnite phase to significantly lower pressures. Finally, irradiation of amorphous silicon dioxide with swift heavy ions changes the short-range ordering of the material, such that it exhibits unique polyamorphism under dense electronic excitation.

M. Lang, F. Zhang, J. Zhang, C.L. Tracy, A.B. Cusick, J. VonEhr, Z. Chen, C. Trautmann, R.C. Ewing, *Nucl. Instrum. Meth. B* **326**, 121 (2014)

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*Speaker

Small Angle X-ray Scattering and X-ray Absorption Spectroscopy Investigations of Ion Tracks in MgAl2O4

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Magnesium aluminate spinel (MgAl2O4) is known as a radiation tolerant oxide, and it has been a model materials for researches of radiation resistance mechanism. High density electronic excitation generated by swift heavy ions produces characteristic defects in insulating materials. In the case of MgAl2O4, transmission electron microscopy (TEM) investigations have reported that ion tracks maintain crystalline and are concentrically composed of multiple regions, such as defective core (_˜1 nm in radius), strained shell (2 nm) and disordered outer-shell (5 nm) [1]. In this study, we adopted two kinds of synchrotron x-ray techniques, small angle x-ray scattering (SAXS) for nano-meter sized structures and x-ray absorption spectroscopy (XAS) for local atomic coordinations, to further understand the structure of ion tracks in MgAl2O4.
Polycrystalline MgAl2O4 samples were irradiated with 100 or 200 MeV Xe ions by using a tandem accelerator at Japan Atomic Energy Agency-Tokai. SAXS measurements were carried out at the beamline 06 in Kyushu Synchrotron Light Research Center using an X-ray wavelength of 0.15 nm and a camera length of 0.5 m. Images were taken in transmission geometry with using a 2D detector. XAS measurements on the Mg K-edge and Al K-edge were performed using beryl double crystal monochromator at the beamline 2A in UVSOR. The photo-absorption spectra were recorded in total electron yield mode, with use of an electron multiplier detector.

Under a condition of tilted X-ray beam incidence, SAXS images of irradiated samples showed curved intensity streaks, indicating the formation of anisotropic cylindrical defects of the ion tracks with a high aspect ratio. The profiles obtained by circular integration of SAXS images taken from a direction parallel to the incident direction of ions showed a broad peak, and the intensities were increased with increasing ion fluence. The peak position in scattering vector q indicated that a 10 nm-sized structure was formed in MgAl2O4. The size was in accordance with the disordered region detected by TEM analysis, which suggests an increase in atomic density within the region. The XAS of the irradiated sample were a different spectrum from the non-irradiated one. Theoretical absorption spectra with using DFT method have suggested disorder between Mg and Al sites due to ion irradiation. These results are also compared with microstructure observations obtained by TEM.

K.Yasuda, T.Yamamoto, M. Etoh, S. Kawasoe, S.Matsumura and N.Ishikawa, *Int. J. Mat. Res.* 102 (2011) 9.

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Session III

Swift Heavy Ion shaping of oxide-structures at (sub)-micrometer scales

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Many amorphous (and also a few crystalline) solids exhibit anisotropic deformation when irradiated with swift heavy ions, such that they shrink along the beam direction and expand perpendicular [1]. In this presentation we will show that this hammering-effect can be utilized as a tool for reshaping of (sub)micrometer-sized oxide structures. Using FIB we have pre-structured 100 nm thin NiO- and ZnO-films into small platelets of 100 – 5000 nm side-lengths on oxidized Si-substrates. The development of the platelets under swift heavy ion irradiation was monitored using our "High Resolution In-Situ Scanning Electron Microscope" installed in the beam line of the UNILAC ion accelerator at the GSI Helmholtz Centre for Heavy Ion Research [2]. This instrument allows us to *in-situ* investigate the structural and compositional development of individual objects in the (sub)micrometer-range under swift heavy ion bombardment, from the very first ion impact up to fluences of some 10ˆ15 cmˆ-2. The sample is irradiated in small fluence steps and in between SEM-images (and EDX-scans) of one-and-the-same surface area are taken. The irradiation can be carried out at any incidence angle between 0deg and 90deg and under stepwise or continuous azimuthal rotation of the sample.
Swift heavy ion irradiation at small incidence angles (5deg – 10deg) and azimuthal rotation results in lateral shrinking and vertical growth of the platelets. At intermediate fluences additional rounding of edges and corners can be observed. At high fluences the deformation finally saturates. The deformation of the platelets is accompanied by huge sputtering of the exposed SiO2-layer, which due to the retreating edges of the platelets results in a pyramidal-like base underneath of them. In our presentation we will illustrate and discuss the reshaping mechanisms and underlying driving forces.

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*Speaker

Damage in LiTaO3 induced by high energy heavy ion irradiation: from nuclear to electronic damage

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Lithium tantalate (LiTaO3) is an interesting material for photonic applications, offering some advantages regarding submicron ferroelectric domain engineering, compared to the more studied lithium niobate (LiNbO3) [1]. There is a high interest in combining its attractive properties with optical waveguide structures. Swift heavy ion irradiation has been shown in the past to be an excellent route to produce unique high contrast optical waveguides in many crystals [2,3]. Comparing the ion damage formation in LiTaO3 with that in LiNbO3 is very attractive for the subsequent modeling and analysis because both materials, being quite similar regarding many structural properties, have significantly different melting points and band gaps.
We have made a systematic study of the damage created in LiTaO3 by ion irradiation in conditions that create a buried damage layer (i.e. producing an optical waveguide), exploring the cases of C 15 MeV, F 20-30 MeV and Si 40 MeV at several fluencies to follow in detail the damage kinetics. Optical waveguide characterisation allows the determination of the refractive index (in-depth damage) profiles. On the other hand, with Br ion irradiation at 40 and 25 MeV we have explored irradiations that are above the (individual track) amorphization threshold. In situ optical measurements (reflectance and transmittance) have been made to monitor the continuous damage kinetics. DC electrical measurements using the four and two-point probe methods, between 295 and 490 K, were used to characterize the electrical conductivity of damaged layers at the surface [4]. Like similar measurements in LiNbO3, they suggest a thermally activated process. The I-V characteristics reveal an ohmic behaviour trend of the electrical contacts in damaged layers, in contrast to the blocking contacts in undamaged regions.

Interestingly, for the same "subthreshold" irradiation (F 20-30 MeV) having similar electronic stopping power (Se) in both materials, the fluence needed for causing amorphization is one order of magnitude larger for LiTaO3, what would be consistent with a thermal-spike model. The damage in LiTaO3 first appears at low fluence (_˜1e14 cm-2) being caused by nuclear interac-

*Speaker

tions and moves towards "electronic damage" regime for higher fluences (_˜1e15 cm-2).

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Role of atomic-level defects and electronic energy loss on amorphization in LiNbO3 single crystals

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Understanding the complex non-equilibrium defect processes where multiple irradiation mechanisms may take place is a long standing subject in radiation material science. Understanding the separate and combined effects of elastic and inelastic energy loss is a very complicated and challenging endeavor.
LiNbO3 oxide has been extensively studied for decades, since it exhibits a variety of interesting properties that make it suitable for many applications, specifically for photonic devices (optical waveguides, lasers). In this work, LiNbO3 has been irradiated with 0.9 MeV Si and 8 MeV O ions, which are representative of nuclear (Sn) and electronic (Se) energy loss regimes, respectively. The damage evolution has been investigated by Rutherford backscattering spectrometry combined with a channeling technique. Irradiation with an ionizing beam of 8 MeV O ions, where Se is about 3 keV/nm and almost constant near the surface region, induces a crystalline to amorphous phase transition at high ion fluence, even below the amorphization threshold (Se,th = 5-6 keV/nm). Moreover, a strong synergistic behavior of the electronic energy loss with the nuclear energy loss is evident in the sequential Si and O irradiations. The pre-existing damage strongly promotes damage production, showing a non-linear additivity behavior. The damage build-up kinetics for subsequent high-energy irradiation on undamaged and pre-damaged LiNbO3, reveal an increasing reduction of the O ion incubation fluence for amorphization with increasing pre-existing damage.

The results highlight the important role of the atomic-level defects on lowering the threshold for electronic energy loss induced amorphization. Controlling the pre-damage amount prior to high energy irradiation is an interesting approach to tune the optical properties for photonic devices applications.
This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

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Molecular Dynamics study of hillock formation under grazing angle SHI irradiation:

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Previous studies have shown that in layered crystals such as SrTiO3 or Mica, SHI irradiation under grazing incidence can produce chains of hillocks on the surface of the material. These structures have length scales of tens of nanometers and were associated with the local electron density along the ion track [1, 2, 3].
In our work, we apply an up-to-date theoretical model to calculate the energy deposited on atoms in layered materials by SHIs under grazing incidence. We combine the energy profiles with inelastic thermal spike Molecular Dynamics (MD) simulations in order to reveal the mechanism of hillock formation. We calculate the stopping power and simulate the SHI-induced electron cascades at different points along the ion trajectory to study the energy distribution and its dependence on the local electron density. We observe along the track periodic peaks of energy deposited with the same length scale as the hillocks observed experimentally [1]. Moreover, we apply TREKIS code to calculate the electronic cascades near surface to estimate more accurately the energy deposited in the near-surface layers. The simulations show good correlation of surface behavior (formation of rims and hillocks) in the simulated structure to the experimental observations.

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Session IV

Tailoring through ion implantation of the near-field coupling of Er3+ emitters with plasmonic and pre-plasmonic nanostructures

Tiziana Cesca *† [1], Boris Kalinic [1], Niccolò Michieli [1], Chiara Maurizio [1], Carlo Scian [1], Giovanni Mattei [1]

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Ion implantation is a very versatile technique for local doping on predefined patterns of functional substrates.
This is of paramount importance for instance when investigating optical phenomena arising from the near-field coupling of atomic-like emitters with plasmonic nanostructures, i.e., in which a highly controlled positioning of the emitters with respect to the metal nanostructures is required.

In this talk, we will exploit such capabilities to efficiently couple Er3+ ions in silica (emitting at 1.5 microns at room temperature) to suitable plasmonic nanostructures, for controlling and enhancing the emission efficiency of the rare-earth ions. Two classes of metal nanostructures will be investigated: (i) pre-plasmonic sub-nanometric metal clusters and (ii) fully-plasmonic ordered arrays of metal nanostructures. For type (i), recently we demonstrated that ultra-small metal clusters, made of 5-20 atoms, can boost the Er3+ photoluminescence (PL) with an enhancement of the effective excitation cross-section by 2-3 orders of magnitude [1,2]. For type (ii), the emission efficiency is enhanced through the control of the energy relaxation rates. Here, we will show how ordered arrays of plasmonic nanostructures, as nanohole arrays (NHA), can be effectively employed to this aim. Particularly, we demonstrated, both experimentally and by FEM simulations, that Au NHAs can remarkably shorten the radiative emission lifetime (up to a factor of 2) with limited dissipation in the NHA, leading to a net increase in the far-field photon flux.

Finally, a highly efficient synergistic effect is further obtained by combining the two approaches, i.e., by using both sub-nanometric clusters for the excitation cross-section enhancement and ordered plasmonic nanostructures for the emission rate control, and an enhancement of more than 2 orders of magnitude in the Er3+ PL intensity at room temperature is demonstrated in this way.

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Formation of three-dimensional interconnected network of nanowires by ion beam irradiation

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Formation of three-dimensional interconnected network of nanowires by ion beam irradiation
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The one-dimensional form of nanomaterials has been very popular for their high aspect ratios and usefulness in the applications where high surface area is a prime requirement. In most of the cases nanowires/nanotubes are placed on two-dimensional planes. However, a three-dimensional network of interconnected nanowire might have huge potential for making device as it covers large surface as well as volume. For instance, such 3D structure could be useful in sensing, catalysis or in filter applications. In this work we show that simple ion irradiation can be a useful tool to make such 3D structure with solid joining between two nanotubes. Such networking is possible even for ceramic nanowire/nanotubes with higher melting points than metals. Several studies have been performed earlier on 3D junction formation of CNTs, which was achieved using chemical based techniques.[1],[2] 3D ZnO nanowire network was done by high temperature solid–vapor deposition process.[3] There are also numerous studies in which 3D Ti foams[4] and porous titanium scaffolds[5] having relative densities and high strength than those of human bones alike, can be used as implant materials and coating materials in stem cells which can be helpful in bone tissue engineering applications. In this work we have synthesized hydrogen titanate nanotubes using hydrothermal method and produced 3D assembly. These nanotube assembly was irradiated with low energy argon and sodium ions at various fluences. After the irradiation, the nanotubes form a complex network of interconnected tubes, establishing a three-dimensional (3D) porous structure by ion induced welding. Earlier we have shown formation of 2D large-scale network structure of hydrogen titanate nanowires induced by nitrogen ion irradiation.[6] This technique can also applied for other ceramic based nanostructures as well as metals. The formation of 3D web of titanate nanotubes may be considered for the development of micro electro-mechanical devices.

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The effect of local structure in the ion beam modification of PECVD and LPCVD silicon nitride: ion track formation and nanoparticle synthesis

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Silicon nitride is of particular interest due its physical properties such as high dielectric constant, high chemical inertness, resistance to moisture penetration and compatibility with Si-based devices. Chemical vapor deposition methods (CVD) are among the preferred techniques, among which plasma enhanced (PECVD) and low pressure (LPCVD) are the most commonly used techniques in device processing. While both techniques provide with highly uniform films with controllable stoichiometry, the temperature and synthesis process has a major impact on the local structure of such materials. In this work, we report on the role of short-range order on the ion beam material modification of amorphous silicon nitride layers. For this purpose, we present the material response of PECVD and LPCVD silicon nitride layers under two experimental conditions: after being irradiated with 185 MeV Au ions at low fluences; and the synthesis of metallic nanoparticles resulting from Au implantation at 2 MeV with a fluence of 5×1016 cm-2. The pre-characterization with Fourier transform infrared spectroscopy demonstrated the appearance of Si-H and N-H bonds for the sample prepared by PECVD, deviating the local structure from the LPCVD near-ideal amorphous silicon nitride. Synchrotron based small angle X-ray scattering (SAXS) measurements demonstrate the presence of an ion track morphology resembling an under dense core surrounded by a thick over dense shell with a smooth transition between the two regions. In the case of the PECVD sample, we determined an ion track radius of 4.2 ± 0.1 nm while for the LPCVD nitride, the radius was 4.9 ± 0.2 nm. Furthermore, a higher absolute density change (-8.5 ± 0.5%/2.2 ± 0.3%) was deduced for the first, contrasting with the density change of -1.5 ± 0.3%/0.13 ± 0.02% of the later. In order to promote Au Np formation and growth, post-implantation thermal annealing processes at 1000∘C and 1100∘C in air and N2 were carried out. Transmission electron microscopy (TEM) and SAXS show a high density of small NPs (R < 2 nm) in the PECVD sample while for the LPCVD nitride a high diffusion of Au towards de Si interface induced by the crystallization of the nitride was observed. Grazing incidence X-ray diffraction confirmed the amorphous to alpha phase transition in the

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LPCVD sample while the PECVD remained amorphous. The results are discussed in terms of the density of point defects inherent to the deposition process.

Recent Developments on Nanostructures Fabricated by Ion-Track Technology for Photoelectrochemical Applications

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The implementation of nanowires and nanotubes for applications such as thermoelectrics, catalysis, solar cells, and photoelectrochemical water splitting for hydrogen generation requires a successful assembly of the nanostructures into 2-D and 3-D architectures. Fabrication of 3-D nanowire superstructures by vapour–liquid–solid processes has been reported; however, revealing a limited tunability of the relevant parameters. By swift heavy ion-track technology mechanically stable 3-D networks consisting of well-defined interconnected nanowires can be produced. The networks are fabricated by electrodeposition in polymeric etched ion-track membranes. The membranes with nanochannel arrays tilted at various angles are produced at GSI by GeV ion irradiation of polymer foils at several incident angles in consecutive steps, followed by chemical etching. Nanochannel density, as well as diameter and geometry, are adjusted by the irradiation and etching conditions, respectively. Subsequent electrodeposition in the nanochannel network results in highly ordered 3-D nanowire ensembles. [1,2]
In this talk, recent developments achieved on the production of semiconductor (ZnO and p-Cu2O) nanowire arrays and nanowire networks will be presented. The structures exhibit high mechanical stability after the membrane dissolution and can be easily handled and investigated as photoanodes and –cathodes for photoelectrochemical water splitting. The one-dimensional shape and geometrical orientation of the nanostructured photoelectrodes foresees more efficient charge carrier separation and transport to the surface of the electrode as compared to bulk materials. The semiconductor nanostructures are additionally coated with TiO2 by atomic layer deposition to protect them from corrosion in aqueous electrolyte. Their photoelectrochemical performance is measured and compared to that of their film counterparts.

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Tuning ferromagnetic semiconductors by ion irradiation

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Ion irradiation has been widely used to render a semiconductor layer highly resistive through the creation of carrier-trapping centers. In Mn doped III-V compound semiconductors, which are candidates for spintronic applications, free carriers play deterministic roles for the magnetic properties. However, Mn substitutes the cation in III-V and acts as an acceptor, resulting in the difficulty to independently change the local-moment and hole concentration. In this contribution, we show how the carrier concentration in (III,Mn)V and consequently the magnetic properties can be precisely tuned by ion irradiation [1, 2].
On one hand, we investigate fundamentally how magnetic properties change upon shifting the Fermi level by hole compensation via ion irradiation. We monitor the change of Curie temperature (Tc) and conductivity. For a broad range of samples including (Ga,Mn)As and (Ga,Mn)(As,P) with various Mn and P concentrations, we observe a smooth decrease of Tc with carrier compensation over a wide temperature range while the conduction is changed from metallic to insulating. The existence of Tc below 10 K is also confirmed in heavily compensated samples. Our experimental results are naturally explained by assuming that the Fermi level resides in the valence band being merged with the Mn-derived impurity band [2].

On the other hand, we explore the application potential of ion irradiation in semiconductor spintronics. In the light compensation regime by ion irradiation, the magnetic easy axis of (Ga,Mn)(As,P) can be gradually changed between in-plane and out-of-plane directions [3]. Combined with the possibility of lateral patterning [4], such an approach allows for developing new concepts for spintronic devices.

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Session V

Investigating Radiation Effects in Materials by Neutron Total Scattering

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We present neutron total scattering with pair distribution function (PDF) analysis as a new strategy for the characterization of radiation effects in materials. Key to this approach is the use swift heavy ions with a very high penetration depth to produce sufficiently large irradiated sample mass (_˜150 mg). Irradiation experiments were performed at the UNILAC accelerator of the GSI Helmholtz Center with ions of specific energy of 11.4 MeV/u. Samples were characterized after irradiation at the Nanoscale Ordered Materials Diffractometer (NOMAD) beamline at the Spallation Neutron Source (Oak Ridge National Laboratory). We have investigated various ion-induced structural modifications, such as defect formation (CeO2 and ThO2), disordering (Er2Sn2O7), amorphization (Dy2TiO5), and changes in the atomic arrangement of glasses (vitreous SiO2). Neutrons scatter strongly from low-Z elements, permitting a detailed analysis of both cation and anion defect behavior. PDF analysis elucidates the local defect structure, including changes in site occupation, coordination, and bond distance. This is particularly important for characterizing radiation effects in oxides, as structural modifications induced by ion-beam irradiation are seldom ordered over long length scales and in extreme cases result in complete loss of long-range order (*i.e.,* amorphization).

*Speaker

Latent tracks and surface hillocks in high resolution: A study of simple oxides

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Studying the structure of SHI induced latent tracks in materials gives insight into the mechanisms responsible for their creation. A reasonably large pool of data on track diameters in various materials is available in the literature but most of this data represents average values of a large number of tracks sampled simultaneously through indirect methods such as RBS/c, SACS, m'osbauer spectrometry etc. TEM gives the unique ability to directly image latent tracks in both plan view and cross section at atomic resolution. The majority of the already limited TEM obtained track parameter data available in the literature is mostly limited to plan view sections containing the irradiated surface, forcing one to make assumptions on the nature of the latent track in the bulk of the material based on observations of the track 100 nm or less from the irradiated surface. While the assumption of continuous cylindrical tracks is valid for certain materials such as pyrochlores and garnets, we have recently recently shown that this assumption does not hold for the more simple oxides such as TiO2, Al2O3, YSZ and CeO2. The morphology of surface hillocks produced during SHI irradiation is also of interest in order to understand their formation. Literature data on hillock size and shape is almost exclusively obtained by AFM although this technique can not distinguish between crystalline and amorphous hillocks. The biggest limiting factor for surface hillock investigation by TEM is the production of electron transparent sections of the hillock containing crystal in cross section without destroying the hillock itself. Newly obtained data on the morphology of surface hillocks and the near-surface track region in selected simple oxides will be presented and discussed including temperature dependent feature sizes.

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Ion irradiation induced absorption band in the transparent UV range of AlN: real synergetic effect between electronic excitations and nuclear collisions

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AlN, because of its large band gap (6.2 eV), is used as a substrate for ultraviolet light emission and laser diodes, particularly for AlxGa1-xN (x $\neq$ 1) based technology in order to avoid the lattice mismatch with the classical substrates like sapphire and SiC [1]. However, an optical absorption band at 4.7 eV have been observed below the band gap of AlN. It affects the UV transparency and may spoil the UV optoelectronic applications. This absorption band is linked to defects either created during the AlN material growth [2] or induced by ion irradiation [3]. In the latter case, it was demonstrated that the creation mechanism is ruled by an unprecedented synergy between electronic excitations (Se) and nuclear collisions (Sn) [4]. The coefficient of synergy highly depends on Se, and can be increased by three orders of magnitude with the sole effect of Se.

We performed different sequential irradiations to study the synergy mechanism by paying great attention to the spatial superimposition of nuclear collisions and electronic excitations. Different hypotheses for the synergy mechanism were tested. It appears from our study that the defects linked to the absorption band are created by a real positive synergy between electronic excitations and nuclear collisions. The two phenomena (Se and Sn) must be spatiotemporally simultaneous, at least at a macroscopic scale, so that the synergy occurs. In fact, there is a mutual assistance between Se and Sn for a direct creation of optical defects. This would be a complex phenomenon as nuclear collisions and electronic excitations are not, at a microscopic scale, really simultaneous ($\approx$100 fs delay). Furthermore, the radial distributions around the ion path of Se and Sn may be very different. This opens new research perspectives (experiment and simulation) in the field of synergy phenomena which is gaining more and more attention in our community.

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Response of pre-damaged strontium titanate to electronic energy loss

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The interaction of ions with solids results in energy loss to both electrons and atomic nuclei in the solid. Additive [1-4], competitive [1,4-6] and synergistic [7] effects of electronic and nuclear energy loss for intermediate energy ions have been demonstrated in different ceramics. We have previously demonstrated a unique synergistic effect of electronic loss from 21 MeV Ni ions (9.9 keV/nm) with pre-existing damage in single crystal SrTiO3 [7] that resulted in amorphous track formation. In the present study, the response of single crystal SrTiO3, pre-damaged with 900 keV Au ions at 300 K, is examined as a function of electronic energy loss using ions of different energies and high electronic-to-nuclear stopping ratios. Pre-damaged and irradiated single crystals were characterized by channeling Rutherford backscattering spectrometry and transmission electron microscopy. The threshold for track formation in SrTiO3, pre-damaged to a relative disorder fraction of 0.10 to 0.15 at the damage peak, is about 6.6 keV/nm, and the track diameters range from 1.6 nm for 12 MeV Ti to 8.5 nm for 640 MeV Xe. This threshold for track formation decreases with increasing pre-existing disorder. Below this threshold, defect annealing is demonstrated with 12 MeV O ions (3.0 keV/nm) in pre-damaged SrTiO3. Molecular dynamics simulations [8], based on the two-temperature model, are consistent with the experimental observations.

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Poster session A

AlN influence on the radiation damage of Ar and Xe implanted AlGaN

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Implanted III nitride compounds are currently attracting considerable research interest due to the large potential for application in opto-electronic technology. Ion implantation is an ideal technique for selective area doping and control of dopant depth distribution. However implantation damage is still not well understood in these alloys, despite all the research efforts. In this work AlxGa1-xN alloys covering the entire compositional range ($0 \leq x \leq 1$) were implanted with both 200 keV Ar or 300 keV Xe ions, to fluences ranging from 1×1013 to 2×1016 at/cm2 at RT. The created damage build up were studied and the role of AlN content on radiation hardness studied in detail. Unexpectedly it was observed a high radiation damage for high AlN containing alloys implanted with Ar ions. To understand the influence of collision kinematics we also implanted Xe ions. The damage profiles were studied using Rutherford backscattered spectrometry channelling (RBS/C) and High resolution X-ray difraction.
Furthermore we used Heavy Ion Elastic Recoil Detection Analysis (HIERDA) to complement the detailed study of Argon (Ar) implantation into AlGaN alloys to measure the depth distribution of the light element like N and Al. Quantitative depth profiles of all elements in the sample surface region were acquired and the influence of ion implantation on the elemental distribution studied.

*Speaker

Defect interaction in ZnO investigated by sequential implantation of ions and subsequent annealing

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ZnO is a wide and direct band-gap semiconductor belonging to the group of so-called "radiation-hard materials" where amorphization is strongly suppressed even for heavy ion bombardment at cryogenic temperatures [1]. In contrast to the ballistic processes of defect formation, occurring on a very short time scale (_˜1e-12 s), dynamic defect annealing processes have several orders of magnitude larger characteristic time scales. The understanding of the latter processes is limited due to complexity and they are also challenging to molecular dynamic simulations because of the long time scales [2].
In the present contribution, we demonstrate that Ag ion implantation performed in channeling direction of ZnO, results predominantly in the formation of extended defects. This is in direct contrast to implantations at random directions. Aligned Ag implantation has then been used to form a dense band of extended defects peaking at a depth of 350-450 nm, followed by implantations with elements such as B and N having their profile peak in the region between the sample surface and the Ag peak. In addition, the diffusion of residual Li atoms during the post-implant anneals was monitored to trace the presence and migration of Zn interstitials [3]. Hence, correlating diffusion and structural data obtained by RBS and SIMS measurements it is revealed that extended defects in ZnO act as efficient traps for mobile Zn interstitials during post-implantation annealing [4]. In its turn, the role of the pre-existing extended defects on the dynamic defect annealing during subsequent implantations has also been studied by in-situ RBS/C measurements of co-implanted samples. In particular, the results show that high density bands of extended defects could be beneficial to enhance the radiation tolerance of ZnO.

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Behavior of white pigments under ion irradiation

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Non-destructive analytical techniques using photon and ion beams produced by particle accelerators and synchrotrons are increasingly being applied to study artefacts from Cultural Heritage. While radiation effects have been investigated for a long time in the field of material sciences, few studies have addressed the potential consequences on works of art.
In this study, we have investigated a major compound of art: the white pigment. White pigment is present in most of the paintings and is particularly sensitive to irradiation and color modification. Various types of white pigment – lead white (hydrocerussite and basic lead sulfate), gypsum, calcite, zinc white (zinc oxide) and titanium white (titanium oxide) – have been irradiated with an external 3 MeV proton micro-beam to reproduce irradiation conditions of conventional ion beam analysis (with the AGLAE accelerator of the Centre de recherche et de restauration des musées de France C2RMF, Paris, France). We have observed various sensitivities depending on the pigment.

No visible change occurs for calcite and titanium oxide, whereas zinc white and lead white pigments are optically modified. Modifications in lead white pigments were studied by micro-Raman and XPS. Structural modifications and dehydration were detected. Damage recovery was observed under UV-light irradiation. Zinc white shows little change after proton irradiation. In order to further investigate the damage formation in that material, complementary irradiations in vacuum with proton and gold ions were conducted at the multi-ion irradiation platform of JANNUS-Saclay (CEA, France). Modifications were characterized by *ex situ* and in situ μ-Raman and XPS. Gold ions induce an important damage characterized by a decrease in the 438 cm-1 band assigned to the wurtzite structure and an increase in the broad band at 540-580 cm-1 associated to disorder. Au ions irradiation also induces a strong yellow coloration of the pigment. Conversely, protons seem to have a very light effect on the structure and on the color, showing safe conditions for applying IBA to 19th century paintings.

*Speaker

ELECTRON DENSITY CHANGIES IN THIN SUPERCONDUCTIVE NbN FILMS UNDER LOW ENERGY OXYGEN IRRADIATION

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Thin niobium nitride film is a promising material for use in various devices (SSPD, HEB, etc.) and also for cryo-electronic application elements: capacitors, resistors, inductance elements, Josephson junctions. One could use ion beam irradiation to control chemical composition and properties of thin superconductive NbN films[1]. These radiation technologies for creating functional nanoelements has been actively developed in NRC "Kurchatov Institute" during the past ten years, implying impact of low-energy ion beams of different composition (protons, oxygen, nitrogen and other ions) at various doses [2,3].
In this work, the radiation-induced changes of free electron density state at Fermi level were investigated by electron energy-loss spectroscopy (EELS) in low-loss region of energies. FIB prepared cross-section samples of NbN films irradiated by + ions with energies (0.1-4) keV in a dosage range (0.034-0.14)*10ˆ18 cmˆ-2 were investigated in STEM using plasmon EELS peak. Energy of plasmon is Ep=(h/2π)*ω=(h/2π)((neˆ2)/(ϵ0*m))ˆ0.5≈20eV, were n–the free-electron density. The energy-loss function was expressed by the complex dielectric function ϵ=ϵ1+iϵ2, where ϵ1–was characterized the polarizability of the electron system, and ϵ2 described the measure for absorption occurring in the electron system. The plasmon loss energy corresponded to value ϵ1=0, determined by the Kramers-Kronig transformation.

The energy of oxygen ion was chosen to modify the NbN thin film not to the full depth- to keep bottom layer close to the substrate in virgin state. The free-electron density have been measured in the modified (upper) region of the film and at the bottom region. It was shown that, with increasing of irradiation dose, the free-electron density decreased from 3.35*10ˆ29 to 2.65*10ˆ29mˆ-3 for bottom region and from 1.55*10ˆ29 to 1.36*10ˆ29mˆ-3 for upper region, which was caused by replacing nitrogen atoms by oxygen ones and transformation of superconductive NbN into insulator Nb2O5 under irradiation.

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High-temperature annealing effects in carbon ion irradiated α-KY(WO4)2

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KY(WO4)2 has gained interest in recent years as an excellent gain material for the realization of integrated optical amplifiers [1] and lasers [2], due to the high absorption and emission cross-section of rare-earth ions doped in it, and its capability of supporting high rare-earth ion doping concentrations [3]. Swift carbon ion irradiation [4] is currently being investigated as a method for the fabrication of high-contrast waveguides in KY(WO4)2 by inducing a damage-related, graded refractive index profile in the crystal. An annealing step needs to be introduced after irradiation to reduce scattering losses in the optically guiding region of the crystal. In this study, the effect of high-temperature (above 450∘C) annealing of irradiated KY(WO4)2 has been investigated using a combination of micro-Raman, SEM and refractive index measurements. Non-permanent damage is almost fully recrystallized after annealing above 450∘C. However, in the regions in which the amorphization threshold is exceeded, micro-Raman and SEM measurements show the conversion of the amorphous layer into a polycrystalline structure, with distinctively different characteristics from α-KY(WO4)2. The ion fluence and annealing temperature can therefore be used to tune the refractive index contrast in the range of 0 to 0.2 and the shape of the refractive index profile.

Figure 1: SEM images of 550∘C annealed 12 MeV carbon irradiated KY(WO4)2. Energy selective backscattering (a) indicates the presence of a crystalline structure at 4.5 μm depth surrounded by partially damaged KY(WO4)2, while scattered electron imaging (b) shows the difference in crystalline structure.

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Novel Experimental Investigations on Radiation-Enhanced Diffusion in Insulators

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Radiation-enhanced diffusion (RED) can be several orders of magnitude faster than thermal diffusion and allows atomic movements and the ensuing modifications of materials properties at temperatures where they are usually inexistent (corrosion and oxidation, deformation, phase transitions, grain boundary segregation, etc.). Nowadays, the use of insulators in nuclear industry is important since it concerns critical points (e.g. radioactive waste storage glasses, nuclear fuel) and will be massive in the future (e.g. matrices for radioactive waste burial or transmutation, insulators and diagnostic windows for fusion reactors, nuclear fuel, fuel cladding, reactor structure elements, etc.). While RED is well documented and understood in metals, it is largely unexplored in inorganic insulators. The rational understanding and control of the properties of current and future materials of nuclear industry thus require a fundamental understanding of RED in ceramics.

We initiate experiments on dedicated samples allowing not only the investigation of volume RED but also grain boundary RED. This is of crucial importance since most of materials are and will be polycrystalline or composite with a high density of inter-phase or grain boundaries (e.g. nano-ceramics, fiber matrices). For instance, Mg2SiO4 olivine bi-crystals coated with Ni2SiO4 olivine thin films are irradiated at high temperature in order to measure the enhancement of Ni2+↔Mg2+ inter-diffusion between the film and the bi-crystal, in volume and at grain boundary.RED was evidenced during preliminary experiments using 12-MeV-C ion beam at GANIL, especially at grain boundary where the enhancement appears greater than in volume.

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Zirconia ceramics processing by intense electron and ion beams

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Processes zirconia ceramics properties modification under intense electron and ion beams action are investigated.

Experimental method. Zirconia ceramics was sintering by thermal method. The specimens were irradiated in vacuum. For electron processing we used electrons beam having the following parameters: =15 keV, current density per pulse – 18 A/cm2, pulse duration – 50 μs, and pulse repetition rate – 0.1 Hz. For Ion treatment we used C+ ion beam with the following parameters: energy of accelerated ions, 200 keV; current pulse duration, 100 ns; and pulse current densities, 40 and 150 A/cm2.

Experimental results. The effect of electron beam on the structural state of near-surface layers of composite ceramics of ZrO2 (Y) – Al2O3 with different levels of porosity is investigated. It is shown that electron-beam treatment leads to melting and subsequent crystallization of ceramic near-surface layer thickness of 30 – 40 μm. SEM analysis of the microstructure surface and cross section of the modified electron beam layers of ceramic samples was carried out. It is shown that in the irradiated surface layer of all the types of ceramics pores and grains of corundum phase are practically absent. It was found that irradiation by electron beam of ceramics material results in decrease of grain size and formation of texture in near-surface layer. It is shown that the surface layer modified by an electron beam is characterized by elevated microhardness as compared with the initial state.

Modification of the structural phase state of the surface layer of 97ZrO2–3Y2O3 (mol %) zirconium ceramics irradiated by high-power pulsed beams of carbon ions is revealed using X-ray phase and SEM analysis. The analysis of roentgenograms indicates efficient formation of the high-temperature cubic modification of zirconium dioxide. The study of the depth distribution of oxygen ions using the secondary ion mass spectroscopy yields deficit of oxygen in the surface layer of the irradiated ceramics. A violation of the oxygen stoichiometry leads to a significant (by several orders of magnitude) increase in the conductivity of the samples under study. Mechanical characteristics of the zirconium ceramics are determined after processing with high-power pulsed beams. It is shown that the ion processing of the ceramic materials leads to a decrease in the mechanical characteristics of the surface layers (micro- and nanohardness and Young modulus).

*Speaker

Stabilization of nitride phase upon Swift Heavy Ion irradiation of 100 MeV Au8+ ions in Si rich a-SiNx:H thin films

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Amorphous hydrogenated silicon nitride thin film are used for a broad range of applications such as LEDs, non-volatile memories [1].It has also led to the interest in Si-QD's embedded in dielectric matrix, which provide passivation to Si QDs and also the ability to tune the photoluminescence (PL). Recently enormous attention has been paid to the silicon nanoparticles embedded in silicon nitride matrix, which show relatively lower barrier for carriers than those of silicon oxide making it a better candidate for photonics and photovoltaics devices. This also opens up the possibility of fabricating silicon based optoelectronic devices such as tandem solar cells [2]. The general recipe to procure Si nanostructures embedded in Si3N4 is to grow Si rich amorphous hydrogenated Silicon Nitride (a-SiNx:H) followed by post deposition treatments. In this study Si rich a-SiNx:H thin films grown by Hg sensitized Photo-CVD were irradiated using 100 MeV Au8+ ions (dominant electronic energy loss regime) with various fluences of 1×1011, 5×1011 and 1×1012 ions/cm2. The ion beam and materials interaction is understood with the help of Thermal spike model [3]. We present a detail study of emanate modifications in properties upon Swift Heavy Ion (SWI) irradiation on Si rich a-SiNx:H. In order to explain the effect of irradiation on bonding configuration and composition of the thin films Fourier transform infrared spectroscopy (FTIR) and X-ray photoelectron spectroscopy (XPS) will be discussed in particular. XPS and FTIR study shows the stabilization of silicon nitride phase upon irradiation. FTIR depicts increase in Si-N bond density upon irradiation also decrease in Si-H bond density was observed which shows support the out-diffusion of hydrogen from lattice upon irradiation [4]. Also a significant change in reflection minimum and refractive index of films upon irradiation towards lower wavelength region is observed, which signifies the increase refractive index in films upon irradiation, ellipsometry also confirms the increase in refractive index of films from 2.02 to 2.74 upon irradiation which implies the dominate nitride phase upon irradiation .

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Desorption kinetics of ultra thin NaCl films on Ag(001) upon electron irradiation

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Electron-induced modification of alkali-halide bulk crystals has been widely investigated, mostly using Auger electron spectroscopy, low-energy electron diffraction, and scanning tunneling microscopy. At primary electron energies typically less than 10 keV, electron irradiation is known to induce layer-by-layer alkali halide desorption, through a mechanism that involves the creation of halogen atom vacancies in the bulk, followed by their migration to the crystal surface, and the agglomeration of alkali metal atoms at step edges. Comparatively, the effects of electron irradiation on thin alkali-halide films have rarely been considered; in particular, the case of *ultra-thin* alkali-halide films composed of one or two monolayers, grown on fcc metals has never been addressed. This is all the more surprising since such alkali-halide films are increasingly used as spacers to electronically decouple organic molecules from metallic substrates in atomically controlled systems for single molecule spectroscopy measurements.
In the ultra-thin film case, the limited amount of reactants and the interactions with the substrate are crucial, leading to different reaction kinetics, compared to the bulk crystal or thick film case. The outcomes may be different too, since the products of alkali-halide dissociation may adsorb or even react with the metallic substrate, whereas on bulk crystals and thick films the dissociation products inevitably adsorb on the same alkali-halide material.
Here, we report on the desorption of ultra-thin NaCl films grown on Ag(001) upon electron irradiation using low energy electron diffraction (LEED) and Auger electron spectroscopy (AES), with primary electron energies of 52-60 eV and 3 keV, respectively. LEED and AES are used both to modify the NaCl films and to investigate the reaction kinetics and the outcome of any modification. We observe that Cl depletion follows first-order reaction kinetics, in contrast with previous studies on thick NaCl films and bulk crystals. Na atoms produced from NaCl dissociation diffuse to bare areas of the Ag(001) surface, where they form Na-Ag superstructures that are known for the Na/Ag(001) system. A model for electron-induced desorption of ultra-thin alkali-halide films from metallic surfaces is proposed, and future applications in the production of nanoscale chemical templates are discussed.

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Investigating radiation damage in inorganic 2D materials caused by accelerated helium ions

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Recent discovery of graphene has opened a new research field exploring a variety of exceptional properties of this as well as of many other two-dimensional (2D) materials [1]. Currently, 2D-based technology is proposed for various applications, including flexible electronics with potential use in nuclear environments, e. g. as radiation dosimeters [2, 3]. Furthermore, the study of radiation effects is valuable for 2D-based electronics and sensors to be used in outer space, where a significant exposure to energetic ions may occur. Additionally, focused ion beams represent one of the most promising approaches for etching and patterning of 2D compounds. Ionising radiation introduces structural defects in 2D materials [4-6] and provides a versatile tool for manipulating their physical properties. While the interaction of particle radiation and solid compounds has been well studied, their effect on single-layer materials is expected to be quite different from that of bulk materials.
Here we experimentally investigate the mechanisms of alpha radiation damage in the transition metal dichalcogenides, such as MoS2 and WS2. To contrast the properties of few-layer vs. bulk materials, MoS2 and WS2 have been irradiated in liquid-phase exfoliated form and in as-received bulk condition. The extent of radiation damage in these materials has been studied as a function of a variable adsorbed dose at constant ion beam energy (5.5 MeV). Irradiated samples have been characterised using FTIR Spectroscopy, Raman Spectroscopy, Scanning Electron Microscopy, Energy Dispersive X-Ray Spectroscopy, Atomic Force Microscopy and Transmission Electron Microscopy. This work represents the initial step of our endeavour to understand fundamental mechanisms of radiation damage in inorganic 2D materials.

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Emission of the ferrocene molecules encapsulated in single-walled carbon nanotubes by X-ray irradiation

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Single-walled carbon nanotube (SWNT) is hollow material that can encapsulate various molecules. Hence, there are proposals for utilising SWNT as a molecular arrangement template or a carrier of Drug Delivery System (DDS). Although the encapsulations of various guest molecules in SWNT have been reported, there are few studies on the extraction of the guest molecules from SWNTs. Previously, we reported that X-ray irradiation of SWNT induces the formation of lattice defects efficiently in SWNT and that the structural modification of SWNT is triggered by X-ray induced defect formation. [1, 2] The X-ray induced defect formation of SWNT would be utilized for extraction of the molecules encapsulated in SWNT. In the present paper, we report the results of the study of the X-ray irradiation effect of SWNT filled with ferrocene (Cp2Fe) as a model material for confirming the feasibility of our proposal. We concluded that X-ray irradiation reduced the Fe concentration of Cp2Fe-filled SWNT (Cp2Fe@SWNT). The result showed that X-ray irradiation triggered release of guest molecules encapsulated in SWNT.

In order to prepare Cp2Fe@SWNT, SWNT thermally treated for removing end caps was sealed with the powder of Cp2Fe in a glass tube under vacuum and annealed at 200 ^{o}C by 12 hours. The Cp2Fe@SWNT thus prepared was irradiated by 1.2 keV X-ray in an evacuated chamber. Raman scattering spectra of the sample at each step in the procedure were measured by a conventional microscopic Raman scattering spectrometer with the probe laser of 532 nm (JASCO NSR-3100). The Fe concentration of the samples was evaluated by energy dispersive X-ray spectrometry (EDS) equipped with aconventional scanning electron microscope (JEOL JEM-7610F). The Cp2Fe@SWNT showed radial breaking modes (RBM) shifted to higher wave-number side from that of pristine SWNT by 5 cm-ˆ{1}. While X-ray irradiation of Cp2Fe@SWNT resulted in an increase of the intensity of the defect-related band, D band, in the Raman scattering spectrum, the RBM peak position was not changed. After washing the irradiated sample by diethyl ether, which is a good solvent of Cp2Fe, the EDS spectrum was measured and compared with the sample without irradiation. We found that the X-ray irradiation decreased the intensity of the peak around 6.4 keV, which is attributed to Fe. The decrease of the peak intensity corresponded to the Fe concentration change from 0.24 % to 0.15 %. The result shows that the X-ray irradiation leads to partial emission of Cp2Fe encapsulated in SWNT. The irradiation gave an inconsiderable change of the RBM peak shift, which is induced by the encapsulation. This is consistent with the result that only a quarter of the Cp2Fe molecules were released.

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Nanostructures formed in single-walled carbon nanotube by thermal annealing after X-ray irradiation

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Previously, we reported that X-ray irradiation leads to formation lattice defects in hexagonal carbon lattice of SWNTs efficiently. [1] Since the recovery of the X-ray induced defects was well explained by second order kinetics, the defect is a distant pair of a vacancy and an interstitial carbon atom. [2] Thermal annealing of the X-ray irradiated SWNTs activates the diffusion of the interstitial atoms and also vacancies, and would form new nanostructures in SWNT as a consequence. In this context, we have studied the effects of the thermal annealing of the X-ray irradiated SWNTs. In the present paper, we describe the results of the Raman scattering spectroscopic study of the products of the annealing of the X-ray irradiated SWNTs synthesized by a conventional alcohol chemical vapor deposition and by CoMoCat method and discuss the origin of these peaks.
SWNT films on silicon substrates were irradiated by 1.2 keV X-ray in an evacuated chamber. The irradiated samples were annealed at several temperatures in argon atmosphere. Raman scattering spectra of the samples before and after the irradiation and also after the annealing were measured by microscopic Raman spectrometers with the probe lasers of 532 nm and 633nm. The X-ray irradiation leads to the enhancement of the defect-related peak, D band, in the Raman scattering spectra, and the following thermal annealing reduced the intensity of the D bands. In the case of the conventional CVD SWNT films, the thermal annealing gave rise to increase of a Raman scattering peak at 1870 cmˆ{-1}, in addition to the D-band intensity decrease. The peak was characterized by the probe-laser energy dependence of the peak intensity Comparing the result with the previous reports, we concluded that the peak is ascribed to one-dimensional carbon chains. [3] Meanwhile, in the case of the CoMoCat-SWNT films, a peak at 1130 cmˆ{-1} but not the 1870 cmˆ{-1} peak was grown by the annealing. The 1130-cmˆ{-1} peak started to grow at a lower temperature than that found in the 1870-cmˆ{-1} peak in the CVD SWNTs. The peak position shifted to higher wavenumber side with the increase of the Raman probe laser energy. The dependence of the peak position on the probe-laser energy is almost identical to that of the peak due to poor quality CVD-diamond. [4] The CoMoCat SWNT has a larger number of preexisting defects than the conventional CVD SWNT. The 1130-cm-1 peak is conceivably relevant to the bond alternation around the preexisting defects.

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Mechanical properties of swift heavy ion irradiated Y3Al5O12 single crystal

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Yttrium aluminium garnet Y3Al5O12 (YAG) is used in several applications due to its optical and mechanical properties. It is also inert matrix fuel candidate due to its radiation resistance. In our previous work, radiation damage induced in this material by swift heavy ions and reactor neutrons irradiation were investigated using numerous techniques, spectrophotometry UV-visible, photoluminescence, X-ray diffraction (XRD), profelometry and atomic force microscopy (AFM) techniques [1-3]. In the present experiments, we used nano-indentation technique to study the nanomechanical properties evolution of Y3Al5O12 under swift heavy ions irradiation.
The irradiations were performed at GANIL, accelerator, Caen, France with 561 MeV 51Cr, 90 MeV 51Cr ions, 278 MeV 128Te, 193 MeV 208 Pb and 885 MeV 238U ions beams. The electronic stopping power Se range from 6 keV/nm to 46 keV/nm.

The nano-indentation tests reveal that both hardness and Young's modulus decreases with fluence. It is found that for approximately the same displacements per atom (dpa) value, the Young's modulus decreases linearly with the electronic stopping power. Taking into account Sickafus et al. [4] findings, where the elastic modulus, is a sensitive indicator of radiation-induced phase transformations, and from the comparison with XRD, profilometry and AFM measurments, we conclude the swift heavy ion irradiation induces amorphization of Y3Al5O12 single crystal.

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Structural and functional modifications of rubbers induced by ion irradiation

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Ion irradiation offers multiple possibility to modify structural and functional properties of various solids. The ever continuing search for new materials having new, specifically designed properties becomes more and more important. Ion beams have been used first for doping of semiconductors, then modification of metals, ceramics and, finally, polymers. Among this last class of materials elastomers, commonly known as rubbers, are potentially very attractive objects for ion beam modification. First of all elastomer sealings are very commonly used in almost any mechanical construction. Secondly, currently used elastomers were optimized mainly for their bulk properties: resistance to various fluids, temperature and oxidation. The drawbacks of them are mainly high friction coefficient and sometimes too low wear resistance. These properties are surface-related, hence the obvious solution is to use an appropriate method of upper layer modification, what should allow for combination of most advantageous bulk properties with improved surface characteristics.

The main objective of the current work is to develop method of surface modification of elastomers allowing to improve their mechanical properties. In the presentation we will discuss the structural modifications induced by ion beams in rubbers, massive hydrogen loss is the main structural effect of irradiation. Then, surface morphology comparison of pristine and ion-irradiated elastomers will be discussed. Finally, we will present the results of the analysis of functional properties: hardness, friction coefficient, wear resistance and surface wetteability. A short discussion of the possibility to reinforce elastomers by using graphene filler will also be included. The presentation will be concluded with some examples of practical applications of new sealings.

*Speaker

Proton irradiation induced radiation effects in dose gels

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Radiation processing of dose gels using high energy particle beams plays an important role in development of the new dosimetry methods for industrial and medical applications [1,2]. Typical gel dosimeter (dose gel) consists of water, gelatin, monomers and a cross-linker co-monomer. The solution may contain also an antioxidant playing the role of oxygen scavenger and some dose sensitizers enabling radiation induced polymerization of dose gels under normal atmospheric conditions.
The aim of this work was to investigate the radiation induced effects in polymerized dose gel structures after the low dose proton irradiation. Three different batches of experimental, modified gels: nPAG (acrylamide based), nMAG (methacrylic acid based) and VIPET (N-Vinylpyrrolidone based) were prepared following routine procedure of hydrogel fabrication [3,4]. Experimental gel samples were irradiated in proton accelerator IBA PROTEOS C230 to doses from the interval of 0.5Gy to 5.0 Gy at OncoRay Clinic in Dresden.

Characteristics, related to the proton irradiation induced polymerization processes in gels (monomer and crosslinker consumption rates, polymerization rate) and also processed gel structure and its physical/chemical properties were investigated applying Raman spectroscopy and UV-VIS spectrometry. Taking into account that polymerization processes in dose gels depend on the initial gel content and irradiation conditions, the characteristics of post irradiated dose gel structures strongly relay on irradiation dose and dose rate.

Investigated nPAG, nMAG and VIPET gels recorded different radiation sensitivity to proton irradiation, however it was possible to calibrate at least their optical characteristics according to the applied irradiation doses.

Performed investigation revealed that acrylamide and methacrylic acid based gels were more sensitive to low doses, than VIPET, showing a potential of nPAG, nMAG dose gels in low dose clinical proton dosimetry.

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Free standing dose gels: first approach to ionizing radiation based 3D printing

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The interest to application of 3D printing issues is growing up, since this technique might be used for the fabrication of differently shaped and very complicated objects, including medical phantoms and applicators. However, to produce any shape one needs to have 3D printer, object related printing algorithm and printing material, which is not tissue equivalent.

Nearly tissue equivalent dose gels are known and used for a long time in high energy external radiotherapy for *in situ* dose assessment and as the phantoms - tumour imitators, for securing quality of the treatment procedure. When irradiated to high energy beams, free radicals created in the gel induce polymerization within restricted region thus forming volumetric shapes of the polymerized gels. The properties of polymerized gels depend on chemical components and their concentrations as well as on gel production technology and irradiation conditions. It is needed to notice that polymerized gel shapes are created inside the tightly closed vessel and are surrounded by gelatine matrix. Assessment of the created polymerized gel shape and dose distribution in it is usually performed taking the whole gelatine volume into consideration, thus contributing to the enhancement of measurement uncertainties and limiting their application in clinical field.

The aim of this work was to develop ionizing radiation based 3D printing method for fabrication of nearly tissue equivalent free standing 3D dose gel medical phantoms (tumour imitators) having the size and shape of a real tumour. (Concept of this method was firstly proposed in our previous publication in 2015 [1].

Special dose gels (patent is pending) were used as printing material" for the processing of free standing dose gel shapes. There was no any request for a special 3D printing equipment or development of the additional object formation algorithm. Varying dose gel content and selecting radiation processing parameters of radiation treatment facility in accordance with a pre-planned cancer patient irradiation procedure, 3D shapes of the polymerized gel volume, corresponding to the real size of the irradiated (treated) volume were fabricated (3D printing) in gelatine. Polymerized gel volume (tumour imitator) representing free standing object was easily separated from the gelatine, thus making direct measurements of dose gel physical and chemical characteristics possible. Investigation results on these issues will be provided and discussed.

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Modification of silver-carbon nanocomposite film by SHI irradiaton

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Carbon-based thin films have attracted a lot of attention as they possess many useful properties. It is well established that macroscopic properties of carbon film strongly depend on relative content of sp3- and sp2-hybridized carbon bonds and doping of the carbon matrix. Hence, one can tune film properties to some particular needs by choosing proper growth technique. Several film preparation techniques were successfully developed to grow carbon films. Irradiation of DLC film with swift heavy ions (SHI) results in the formation of conducting graphitic nanowires of about 8 nm in diameter embedded within the insulating diamond-like matrix.
Films were grown on highly conductive P-implanted (100) Si substrate using single charged filtered C60 beam (99.5 % purity, NeoTechProduct, St. Petersburg, Russia) accelerated to 3 keV. Ag was simultaneously evaporated from nearby placed effusion cell in order to get 1 to 15 at% composite. Nanocomposite films with Ag nanoparticles (NPs) formed inside and on top of the doped samples were obtained. Films were then irradiated at IUAC at room temperature with 100 MeV Ag7+ ions to the fluence 2*1010 cm-2. All films became more conductive after SHI irradiation. Silver NPs fully disappear from the film surface, whereas are still present in the matrix. SEM shows that silver clusters became smaller in size. C-AFM investigations reveal formation of tracks with metallic type of conductivity.
This work was supported by Russian RFBR (grant 17-58-45142) and DST of India.

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Single and molecular ion-irradiation-induced effects in GaN

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Irradiation-induced effects in Si doped wurtzite (0001) GaN bombarded with atomic (B, F, Ne, P, Ag) and molecular (BF2, PF2, PF4) ions with an energy of 0.6-2.1 keV/amu were studied. Irradiation was performed 7degr off the (0001) direction to minimize channeling at 300 K. Samples were investigated by RBS/C and AFM techniques; photoluminescence (PL) spectra as well as time resolved PL decay integrated over 360 nm band were also measured. As it follows from the experiments, molecular ion irradiation produces thicker surface amorphous layer compared to its constituent atomic species, whereas almost equal amount of damage appears in the bulk. Heavy Ag ions, having approximately the same mass as the PF4 molecule, are even more efficient in bulk damage formation than both light atoms and molecules. The thickness of the surface amorphous layer produced by Ag ions exceeds that of light ions, but it is below the one produced by molecular PF2 and PF4 ions. Surface roughness and height of the step between virgin and irradiated areas of the target shows threshold behavior.
Irradiation efficiently suppresses PL intensity and shortens PL decay time. At relatively low fluence, molecular ions are more efficient in PL quenching than any constituent light atomic ions. Heavy Ag ions are most efficient in PL quenching. In all cases PL decay time goes to almost same value of 40 ps with the dose increase. We explain decrease of this time in terms of surface recombination of photo-excited carriers on the interface between damaged and undamaged regions.
Work was partly supported by RFBR (grant 17-52-45145) and DST of India. Value is Irradiation-induced

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Dosimeter Properties of C Ions Doped Al2O3 Transparent Ceramic

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Dosimeter materials are often utilized as periodic radiation monitors for people working in the radiation environment to monitor the cumulated dose, and most dosimeter materials are insulators with a wide band gap. Aluminum oxide doped with carbon (Al2O3:C) as optically stimulated luminescence dosimeters (OSLDs) are now well established in personal dosimetry, having been already used commercially for almost a decade [1]. In this case, it is known that Al2O3:C powder smashed single crystal emits 410 nm photons caused by F centers with stimulation light at 530 nm. Carbon ions are used to enhance the defect creation due to the charge unbalance because a main emission of Al2O3 is caused by several defects. On the other hand, with advancement of ceramic fabrication techniques, transparent ceramic form of Al2O3 was reported [2]. However, no reports can be found about radiation responses of Al2O3:C transparent ceramic material. We expect to radiation response properties of transparent ceramic superior to these of single crystal since defect amounts of transparent ceramic are generally more than those of single crystal.

In this study, we prepared Al2O3:C transparent ceramics by the spark plasm sintering method. Then, we investigated dosimeter properties of the transparent ceramic samples. In addition, we also studied scintillation properties. Recently, it was pointed out that scintillation and dosimeter are complementarily related in some materials [3, 4] so investigations of both properties are important to understand the luminescence phenomena induced by ionizing radiations.

In the thermally-stimulated luminescence (TSL) glow curves, Al2O3:C transparent ceramic showed glow peaks around 50, 75, 150 and 200 ∘C. Among these four peaks, the glow peak at 75 ∘C was not clearly detected in TSL glow curve of undoped Al2O3; therefore, it is implied that C-doping generated the new trapping center.

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Depth profiles of aggregate centers in LiF irradiated with swift heavy ions

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Depth distribution of F type aggregate centers in LiF irradiated by 0.4÷3 MeV/nucleon C, Ar, Kr, Xe and Bi ions have been studied using laser confocal scanning microscopy (LCSM) and microluminescence techniques. It was found that luminescence signal ascribed to F2 and F3+ centers measured across thickness of irradiated layers correlate with ionizing energy loss profiles at fluences corresponding to ion track non overlapping regime. Direct proportion of the luminescence intensity to the total absorbed dose allowed us to quantify the depth profiles of corresponding color centers knowing their total concentration from optical absorption spectra. Experimental data have revealed that the luminescence yield at high ion fluences is associated with radiative decay of F2 and F3+ centers formed in elastic collisions in the end of range area while their emission in the rest of irradiated layer is totally suppressed due to ion track region interference.

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Comparison of thermoluminescence properties of YAG:Ce after X-ray and UV irradiation

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Thermoluminescence (TL) is caused by the metastable trapping of electrons and holes at defect sites. In UV-induced TL, the trapping process occurs via the photoionization of impurities. However, X-ray irradiation has been proposed to induce TL by causing the migration of electrons and holes to different sites. In this study, we characterized the TL properties of YAG:Ce and compared its TL properties after X-ray or UV irradiation. In addition, we compared the TL properties of YAG:Ce single crystals and transparent ceramic.
The TL glow curves were measured after X-ray or UV irradiation at two different heating rates (1 K/s and 0.1 K/s). The lower heating rate was used for the detailed comparison of the glow curves. The TL spectra were recorded at the peak temperatures of the glow curves using an optical multichannel detector.

A prominent band was observed at ¯˜550 nm in the TL spectra of YAG:Ce single crystals after X-ray or UV (254 nm) irradiation at 450 K. This was attributed to the 5d–4f transition of Ce3+, and suggested that in X-ray- and UV-induced TL, the final stage of the process is the intraionic transition of Ce3+.
Three peaks were visible at 380, 440, and 540 K in the TL glow curves of YAG:Ce single crystals after X-ray or UV irradiation. The peak temperatures of the curves were similar in both samples. In the X-ray-irradiated samples, electrons and holes were trapped separately at different sites. In contrast, UV irradiation induced photoionization of Ce3+ ions, resulting in the formation of Ce4+ ions. This process is similar to systems in which holes are trapped at Ce3+ ions, forming Ce4+. When the differences in the trap processes of X-ray- and UV-induced TL are accounted for, the glow curves are similar. This indicates that the hole trapping sites formed during X-ray irradiation are Ce3+-related centers.

*Speaker

Scintillation and Dosimeter Properties of Ca2+-doped MgO Transparent Ceramics

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MgO is a common insulator material with a wide band gap, and have attracted much attention from the viewpoints of a simple oxide system with a rocksalt (fcc) structure and structural defects, producing a variety of optical and radiation detection properties [1-3]. The dosimeter properties of undoped MgO were discovered in the 1970s under X-ray exposure [1]. Two thermally stimulated luminescence (TSL) glow peaks were found around 90-100 and 140∘C, when MgO powder was irradiated by X-rays, γ-rays and UV lights [1]. Recently, dosimeter applications of MgO have been actively since it shows a wide range of dose response from 0.1 mGy to 1 Gy under X-ray exposure [3].
We focused attention on Ca2+ ion because Ca and Mg are the same group elements and the radius of Ca2+ ion is bigger than that of Mg2+ ion; the former is 9.9 nm and the latter is 6.6 nm. We thought if Ca2+ ion is added to MgO structure, and the difference of these radiuses will produce additional lattice defects which will improve the dosimeter properties since the defects play an important role to remember the initial radiation dose as form of carrier trapping. Until now, the physical, catalytic or optical properties of Ca2+-doped MgO (Ca2+:MgO) powders [4], nanocrystals [5] and transparent ceramics [6] were reported, but radiation detector properties such as scintillation and dosimeter properties of them could not be found. So in this study, we synthesized Ca2+:MgO transparent ceramics and evaluated their scintillation and dosimeter properties.

MgO transparent ceramic samples doped with Ca2+ ion (0.001, 0.01 and 0.1%) synthesized by a SPS method were visually transparent. Under UV lamp excitation (254 nm), a bright yellow-green emission was seen by naked eyes from all samples at room temperature. We detected the TSL glow curves of Ca2+-doped MgO samples after 0.54 Gy X-ray exposures by using Nanogray TL-2000. All Ca2+:MgO samples showed a sharp single glow peak around 130 ∘C. In order of decreasing Ca2+ ion concentrations, the TSL peak shifted to high temperature so in these results, 0.001 % Ca2+:MgO samples showed the highest stability among all samples. On the other hand, 0.1% Ca2+:MgO showed the highest TSL intensity, and the storage ability of carriers was enhanced by Ca-doping as we expected. We are also planning to research scintillation and other dosimeter properties such as optically stimulated luminescence.

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The effect of X-ray irradiation on the magnetic properties of ReBa2Cu3Oy (Re = Y, Nd, Gd)

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Introduction

Studies on superconductors have become more popular since the discovery of high-Tc cuprate superconductors having a Tc above the liquid nitrogen temperature (77 K).[1] The discovery of photo-induced superconductivity on thin films of high-Tc cuprate superconductors using visible laser irradiation has enabled the enhancement of Tc and the doping of carriers without any chemical processes.[2] This suggests that irradiation of ionizing radiation brings about a similar change not only in thin films, but also in bulk materials because of its high permeability and energy.

In this work, we used the change in magnetic susceptibility to study the effect of X-ray irradiations, which are known to have higher energy and permeability, on bulk ReBa2Cu3Oy (ReBCO).

Experiment

We synthesized ReBCO (Re = Y, Nd, Gd) using a solid-phase method and fired its pellets for 10 h at 900∘C under atmospheric pressure, and annealed under various conditions. The samples were irradiated with X-ray (Cu K-α) at room temperature. The Cu X-ray tube was operated at 40 mA and 40 kV.

For measuring the magnetic susceptibility, SQUID was used with an applied magnetic field of 5 Oe and a temperature range of 10–100 K (the sweep rate: 0.5 K/min).

Results and Discussion

The magnetic susceptibility of YBCO fell sharply at _˜90 K. This suggests that YBCO shows strong diamagnetism corresponding to the superconducting state below 90 K. All values of the Tc were almost identical and did not change even after irradiation. The magnetic susceptibility just after irradiation is lower than before irradiation, and the temperature dependence of the magnetic susceptibility after 3 h was similar to that of the original state. The results show that in YBCO, X-ray irradiation enhanced the superconductive properties and the effect was maintained for at least 3 h.

*Speaker

In NdBCO, the magnetic susceptibility fell sharply at _˜50 K. This suggests that NdBCO shows diamagnetism corresponding to superconducting state below 50 K. All values of the Tc were almost identical and did not change even after irradiation, similar to YBCO. The magnetic susceptibility just after irradiation was higher than before irradiation. The results show that in NdBCO, X-ray irradiation weakened the superconductive properties.

In the case of GdBCO, the trend in Tc and magnetic susceptibility were similar to that of YBCO.

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Kinetics of dimer F2 - type center annealing in ionic solids

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Primary radiation defects in ionic solids consist of Frenkel defects-pairs of anion vacancies with trapped electrons (F-type centers) and interstitial ions. Upon temperature increase after irradiation, the electronic F-type centers are annealed due to recombination with mobile interstitials. Analysis of the recombination (annealing) kinetics allows us to obtain important information on the interstitial migration (e.g. in corundum [1] and alkali halides [2]). At high radiation doses more complex dimer F2-type centers are observed in several charge states, which are well distinguished spectroscopically [3].
In this paper, we analyzed available experimental kinetics of the F2-type center annealing in a wide temperature range (300-1000 K) in three different neutron-irradiated ionic solids: MgO, MgF2 and Al2O3 (corundum) [4]. The phenomenological theory takes into account the interstitial ion diffusion and recombination with the F2-centers as well as mutual sequential transformation with temperature growth of three types of experimentally observed dimer centers: F2 (1); F2 (2), F2 (3) (which differ tentatively by charges with respect to the host crystalline sites : 0. +1, +2).

As the result, the relative initial concentrations of three types of electronic defects before annealing are obtained, along with energy barriers between their ground states and the relaxation energies [4]. Surprisingly, these parameters are similar in three different types of materials. The results are compared with available experimental data and theoretical calculations.

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STRUCTURAL DEFECTS CAUSED BY SWIFT IONS IN FLUORITE SINGLE CRYSTALS

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Pure and doped with cation impurities CaF2 crystals (the gap of 12.2 eV) are used for various applications: as lenses and windows in vacuum ultraviolet laser lithography, as laser media, radiation detectors and dosimeters, elements for navigation/orientation. Oxygen contamination and structural defects induced during irradiation strongly affect the functionality of fluorite. Therefore, the clarification of defect creation mechanisms and the increasing of radiation resistance are of fundamental importance.

The paper presents a comparative study of radiation damage in oxygen-free CaF2 single crystals induced at 295 K by swift heavy ions (SHIs: Xe132 ions, 0.23 GeV, e14 Xe/cm2, ion range 18 mm, DC-60 cyclotron in Astana or Bi209, 2.38 GeV, 3e11 Bi/cm2, 90 mm, UNILAC accelerator in Darmstadt) and 100-keV hydrogen ions (KIIA 500 kV implanter, Helsinki). The damage was analyzed via radiation-induced optical absorption (RIOA) measured from 1.4 to 10.5 eV in a stepwise regime after preheating of the irradiated samples to different temperatures (295-1100 K). Protons caused the damage of _˜0.2 dpa within a _˜0.8-mm irradiated layer, while SHIs spent _˜95% of their energy on the formation of electronic excitations (EEs) along cylindrical tracks (> 20 keV/nm).

Similar to additively colored CaF2, a wide RIOA band at _˜2.2 eV in ion-irradiated samples is related to different electron F-type aggregates (without single F centers) and Ca-colloids. The main annealing stage of these centers occurs at 480-580 K due to the release of mobile holes from trihalide quasi-molecules and their aggregates (RIOA at _˜6-7 eV) and is accompanied by thermally stimulated luminescence. On the other hand, a complex RIOA band peaked at _˜9.8 eV was detected for the first time only in the crystals irradiated with SHIs (but not with protons or 50-kV X-rays). The band is related to EEs localized near SHI-induced structural 3D defects stable until the disordering starts in an anion sublattice (_˜1100 K). These defects involve many host ions, impede the movement of dislocations to the surface, facilitate the cracking and brittle destruction of irradiated crystals and are tentatively created via a joint action of the impact (knock-out, acoustic shock waves) and nonimpact mechanisms (decay/recombination of EEs) under SHI-irradiation. Notice that Bi ions (nuclear spin 9/2, electrical quadrupole moment

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-0.4) cause extremely efficient cracking and fracturing of CaF2 single crystals into pieces with (111) faces.

Insights into the radiation behavior of Ln2TiO5 (Ln = La-Y): based on defect energetics

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First-principles calculations have been performed to study the structural and energetic properties of orthorhombic Ln2TiO5 (Ln = La, Pr, Nd, Sm, Gd, Dy and Y). Both mean and bond lengths increase slightly with increasing Ln cation radius from Dy to La. The calculation results of point defects formation energies suggest that Ln2-Ti antisite defect is the most easily formed defect type for Ln2TiO5 under radiation. The trend of Ln2-Ti antisite defect formation energy of Ln2TiO5 is consistent with the experimental results, which indicates that the formation of Ln2-Ti antisite defect may has a significant influence on the radiation behavior of Ln2TiO5.

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Microstructure damage to Silicon carbide fiber induced by 246 MeV Ar ions irradiation

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Silicon carbide (SiC) fiber possesses high thermal stability, low density, high specific strength, good oxidation-ablation resistance, high specific modulus, especially improved flaw tolerance and non-catastrophic mode of failure [1]. Therefore, silicon carbide fiber is widely used in aerospace, aviation and nuclear industry etc. fields. The irradiation damage that silicon carbide fiber will be subject to is inevitable although it is immune to various environments. In this work, the third generation SiC fibers, with a diameter of about 10 μm, they are irradiated by Ar15.8+ with an energy of 246 MeV at different fluences at LN2 atmosphere. The Ar ions beam was extracted from Heavy Ions Research Facilities in Lanzhou (HIRFL). After irradiation, the microstructure damage of silicon carbide fiber was investigated by means of Raman scattering spectroscopy (Raman), scanning electron microscopy (SEM) and X-ray diffractometer (XRD).
Raman spectra reveal that the β-SiC fibers have strong carbon cluster peaks located at 1363 and 1590 cm-1 and sharp SiC characteristic peaks, they are E2(TO), E1(TO) and A1(LO), centered at 763, 792 and 964cm-1, respectively. Two carbon cluster peaks are near to the D (1332 cm-1) and G (1580cm-1) peaks of C-C sp3 and C-C sp2 hybridization, corresponding to A1g mode of the diamond and E2g mode of the graphite, respectively. Compared with the bulkβ-SiC, three vibration modes of β-SiC fiber exhibit a redshift due to quantum confinement effects. After irradiation, with the increase of the dose, the intensity of all the vibration peaks first decreases gradually and then increases, indicating that the material experiences the recrystallization. SEM analysis shows that the diameter of irradiated SiC fibers first reduces and then increases as the ions fluence rise successively, and finally the irradiated SiC fibers were broken. XRD curves display the (111), (200), (220), (311) and (222) crystalline plane ofβ-SiC [2] and with increasing ions fluence, diffraction peaks FWHM of all crystalline planes first decreases and then increases due to the occurrence of recrystallization.

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He ION IRRADIATION EFFECTS ON THE MICRO-STRUCTURE AND MECHANICAL PROPERTIES OF α-Al2O3 FILM PREPARED BY SAPS

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α-Al2O3 films was prepared on China Low Activation Martensitic steel CLAM substrates by supersonic atmospheric plasma spraying (SAPS). The preparation method was adopted for the low substrate temperature and high deposition efficiency of the SAPS and for the fine microstructure and high bonding strength (52 $\pm$ 4 MPa) of the SAPS-coating. The obtained Al2O3 films consisted of α-Al2O3 mostly and γ-Al2O3 partly. The samples were then subsequently irradiated by 60 keV He+ ions at ion doses range from 5×1019 to 5×1022 He+/m2 at ambient temperatures. The irradiation impact on the microstructure and mechanical properties of the α-Al2O3 films were investigated. He bubbles and radiation-reduced defects among the α-Al2O3 films were observed after the irradiation, and they got more obviously at raised irradiation doses. The grain size of the α-Al2O3 films varied with the irradiated doses, thus resulted in the density variation. The radiation hardening appeared after the radiation, which may resulted from the radiation-reduced defects mainly and from He bubbles partly. The results experimentally show the resistance of the α-Al2O3 films to radiation damage.

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Tracks induced by high energy mono-atomic and cluster ions in fluorapatite

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Durango apatite, containing trace amounts of uranium isotopes, has been employed as an age-dating standard in fission-track laboratories. In this work, we have compared the latent tracks produced by high energy mono-atomic and cluster ions. The single-crystals of Durango fluorapatite (Mexico) were exposed to mono-atomic ion beams of Cr, Kr, Pb, Bi and U of energy GeV provided by the HIRFL accelerator, Lanzhou and the LINAC accelerator of GSI, Darmstadt, respectively. The cluster ions of C60 were provided by the tandem accelerator of IPN, Orsay. The irradiations were performed at room temperature, applying fluences between 1×10ˆ10 and 1×10ˆ13 ions/comˆ2. The ion tracks were observed by transmission electron microscopy (TEM) and scanning probe microscopy (SPM). A detailed analysis of the Raman spectra as a function of the ion fluence and the electronic energy loss (dE/dx)e will be presented.

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Damage evolution behavior in YAlO3 crystal irradiated with low-energy and swift-heavy ions

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During ion irradiation process, irradiated ion with low energy will mainly interact with target nuclei and lose energy via nuclear energy deposition (elastic collision) process, and produce permanent atomic-scale defects in crystal materials; irradiated ion with high energy will primarily interact with target electrons and lose energy via electronic energy deposition (ionization and electronic excitation) process, and produce ion track containing partially or completely amorphous volume in crystal materials based on thermal spike model. In this work, yttrium orthoaluminate (YAlO3) functional crystal samples have been irradiated with respective low-energy (1.0 MeV) Au-ion and swift-heavy (200.0 MeV) Kr-ion to different fluences. The related lattice damage behaviors in YAlO3 crystal induced by respective nuclear or electronic energy losses have been studied comparatively through Rutherford backscattering/channeling spectroscopy, transmission electron microscopy and X-ray diffraction. YAlO3 crystal has also been irradiated with sequential low-energy (1.0 MeV) Au-ion and swift-heavy (200.0 MeV) Kr-ion in order to discuss the effect of intense electronic energy loss on damage production and evolution in pre-damaged YAlO3 crystal owing to the presence of nuclear-energy-loss induced defects.

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Electronic excitation effects on Fe2O3 films by high-energy ions

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Electronic excitation effects on Fe2O3 films by high-energy ions
For better understanding of electronic excitation effects on materials with small bandgap, we have extended measurements to Fe2O3 (hematite) films (bandgap=3 eV). Applying carbon-film (100 nm)-collector method [1], we have measured amounts of Fe in the C-collector as a function of fluence of 198 MeV Xe, 99 MeV Xe and 89 MeV Ni ions with the equilibrium charge. From the slope of Fe amount vs ion fluence with the efficiency fc of C-collector (taken as 0.3, average of fc for Ti, Cu and Zn [2]), total sputtering yields Y are obtained to be 83, 57 and 39 by these ions. Here, stoichiometric sputtering is assumed. It appears that the sputtering yields are much larger than the calculated sputtering yields based on the elastic collisions. We obtained Y=BSen with n=1.3 and B=1.1, Se being the electronic stopping powers. Y(Se=15 keV/nm) is obtained to be 35 and this value is somewhat larger than that of TiO2 with bandgap similar to Fe2O3. Also, we have studied modifications of atomic structure in terms of X-ray diffraction and optical absorption. Electronic excitation effects on modifications of these properties as well as the electronic sputtering will be discussed.

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Ion irradiation effects on WNxOy thin films

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We have investigated ion irradiation effects on modifications of electronic- and atomic-structures of WNxOy films on C-plane-cut-sapphire (C-Al2O3) substrate. Rutherford backscattering spectroscopy (RBS) of 1.8 MeV He+ ions leads to the composition, x=1.1±0.1 and y=0.4±0.2. X-ray diffraction (XRD) with Cu-kα shows a strong peak at the diffraction angle (2
theta) ≈37 º and a weak peak at ≈78 º. These peaks are assigned as hexagonal-WN and no peaks were observed other than WN and C-Al2O3 (2
theta=41.7 º). It is found that the electrical resistivity of unirradiated film (25x10-3 Ωcm) is reduced to 4x10-4 and 2x10-3 Ωcm by 100 MeV Xe ion irradiation at 4x1014 cm-2 and 100 keV N at 1016 cm-2, respectively, and that the resistivity of unirradiated film increases with decreasing temperature from RT to 30 K like semiconductor and irradiated film shows very weak temperature dependence. It also appears that the XRD intensity decreases by more than a factor of 10 under these ion irradiation, and lattice expansion of _˜1% at low ion fluence turns into lattice compaction for further ion irradiation. Optical absorption monotonically decreases with increasing the wavelength from 200 to 2500 nm, implying that the bandgap does not exist in the region of 0.4- 6 eV and the optical absorption at 310 nm decreases by _˜10 % by the ion irradiation.

*Speaker

Channeling study of defects accumulation in Er-implanted ZnO

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In spite of the extensive study over the last three decades, a lack of complete understanding remains on the mechanism of damage buildup in semiconductor compounds. In the majority of compound crystals structural transformations at specific fluencies occur, which can be visualized as steps in the defect accumulation curve. RBS/c technique was typically used for structural analysis of structural properties of ion implanted crystals by many authors. However, over-simplified methods of spectra analysis (two beam approximation) have been typically applied, which preclude insight in the real structure of implanted crystals. The crucial effect occurring upon ion bombardment is the stress mediated plastic deformation. Once the critical ion fluence for plastic deformation is surpassed the subsequent defect annealing is hardly possible. ZnO is a very promising material for semiconductor device applications. In order to tune the optical emission from ZnO into the visible spectral range the optically active centers have to be formed. It is expected that implantation of different REs (rare earth) ions can be used for fabrication of white light emitters. ZnO single crystals were implanted with 300 keV Er ions to fluencies ranging from 1e14 to 5e16 at/cm2 encompassing the region of plastic deformation. Quantitative analysis of the damage has been carried using the Monte Carlo simulation code McChasy. It can differentiate between various types of defects, which allows to follow their evolution as a function of ion fluence. Basing on these observations the model of structural transformations has been conceived.

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Swift heavy ion irradiation inducing climb of dislocations in AlN

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Aluminum nitride (AlN), part of the III-nitride semiconductor family, presents interesting properties for use in deep ultraviolet optoelectronics and in high-power applications [1]. It may be subjected to ion irradiation for achieving n or p doping, or when it is used in radiative environment. For instance for space applications, high energy particles from solar winds and cosmic rays can induce by electronic excitations (electronic stopping power, Se) structural defects that affect the functioning of devices. But AlN had been considered insensitive to Seeffects because of the non-creation of tracks by monatomic Swift Heavy Ions (SHI). Tracks only appear after fullerene irradiations which allow reaching Se values higher than the maximum obtained with monatomic SHI. However, recent studies have shown a huge effect of Se on the creation of point defects in AlN even under the Se threshold for track formation[2].
We address here an indirect observation of a new effect of electronic excitations in point defect production in AlN. Unprecedented climb of screw dislocations after interaction of point defects in irradiated AlN was studied by means of TEM observations (Fig. 1). A detailed analysis after many SHI irradiations demonstrated that point defect creation and/or mobility at the origin of the dislocation climb is ruled by electronic excitations. It happens above an electronic stopping power threshold, whose value is between 8 keV/nm and 17 keV/nm. Above this Se threshold, the dislocation line transformation may result in a zigzag or a helical structure depending on the irradiation fluence.

*Speaker

Analysis of electron and hole trap states in novel storage phosphors: Undoped, Eu-doped, and Ce-doped CsCaCl3 ceramics

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Under irradiation, complementary defects, electron or hole trap centers, are generated in storage phosphors. Subsequently, the trapped electrons can be stimulated thermally and they recombine with holes. The recombination energy is emitted as light called thermally stimulated luminescence (TSL) [1].
The TSL glow curve, which plots the TSL intensity versus temperature, is used to analyze the states of trapped electrons or holes. One of the methods for analyzing TSL glow curves is called the initial rise method, and it is used to determine the trap depth which is the thermal energy required to release trapped electrons or holes [2].

The purpose of our study is to analyze the states of electron and hole trap centers formed in storage phosphors during irradiation. We aimed to determine the trap depths in novel scintillator materials, namely, undoped, Eu-doped, and Ce-doped CsCaCl3 [3]–[5], which are also novel storage phosphors that exhibit efficient TSL.

The undoped, Eu-doped, and Ce-doped CsCaCl3 ceramic samples (1 g) were prepared. All samples were sintered at 673 K under vacuum. The samples were irradiated at room temperature with X-rays (Cu target, 40 kV, 40 mA) at 45 Gy and the TSL glow curves were measured at a heating rate of 0.5 K/s.

The TSL glow curve of undoped CsCaCl3 had two peaks at 360 and 400 K and some shoulders around of 380, 460, 520, and 560 K. The calculated trap depth corresponding to the peak at 360 K was 0.81 eV. The TSL glow curve of Eu-doped CsCaCl3 had three peaks at 400, 470, and 530 K and some shoulders around 360, 580, and 610 K. The calculated trap depth corresponding to the shoulder around 360 K was 0.83 eV. The TSL glow curve of Ce-doped CsCaCl3 had a peak at 360 K and some shoulders. The calculated trap depth corresponding to the peak at 360 K was 0.80 eV.

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Structural and optical properties of nano-porous GaSb prepared by swift heavy-ion irradiation

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GaSb is a narrow band gap semiconductor used in many optoelectronic devices such as light emitting diodes, photodetectors, and diode lasers. We have recently discovered the evolution of fascinating nano-porous structures in GaSb following swift heavy ion irradiation. Porous semiconductors differ significantly in their physical and chemical properties from their bulk counterparts, due to their microstructure. Porous silicon, for example, shows an intense, spectrally tunable luminescence while no optical activity is observed for bulk silicon. The controlled fabrication of porous semiconductors thus paves the way for the development of new materials with application specific properties.
We are investigating the structural and optical properties of nano-porous GaSb formed by swift heavy ion irradiation using a combination of high resolution structural characterization techniques including synchrotron based small- and wide-angle x-ray scattering (SAXS/WAXS), extended x-ray absorption fine structure (EXAFS), as well as optical measurements like Raman and photoluminescence spectroscopy.
GaSb films with a thickness of 2 μm, grown on InP substrates as well as bulk specimens were irradiated with different fluences and incidence angles with 185 MeV 179Au ions at the ANU Heavy Ion Accelerator Facility. In contrast to nano-porous GaSb prepared by low energy ion irradiation, the swift heavy ion irradiated samples do not show any sign of homo-polar bonding typical for amorphous materials in EXAFS- as well as in Raman-spectroscopic measurements despite the observed significant structural disorder. Furthermore, x-ray diffraction and Raman-spectroscopy reveal the presence of small ($<$ 10 nm) crystallites inside the pore walls. The microstructure of the porous material is highly dependent on the incident angle of the ion irradiation.

*Speaker

Radiation-Induced Correlated Disorder and its Impact on Ionic Conductivity

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It is well known that defects and structural disorder can strongly influence a material's physical properties. High-energy ion beams induce a wide range of radiation effects and provide a unique means for manipulating the structure of a material. We have established an experimental strategy that characterizes the short-range and long-range structural modifications created in a material by swift heavy ions and analyzes their impact on ionic conductivity. Irradiation experiments were performed on Gd2Ti2O7 and Dy2Ti2O7 pyrochlore oxides with 2.2 GeV Au ions at the GSI Helmholtz Center in Darmstadt, Germany. The samples were analyzed after irradiation by means of neutron total scattering with pair distribution function (PDF) analysis at the Spallation Neutron Source at Oak Ridge National Laboratory. Sampled over longer length scales, cations and anions in amorphous titanate pyrochlores appear randomly arranged [1]; Neutron PDF revealed in Dy2Ti2O7, however, atomic correlation at the sub-nanometer scale. This radiation-induced correlated disorder is manifested in the local structure as ordered orthorhombic weberite-type units [2] and this unconventional disordering mechanism significantly impacts the transport properties in these complex oxides. High temperature broadband dielectric spectroscopy revealed a significant increase of ionic conductivity in amorphous Gd2Ti2O7 which can be explained by modifications of both the short- and long-range structure. The application of advanced characterization techniques, in addition to physical property measurements, provide the basis for a better understanding of structural modifications induced by swift heavy ions. [3] Park, S. *et al.* Response of Gd2Ti2O7 and La2Ti2O7 to swift-heavy ion irradiation and annealing. *Acta Mater.* **93,** 1–11 (2015).

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*Speaker

Radio-photoluminescence observed in MgF2:Sm ceramics

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Radio-photoluminescence (RPL) is a radiation-induced effect observed in phosphor materials that new luminescent centre is generated by irradiation of ionizing radiation. The signal can be easily read via photoluminescence (PL) and the intensity corresponds to the number of luminescent centres, thus the incident radiation dose accumulated. The signal is, in general, so stable that fluorescent microscope, e.g. confocal microscope, can be used to read out the signal without fading of signal. For this reason, RPL can be used for dosimetry applications requiring sub-micrometer resolution. Unlike usual storage luminescence such as thermally- and optically stimulated luminescence (TSL and OSL, respectively), RPL has been relatively recently recognized, and there are not so many materials known to show RPL today. In this paper, we report RPL observed in MgF2:Sm ceramics. MgF2 as a host material has a low effective atomic number (Zeff = 10.96) and thought to be equivalent to biological tissue. Therefore, it is of great interest for use in dosimetry applications. In the MgF2 host, we have found, in this study, that the Sm ion exhibits valence change by X-ray irradiation (Sm3+→Sm2+). In this context, Sm2+ ion is generated by irradiation as new luminescent centre, so Sm2+ feature is observed in PL appearing in the near infrared range after irradiation, which is an indication of RPL. The PL intensity of Sm2+ increases as a function of irradiation dose. In addition to the RPL by Sm ion, RPL due to luminescence of radiation-induced M-centre generated in the MgF2 host is observed. However, the RPL signal by Sm is much more stable than that of M-centre. Further discussions will be made with supporting experimental data in the presentation.

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Influence of gamma-ray irradiation on mechanical property of YSZ for oxygen sensor in ADS

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In order to reduce the long lived radioactive waste in spent nuclear fuel, R&D for the accelerator driven system (ADS) has proceeded energetically, especially in Japan, after the Fukushima accident. The ADS consists of high power proton accelerator and non-critical reactor, which spallation target and coolant is lead-bismuth eutectic (LBE), to transmute the minor actinides in spent fuel by spallation neutrons. Material life time of the beam window, which is the most important boundary between the accelerator vacuum line and reactor core, is dependent on the oxygen concentration in LBE. The developing of durable and trusted oxygen sensor, which can work around 300 to 550 deg.C, is necessary for the control of oxygen concentration in ADS. The sensing element of yttria-stabilized-zirconia (YSZ) is irradiated by gamma-ray in activated LBE under ADS operation.
The mechanical property of ZrO2 is known to be modified by doping of Y2O3. Especially, the 3 mol% Y2O3 (3Y) doping YSZ shows much higher strength than 8 mol% (8Y)-YSZ. Partially stabilized zirconia, like a 3Y-YSZ, has high strength for 3 or 4 point bend types of fracture tests due to the stress induced phase transformation from tetragonal (T)-to-monoclinic (M) phase. It is known that gamma-ray irradiation causes oxygen deficient defects in ceramics. The mechanical properties of YSZ specimens after gamma-ray irradiation, thermal aging and immersion in LBE are reported with the structural change evaluated by X-ray diffraction measurements.

In the case of 8Y-YSZ, the 4-point bend strength did not change even after gamma-ray irradiation of 1MGy and thermal aging at 450 deg.C for 1000 hrs. The 3Y-YSZ, however, showed that the strength was about 50% decreased by the gamma-ray irradiation, thermal aging and also immersion in LBE at 450 deg.C for 1000 hrs. The fracture surface of pristine specimen showed M phase and it had high strength around 500 MPa. The side plane surface of the specimen processed by gamma-ray irradiation and immersion in LBE showed M phase and they had lower strength around 200 and 300 MPa. The results suggest that the process of gamma-ray irradiation and thermal process around 450 deg.C cause phase transformation from T to M, which leads to volume expansion previously and results in lower strength.

*Speaker

Bi and Bi(2+x)Te(3-x) Nanowires Modified by 400 keV and 1 MeV Au ions

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Bismuth and bismuth tellurides are materials known for their high thermoelectric effects, especially when in the form of nanowires [1]. Doping and defect creation by means of ion implantation and/or irradiation is a possible route to modify the transport properties of such materials and therefore tailor their thermoelectric behavior. In this work, we report on implantation and irradiation effects on the structure and morphology of Bi and Bi(2+*x*)Te(3-*x*) nanowires exposed to Au+ beams of 400 keV and 1 MeV. The wires were grown by electrodeposition from aqueous electrolytes into polycarbonate templates and have a smooth surface with diameters of 30, 100, and 130 nm. The composition of the nanowires depends on the deposition potential. Bi-rich compounds are obtained at *-200* mV, using a saturated Ag/AgCl electrode. Almost stoichiometric nanowires are obtained at *0* mV. XRD measurements revealed a polycrystalline structure, with a strong peak at the (015) planes for Bi-rich wires, and a preferential (110) diffraction for the Te-rich compounds. The ion energies were selected based on simulations by SRIM and Iradina to either implant the ions in the middle of the thickest wires (130 nm diameter) or to cross over their diameters. The irradiations were performed with the wires deposited in transmission electron microscopy (TEM) grids. TEM observations reveal that the irradiated nanowires present an amorphized structure, containing an embedded dispersion of small spherical crystallites. Both beams generated rough wire surfaces, sometimes presenting a "wavy" morphology. A distribution of nanoparticles dispersed in the vicinity of the irradiated wires was also seen on the TEM grids, formed most probably from material redepositing due to sputtering. The 400 keV and 1 MeV Au ions have comparable stopping powers. However, for irradiations at 1 MeV the material underwent a greater erosion process, resulting in the formation of holes through the wires. The observed morphologic modifications are discussed considering sputtering and radiation induced surface diffusion effects.

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Time-resolved spectroscopy of YAG and YAG:Ce phosphors under e-beam excitation

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Yttrium aluminum garnet Y3Al5O12 (YAG) are widely used as hosts for doping with different rare-earth ions for use in different applications like laser crystals, fast scintillators, phosphors in LEDs, dosimeters for ionizing radiation etc. [1,2]. Although this material is widely used under various radiation conditions, the role of defects in the relaxation processes of electronic excitations in electron irradiated YAG crystals is not understood in detail.
The powders Y3-xAl5O12xCe (x=0.02, 0.04, 0.06, 0.08 and 0.1) were synthesized by high-temperature solid-state reaction under reducing atmosphere with the addition of BaF2. The morphology of phosphor particles was investigated by using a scanning electron microscope (SEM, Quanta 250, FEI, USA. The crystalline phases were characterized by powder X-ray diffractometer, (TD-3500, Dandong) using Cu Kα radiation at 30 kV and 20 mA. The absorption spectra were measured by UV-Vis-NIR spectrophotometer. Electron accelerators with air-filled gas diode operating at atmospheric pressure [3] and with vacuum diodes [4] were used for generation electron beams with pulse duration 150 ps and 10 ns respectively. Time-resolved spectra of cathodoluminescence (CL) and the luminescence decay kinetics been investigated by photomultiplier tube (FEU-84-6) and digital oscilloscope LeCROY-6030 (350MHz). The integrated spectrum CL were recorded using fiber spectrometer AvaSpec-2048.

In work the relaxation processes in YAG after influence electron irradiation are studied. Influence of cerium concentration on luminescent properties of YAG was studied. The decay kinetics of luminescence at different exposure conditions was investigated. The mechanisms of luminescence and processes of formation of defects in pure and cerium-activated garnet are discussed.

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Thermal annealing of F-type color centers in irradiated oxides: A critical analysis of experimental and theoretical results

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The radiation-resistant oxide insulators (MgO, Al2O3, MgAl2O4, BeO etc) are important materials for applications in fusion reactors. It is very important to predict/simulate not only the kinetics of diffusion-controlled defect accumulation under neutron irradiation, but also a long-time defect structure evolution including thermal defect annealing after irradiation.
After introducing some basics on the radiation point defects in halides, binary oxides and oxide perovskites as well as the mechanisms of point defect and metal colloid formation in thermochemically reduced samples or under particle irradiation (neutron, ion, proton, electron), the current understanding of their thermal annealing is briefly reviewed. We will shortly describe new theoretical approach based on the formalism of the correlation functions, describing spatial distribution of both similar (F-F centers) and dissimilar defects (a Frenkel pair of defects: an F center – an interstitial Oi ion) which suits for the study of defect kinetics and aggregation much better than generally accepted rate equations or simple first order kinetics.

In particular, the kinetics of the F-type center annealing after electron, heavy ions or neutron irradiation was treated as the bimolecular process with equal concentrations of the complementary F and Oi defects. It is controlled by the interstitial oxygen ion mobility, which is much higher than that of the F centers. The F center annealing begins in binary oxides at temperatures 500-700 K, when both F and $F+$ centers are practically immobile, due to the recombination with mobile Oi defects. It is demonstrated how the shape of the F-annealing curves is determined by two control parameters: Ea and effective pre-exponential factor and strongly depends on irradiation conditions.

The appropriate migration energies were obtained from available from literature annealing kinetics for electron, neutron and ion irradiated MgO, Al2O3, MgAl2O4, BeO, ZnO, PLZT etc. The results obtained are compared with recent *ab initio* calculations of interstitial oxygen migration. Another type of experiments, such as F-type center annealing in thermochemically reduced samples, was also simulated.
Special attention is paid to: (1) dose effects on F center annealing in neutron and fast electron irradiated MgO and MgF2; (2) a detailed comparison of diffusion-controlled F center thermal annealing in neutron, electron and heavy-ion irradiated MgO, MgF2, Al2O3, ZnO and

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MgAl2O4; (3) the F center annealing and metal colloid formation in thermochemically reduced MgO, Al2O3 and BeO.

Use of low energy ion beam irradiation to transform superconductive NbN thin film to metal or insulator

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Low temperature superconductive NbN with 4-5 nm thickness are very attractive to use in modern devices (SSPD, HEB, etc.) due to high transition temperature (_˜12 K) and high critical current density _˜(8-20) MA/cm2. Our idea was to use ion beam irradiation through the micro or nano-mask to change the atomic composition of the material by a control way to get metal or insulator state and build up resistive or capacity elements integrated on the chip.
It was shown [1] that low energy middle dose composite ion beam irradiation by hydrogen and oxygen ions at the same energy could be used to transform NbN thin film to NbNO crystal phase, that characterized by the metal-like electrical conductivity at 4.2K[2]. One could build up any value of the resistance by playing of the resistive area topography. We have demonstrated formation of big range of resistive elements from a few ohm to a few megaohm.

The above mentioned NbNO formation from NbN under composite ion beam irradiation were taking place in a dose range from _˜1 d.p.a. to _˜4 d.p.a. and took place not at the same time in all grains. We had found the rest of superconductive phase up to dose of _˜2 d.p.a. by structure analysis and also on IV curves at low currents and small gaps between superconductive islands the percolation effect could took place.

With increasing of the dose of composite ion beam irradiation [3] or using high dose oxygen ion beam irradiation [4] the insulator Nb2O5 could be formed from initial NbN under irradiation. The latter way was more useful due to the high dose rate but slightly more complicated due to the radiation stable mask design. This Nb2O5 could be used to form on chip planar capacity elements.

Taking into account that long superconductive wires characterized by kinetic inductance, all basic cryo-electronic elements could be integrated on the chip under ion beam irradiation.

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Strain detection in crystalline GaN-based heterostructures using bidimensional blocking patterns of channeled particles

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Ion implantation can induce a large variety of defects in crystals. These defects often lead to a lattice expansion along the surface normal for high fluences, which is especially relevant in GaN or ZnO semiconductors, where polarization effects are strongly linked to the strain in the hexagonal lattice [1]. Such strain is frequently analyzed by means of X-ray diffraction (XRD) and, quite recently, the development of new analytical tools has allowed the determination of strain depth profiles [2]. An excellent complement to XRD analysis is Rutherford backscattering spectrometry under channeling conditions (RBS/C), a powerful technique to perform strain profiling with the additional advantage of the mass resolution [3]. In addition to the conventional measurement through angular scans (detecting the angular shift between the layers), the development of 2D detectors in the last years has opened a new and more detailed way to extract this structural information.

In this work, we analyze the accuracy of RBS/C for the quantification of strain in GaN-based heterostructures with different strain states (ϵ, from -1% to 1%) and different thicknesses (from 50 to 250 nm). The blocking patterns in the vicinity of the axis were recorded with a position sensitive Timepix pixel detector developed at CERN [4]. The obtained values present deviations from the XRD data, depending on both the strain state and the thickness of the layers, confirming the importance of steering phenomena in the strain determination by RBS/C [5]. These effects, however, can be taken into account with Monte Carlo simulations and controlled by means of the experimental parameters (e.g., the beam energy) [6]. We demonstrate the good agreement between both the experiment and the simulation when those effects are corrected, showing the general applicability of this method.

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Structural modifications induced by swift heavy ions in α-Al2O3 substrate

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Sapphire is a common substrate for nitrides due to its optical transparency and for its hexagonal structure making easy epitaxial growth. Indeed nitride semiconductors are mostly epitaxial films, thick of few microns deposited on insulating substrate for applications in high power and high frequency optoelectronic devices. In real world conditions, these devices can be exposed to ion irradiation as in space or accelerator environment. Thus it is necessary to study under ion irradiation the behaviour of nitride layers and sapphire substrate, of which the evolution of structural properties influence the features of the epitaxial top layer.
In this work, defect formation and structural modifications of a-Al2O3 induced by swift heavy ion irradiation are investigated. (0001) Al2O3 single crystals have been irradiated along the c-direction by 92 MeV Xe at room temperature. The irradiation experiments have been performed at GANIL facility (Caen) on IRRSUD beam line. The ion beam energy is 0.7 MeV/A, where along the ion path the electronic stopping power dominates near the surface compared to nuclear stopping power, whereas an inversion of energy deposition processes is observed at the end of the projected range (around 8μm). High resolution X-ray diffraction and in-plane diffraction are used to characterize samples with various sensitivities to surface and to deep thickness. Using different fluences, the mechanisms of structural modifications are investigated.
In the communication, the evolution of the X-Ray patterns recorded in the two configurations for several reflections will be shown, discussed and compared to literature results. A careful study of the reflection characteristics will be detailed to highlight the material damaging through strain and amorphization. The kinetics of these processes with the ion fluence increase will also be discussed. We will show how much the c-parameter (parallel to ion beam) and the a-parameter (perpendicular to ion beam) are affected by irradiation in the MeV range. The biaxial and hydrostatic strains, linked to defect formation with fluence increase, are estimated. Finally a depth profile will be purposed as an explanation for the structural behaviour of Al2O3 under 92MeV Xe irradiation. Complementary TEM results will be shown to improve the understanding of the modifications under irradiation.

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Radiation effects in nitrogen and methane "ices"

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The keen interest in research of radiation effects in N2 and CH4 ices" is associated with their significant presence on several planets in the solar system. N2 solids attract also much attention as environment-friendly high energy density materials. Solid CH4 is actively used as a moderator for a pulsed cold neutron sources. Radiation-induced chemical modification of solid CH4 andN2 has been studied extensively however the role of the charge states in the relaxation of excitations is just beginning to be studied. Only recently the hole self-trapping – formation of N4+,[1] and creation of N3+ [2] in irradiated solid N2 were found. Different channels of ionization and dissociation at electron degradation in CH4 gas were modelled by the Monte Carlo simulations [3].
Here we present new trends in the study of radiation effects in N2 and CH4 solids with a focus on relaxation phenomena in the preirradiated with an electron beam films. During a controlled warm-up of the ices three thermally stimulated effects were monitored: a VUV and visible photon emission, an exoelectron emission, and the ice‘s particles ejection. Dynamics of cathodoluminescence CL under beam was detected in the visible and VUV ranges. The dose dependence of CL bands in solid N2, fitted by the exponential function: $I(t)=I\mathrm{sat}[1\text{-}\exp(\text{-}t/tau)]$, evidenced accumulation of N3+, N4+ species and N radicals. N3 radicals efficiently formed N3- centers by electron attachment. CL of solid CH4 steeply increased at switching on the beam, reached maximum and then decayed exponentially, indicating radiation-induced chemical modification of the film. On completion of the exposure to an electron beam afteremission of electrons was detected pointing to an electrostatic charging of both films. Thermally stimulated exoelectron emission TSEE (two peaks at about 18 and 43 K) was detected from solid CH4 for the first time and trapping parameters were estimated. In contrast to solid N2 [1] no thermally stimulated luminescence TSL was observed from pure solid CH4 in the visible and VUV range. Strong peaks of particle ejection (post-desorption) were found in solid N2 and CH4 at temperatures much lower than the characteristic sublimation temperatures. Possible mechanisms of low-temperature post-desorption are discussed.

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Local Order in Disordered and Amorphous Pyrochlore Oxides

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Complex oxides such as pyrochlore (general formula A2B2O7) are candidate materials for a wide range of engineering applications, such as solid electrolytes for fuel cells, host materials for nuclear waste containment, and thermal barrier coatings for gas turbine jet engines. Predicting the retention of incorporated actinides is important for their safe use as nuclear waste forms and requires a detailed knowledge of how the atomic structure responds to self-irradiation. When subjected to extreme environments, such as high temperatures or highly ionizing radiation, many of these compounds (at least partially) lose their long-range crystal structure. The specific structural response of a pyrochlore composition under irradiation (disordering *vs.* amorphization) depends on its cation ionic radii ratio, $r\mathrm{A}/r\mathrm{B}$. In general, compositions that easily form cation antisite defects (small $r\mathrm{A}/r\mathrm{B}$) will disorder to a defect-fluorite phase while those for which these defects are energetically expensive (large $r\mathrm{A}/r\mathrm{B}$) will instead amorphize as atoms are displaced to interstitial positions. The nature of the local atomic arrangement in these two final radiation states is not well understood. We have used neutron total scattering with pair distribution function (PDF) analysis to elucidate the local defect structure in pyrochlore samples that were irradiated by swift heavy ion irradiation. Measurements were performed at the Nanoscale Ordered Materials Diffractometer (NOMAD) beamline at the Spallation Neutron Source (Oak Ridge National Laboratory). Two pyrochlore samples, one that is known to disorder (Er2Sn2O7) and the other to amorphize (Dy2Sn2O7), were irradiated with 2.2 GeV Au ions at the GSI Helmholtz Center in Darmstadt, Germany. Neutron PDF analysis performed after irradiation revealed that the A- and B-site cations in the disordered pyrochlore are not randomly arranged at the atomic level as previously assumed, but only appear so when sampling over longer length scales. The local defect structure in disordered pyrochlore analyzed over short length scales ($<$ 10 Å) consists of orthorhombic, weberite-type structural units, which are arranged with pseudo-translational symmetry to form the well-known defect fluorite structure over longer length scales [1]. This local order is also present in the amorphous pyrochlore, de-

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spite the contrasting long-range behavior. Thus, neutron PDF analysis shows that the ability to stack these local structural units to maintain partial long-range order is a key parameter in describing the radiation response of pyrochlore. [1] Shamblin, J. *et al.* Probing disorder in isometric pyrochlore and related complex oxides. *Nat. Mater.* **15**, 507-512 (2016).

Optical and Structural Modifications of Cu-C70 Nanocomposite Thin Film under 350 keV Ar Ion Irradiation

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Metal based fullerene nanocomposite is an interesting area for the researchers due to their enhanced optical, electrical and mechanical properties in comparison to pure fullerene thin film. Fullerene, in the form of thin film, is itself a multi-application system and its application can be further enhanced by adding small amount of metal as nanoparticulates in it. The present study deals with the enhanced absorption of fullerene C70 on incorporating Cu nanoparticles into it due to plasmonic resonance. Cu-C70 nanocomposite thin films are synthesized by thermal co-deposition technique on glass and silicon substrates. These films are irradiated with 350 keV Ar ion beam at different fluences ranging from 1×1013 to 3×1016 ions/cm2 using ECR ion source based accelerator facility at Inter University Accelerator Centre New Delhi. The optical and structural studies on pristine and irradiated films have been performed using UV-visible absorption spectroscopy and Raman spectroscopy, respectively. Optical studies reveal that there is no signature of surface plasmon resonance band (SPR) in pristine Cu (10%)-C70 thin film which may be due to low concentration of Cu in fullerene C70 matrix. With increasing fluence of 350 keV Ar beam, signature of SPR band is clearly visible at ¯ 627 nm for a dose of 1×1015 ions/cm2. With further increase in dose, SPR band is shifted to lower wavelength. At fluence 3×1016 ions/cm2, a blue shift of ¯ 24 nm is obtained and a comparatively sharp SPR band is observed at ¯ 603 nm. Raman spectroscopy on pristine and irradiated sample of Cu-C70 nanocomposites confirms the transformation of fullerene in amorphous carbon (a-C) at fluence 3×1014 ions/cm2. The blue shift of Cu nanoparticles in fullerene C70 matrix is explained in terms of Maxwell-Garnett Effective medium theory.

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Structural changes and defects evolution in Ti3AlC2 induced by 500 keV He-ions irradiation

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The MAX phases, and more particularly Ti3AlC2, combine the properties of metals with those usually attributed to ceramicssuch as excellent mechanical properties and high-temperature stability (> 1000 oC). These properties, arising from their specific structure composed of ceramic octahedral (i.e. TiC8) and a single intercalated metallic layer (i.e. Al layer), make them ideal for applications under extreme radiation conditions. Therefore, it may be used as not only the first-wall candidate material in the fusion reactor (ITER) but also the structural material in the fission programmes (ADS and Gen IV).
The studied samples consisting of about 99.5% Ti3AlC2 were obtained with a hot isostatic pressing (HIP) method. And irradiation experiments with He2+ of 500 keV were performed at different temperatures and influences under 320 kV multi-discipline research platform in the Institute of Modern Physics, ChineseAcademy of Sciences (IMP, CAS), Lanzhou. All the samples studied in this work were characterized by low-incidence X-ray diffraction and analyzed by Positron Annihilation Spectroscopy (PAS), respectively.
The observed diffraction patterns revealed apparently the formation of new phases such as TiCx and Ti3Al within the matrix caused by irradiation. Moreover, the change in peak broadening was also indicative of the presence of a disordered phase, but the amorphous phase didn't occur in all the irradiated samples even at the fluence of 1.0×1018 ions/cm2. Besides, an expansion of the hexagonal close-packed lattice along the c axis increases with the influence at the same temperature. In addition, for the sample irradiated by He2+ with a fluence of 1×1018 ions/cm2S parameter was higher than that for all the other samples including the virgin one, which clearly indicates that positrons detect the presence of vacancy-type defects generated during irradiation of He in Ti3AlC2. Meanwhile, the combination of He-Vacancy was related to the lower density of defects induced by irradiation. Moreover, the recovery phenomenon of defects was evidently at high temperatures.

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Swift heavy ion irradiation modification in Fe-based amorphous alloys

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Amorphous alloy (also known as metallic glass) is a kind of new alloy material synthesized by using modern rapid solidification metallurgical technology, owning excellent mechanical, physical and chemical properties that general metal and glass have. The unique glassy structure makes metallic glass have some high performances such as high strength, corrosion resistance, great ductility, and having a wide supercooled liquid region, etc. which usually belong to the high-quality magnetic functional materials, and hence showing enormous potential for development and application in the fusion reactor [1-2]. In this work, SHI irradiation as a kind of special non-equilibrium and exogenous energy deposition process will be applied to the study on modification of the structural and magnetic properties of the amorphous alloys.

Amorphous FeSiNbZrB alloy ribbons were prepared by melt spinning, and then the amorphous ribbons were irradiated at RT with 2.01 GeV Kr26+ ions for fluence range from 1×1011 to 1×1014 ions/cm2 on the materials research terminal of the HIRFL-SSC (IMP, Lanzhou). X-ray diffraction (XRD), transmission electron microscopy (TEM), vibrating sample magnetometer (VSM), superconducting quantum interference device (SQUID) and m´ossbauer spectra (MS) were used to measure the structural and magnetic properties of the pristine and irradiated samples.

It's obviously that before and after SHI irradiation, such amorphous FeSiNbZrB alloy systems do not have a long-range order in atomic arrangement and exhibit only a short-range order. Under SHI irradiation at RT, local crystallization phenomenon of amorphous FeSiNbZrB alloy ribbons has been confirmed and formation of finer α-Fe(Si) phases precipitations with diameter of 1-2 nm has been observed. In addition, after irradiation, magnetic anisotropy considerably changes from its original in-plane direction. Possible mechanism of structural and magnetic properties modification after SHI irradiation is discussed briefly.

*Speaker

Ion irradiation-induced crystal structure changes in spinels: MgAl2O4, MgGa2O4, and MgIn2O4

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Irradiation-induced structural evolution in many spinel compounds (AB2O4), especially MgAl2O4, has been extensively studied under various radiation environments. However, systematic studies that allow for a clear identification of the role of cation chemistry, and thus tendency for inversion/cation disorder x, are limited. In this study, three spinel oxides with varying tendencies for inversion – namely normal spinel (x˜0) MgAl2O4, half-inverse (x˜0.5-0.6) MgGa2O4 and fully-inverse (x˜1) MgIn2O4 – were selected to examine the influence of cation disordering on radiation tolerance in spinel. Here x is the inversion parameter measured as the fraction of B cations that reside on A lattice sites. These three spinels were irradiated with different ion species (Kr, Ne, He) at cryogenic temperature (100 K). The structural changes after irradiation were characterized using X-ray diffraction and transmission electron microscopy. We have observed, for the first time, the formation of a rocksalt phase in spinel structured materials by 600 keV Kr and 400 keV Ne ion irradiations. This transformation involves not only disordering of cations, but a rearrangement of cations onto interstices that are normally unoccupied in spinel. On the other hand, a phase transformation from inverse spinel (x˜1) to random spinel (x˜2/3) structure is observed in MgIn2O4 under 200 keV He ion irradiations. Most importantly, varying tendencies to amorphize under irradiation are observed for the three different spinels; this amorphization resistance correlates directly with the energy to disorder the structure. These results indicate that several different crystal structure changes are possible in irradiated spinels and provide new insight into the behavior of complex oxides under irradiation environment. Also, possible spectrum effects on the irradiation-induced microstructural evolution will be discussed.

*Speaker

Swift Heavy Ion Irradiation induces enhancement in electrical conductivity of LiTaO3 and LiNbO3 crystals

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Swift heavy ion irradiations (SHI) of insulators have long been known to create macroscopic structural modifications such as a buried damage layer in bulk, due to the ion energy loss, being thus an attractive method to produce optical waveguides in LiNbO3 [1,2]. The electrical conductivity in LiNbO3 single crystals with a certain amount of deficit of lithium (specific intrinsic defects) is determined by electrons or by electron lattice interactions (polarons) released from neutral oxygen vacancies, the hopping conduction being the dominant mechanism of charge transport. However, it is not clear that for high concentrations of oxygen vacancies together with structural disorder, Mott's variable range hopping with a Tˆ(-1/4) dependence to the temperature remains the most important mechanism.
In this work, we have investigated and related the results from the optical waveguide characterization to the changes in electrical conductivity due to damage by SHI in LiTaO3 and LiNbO3 single crystals. In particular, we use Si and Br ions, with energies in the range from 20 to 40 MeV and fluences within (0.1-10)xˆ14 ions/cmˆ2, to carry out an extensive study of damage accumulation in the buried layer. We account for the changes in the electrical behavior of the Al-[LiTaO3/LiNbO3] interface, such as that in conductivity with temperature in the damaged layer, up to irradiation levels close to the amorphization threshold in individual tracks. Direct current electrical measurements between 296 and 445 K were used to characterize the electrical conductivity of the irradiated region in LiTaO3 and LiNbO3 single crystals [3,4] before and after removing successive thin layers from the surface by etching. Preliminary results in LiNbO3 samples irradiated with Br ions, with an energy of 40 MeV suggest thermally activated processes with activation energies of about 0.56 eV, probably associated with the intrinsic defects created by the irradiation, rather than with the Br ions themselves.

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High energy heavy ion irradiations in LiTaO3: damage characterization and optimization of optical waveguides

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Lithium tantalate (LiTaO3) is a nonlinear optical material with interesting properties for optical waveguide structures and potential advantages, regarding ferroelectric domain engineering, compared to lithium niobate (LiNbO3) [1], which has been studied more in depth. Unique high contrast optical waveguides have been successfully fabricated in LiNbO3 and other crystals by means of swift heavy ion irradiation [2,3]. Furthermore, the comparison of ion damage in both materials is very attractive for the subsequent modeling and analysis.
A systematic study of waveguide fabrication by swift heavy ion irradiation is addressed, exploring the cases of C 15 MeV, F 20-30 MeV and Si 40 MeV at several fluencies in LiTaO3. In order to optimize the propagation losses of the generated waveguides, the influence of post-irradiation annealing has been investigated in the range 150-350°C. The optimum propagation losses (0.8 dB/cm) have been obtained after a 225°C annealing for nuclear-regime waveguides, in contrast with the results previously obtained in LiNbO3 [4]. In addition, optical in situ measurements have been performed in order to study the damage kinetics for different F, Si and Br energies in LiTaO3, and compared with those in LiNbO3.

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Studying the annealing effect of swift heavy ion irradiation on Graphene oxide film

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Single layer graphene is a semi-metal with zero band gap with only sp2 hybridization [1]. However, it's functionalized form, graphene oxide (GO), is an insulator due to the presence of oxygen-containing functional groups (-COOH, -OH, -O-) on edges and basal planes. Therefore the GO sheets contain a ratio of both sp2 and sp3 hybridization due to the presence of disrupted sp2 network bonding. Since the stoichiometric ratio is not fixed, its structure is still under debate. GO, due to its functional groups, has good dispersibility in most of the organic solvents and also provide a good matrix for nanocomposites [2]. Reduction of GO leads to reduced graphene oxide which is similar in properties to pristine graphene. Swift heavy ion (SHI) irradiation can also be a method of reduction [3]. Our group has observed an interesting result [4-7] of annealing of defects in carbon nanostructures (fullerene, CNT, and graphene) at lower fluences of SHI. In the present work, we carried out a study on the defect annealing of the GO film at the low fluence of SHI. The graphene oxide films were irradiated with Gold ion beam of energy 120 MeV and the X-ray diffraction, Raman microscopy, UV-Vis spectroscopy and Fourier transform infra-red spectroscopy were performed for pristine and irradiated films. Disorder parameter, ID/IG (calculated from Raman spectra) decreased indicating the annealing of films till the fluence 3x1011 ions/cm2.
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Strain Induced modifications in Structural and Magnetic behaviour of NdMnO3 thin films: 200 MeV Ag+15 Ion Irradiation Study

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We report the results of the 200 MeV Ag+15 ion irradiation on the modifications in structural and magnetic behaviour of pulsed laser deposition (PLD) grown NdMnO3 (NMO) manganite thin films on (100) substrate of single crystalline (LaAlO3)0.3 (Sr2AlTaO6)0.7 (LSAT). Irradiation of films with different ion fluences (5 x 1010, 5 x 1011, 1 x 1012 ions/cm2) results in modifying the structure and magnetic response of the films. Structural strain was quantified using XRD, Reciprocal Space Mapping (RSM) and Raman Spectroscopy. Rutherford backscattering (RBS) measurements were performed on pristine NMO film to conform the elemental composition, thickness and oxygen content. Magnetic measurements performed on all the NMO/LSAT films show that both magnetization and coercive field are sensitive to different Ag-ion fluences and exhibit the ferromagnetic behaviour below 10K. Pristine and Irradiated NMO films are antiferromagnetic and a shift in Neel Temperature (TN) which has been observed with increase in irradiation dose is attributed to the irradiation induced increase in strain at the interface in the thin films.

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Size effect in AlN/SiN multilayered films irradiated with helium and argon ions

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Nanostructured materials are reported to have unique properties that are not characterized for their bulk analogous. This mainly appears due to a big fraction of interfaces arising between different phases or grains. The interfaces can also sufficiently serve as sinks for structure defects annihilation including radiation defects. Since, nanostructures can be considered as promising class of materials with enhanced radiation stability. In the present work the radiation effects in the AlN/SiN multilayered thin (300 nm) films after irradiation with helium (He+, 30 keV) and argon (Ar+, 180 keV) ions are discussed.
The AlN/SiN multilayered thin films were synthesized by magnetron sputtering, the AlN as well as SiN layers thicknesses being varied in the range from 2 to 10 nm. According to the XRD results the AlN layers are crystalline meanwhile the SiN layers are amorphous. The obtained multilayered films were irradiated with He (30 keV) and Ar (180 keV) ions with a dose of 5E16.

After the irradiation with both types of ions a decrease in the lattice parameter of the AlN phase was revealed. With decrease in AlN thickness (from 10 to 2 nm) the role of the interfaces between AlN and SiN layers increases and the radiation defects, like vacancies and interstitials, produced by the impurities migration towards the interfaces with a subsequent annihilation and redistribution in the amorphous SiN phase. So, the increased vacancies concentration in the SiN layers provides accumulation of the implanted ions inside. The implanted ions (He or Ar) are clustered and form bubbles with an average size of 2 – 3 nm. The bubbles growth preliminary inside the amorphous SiN layers and produce addition pressure on the neighbor AlN crystal phase resulting in decreasing the lattice parameters.
The mechanism of structure changes in dependence on the layers thickness and ions type are discussed in the work.

*Speaker

Electronic structure of nanoscale phases CoSi2 and SiO2 were formed in different depths of Si

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Multilayer thin film nanostructures containing layers of SiO2 and CoSi2 have prospects in the creation of metal-insulator-semiconductor (MIS) -, semiconductor-insulator-semiconductor (SIS) -structures, ohmic contacts, barrier layers, electronic and magnetic storage devices. One of the prospective methods for creating nanostructures on the surface and near-surface region of semiconductor and dielectric films is a low-energy ion implantation.
In this paper, we first attempted to obtain nanoscale phase SiO2 and CoSi2 in different depths Si by ion implantation in combination with annealing. These phases we obtained by implantation of ions O2+ and Co+ on Si, varying the ion energy (1.0 to 30 keV) and a dose of (D = 5·1013 - 5·1015 cm-2), followed by heating T = 800- 1000 K. The experimental results showed that the volume of each nanocrystalline phase created with the same dose of the ions in the surface layers and as well subsurface layers are about the same. If CoSi2 obtained at D = 1015 cm-2 the volume of each crystalline phase be within _˜ (1.5 - 2) × 10-18 cm3, and they formed epitaxially. By varying the ion dose in the range of about 5·1014 - 5·1015 cm-2 may be controlled to change the volume of the nanocrystalline phase in the range of _˜ 10-19-10-18 cm3. The width of the forbidden zone CoSi2 decreases monotonically from _˜1 to _˜0.6 eV. When D $\leq$ 1014 cm-2 we did not find the formation nanocrystalline phases of CoSi2 with good stoichiometry. Also due to the low concentration of Co atoms on the dependence of $I(hn)$ no appreciable decrease in the intensity of the transmitted light up to energy hn _˜ 1 eV. When D > 5·1015 cm-2 observed overlapping boundaries of separate cluster phases.

In contrast to the CoSi2 in the case of SiO2 failed to obtain the epitaxial formed crystalline phases. This is primarily can be due a substantial difference between the parameters lattices of Si (a = 5,48 Å) and SiO2 (a = 7Å). We determined optimal modes of ion implantation and annealing of the nanocrystals to obtain SiO2 and CoSi2 of two different depths in monocrystal Si (111). After each cycle of implantation, the sample was heated at an appropriate temperature during 30 minutes.
Results of the experiments showed that after annealing Si, implanted ions of Co+ with energy E0 = 30 keV nanocrystalline phase in the form of spheres formed at a depth of 26 - 30 nm. When D = 5 · 1014 cm-2 average diameter nanocrystals 5-6 nm, and at D = 1015 cm-2 – 10 - 12 nm. In the case of E0 = 15 keV nanocrystalline phase formed at a depth of 13-15 nm in diameter and the phases differ little from those of E0 = 30 keV. In the case of E0 = 15 keV nanocrystalline phase formed at a depth of 13-15 nm and their diameters differ little from those

*Speaker

for E0 = 30 keV. In the case of O2+ ion implantation in Si with energy E0 = 30 keV after heating at T≈900 K nanophases SiO2 formed at a depth of 18-20 nm. Research in this area continues.

FORMATION OF NANOSIZED STRUCTURES ON THE SURFACE OF FILMS MgO AT BOMBARDMENT BY IONS LOW ENERGY

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Creation of nanosized structures with new physical properties on the basis of dielectric films is one of the primary goals modern micro - opto - and nanoelectronics. In particular, films MgO are characterised by high energy of communication that defines its chemical stability and wide forbidden zone. These films in a combination to metal and semi-conductor films are used in creation of unique electronic devices. The work is devoted to studying of structure and electronic properties of nanosized structures formed on surface layer MgO at bombardment by ions Ar +. Ion bombardment, researches of structure, profiles of distribution of atoms on depth and electronic structure were spending in the same over highly vacuum device consisting of two adjacent chambers.

Spectra characteristically lost energy of electrons of amorphous film MgO received after bombardment by ions Ar+ with 0 = 1 keV by different doses have shown bombardment by ions Ar + led to change of intensity and position of spectrum peaks. The joint analysis with results Auger electron spectroscopy have shown that it is caused with decomposition of communication Mg - O and occurrence on a surface of atoms free Mg. Already at D = 1015 cm-2 are formed clustered sites of magnesium which form communications of type Mg - Mg, and atoms (molecules) of oxygen from these sites are almost completely sprayed. With the further growth of a dose of an irradiation reduction of intensity of peaks and oxide magnesium, occurrence and increase in intensity of peaks of plasma fluctuations characteristic for Mg is observed. The increase in the last is equivalent to increase in superficial concentration Mg. These changes occur to D = (4 - 6) ×1016 cm-2. Further increase D does not lead to appreciable change of spectrum characteristically lost energy of electrons. Results of analysis from SEM and the AFM-images of a surface have shown, at D = 1015 cm-2 the superficial sizes clustered sites Mg make 50 - 100 nanometers, and their height - 20 - 25 nanometers. With growth of a dose of an irradiation the superficial sizes of these sites increase and at D = 6×1016 sm-2 surface MgO completely becomes covered by atoms Mg. Thus the surface becomes more smooth and its roughness does not exceed 0,5 - 1 nanometer.

*Speaker

Near-surface thermal transport studies of swift heavy ion irradiated insulators by picosecond time-domain thermoreflectance

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Radiation-induced thermal conductivity degradation is a critical issue for nuclear reactor materials since the knowledge of thermal transport in reactor's components is of paramount importance for reactor system design and validation. Most of corresponding experimental data on this subject concern neutron irradiation and almost nothing is known about high energy heavy ion irradiation simulating fission fragment impact. At the same time such data are of considerable practical value especially for insulators like AlN and Si3N4 suggested as candidate materials for inert matrix fuel hosts due to large number of fission track recoil in reactor fuels.

We have studied nano- and micro-scale near-surface thermal transport in several swift heavy ion irradiated polycrystalline ceramics (Si3N4, AlN, ZrN) and single crystals (Al2O3, LiF). These materials were irradiated at T $<$ 60oC with 1 - 3 MeV/nucleon Ar, Bi, Xe, Kr ions with fluences ranging from 109 to 1014 cm-2 at IC-100 and U-400 FLNR JINR cyclotrons.

Thermal conductivities were measured using non-contact, nondestructive ultrafast laser-based pump-probe technique called picosecond time domain thermoreflectance (TDTR) [1]. This method makes use of change of laser pump beam-induced reflectivity of thin Al coating covering studied bulk samples and acting as an optical absorber and temperature transducer, which enables one to sample thermoreflectance with picosecond time scale resolution via scanning probe beam with respect to fixed laser pump beam. Obtained thermoreflectance signal is fitted using solution of the heat diffusion equation for layered (i.e. transducer film - bulk sample) structure [2].

Investigated materials demonstrate substantial degradation of thermal conductivity with increase of the ion fluence. Comparison of thermal conductivity of AlN, Si3N4, Al2O3 and LiF as a function of ion fluence allow us to conclude that latent track associated radiation damage

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play very important role in thermal transport degradation behavior.

Additionally, changing the modulation of the pump laser beam in 1 – 10 MHz frequency range enables us to tune the confinement of modulated thermal wave to the subsurface region of fresh and irradiated insulators, the heat penetration depth of which correspondingly ranges on sub-micron scale. This allows one to probe small volume scales and characterize depth-dependent ion-induced damage. Modulation frequency- and heat penetration depth- dependent thermal transport properties of studied insulators will be discussed in terms of contribution of phonons and ion-induced structural damage.

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Swift heavy ion induced modifications of copper-fullerene nanocomposite thin film

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Metal based fullerene nanocomposites is an interesting field of Plasmonics due to increased absorption in visible region as a result of Surface Plasmon resonance (SPR) of metal nanoparticles. The SPR peak position and width depends strongly on the surrounding matrix in which these noble metal nanoparticles are embedded. Using fullerene to incorporate metal nanoparticles makes it a bi-functional nanocomposite, in which the properties of fullerene as well as of metal nanoparticles can be used simultaneously. The structural and optical properties of these nanocomposite thin films can be engineered using post deposition techniques such as thermal annealing. In order to tune to the properties of nanocomposite thin films spatially, ion beam techniques are the most suitable tool. Swift heavy ion beams can modify the material in nanometer zones by creating ion tracks in their path into the target material. In the present study, Copper (Cu) nanoparticles are embedded in fullerene C60 matrix by thermal co-deposition of Cu and C70 simultaneously on a substrate. These films are irradiated using 120 MeV Ag ion beam at the fluences of 1×1012, 3×1012, 6×1012, 1×1013 and 3×1013 ions/cm2 at IUAC, New Delhi using Pelletron accelerator. In UV-visible absorption spectrum of pristine Cu(15%)-C60 nanocomposite thin film, absorption bands occur at 217 nm, 267 nm, 346 nm and a hump is observed _˜461 nm. Some weak bands are also observed beyond 500 nm. As the fluence is increased, the intensity of absorption bands is diminished. At a fluence of 3×1013 ions/cm2, the band at 267 nm shifts to lower wavelength 248 nm that is a shift about 19 nm is observed. A little shift is also observed in other absorption bands. This is attributed to the ion irradiation induced structural changes in fullerene material. Raman spectroscopy confirms that fullerene C70 is has been transformed to amorphous carbon at a fluence of 3 x 1013 ions/cm2. The D and G bands, characteristics of amorphous carbon are clearly visible in the Raman spectrum for the sample irradiated at 3 x 1013 ions/cm2. The change in the size and shape of Cu nanoparticles is studied using transmission electron microscopy.

*Speaker

Carbon-ion irradiation effect on surface microstructure and optical properties in monolayer WSe2

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In recent years, two-dimentional (2D) layered nanomaterials have attracted much attention due to their unusual physical properties [1]. As a typical semiconducting transition-metal dichalcogenides (STMD), tungsten diselenide (WSe2), has started to attract the numerous attention due to its p-type characteristics [2]. However, there exist only few optical studies on WSe2, and most of them deal with the bulk phase. Here we present a careful investigation of monolayer WSe2 about the spectra properties.

Monolayer WSe2 were prepared on sapphire substrate by chemical vapor deposition (CVD). In this paper, we report the related spectra properties on the monolayer WSe2 with 1.0 MeV carbon ion at fluences of 5.0×1013 ions/cm2 and 5.0×1014 ions/cm2. The surface morphology and binding energy before and after carbon ion irradiation were studied by atomic force microscope (AFM) and X-ray photoelectron spectroscopy (XPS). The change in transmittance were also been studied on these samples. The Raman spectra were measured to study the vibrational and the electronic properties. Photoluminescence (PL) spectra were used to investigate the properties of defect and exciton physics on monolayerWSe2 before and after irradiation.

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Raman monitoring of ion-beam synthesis of ZnSe and ZnSxSe1-x nanocrystals in silicon dioxide films

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Synthesis and characterisation of "ZnSe precipitates + silicon dioxide" nanocomposite is of great interest due to its application potential in optoelectronic devices such as light-emitting diodes, flat panel displays, infrared windows, nonlinear optical devices and sensors. Further, there is particular interest in ternary alloy-based ZnSxSe1-x nanocrystals due to the possibility of band gap variation via the alloy composition. There are many methods to prepare such nanocrystals. The majority of them are multistep and expensive ones. In this report we offer to synthesize ZnSe and ZnSxSe1-x nanocrystals in SiO2 matrix by ion implantation method. The ion implantation is price-acceptable, reproducible and full compatible one with current silicon technology.

In order to form ZnSe and ZnSxSe1-x nanocrystals in dielectric matrix, SiO2 (600 nm)/Si samples were consistently implanted at 500 ∘C with (Zn+Se) and (Zn+Se+S) ions, correspondingly. The energies and fluencies of implanted ions are: Zn (150 keV, 8×1016 cm-2), Se (170 keV, 3.5×1016 cm-2) and S (90 keV, 4×1016 cm-2). After implantation the samples were annealed in Ar atmosphere at 900 ∘C during 30 min. Rutherford backscattering spectrometry, Raman scattering (RS) spectroscopy, transmission electron microscopy and photoluminescence (PL) have been employed to investigate elemental and phase composition as well as light-emitting properties of implanted silicon oxide films.

Raman measurements were performed in backscattering geometry with a Nanofinder High End micro-Raman spectrometer using a UV (355 nm) and blue (473 nm) laser beams as the excitation sources to investigate phase composition of the samples. In the case of double implantation, the LO-, TO- as well as second-phonon modes of ZnSe phase have shown resonance behaviour in the RS spectrum under blue excitation. In the case of triple implantation, there are some features in Raman spectra which prove formation of ternary compound. Firstly, in the case of UV excitation, Raman spectrum of silicon oxide film implanted with (Zn+Se+S) ions exhibits the weak band at _˜570 cm-1 which can be assigned to second-order scattering mixed process involving the ZnSe-like and ZnS-like LO phonons. Using methodology based on the calculation

*Speaker

of integral intensity ratio of LO ZnS-like and LO ZnSe-like peaks from Raman spectra measured with UV and blue excitations, the sulfur content (x $\approx$ 0.4) was estimated. Thus, based on Raman spectroscopy data we can conclude that ZnSe and ZnS0.4Se0.6 ternary alloy-based nanocrystals are synthesized in the SiO2 films by ion implantation. The intensive PL bands for SiO2 films implanted with (Zn, Se, S) and (Zn, Se) were detected in the blue and red spectral ranges, respectively. The interpretation of PL spectra is in a good agreement with the conclusions obtained by RS data.

The stress evolution in silicon carbide during thermal annealing

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As a candidate structural material in nuclear energy system, helium (He) effect in silicon carbide (SiC) is a serious concern, which can induced a buildup of lattice disorder and formation of helium bubbles. In this study, the evolution of stress induced by He in thermal annealing process was investigated. Two SiC samples (4H-SiC) were implanted with multi-energy He ions to produced a plateau in the depth from surface to 1.4 um with the He atom concentration of 3000 (lower than helium bubble formation threshold concentration) and 6000 appm (higher than helium bubble formation threshold concentration). Subsequently, the implanted samples were annealed from 300 to 1100 in vacuum condition. The X-ray diffraction (XRD) measurement was performed for the two samples after implantation and each step thermal treatment. The stress data were extracted from XRD results, and the different behavior of stress evolution during annealing was discussed for the two samples.

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Investigating the effects of ionizing radiation on quantum dots and possible applications in nanodosimetry

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Nowadays, it is accepted by the scientific community that the early radiation-induced damage to cells begins with the damage of DNA segments and it is the result of the spatial distribution of inelastic interactions of single ionizing particles (track structure). For this reason, the radiation damage depends on radiation quality and cannot be accurately described by conventional radiation quantities, such as absorbed dose and linear energy transfer (LET) [1]. The field of nanodosimetry aims therefore to study the stochastic of particle interactions in nanometre-sized volumes with the target of correlating quantities derived from the ionization cluster-size distributions to radiobiological effects. The development of specific apparatus, for example the Startrack [2], allowed the investigation of the ionization cluster-size distributions of different particles and ions on a nanoscopic DNA level. Experimental investigations combined with Monte Carlo simulations demonstrated the possibility of a new metrology of ionizing radiation based on nanodosimetric descriptors [3]. With the growth of nanodosimetry, many applications including radiation protection and medical radiation treatment would benefit from the development of portable nanodosimeters, i.e. relatively compact and light devices that quantify the energy released by ionizing radiation within nanometric volumes. A possibility could be the use of Quantum Dots (QDs) as active material, since their size is comparable with those of the most probable radio-sensitive volumes of biological systems [4]. The development of such devices depends therefore on a deep understanding of the physical interaction mechanisms between ionizing radiation and QDs. In this preliminary work, CdSe/ZnS core-shell QDs dispersed in a polysiloxane matrix are irradiated with proton and helium beams at different fluences and at energies of 2 MeV. Emission and excitation spectra are collected with a Jasco FP spctrofluorimeter. Absorption spectra are measured with a Jasco V-570 spectrophotomer and in diffuse reflectance mode with a QE65000 Ocean Optics spectrometer equipped with a silica fiber bundle. Luminescence spectra and lifetimes before and after irradiation are measured with different pulsed lasers at 355, 405 and 470 nm and with a time correlated single photon counting (TCSPC) system connected to a focusing lens. Optical images of irradiated and unirradiated regions are collected with a wide-field microscope equipped with a CCD camera. Experimental results are then correlated with the released dose and with the track structure of the ionizing particle within the QD-matrix complex.

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Defect production and its impact on photoluminescence in GaN irradiated with energetic heavy ions

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Gallium Nitride (GaN) is an important material for the development of novel photonic or electronic devices. Ion implantation/irradiation is an efficient method of doping or etching of the material. Damage production in crystal in the case of ion-implantation is an important concern.
In the present work, we studied the damage production in GaN by keV and MeV heavy ions and its effect on the photoluminescence (PL) character of GaN epi-layers (n-type doping, grown on sapphire substrate by MOCVD). Some specimens were irradiated with Fe+ ions of 110 keV to three successively increasing fluences of 2x10ˆ15, 1x10ˆ16 and 5x10ˆ16 ions/cmˆ2, which correspond to peak damage levels of 2, 10 and 50 dpa (displacement per atom), respectively. For each dose the specimens were kept at different temperatures from 300 K to 650 K during irradiation. Other specimens were irradiated with 2.3 MeV Ne ions at room temperature to successively increasing fluences from 1x10ˆ12 to 1x10ˆ16 ions/cmˆ2, in which case energy deposition from atomic excitation and ionization is a concern.

The specimens were subsequently investigated by RBS spectrometry in channeling geometry (RBS/c), high-resolution XRD, Slow positron beam with Doppler Broadening spectroscopy (PAS), and Raman scattering spectrometry. The photoluminescence of specimens in all the conditions were tested.
It is observed from RBS spectrometry that an enhanced lattice disorder occurs at the mediate irradiation temperature of 410 K for the mediate and highest Fe-ion fluence. Doppler Broadening spectroscopy of Slow positron beam shows that defect structure is different in the specimens irradiated at different temperatures. The heavily damaged layer results in a sharp PL peak at 363 nm, which intensity increases significantly when the relative disorder is higher than 0.4. In the case of MeV Ne ion irradiation, a homogenous lattice expansion was observed at low doses, while a damage gradient was built up at the highest dose. Mechanisms underlying damage production is discussed.

*Speaker

Defect evolution and its effect on surface hardness in helium-implanted silicon carbide

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Effects of radiation damage and accumulation of helium in silicon carbide have been important concerns for the use of silicon carbide in advanced nuclear energy systems. In the present study, defect production and change of nano-hardness in silicon carbide implanted with helium ions is described. Implantation of silicon carbide (4H, 6H types) with helium ions with single or multiple kinetic energies ranging from 15 keV to 480 keV was performed at two temperatures (300, 600 K) respectively. The fluences of ions were selected to be in the range from 1x10ˆ15 to 1x10ˆ17 ions cmˆ-2. The evolution of defects in the specimens with annealing temperature (from 773 to 1473 K) was investigated with slow positron beam annihilation technique (PBA), high-resolution X-ray diffraction spectrometry (HRXRD) and transmission electron microscopy (TEM).

The study shows quite different annealing behavior of the helium-implanted layer below or above the dose necessary for the formation of helium bubbles. The bubble planar clusters were regarded as the precursor for the long-range ordering of bubbles. Formation mechanism of He-vacancy clusters was discussed to describe the feature of microstructures.

In addition, nano-indentation test of the helium implanted specimens were performed. The dependence of the nano-hardness on dose and annealing temperature was discussed in light of our understanding about the microstructures.

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Projectile fragment emission in the fragmentation of 20Ne on C, Al and CH2 targets at 400 A MeV

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The emission angle and the transverse momentum distributions of projectile fragments (PFs) produced in fragmentation of 20Ne on C, Al and CH2 targets at 400 A MeV are measured. It is found that the average emission angle and transverse momentum increase with the decrease of the charge of PFs for the same target, and no obvious dependence of angular and transverse distribution on the mass of target nucleus is found for the same PF. The cumulated squared transverse momentum distribution of PF can be well explained by a single Rayleigh distribution, the temperature parameter of PFs emission source is obtained, which is about 2.0 MeV and do not depend on the size of PF and mass of target for PF with charge of 5

*Speaker

In-cascade Defect Production and Annealing in Silicon Carbide

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Coupled energy processes in electronic and atomic subsystems and subsequent defect evolution in SiC are investigated under ion irradiation with energies in the intermediate energy regime where ionization and displacement events occur simultaneously. Various energetic ions are utilized to evaluate ionization effects due to the electronic energy deposition and displacement events due to nuclear energy deposition. In-cascade damage processes are revealed through temporal and spatial coupling of ionization with cascade events in SiC. While depending on the lattice temperature raise, recoil and cascade distributions and defect configurations, in-cascade ionization can induce local temperature increases from the energetic ions in the intermediate regime that effectively anneal defects and suppress damage accumulation. Insights on the complex electronic and atomic correlations on extreme energy deposition may provide a basis to better control and predict SiC and other ceramic material properties in extreme radiation environments. This work was support by U.S. DOE, BES, MSED.

*Speaker

Lattice damage effects of H ion irradiation on 4H-SiC crystal

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Silicon carbide (SiC) is of potential use in first wall of fusion reactors because of its excellent physical and chemical properties such as it has high thermal conductivity, good thermal shock resistance, small neutron capture cross-section and high chemical stability. In our work, we research the damage behavior of 4H-SiC crystal by H ion irradiation. The samples irradiated with 100-350 keV H ions at room temperature with fluence of 5 × 1014 ions/cm. A series of heat treatments at temperatures ranging from 200° to 800° in an air atmosphere were used to investigate the thermal stability of our ion-implanted 4H-SiC crystal. RBS/channeling (RBS/C) has been used to study the formation and recovery of disorder on the lattice in 4H–SiC single crystals before and after annealing treatment. Micro-Raman imaging is a powerful nondestructive approach to examine lattice modification and local micro-structural change. We performed confocal micro-Raman measurement and it is used to provide the information about the crystal structure of SiC crystal after H ion irradiation. The changing trend of damage profile with annealing temperature was given also. The damage profile of H ion irradiation SiC crystal is also calculated by SRIM 2010 software. This work could provide useful information for fusion reactors device based.

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NANO GRAPHITE CRYSTAL FORMED IN 4H-SIC

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As emerging material, graphene combined with a substrate has shown explosive application in electronic industry. To become a viable technology, graphene need to be grown on or embedded in a substrate. Graphene epitaxial grown on SiC substances has been extensively studied. Here we explore formation of graphene embedded in SiC matrix utilizing ion implantation and annealing. Raman spectra and transmission electronic microscope (TEM) were used to analysis the formation of nano graphite crystal in 4H-SiC. The 4H-SiC specimens were implanted with 110 keV C-ions and then irradiated with 230 MeV Pb-ions and subsequently annealed at different temperatures in vacuum. Raman spectra detected the mode graphite after high temperature annealing. TEM verified that nano graphite crystal exit in the layer of carbon precipitation. This exploration provides a potential way to form graphene multilayer embedded in SiC.

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Colossal enhancement in magnetic moment of ferrimagnetic NiCo2O4 via irradiation induced strain-doping

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Strain doping has emerged as a powerful technique for efficient control of single axis lattice expansion to fine tune and modulates the inaccessible complex correlated phases in the oxide thin films. We report the fine tuning of the magnetic moment and insulator-metal transition in the ferrimagnetic NiCo2O4 inverse-spinel oxide by creating oxygen deficiencies employing high energy He-ion irradiation. Application of the uniaxial tensile strain, less than 1%, can effectively tune the oxygen vacancy driving the system in the colossal increase of the magnetic moment by two-factors in magnitude. This magnetic moment shows scaling with the He-ion irradiation fluence. Our results corroborates well with the X-ray absorption spectroscopic data which shows the peak-height changes and energy shifts of Co-L2,3 and Ni-L2,3 edge driven by the oxygen vacancy. These results demonstrate a new pathway of decoupling the oxygen content from its typical crystal environment via He-ion irradiation, useful for designing new functionalities in other spinel oxide thin films.

*Speaker

Session VI

Investigation of 2D-hBN and graphene after swift heavy ion irradiation

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The irradiation with ions opens up the opportunity to modify materials on the nanoscale, hence this technique is also of considerable interest for the modification of 2D materials. Depending on the kinetic energy and the charge state of the projectile, the initial energy deposition can be tuned: While slow, singly charged projectiles basically interact via direct nuclear collisions, the major channel for energy deposition of swift heavy ions (SHI) and highly charged ions (HCI) is by electronic excitations and ionizations [1,2], for a comparison and review see [3].
One essential difference between the latter two projectiles is the depth of excitation. In contrast to HCIs, SHIs do not just excite the (near-)surface atoms, but excite the electronic system and ionize target atoms along their whole trajectory, which may extend up to several microns deep. By tilting the SHI beam, this can be exploited to effectively introduce extended defects even in 2D materials [4,5].

Graphene is one of the most investigated 2D materials and as such there are many studies dealing with the interaction of SHIs and graphene, focusing mainly on the characteristic, structural modification of graphene, see e.g. [6]. Since graphene is unique with respect to its electronic properties, the question arises, how the defect creation is connected to these properties. We therefore study structural modifications after intense electronic excitation in 2D hexagonal boron nitride (hBN), often called "white graphene", an insulating material which is regularly used as a building block for van der Waals-heterostructures together with graphene or other semiconductors.

In our study we determine the efficiency (i.e. the number of ions needed to create one defect one average) and show that the efficiency for graphene is one for single layer graphene, but decreases down to zero very fast, with increasing number of layers. We find that for two to three layer hBN the efficiency is higher than for two to three layer graphene. We also compare the efficiency of defect creation for graphene and hBN exfoliated on different substrate materials.

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Conical etched ion tracks charaterised by small angle x-ray scattering

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When a highly energetic heavy ion passes through a target material, the damaged region left in its wake often exhibits preferential etching over the bulk. The etching process can create very high aspect ratio channels of up to tens of microns in length, with pore diameters as small as a few nanometers. Using this technique, so called "ion track etched membranes" can be fabricated in a variety of materials including polymers and some of the thin films typically used in semiconductor processing such as silicon dioxide (SiO2) and silicon nitride (Si3N4). Pores formed by this method are highly parallel-oriented with very narrow size distributions. The morphology of the pores can be cylindrical, conical or double conical, depending on the etching conditions.

We are seeking to develop a better understanding of the ion track etching process and its dependence on the un-etched track structure through a unique combination of complementary characterisation techniques including synchrotron based small angle x-ray scattering (SAXS) combined with Monte-Carlo simulation, and advanced electron microscopy. The combination of these techniques enables an accurate reconstruction of the size and shape of the pores.

Freestanding SiO2 and Si3N4 membranes were irradiated with 185 MeV 179Au ions at the ANU Heavy Ion Accelerator Facility. SiO2, and Si3N4 films were irradiated with 1.1 GeV 179Au ions at the GSI UNILAC in Darmstadt, Germany. Low irradiation fluences of the order 1x108 ions/cm2 were chosen to avoid significant overlap of the pores during etching. This study focuses on the influence of the etching time and etchant concentration on the pore morphology for ion tracks etched in SiO2. We have determined the track etch rate and cone angle as a function of these parameters. This is necessary for reproducible fabrication of porous membranes for specific functions in the future.

*Speaker

Track-associated radiation damage in Y-Ti-O nanoparticles in ODS alloys

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Swift heavy ion induced structural changes in oxide nanoparticles in metallic matrices remain much less studied compared to metal and semiconductor nanoparticles embedded in oxides. The aim of this report is to review recent experimental data on the morphology of swift (167 and 220 MeV) Xe ion induced latent tracks in Y2Ti2O7 nanoparticles within oxide dispersion strengthened (ODS) alloys as a function of ion fluence, irradiation temperature and post-irradiation heat treatment. It was found that high energy heavy ions induce amorphous latent tracks in Y-Ti-O nanoparticles for ions exceeding the threshold electronic stopping power of about 8 keV/nm [1]. Track diameters measured at a specific energy loss are similar throughout the temperature range of 300 - 1000 K. Ion track overlapping results in complete amorphization of nanooxides irrespective of irradiation temperature and no recovery to the crystalline state was observed after post-irradiation heat treatment [2]. However, recrystallization of amorphous track regions was observed after annealing samples irradiated in the ion track non overlapping regime. The structural recovery of latent tracks was found to be dependent on particle size and its coherence with the metallic matrix.

*Speaker

Competition between annealing and damage in carbon nanostructures by swift heavy ions

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We have observed annealing effects at lower fluences in carbon based materials (such as fullerenes, carbon nanotubes, graphene and graphene oxide), whereas defect production at higher fluences is observed. The inelastic thermal spike model calculations are used to show that an ion track core is formed which is surrounded by a halo. The high transient temperature above melting point in track core results in damage, whereas lower temperature in track halo is responsible for annealing. Swift heavy ion (SHI) irradiation induced annealing and purification effects in graphene and graphene oxide films using Raman studies after irradiation with Ag, Au and other ions show that the disorder parameter α, defined by ID/IG ratio, decreases at lower fluences but increases at higher fluences beyond 1e12 ions/cm2. The radiation stability of graphene under Au ion irradiation using Raman and XRD characterization techniques will be discussed. It is shown that graphene sustains irradiations at high fluence and energy without showing significant damage or amorphization.

*Speaker

Effect of an initial lattice state on the kinetics of Al2O3 excitation in tracks of swift heavy ions

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This report presents theoretical study of swift heavy ion (SHI, $M >$ 20 amu., $E >$ 1 MeV/nucl) tracks formation kinetics depending on the initial state of an irradiated material. This research is stimulated by so far an open question how the lattice structure or temperature affect material excitation process. To investigate this problem, we apply a new version of TREKIS code [1,2] for description of excitation of alumina in the nanometric vicinity of trajectories of SHIs decelerated in the electronic stopping regime.
TREKIS code is based on a Monte-Carlo algorithm describing kinetics of fast electrons and valence holes, which appear due to material ionization, as well as their interaction with the lattice up to ~100 fs after the projectile passage. Building cross sections within the dynamic structure factor/complex dielectric function (DSF-CDF) formalism [3], this model takes into account collective response of the electronic and ionic subsystems to excitation which can be of principal importance for realization of unusual pathways of the extreme track kinetics.

To describe interaction of excited electronic subsystem with the lattice, the presented upgraded version of TREKIS uses cross sections based on the DSF of the lattice, calculated with an in-house molecular dynamic code. The DSF of Al2O3 lattice was calculated for the wide range of temperatures (80-1000 K), that enables to investigate effects of initial states of this target on the SHI track kinetics. In particular, a sharp increase of mean free paths of electron scattering on the lattice is found in simulations when the temperature of Al2O3 crystals is below 200 K.

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Session VII

Quantum dot synthesis by ion beam mixing in Si-SiO2 heterostructures and nanopillars

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Semiconductor quantum dots self-assembled within an insulating nanolayer are promising for a significant advance in nanotechnology: design and building single electron transistors (SET) working at room temperature [see, e.g. Nano lett. 14(2014)71]. The key step for building well-separated quantum dots requires a self-assembly process in strongly restricted regions. It was previously shown that a reliable formation of nano-dots can be achieved by controlled self-assembly during phase-separation of meta-stable SiOx, which was obtained via ion mixing by irradiating Si-SiO2-Si sandwich structure. However, such phase separation has been resulting in a quantum dot chain with only small space separation.
In the current work, we examine two suggested scenarios how to restrict the volume of metastable SiOx, where a single quantum dot can be formed: either using highly focused ions provided by Hellium Ion Microscope to irradiate a flat Si-SiO2-Si sandwich structure or irradiate with the broad ion beam the Si-SiO2-Si nanopillars. Both scenarios are expected to restrict the volume of ion mixing creating well-separated intermixed regions of SiOx phase. The physics of ion irradiation in both cases, however, may not be exactly the same. Straggling of the ion beam during the irradiation may lead to significantly larger regions of ion mixing in the focused ion irradiation. On the other hand, large surface areas of nanopillars can also affect the formation of SiOx layer in a non-intuitive manner.

Here, we present a comprehensive computer simulation model on the formation of SiOx restricted volumes by ion beam mixing of Si into a thin SiO2 layer embedded in Si in a sandwich-like manner in both flat and nanopillar samples at experimental fluences. Atomic cascades initiated subsequently by thousands of energetic Ne+ or Si+ ions in a volume of approximately 10x10x5 nmˆ3 are needed to provide sufficient mixing of Si recoil atoms into SiO2, for self-assembly of the 2-3 nm wide quantum dots.

An accelerated molecular dynamics (MD) method, utilizing the ZBL potential for high energy and the Munetoh or Watanabe potentials for low energy interactions, was used to simulate the formation of the SiOx volume. The two cases of restricted regions of ion mixing in flat interfaces and nanopillars are calculated and compared. The MD results are also compared to the ones obtained by 3D-TRIDYN and the concentration profiles of SiOx from our MD model was used for phase separation simulations by KMC model.
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*Speaker

Cathodoluminescence analysis of damage build-up in irradiated spinel mono- and polycrystals

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One of the still unresolved problems of the analysis of radiation build-up in various materials is the lack of quantitative method to determine damage level in polycrystalline solids. This analysis is crucial for modelling of structural transformations upon irradiation. The obvious method of choice used for quantitative evaluation of the extent of damage is Rutherford Backscattering/Channeling (RBS/C). This technique, however, applies only in single crystals therefore correlation of the results obtained for single and polycrystalline crystals is not straightforward, as numerous mechanisms may influence defect formation in polycrystals. The most evident mechanism is defect annihilation at grain boundaries and small size of crystalline domains (grains) what may facilitate their structural transformation. The very recent concept is to use luminescence techniques to measure the level of disorder in polycrystals, as it may be applied to both single and polycrystalline solids. The experimental method described in this work relies on a comparative analysis using quantitative cathodoluminescence (CL) measurements of irradiated single crystals, correlated with well-established RBS/C technique to validatethe cathodoluminescence data. Additionally, cathodoluminescence analysis provides an insight into differences between damage accumulation in single- and polycrystals. MgAl2O4 samples were irradiated with 320 keV Ar+ ions at fluencies ranging from 1e12 to 2e16 cm-2 in order to create various levels of radiation damage. Cathodoluminescence measurements were performed on an Attolight Rosa 4634 CL microscope, which tightly integrates an achromatic reflective lens within the objective lens of a field-emission gun scanning electron microscope (FEG-SEM). The spectrally resolved raw signal for each sample with different fluencies of Ar+ ions was analyzed in terms of signal intensity of the selected band. Additionally, for single crystals, the damage-build up as a function of accumulated ion fluence was established through RBS/C as a control. The results were then processed using Multi-Step Damage Accumulation (MSDA) model, allowing determination of damage build-up kinetics, and finally cross-sections for radiation damage build-up in polycrystals. The phenomena responsible for the rapid decrease of the cathodoluminescence of the material are different than those related to the creation of displaced atoms present in the crystal channels. The rate of changes resulting from the formation of non-radiative recombination centers is very different than that resulting from the creation of single defect clusters or dislocations. Consequently, CL technique appears as a complementary tool that opens a new pathway in damage accumulation studies in single- and polycrystalline materials.

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Radiation Effects and Quantum Well Intermixing in InGaN/GaN Multi Quantum Wells

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The efficiency of InGaN-based light emitting diodes (LEDs) decreases dramatically in the green spectral region, leading to an output deficiency commonly known as the "green gap". In addition, the loss of efficiency at high injection current, commonly called 'droop', worsens in this important spectral region for solid state lighting applications. Following work on 'super-bright' core-shell quantum dots with deliberately graded interfaces, compositional grading by irradiation and annealing of InGaN/GaN multi quantum wells (MQW) was proposed to mitigate polarization effects and Auger losses and improve the internal quantum efficiency of green LEDs [1]. Quantum well intermixing (QWI) was successfully applied to III-V arsenide and phosphide MQW to introduce such gradients with the possibility of monolithic lateral patterning [2]. In III-nitride MQW, however, little is known on the effects of irradiation and annealing on structural and optical properties.

I will review our recent work on QWI in InGaN/GaN MQW. Annealing up to 1400 °C, well above typical MOCVD growth temperatures, resulted in negligible interdiffusion of QWs and barriers revealing a surprising thermal stability [3]. The defect formation upon nitrogen implantation was studied in detail [4]. Despite strong dynamic annealing effects, which keep structural damage low, the created defects strongly quench the QW luminescence even after annealing. Diffusivity remains low while implantation damage promotes the formation of voids and In-rich

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zones inside the quantum wells during annealing. First results will be presented on using swift heavy ion irradiation for QWI and hint at a more efficient intermixing process in this high-electronic-energy-loss regime.

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Swift Heavy Ion Track Dynamics in Gallium Nitride

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Group III-nitrides have been the materials of choice of some of the most important achievements in the semiconductor industry of the last decades. Applications based on their wide band gap abound, ranging from light emitting diodes to high-power transistors. More recently, there has been an increasing interest in understanding the response of this group of materials to the so-called Swift Heavy Ion (SHI) irradiation. Group III-nitrides appear to be strong candidates for radiation hard electronics to be used in extreme environments such as space or nuclear reactors. Moreover, the possibility of using SHI for structural modification and bandgap engineering in heterostructures has been studied. It is thus paramount to understand the dynamics of the crystal upon the passage of the SHI, namely the conditions for ion track formation, defect creation, dynamic annealing and recrystallization effects.
In this work, we aim at understanding the SHI interaction with hexagonal c-plane GaN using Molecular Dynamics (MD) simulations along with the Thermal Spike (TS) model backed by experimental data. A time-dependent study of the track morphology is presented. It is shown that, above an energy deposition threshold, at least two phase transitions can occur, the decomposition of GaN into Ga and N2 and the congruent melting of GaN. While in the former the phase transition is irreversible, in the latter it is not. This leads to a partial recrystallization of the amorphous track during the cooling of the crystal. The thermodynamics of this recrystallization is inspected and a pressure-temperature study is shown. Furthermore, the depth dependence of the track morphology is discussed under this thermodynamic approach.
A comparative study of these simulations with experimental results is also presented. GaN samples irradiated with various fluences of 185 MeV Au ions are characterized with Rutherford Backscattering Spectrometry/Channeling (RBS/C). A statistical model for the lattice damage, taking in consideration the recrystallization effect, is derived and applied to the RBS/C spectra. The resultant track radius is in very good agreement with the simulation results. Finally, upper and lower bounds for the electron-phonon relaxation time, the only fitting parameter of the TS model, are estimated.

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Radiation hardness of Kr+ ion implanted BaWO4 at room temperature

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BaWO4 is an interesting material which has a wide band gap of about 4.8 eV and a correspondingly high transmission of light in the visible spectral range. This makes this material a possible candidate for the formation of optical devices. In several oxidic materials ion implantation was successfully applied to build wave guides or other optical devices (see e.g. [1]). Furthermore, BaWO4 may be useful as detector or in nuclear waste management. BaWO4 has the same lattice structure as PbWO4 which is well known as detector material [2]. For all these applications sufficient knowledge about the behaviour of the material during irradiation with energetic particles is necessary.
In this presentation, we report on 370 keV Kr+ ion implantion into BaWO4 with ion fluence ranging from 1×1012 to 4×1016 ions/cm2 at room temperature. The quasi *in situ* damage built-up in Kr-implanted BaWO4 was investigated by Rutherford backscattering spectrometry in channelling configuration (RBS/C) using a two-beam chamber. No amorphization is observed in Kr-implanted BaWO4 up to the highest ion fluence applied. The shape of the RBS/C spectra indicates the formation of extended defects. Additionally, a significant increase of the surface peaks of Ba and W is observed. Damage formation at depth proceeds in two steps which can be attributed to point defects formation and recombination and formation and saturation of extended defects [3, 4].

Our results indicate that BaWO4 is less radiation resistant than PbWO4 in which extended defects were found only locally after irradiation under extreme conditions [2]. This is a remarkable result because both materials have the same crystal structure. Annealing for the highest fluence of 4×1016 ions/cm2 was performed at temperatures from 300 up to 600∘C for 60 min. Close to the surface strong damage annealing takes place. However, much less annealing is observed within the implanted layer. Further work is in progress for investigating the defect structures produced in more detail. Additional ion implantations will be performed at lower temperatures, which will lead to better understanding of the primary effects in ion implanted BaWO4.

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Session VIII

Microstructure of Si3N4 and AlN Irradiated with Swift Heavy Ions at 80-1000 K

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Si3N4 and AlN are not only important semiconductor materials but are also under consideration for use as candidate-inert-matrix-fuel-hosts (IMs) for the burn-up of plutonium and other minor actinides [1,2]. IMs are envisioned as one possible means to close the nuclear fuel cycle in an effort to reduce the amount of high level waste materials which require long-term storage [3]. The physical properties of these materials make them well suited to reactor conditions [2]. However, in order to prove the viability of these materials for nuclear applications their radiation stability must be tested.
In this study swift heavy ions (SHIs) are used to simulate the effects of fission fragments on the microstructure of Si3N4 and AlN. Polycrystalline specimens were irradiated with Xe and Bi ions, with energies ranging from 167 to 1030 MeV at temperatures ranging from LNT to 1000 K. Such experimental parameters allow for the determination of electronic energy deposition and irradiation temperature effects within the aforementioned materials. Since the mechanisms involved in the process of latent track formation in ceramics are still unconfirmed it is important, from a fundamental point of view, to obtain experimental data from a wide range of materials so that an accurate model for latent track formation can be developed.

TEM lamellae from irradiated ceramics were prepared using an FEI Helios Nanolab 650 FIB. Specimens were analysed using either a JEOL JEM 2100 LaB6 or ARM 200F TEM.

It was found that latent tracks are registered in Si3N4 at all ion energies and track diameters increase with the irradiation temperature and electronic stopping power opposed to AlN, where no indication of latent tracks was observed.

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*Speaker

Radiation tolerance of Yttria stabilized Zirconia against SHI irradiation: Effect of grain size and temperature

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Materials employed in the nuclear industry are prone to un-desirable damages since they are subjected to an extremely harsh environment consisting of extensive radiation and high temperatures. It is therefore vital to understand the behavior of these materials under such extreme conditions for the design of durable and efficient nuclear energy systems. Recent studies [1-3] suggest that materials in nano-dimension should exhibit enhanced radiation tolerance as compared to their bulk counterparts. However, as illustrated in several reports[4, 5], going to a highly nano-crystalline state might not always be advantageous for improving the radiation stability. Hence, the radiation stability of nano-materials in comparison to bulk materials is still a matter of debate.

To address the aforementioned issues, Yttria stabilized Zirconia (YSZ) pellets, with grain sizes ranging from _˜ 30 nm up-to few microns, were irradiated with 80 MeV Ag6+ ions at room temperature and 1000 K for a systematic understanding of the dependence of radiation stability on the grain size and temperature under high energy irradiations. These ions were chosen so as to effectively simulate fission fragments; while the irradiations were performed at typical reactor temperature of 1000 K to better simulate a nuclear reactor environment. At room temperature, the nano-crystalline samples suffered maximum damage while the sample with micron sized grains was most stable – this result being contradictory to a previous study [6] investigating the dependence of radiation stability of YSZ on grain size under low energy irradiations. In case of irradiations at 1000 K, the damage for all grain sizes was found to be reduced as compared to that at room temperature; the reduction in damage being significantly greater for the nano-crystalline samples in comparison to the bulk sample. Variation in the damage production mechanism depending on the energy of irradiations coupled with the role of grain boundaries/grain size and temperature in determining the overall irradiation induced damages will be discussed in detail to explain the observed results and its contradiction with previous reports.

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Thermal effects in ion irradiated Ti2AlC and Ti3SiC2

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Structural materials in nuclear systems endure a harsh environment, like high temperature, high stress and intense radiation fluxes [1]. MAX phases have been suggested for advanced nuclear reactor applications due to their excellent irradiation tolerance, especially in high temperature irradiation. To better understand the mechanisms of irradiation tolerance of MAX phases and the evolution of defects in high temperature irradiation. Herein, we irradiated Ti2AlC and Ti3SiC2 with 3 MeV Au ions at 25 , 360 and 700 to a dose of 1.5×1016 cm2, and then 360 and 700 thermal annealing was performed for samples irradiated at room temperature. GIXRD, TEM and nanoindentation were used to characterize microstructural evolution and mechanical property degradation. Our results show that ion irradiations induce a structural transformation from initial hcp structure to fcc structure in both materials irradiated at room temperature. No such structural transformation was found in both materials irradiated at high temperature. After annealing room at 360 and 700 , fcc structure caused by irradiation at room temperature was not observed in Ti2AlC. However, fcc structure in the Ti3SiC2 irradiated at room temperature remained after annealing at 360 and 700 . This indicates that the structural defects in Ti2AlC are more instable than Ti3SiC2, resulting in the higher mobility and recombination rate.

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Time-of-Flight Secondary Neutral & Ion Mass Spectrometry Using Swift Heavy Ions

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We report on a new time-of-flight (TOF) spectrometer designed to investigate sputtering phenomena induced by swift heavy ions (SHI) in the electronic stopping regime. In this experiment, particular emphasis is put on the detection of secondary ions along with their emitted neutral counterparts in order to examine the sputtered material with respect to its composition, emission velocity and angular distribution, ion fraction etc. For the detection of neutral species, the system is equipped with a pulsed VUV laser for post-ionization of atoms and molecules ejected from the surface via single photon ionization at a wavelength of 157 nm (corresponding to 7.9 eV photon energy). The instrument has been added to the M1-branch beam line at the Darmstadt accelerator facility (GSI) and was tested with 4.8 MeV/u Bi26+, Au26+ and Ca10+ ions impinging onto various samples including metals, semiconductors, ionic crystals and organic films. These conditions refer to the maximum of the electronic stopping power (around 10 keV/nm), where nuclear stopping is negligible and the projectile induced emission of surface material is dominated by electronic sputtering. The direct comparison of secondary ion and neutral spectra obtained under otherwise identical instrumental conditions allows a mass resolved characterization of the sputtered flux. As a result, we find that the vast majority of the ejected material is emitted in the neutral state. Moreover, the ionization probability measured, for instance, for metal atoms emitted from a clean metal surface appears to be quite similar to that observed in Secondary Ion Mass Spectrometry (SIMS) involving keV ion bombardment. However, the dependence of this quantity on surface conditions like, for instance, an oxygen coverage, is shown to be very different in both cases, thereby clearly indicating a fundamental difference between the ejection mechanism under electronic and nuclear sputtering conditions. Interestingly, we find rather large SHI impact generated neutral sputter yields even from metallic samples, which exceed that measured under 5 keV Ar+ bombardment and are shown to critically depend on the morphology of the bombarded sample. In addition to single atoms, we observe an abundant emission of neutral clusters as well as secondary cluster ions, many of them produced by the adduction of positive (alkali) or negative (halogen) ions. For molecular samples, we find that electronic sputtering produces an abundant emission of intact molecules or quasimolecular ions, respectively, while nuclear sputtering induced by 5 keV Ar+ bombardment leads to strong fragmentation. For a few exemplary cases, it is shown that the sputtered material is entirely dominated by intact neutral molecules, indicating the feasibility of SHI induced sputtering as a soft desorption mechanism for molecular analysis.

*Speaker

Session IX

Anomalous kinetics of diffusion-controlled F center annealing in neutron irradiated sapphire

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Al2O3 (sapphire, corundum) is a promising material for fusion reactors, mainly for diagnostics as a general insulator or optical components. Thus, it is very important to predict/simulate the kinetics of defect accumulation in sapphire under neutron irradiation as well as long-time defect structure evolution. There were numerous experimental measurements of the primary defect accumulation kinetics (first of all, F color centers-oxygen vacancy with two trapped electrons) as a function of radiation dose rate and temperature with subsequent post-irradiation annealing. As is well known, the F center mobility is much smaller than that of the complementary Frenkel defects – interstitial oxygen ions. Thus, at moderate radiation doses and temperatures, the kinetics of the F center annealing is controlled by their diffusion-controlled recombination with mobile oxygen interstitials. Despite numerous experimental data, very few theoretical efforts were devoted so far to the quantitative analysis of available kinetics, in order to extract main kinetic parameters- interstitial migration energy Ea and diffusion pre-exponent Do, necessary for further prediction of the secondary defect kinetics and radiation stability of sapphire and related materials.

Such theory was developed and applied to irradiated insulators in our recent studies [1,2]. In this paper, we analyzed carefully the annealing kinetics for neutron irradiated sapphire available from literature. The extracted migration energies in different experiments vary from 0.8 eV (close to theoretical prediction [3]) down to 0.3 eV, as radiation dose increases. The pre-exponent D0 is also much smaller than the estimate for a regular diffusion in crystalline solids. This could be attributed to a strong spatial correlation of radiation-induced defects along neutron trajectories. Moreover, we have observed a strong correlation between the activation energy Ea and pre-exponent D0 (Ea) which is no longer constant but fits very well to the exponential function of Ea. In fact, as radiation dose increases, *both* the migration energy Ea and Do decrease, as the defect diffusion rate effectively grows. Moreover, this correlation was also observed for several neutron irradiated ionic materials- sapphire, MgO and MgF2. These results are analysed in terms of the Meyer-Neldel rule [4] observed earlier in glasses and disordered materials.

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Mo migration in UO2 under swift heavy ion irradiation

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Mobility of fission products (FP) in nuclear fuels is a key element for understanding and modelling the fuel behaviour during normal and off-normal situations. The present study, realized in collaboration with IRSN, focuses on the molybdenum behaviour in uranium oxide (either stoichiometric UO2 or hyperstoichiometric UO2.1).
Molybdenum is a high fission yield FP (6 %) , poorly soluble in UO2 (Kleykamp 1985) in which it can precipitate either into metallic inclusions or as oxides (MoO2 and MoO3). The redox potential of the Mo/MoO2 couple being very close to that of UO2, Mo might play the role of an oxygen buffer for the fuel (Matzke 1995). In return, the formation of UO2+x increases the release rate of Mo possibly via the formation of molybdenum oxides. Moreover, Mo can interact with other FP, like caesium, barium or strontium to form molybdate MoO42-. The Mo diffusion proceeds by thermal and a-thermal (irradiation-enhanced) mechanisms.

Three main parameters affect the Mo mobility: (i) temperature (up to 1000 or 2200 ∘C in normal or accidental conditions respectively), (ii) the irradiation mode (electronic excitations and/or ballistic damage) and (iii) the deviation from stoichiometry. The aim of our work is to estimate thermal and "athermal" Mo diffusion coefficients in UO2 and UO2+x and to identify the associated mechanisms. Our experimental procedure is the following. Molybdenum is first introduced in UO2 and UO2+x pellets by ion implantation at a mean depth (Rp) of 90 nm and a maximum concentration of 1 at.%. The evolution of its concentration profiles, before and after irradiation/annealing treatments, is followed by Secondary Ion Mass Spectrometry (SIMS) using a rotating sample holder, with a similar methodology used with success in a previous thesis (Xe behaviour in UO2 (Marchand 2012)). The evolution of the sample surface is followed by Scanning Electron Microscopy, and the structural modifications (due to irradiation/oxidation)

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by Raman spectroscopy. The present paper will focus on the Mo mobility in UO2 under swift heavy ion irradiation performed with iodine ions at 60 and 200 MeV and at 600 and 1000∘C.

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Raman scattering spectroscopy and irradiation damage in actinide oxides : From post-irradiation to in situ measurements

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Raman scattering is a powerful tool for characterizing irradiation-induced effects in materials. Whatever the type of irradiation (heavy or light ions, electrons) it can help to monitor and identify the type of induced damage. In fact, in crystallized phases, the most often Raman scattering does not detect the created defects themselves, but their consequences on the selection rules due to the symmetry lowering. This can occur with localized defects, as for amorphized states. One peculiar advantage of Raman is to have a micrometer spatial resolution, allowing to analyze the depth dependence of damage, which can lie in this length range depending on the ion beam characteristics (mass/energy). Moreover, in an inhomogeneous material (ceramics), the analysis can be selective on different grains and their orientations, and between grain cores and boundaries, through Raman imaging. A rapid review will be given on different cases recently studied, illustrating these different situations, for electronic and ballistic regimes: pyrochlores and other rare earth oxides, and actinide oxides. This latter case will be discussed in details, with comparison between UO2, PuO2 and ThO2; for the latter, the Raman spectrum is accessible only through time-resolved Raman scattering, because of a strong luminescence. All types of irradiation induce the same set of Raman lines, which can be assigned to originate from one type of defect, a cationic Frenkel pair. These Raman experiments can be performed classically, as *post-mortem* in a lab spectrometer after irradiation inside an accelerator facility, but they also can be performed during irradiation, as *in situ* measurements. This gives access to the kinetics of damage creation under beam, even with specific sample environment conditions (T, P, atmosphere), then performing *operando* conditions. Besides, this drastically reduces the necessary beam time, as increasing doses can be measured sequentially in the same experiment. Another accessible information is the irradiation-induced heating. All this will be illustrated

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by recent results on actinide oxides (UO2 and ThO2), including comparison of UO2/Argon and UO2/H2O interfaces under He2+ irradiation with radiolysis-assisted damage processes

Formation mechanisms of the high burnup structure in the spent nuclear fuel - in situ experimental simulation with ion beams in urania

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Ever since the early days of the nuclear industry researches devoted to nuclear fuels enlightened the legendary radiation stability of fluorite-structured oxides. Uranium dioxide does not become amorphous under irradiation but exhibits instead a defective structure, whose specific microstructure depends on several parameters (burnup, local temperature, irradiation conditions, incorporated impurities). Although the basic mechanisms of defects production in irradiated solids are well established, considerable experimental and computational efforts are undertaken to better understand the exact role played by the various relevant parameters in the formation of a specific microstructure and on the final destabilization of the solid. In particular, a so-called High Burnup Structure (HBS) is observed at the peripheral region of the UO2 nuclear spent fuel pellets, characterized the formation of sub-micron grains with a size (about 0.2 μm) and the development of fission gas pores [1-4].
Experimental simulations based on the use of monoenergetic ions offer the unique opportunity to investigate the behavior of a material under irradiation. Such an approach was successfully applied to urania single crystals, as a model system, irradiated with low-energy ions to examine the contribution of ballistic damage and the contribution of implanted species to the formation of the HBS structure. Crystals were alternatively (i) implanted at increasing fluence steps with few 100-keV Xe or La ions (soluble and insoluble species in UO2, respectively) at 500∘C (the temperature at the periphery of the fuel) and (ii) characterized *in situ* by Rutherford Backscattered Spectrometry in Channeling geometry (RBS/C) and *in situ* Transmission Electron Microscopy (TEM). Experiments were carried out at the JANNuS-Orsay facility. Two important steps in the disordering kinetics of the solid were established and they were interpreted in terms of the transition from the formation of isolated defects to extended defects at a low dpa number, and due to the aggregation of impurities when their concentration reaches a critical threshold. This second step was solely observed for insoluble specie. The important role played by the temperature will be discussed.

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Session X

In situ SAXS investigation of ion track nano-pore etching in polymer membranes

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Membranes containing nano-sized pores have many important applications in the areas of ultra-filtration, bio- and medical sensing, nano-fluidics, and nano-electronic devices. These applications require pores to be nano-engineered with controlled shapes and uniform sizes. Nano-pore membranes with extremely narrow pore size distributions can be fabricated in a variety of polymers using high-energy ions and chemical etching, yielding so called 'track-etched membranes'. The crucial step for the fabrication of these membranes is the etching process. It determines not only the final size of the nano-pores, but also their uniformity and shape. While the technique is commercially used for the fabrication of nano- and micro-pore membranes, a detailed understanding of the track etching process is still lacking, predominantly due to challenges for characterisation of the high aspect ratio pore morphologies. We have developed *in situ* etching capabilities for synchrotron based small angle x-ray scattering (SAXS) measurements to study the detailed track etching kinetics of nanopores in polymers. In combination with Monte-Carlo (MC) modelling of the SAXS patterns, a reconstruction of pore morphologies such as conical, double conical, or more complex shapes as a function of etching time is achievable. This enables a detailed study of the influence of the etching parameters such as concentration and temperature as well as the irradiation parameters on the track etching process. We will present first results on ion track etching in polycarbonate (PC) using 3M NaOH as a function of the etching temperature. Samples were either etched from one side or from both sides. For example at 50∘C the initial stage is characterised by etching along the highly damaged track with a rate of around 7.5 μm/min, while subsequently the radial etching rate of the pores is 2.9 nm/min. The large difference between the two etching rates of three orders of magnitude leads to the formation of almost cylindrical pores. The presentation will also provide details of the measurement setup and outline future perspectives.

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On the radiolytic efficiency of high-energy ions in ultrathin polymer films

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In this contribution, we will present recent results on chemical damage produced by high-energy ions (2 MeV protons and 2.2 GeV Bi) in PMMA and PVC thin and ultrathin films. The aim was to investigate if the radiolytic efficiency (i.e, the bond-breaking cross sections) of fast ions is altered due to the spatial confinement conditions of ultrathin films, when reducing the thickness of the film from 200 nm down to 2 nm. Chemical effects were evaluated by X-ray photoelectron spectroscopy. Bond breaking cross sections of C-O and C-Cl bonds, were found to be to a large extent insensitive to thickness reductions, even in layers as thin as 5nm. There are limitations to extract damage cross sections from very thin films, because of the non-negligible influence of the adventitious carbon and thinning of the films caused by the ion beam. These findings indicate that most of the bond-breaking induced by the ions is related to short-range events close to the track core. Such observations are in contrast to our recent studies on surface effects induced by swift heavy ions. It was evidenced that mass transport and crater formation are substantially weakened, when individual ion tracks are confined into polymeric ultrathin films, due to the suppression of cooperative effects of excited atoms along the ion track [1]. We also obtained from Monte Carlo simulations with the GEANT-DNA toolkit radial dose profiles due to the delta rays in thin water layers in a thickness range similar to the polymer films. Such simulations are a first approach to rationalize the impact of film thickness on the energy spread by the secondary electrons, and allowed the estimation of expected values for the damage cross sections for the different film thickness. [1] R. M. Papaléo, R. Thomaz, L. I. Gutierres, V. M. de Menezes, D. Severin, C. Trautmann, D. Tramontina, E. M. Bringa, and P. L. Grande, Phys. Rev. Lett. **114**, 118302 (2015).

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Study of writing laser polarization dependence of femtosecond laser induced circular optical properties in silica glass

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From a practical point of view, femtosecond IR lasers can now generate pulses with ultra-high intensity of tera-(1012) or even peta-(1015) W/cm2. This kind of laser leads to radically different laser–matter interaction from that achieved with a conventional laser. Highly non-linear multiphoton processes are observed, so even transparent material can absorb this light when the intensity is high enough. This allows 3D direct writing when the beam is strongly focused into transparent materials, particularly silica-based glasses. The mechanism of interaction of the femtosecond laser light with dielectric materials is not fully understood but one recognized specificity due to the very small pulse duration is that the action of the light on electrons and ions is decoupled. Then, by choosing the correct configuration of the beam (laser polarization, intensity, and phase distribution) for controlling the ponderomotive force, we can imagine forcing the electrons to move to one side of the beam, creating an inhomogeneous plasma. This may be the clue to an innovative aspect in materials science. Many recent works on pure silica have been conducted, and several properties have been demonstrated in this glass: average index changes, linear birefringence LB and linear dichroism LD. We recently revealed a chiral mechanical structure by measuring the surface topography of laser tracks written in opposite directions that could lead to circular properties. Taylor reported highly ordered " chiral-like " nanostructures using circular polarized laser light but no circular optical properties. We recently report on the creation of circular optical properties and non-reversible measurements according to the probe face. Here it is shown that by controlling the laser-writing configuration, we can create a quite high ellipticity of 40deg/mm revealing the creation of a large circular dichroism (CD), a useful range for potential applications. As the writing polarization is adjustable from 0 to 360○, the ellipticity maximum appear for linear polarization oriented at 112○ and 292○. In addition, ellipticity measurements are non-reversible (the values are different when light is propagating from one face to the other and the reverse). This is due to the co-existence of linear anisotropic properties (LB and LD), which exhibit a different spatial distribution from the CD.

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Fluoropolymer-based nanostructured membranes created by swift-heavy-ion irradiation and their energy and environmental applications

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A fluoropolymer, defined as a polymer consisting of carbon and fluorine, has useful properties such as chemical resistance, thermal stability, cryogenic properties, low coefficient of friction, low surface energy, etc. Practical applications for fluoropolymers always exploit one or more of these properties that set them apart from other plastics, in general, spanning all facets of human life from household uses to the aerospace and electronic industries. We have realized the importance of developing micro/nanofabrication techniques for this plastic family in order to further pursue the potential for future applications. My talk is devoted to the following two topics, i.e., ion-track membranes of poly(vinylidene fluoride) and ion-track-grafted electrolyte membranes for fuel cell applications. Both of these include the creation of fluoropolymer-based nanostructured membranes with swift heavy ions mainly from the cyclotron of the Takasaki Ion Accelerators for Advanced Radiation Application (TIARA), QST, and from UNILAC, GSI.

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Session XI

Ion irradiation of nanomaterials and optical waveguides for photonic applications

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Ion irradiation has been widely applied to modify the properties of both nanomaterials and to implement refractive index engineering of optical materials. With tailored features, the nanomaterials, for example, two-dimensional materials (graphene, MoS2, Bi2Se3 etc.) could possess intriguing optical nonlinearities for lasing of ultrashort pulses. Ion beam-induced index modification of optical materials (crystals, glasses) enables optical waveguide fabrication with various geometries. The combination of ion irradiated nanomaterials and optical waveguides may develop novel platforms for photonic applications with tailored properties. In this work, we report on our recent results on the ion beam modification of nanomaterials on single crystalline waveguide systems. This work paves a way to implementation of low-cost, miniature devices by using ion beam techniques.

*Speaker

Fabrication by ion implantation and optical characterization of single-photon emitters in nanodiamonds

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Deterministic single-photon sources are a fundamental tool for several emerging applications in quantum optics and quantum sensing and metrology, where the exploitation of single quantum objects could improve the existing measuring capabilities and define a new generation of standards measuring units. In addition, the availability of nanoscale-sized individual emitters is also of considerable interest as it enables a further integration with external structures or living systems.
In this work, we investigate the role of ion implantation in the production of single-photon emitters based on the nitrogen-vacancy complex (NV center) in nanodiamonds [1,2]. Powders of nitrogen-containing type Ib diamond nanocrystals with a median size distribution of 80 nm were irradiated with 2 MeV protons, with the purpose of creating vacancies and thus promote the formation of NV centers upon a subsequent thermal annealing at 800◦ C. Irradiations were performed in the 1×10ˆ12 – 1×10ˆ15 cm-2 ion fluence range, in order to determine the optimal conditions for the formation of single-photon emitters in individual nanodiamonds.
Following an appropriate chemical treatment, the nanodiamond powders were dispersed on glass cover slips and characterized in their opto-physical properties by means of a single-photon-sensitive confocal photoluminescence microscopy setup. The microscope was equipped with a "Hanbury Brown & Twiss" interferometer enabling the measurement of the the second-order autocorrelation function ($g(2)(t)$) [3].

The optical characterization of the samples enabled to experimentally demonstrate that irradiations in the 1×10ˆ12 – 1×10ˆ14 proton fluence range were effective at fabricating single-photon sources consisting of individual NV centers in nanodiamonds. The best $g(2)(t{=}0)$ value reported is 0.085 (see Figure), which is comparable with the state of the art.
An additional comparison with results obtained from unirradiated nanodiamond samples provided a further insight in the role of the thermal treatment alone in the formation of NV centers in Ib diamond nanocrystals.

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Figure: (**Left)** Confocal photoluminescence map single-photon-emitting nanodiamonds dispersed on a glass cover slip (532 nm pulsed laser excitation). **(Right)** Second-order autocorrelation function (g(2)(t)) acquired from a single-photon emitting nanodiamond. The $g(2)(t{=}0)$ value is reported in the graph.

Magnetic properties and microstructure of metal nanoparticles in oxides induced by energetic ion irradiation

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Materials including metal nanoparticles have become an object of interest among many researchers because of their promising properties. For example, they can provide new magnetic, optical or dielectric properties and so on. Among them, we focus on magnetic properties. The distribution of metal nanoparticles (Fe, Co, Ni) will lead to the modification of the properties. There are several well-known methods to prepare metal nanoparticles in solid. Ion implantation is one of the most suitable techniques for the synthesis of metal nanoparticles in materials. Also, by subsequent heavy ion irradiation, the magnetic property and state of implanted ion may be changed. In the present study, magnetic properties and microstructure of transparent oxides implanted with energetic Fe ions have been studied. Target samples were SiO2, Al2O3, MgO. They were implanted with 380keV Fe ions at various fluences at room temperature by using an ion-implanter at Takasaki Advanced Radiation Research Institute. After the ion implantation, some samples were subsequently irradiated with 16MeV heavy ions or annealed at elevated temperatures. The effects of the implantation and the subsequent high-energy ion irradiation or the annealing on magnetic properties were studied by using SQUID magnetometer. Microstructure of implanted metal nanoparticles was observed by transmission electron microscope (TEM). In order to investigate the states of the implanted Fe ions, the X-ray absorption near edge structure (XANES) and the small angle x-ray scattering (SAXS) measurements were performed at a synchrotron radiation facility of High Energy Accelerator Research Organization (KEK-PF). The magnetization-magnetic field (M-H) curves obtained by the SQUID measurement for Fe-implanted SiO2, Al2O3 and MgO show that the magnetic state of implanted Fe is ferromagnetism or superparamagnetism. Magnetization for one Fe atom implanted in the oxides increases with increasing the amount of implanted Fe ions. The magnetization decreases by the subsequent energetic heavy ion irradiation. In the conference, experimental results of annealing, TEM, XANES and SAXS will also be discussed in detail.

*Speaker

Understanding the ion-induced elongation of silver nanoparticles embedded in silica

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The shape deformation (elongation) of metallic nanoparticles (NPs) embedded in a dielectric matrix produced by irradiation with swift heavy ions is a phenomenon that has been known for many years. The rods obtained in this way have their long axis aligned with the incident ion beam direction, which can be advantageous for many applications. The physics involved in the sphere-to-rod transformation has been extensively studied [1–5] and some phenomenological models exist [1–3], but it is not yet fully understood. One of the reasons that complicate this task is the lack of information concerning the intermediate stages of the deformation mechanism. In this work we have studied the elongation of silver nanoparticles irradiated with 40 MeV Bromine ions by means of *in situ* optical measurements, transmission electron microscopy and molecular dynamics simulations. The localized surface plasmon resonance of silver nanoparticles has a strong dependence on the particle shape and size [6], which allowed us to obtain the geometrical parameters with remarkable accuracy by means of a fit of the optical spectra. Optical results have been compared with transmission electron microscopy images and molecular dynamics simulations and the agreement is excellent in both cases. An important advantage of *in situ* measurements is that they yield an extremely detailed information of the full elongation kinetics. Final NP elongation depends on a complex competition between single-ion deformation, Ostwald ripening and dissolution. Building and validating theoretical models with the data reported in this work should be easier than with the information previously available, due to the unprecedented level of kinetic details obtained from the *in situ* measurements.

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Session XII

Confocal-micro-luminescence characterization of femtosecond laser irradiated silica and borosilicate glasses

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The interaction of ultrafast lasers with silica based glasses has attracted the attention of several researchers both for fundamental and applicative reasons. Indeed, the irradiation of silica with ultrafast lasers allows both the study of non-linear ionization processes, fast heating and quenching phenomena and the photoinscription of Bragg gratings, just to cite some examples [1-3]. In our investigation we present an experimental characterization of the exposure's effects to a focused femtosecond laser (λ=800 nm, pulse duration=150 fs, repetition rate=100 kHz) on pure silica (OH rich) and borosilicate glasses as a function of the laser fluence (from 1-3 J/cm2) and scanning speed during irradiation (10-300 μm/s). Our study has been performed recording confocal-micro-luminescence (laser lines at 633 nm and 442 nm and a 50× objective) data. More in details, we obtained ablated and irradiated samples and we studied the spatial distributions of the different emission signals induced by the laser in both types of glasses. For the pure silica sample our data give the spatial distribution (with spatial resolution of few microns) of the well-known Non-Bridging Oxygen Hole Center [4] and provide evidence of their fading after the irradiation, allowing a deeper understanding of the irradiation and ablation related processes both for the zones where the laser was focused and the surrounding ones. Furthermore, for borosilicate materials we observed differences between the emissions induced in ablated and irradiated samples. Indeed, in the ablated samples we identified two emission bands at _˜560 and _˜670 nm, whereas in the irradiated one we detected only one band peaking at _˜560 nm.

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Monitoring the surface density kinetics of silica irradiated with swift heavy ions by means of in situ reflectance measurements

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In this work we have used a combination of *in situ* reflectance measurements to study structural modifications in silica by ion irradiation (Br ions with energies ranging from 5 to 40 MeV) and a methodology based on Molecular Dynamics (MD) and Finite Element Methods (FEM) to simulate its mechanical response to swift heavy ions. Reflectance measurements allowed us to obtain the detailed kinetics of surface modification and reconstruct the refractive index profiles in the irradiated samples, which lead us to very accurate results for the track radius and irradiation threshold of each ion. From these results we have observed that the refractive index increases at first (for low and medium fluences) but decreases for higher fluences. Finally, with the combination of MD and FEM simulations we obtained the local densification generated by an incoming ion and the strain and stress fields along the material as a function of the irradiation fluence. These results allowed us to reproduce track saturation for the low-medium fluence regime and the final decrease for the high fluence regime, which is produced by the plastic expansion induced by track irradiation during irradiation-enhanced viscous flow.

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Atomistic simulation of radiation damage at interfaces in glass/crystal composites

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High-level waste (HLW) resulting from nuclear fuel reprocessing is commonly immobilised in glass matrices. During vitrification, insoluble compounds precipitate and form crystalline phases with various structures and compositions. The resulting wasteform can effectively be described as glass/crystal composite materials (GCM). The effect of secondary phases on properties and long-term behaviour of nuclear glasses is an active field of research. The presented work attempts at improving our understanding of the effect of radiation damage on the properties and structure of the interfaces between different phases in GCMs. To this intent, atomistic simulations and empirical potentials were used to simulate simplified glass and crystal structures. The resulting interfaces have been subjected to radiation damage in the form of displacement cascades with a range of primary knock-on atom energies. Results shows the effect of damage on thermophysical, mechanical and ion transport properties of the interfaces. These characteristics can in turn have implications on mechanical durability of GCMs by favouring crack nucleation. It can also affect the performance of the wasteforms as immobilisation matrices by enhancing diffusion of radionuclides and leaching.

*Speaker

Rare earth ions environment modification by Electron and femtosecond Laser irradiation in phosphate glasses

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Phosphate glasses are attractive materials in different fields like nuclear industry, batteries, optics and medical due to their low temperature melting. Their high ability to dissolve the rare earth ions is also an advantage for optical applications.
Femtoseconds laser writing is commonly used to modify refractive index in various glassy matrix and can also impact the rare earth ion dopant environment [1]. At integrated doses of GGy, under high energy electrons irradiation, the migration of alkali ions in glasses can lead to a strong modification of the glassy network [2].

We want to provide in this work a better understanding of those structural modifications under radiation in order to control the rare earth environment evolution in metaphosphate and pyrophosphate glasses. Focused femto-second laser pulses (1030 nm) at 50 kHz and 250 KHz were used as well as electrons of 700 keV and 2.5 MeV (SIRIUS Accelerator). The impact on rare earth environment of the expected migration of alkaline ions after electron or high-cadency fs laser irradiation is studied by various characterization techniques. The glass structural changes are studied with Raman spectroscopy, point defects and rare earth environment evolution are investigated with photoluminescence spectroscopy (PL) and electron paramagnetic resonance spectroscopy (EPR). In addition, we played on the composition of metaphosphates and pyrophosphates glasses by adding different alkali ion types (Na, Li and K) to investigate the role of electronic ,thermal processes and the mixed alkali effect on the rare earth environment (Er and Eu). and ions showed contrasted behaviors under fs or electron irradiations. Er local environment is for example modified under fs laser writing, leading to an increase of the emission intensity contrary to Eu3+ ions that remain stable. Europium ions show an evolution of the asymmetry ratio under electron irradiation and a partial reduction into Eu2+. Moreover, only Er doped glasses display a second harmonic generation signal (SHG) under fs laser that we want to investigate.

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Ab initio simulations of tritium release from Li2TiO3

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Lithium ceramic pebbles are attractive tritium breeding materials due to their high lithium densities, high melting points and good chemical compatibility with multiplier and structural materials. However, the extraction of tritium from the material is a complex process. Following transmutation, tritium will be accommodated in the lattice at point defects. It must then diffuse to the pebble surface, where it undergoes isotope exchange reactions with H2 in the He coolant, before being carried away for recovery. The rate limiting step in this process is the diffusion through the bulk of the ceramic. Recent experimental observations have suggested that tritium retention increases with burn-up as irradiation and changes in stoichiometry result in the formation of defect trap sites that may compromise the sustainability of the tritium economy[1]. Therefore, it is essential to understand how the changes in the defect chemistry of lithium ceramics during operation may influence tritium release from the material.
Here results from density functional theory (DFT) simulations of tritium solubility and mobility in lithium metatitanate are presented. Formation energies for the intrinsic defects are calculated and through the manipulation of chemical potentials a prediction of the defect chemistry under conditions relevant to the blanket is made. The results show that the defect chemistry of the material changes dramatically as transmutation proceeds [2]. Next, tritium binding energies at the different trap sites are determined allowing the identification of the dominant accommodation mechanisms and how these change to reflect modifications to the intrinsic defect populations [3]. Importantly, tritium is expected to be be more bound in lithium deficient material in agreement with the experimental observations. Finally, we show how the He generated during the transmutation process is accommodated in the matrix and how this may impact tritium diffusivity [4].

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Microstructural evolution of graphite under irradiation: large scale molecular dynamics simulations

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Graphite response to irradiations has been widely studied in the past because of its importance for nuclear engineering. Despite this fact, the very details of the underlying mechanisms that drive its response to irradiation are still under debate and several scenarios are available [1,2,3]. With molecular dynamics simulations using empirical potentials, we investigate in this paper the microstructural evolution under irradiation of bulk graphite (or HOPG) and polycrystalline graphite with a microstructure similar to nuclear graphite. Both primary damages and dose effects are considered and analyzed.
Primary damage was investigated by displacement cascades. While mainly point defects only survive in graphite single crystal, the nanoporosity of polycristalline graphite modifies the nature of the irradiation damage.

Dose effect was subsequently explored with the Frenkel pair accumulations method in graphite single crystal. Before amorphisation, we show that graphite single crystal follows a three stages evolution characterized by: (1) an increase of point defects (2) a wrinkling and pinning of the graphene planes at small amorphous pockets and (3) an amorphisation by percolation of the small amorphous pockets. Although each of these three stages have already been proposed [2,3], their chronology is evidenced in the present simulations [4].

The relevancy of results and interpretation is largely supported by the similarity between calculated TEM images from simulation configurations and real TEM images obtained experimentally.

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Poster session B

Short ion-track formation and shape-elongation of nanoparticles induced by slow MeV-C60 cluster ion irradiation

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It is known that the shape elongation of metal nanoparticles (NPs) is induced in amorphous SiO2 (a-SiO2) by swift heavy ion irradiations, i.e., those with higher velocities than 0.1 MeV/u. Although 6 MeV C60 ion is very slow as 0.008 MeV/u, the electronic stopping power (Se) deduced from the independent 60 carbon monomer approximation was 15.5 keV/nm in a-SiO2, which was comparable to that of 200 MeV Xe ions (Se = 15.0 keV/nm). In this paper, the irradiation effects of MeV-C60 cluster ions on a-SiO2 dispersed with metal NPs are reported, particularly focusing on the short ion-track formation, enhanced sputtering, and shape elongation of NPs.

To visualize the ion track formation induced by the 6 MeV C60 cluster ion irradiation, a crystalline SiO2 sample was irradiated. Cross-sectional transmission electron microscopy (XTEM) revealed the formation of ion-tracks of approximately 100 nm in length, which were unexpectedly short. Since the nuclear stopping power of 6 MeV C60 ions was estimated as 2.66 keV/nm under the same approximation, the ion energy after traversing through the typical track length of 100 nm in SiO2 was roughly estimated as

Eo - (Se + Sn)d = 6 MeV - (15.5 + 2.66) keV/nm x 100 nm = 4.18 MeV.

The electronic stopping power at 4.18 MeV is _˜13 keV/nm in SiO2, which is far beyond the threshold Se for the track formation. Consequently, this observation indicates that the tracks are terminated not by deceleration below the threshold Se, but by other Se reduction process such as the fragmentation of the C60 cluster ions. Other topics will be reported in the presentation.

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Molecular Hydrogen Formation in the Alpha Radiolysis of the Ion Exchange Resins

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For decades ion exchange resins (IERs) have being used by the nuclear industry for a variety of applications, including reactor coolant demineralisation, radioisotope separation and waste treatment [1].
Ion exchange resins are generally radiation resistant [2]. However, during the long-term storage spent IERs are subject to self-radiolysis due to the presence of accumulated radionuclides; the total absorbed doses often reach several MGy. Such long-term exposure to ionising radiation leads to a significant chemical decomposition of these materials [3]. Furthermore, the presence of residual water is known to enhance degradation of these materials and, therefore, must be carefully investigated.

Majority of the published studies have explored the effects of gamma radiolysis on IERs, but very few investigations dealt with the alpha radiolysis of ion exchange resins [4]. It is expected that high Linear Energy Transfer (LET) radiation (i. e. alpha particles) will produce more molecular products, such as hydrogen, in comparison to low LET radiation (i. e. gamma rays). Hence, in the context of long-term storage of nuclear waste it is imperative to discriminate the effects of high vs. low LET in radiolysis of IERs.

In this work the radiation chemical yields of **molecular hydrogen** formed in **alpha radiolysis** of three polystyrene-based commercial resins have been determined; the extent of radiolytic hydrogen production has been studied as a function of water content in slurries. The beam of accelerated He(2+) ions (5.5 MeV) has been deployed to mimic the effects of alpha radiolysis on chosen IERs.

The polymers studied in this work are: (1) nuclear grade sulfonic strongly acidic cation exchange resin (Purolite^{TM} NRW 1600), (2) strongly basic anion exchange resin (Purolite^{TM} NRW 6000), and (3) a 50:50 combination of these resins in a mixed bed (Purolite^{TM} NRW 3560). These polystyrene-DVB based resins have been selected for this study since they are currently widely used in nuclear industry.

In our presentation the molecular hydrogen formation in alpha radiolysis of ion exchange resin/water slurries as a function of water content will be discussed. These results will be compared to the

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hydrogen yields obtained for the gamma radiolysis of the IERs. Complementary information concerning main water soluble degradation products (sulphate anion, amine compounds, etc) will also be presented and discussed.

In summary, the obtained results have allowed us to gain deeper understanding of the high LET radiolysis mechanisms in IERs. This work aids to create simple guidelines for a safe storage of spent ion exchange resins.

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Noble gas implantation into SiC

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Different noble gases (NG) were implanted at RT and at elevated temperatures into 4H-SiC with a large range of fluences and the effects of subsequent annealing (up to 1400∘C) were studied by using different techniques.
Thermal desorption spectroscopy measurements conducted at 1350∘C on 540keV-Xe-implanted samples showed that from threshold fluence all the gas is trapped in the matrix while at very low fluence all the atoms are released after 1h. These results discussed in light of atomistic calculations using an as-developed empirical potential show that Xe atoms are trapped by vacancy-type defects when available. X ray measurements allowing determining the out-of-plane strain has been conducted at RT and 400∘C in large range of doses (0-10 dpa). The elastic strain buildup has then been modeled by using a phenomenological model assuming that the strain level measured by XRD is made of two contributions. The contribution of defects consists in the first step of single hit process for strain accumulation with the existence of a thermally activated saturation stage in accordance with experimental results. The second contribution results from a cascade overlapping model derived from the Gibbon's model (4-5 cascades must overlap in order to create additional defects that participate to the strain development). However, in the second phase the role of NG can no more be ignored with respect to the stability of defects enhancing the strain development. Subsequent annealing conducted on Xe-1dpa damaged samples shows that the evolution of implantation surface swelling (step height) is correlated with strain recovery. Swelling under implantation is also calculated at the atomistic level.
Specific microstructural investigations (RBS, TEM) were carried out on 400∘C Xe-implanted SiC at high dose (30 dpa, CXe_˜1.2%) before and after high temperature annealing (1400∘C-30min). In particular the formation of cavities all along the ion path has been studied (bimodal distribution of cavities according to the damage and ion concentration). Note also that a huge stacking fault pile-up is observed in the highly damaged region as already observed in light ion implantation. With increasing ion mass (or V/ion ratio) a large band of End Of Range defects are observed beyond the implanted region (up to 100nm).

*Speaker

New classical molecular dynamics force fields to simulate the structure and radiation effects in dry and hydrated SiO2-Al2O3-CaO glasses

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CAS (CaO-Al2O3-SiO2) glasses are representative of the alteration layer [1] formed when the French nuclear glass is exposed to water corrosion. This layer is enriched in radioelements (actinides, lanthanides) and will then be subjected to radiation fluxes.
This work presents new molecular dynamics potentials fitted in order to study irradiation effects in CAS glasses. They have been obtained from *ab initio* molecular dynamics simulations according to the procedure proposed by Salanne and co-workers [2]. The analytical form of the interaction potentials are taken from the previous studies of Mahadevan et al. and Lockwood et al. considering hydrated silica [3-4]. They contain pairwise potentials, three-body terms and the coulombic interactions are treated using fix and diffuse charges. These potentials are compatible with the simulation of self-irradiation in glasses.

It is important to investigate the radiation effects in hydrated glasses because the water molecules can modify the glass behavior when it is subjected to ballistic effects. For example it has been shown [4] that they prevent healing of Si-O-Si bonds when recoil nuclei pass through the structure and create channels where water molecules could enter more deeply inside the glass structure.

We will present here the performances of the fitted potentials to reproduce the CAS glass structures and the first results of radiation effects in dry and hydrated configurations.

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*Speaker

Atomic scale insights on the microstructure evolution of urania under irradiation

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Urania is commonly used as a fuel in nuclear industry. Urania is heavily irradiated during its in-reactor stay, and faces drastic microstructural modifications, including few percents swelling and increase of dislocation density. Dislocations loops nucleate first [1] and transform with increasing fluence into lines. However, the early stages of their nucleation are hardly attainable experimentally. One commonly infers that their nucleation is related to the aggregation of point defects or defects clusters into dislocations.
In the present paper [2], we clarify the first steps of the effect of irradiation on urania by means of molecular dynamics simulations using empirical potentials. The irradiation dose is simulated by continuous accumulation of Frenkel pairs at 600∘C, skipping the cpu-expensive displacement cascades.

Starting from a defectless urania, we observe the nucleation and growth of dislocations under Frenkel pairs accumulation. Detailed analysis shows a four stages evolution : (i) an increase of point defects (ii) then the nucleation of Frank loops 1/3 from the aggregation of point defects, (ii) the transformation of Frank loops into perfect loops 1/2 (iv) and finally their stabilization as lines. Our simulations also show a swelling up to 3.2% during the first stage in which point defects are present. This swelling suddenly decreases to 1.5% in the second stage, as soon as dislocation loops transform into lines.

Both stage (iv) and swelling agree with experimental data [1,3] and therefore strengthen the four stages scenario of the microstructure evolution of urania under irradiation.

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Luminescence of LiF crystals activated by uranium

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Lithium fluoride crystals activated by multivalent ions are effective converters of hard radiation flow energy into emission of visible range. The crystals have potential for using as scintillation materials in medicine, since their density is close to the body tissue density. On the other hand, LiF crystals can be used as model crystals with complex defects. The following crystals were prepared for researches: LiF pure, LiF+2,0 mole% OH, LiF+0,005 mole% U, LiF+0,05 mole% U, LiF+0,05 mole% U+0,5 mole% OH, LiF+0,05 mole% U+2,0 mole% OH. Introduction of the activator (U) and the co-activator (OH) shown in occurrence of additional absorption in the range 260-320 nm. The IR spectrum in crystals containing OH, distinguished characteristic absorption bands at 3725 cm-1. In crystals with an activator (U) are observed in the bands 3550-3580 cm-1, which are responsible, probably, OH ions in the activator. The activated crystals observed with co-activator additional band at 3342 cm-1. The activated crystals luminescence observed in the field of 470- 520 nm when excited by hard and UV radiation. The excitation of crystals with a pulse of high-energy electrons (250 keV) results in the excitation of luminescence of crystals with integral spectra, qualitatively similar to measured ones by photoexcitation. A band at 425 nm excites in pure and OH-doped crystals. Crystals containing U, or U and OH co-activators quantitatively differ from the measured crystals in photoexcitation. A luminescence band at 490 nm is observed in the spectra of all crystals containing U and OH co-activators.

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Zn and Sn based nanoprecipitates deposited in a- SiO2/SI ion track templates

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Amorphous SiO2/Si structures produced by thermal oxidizing of silicon substrate. The thickness of oxide layer is 600 nm. Samples were irradiated on cyclotron DC-60 (Astana, Kazakhstan) with Xe ions (E=133 MeV $\Phi = 1\times109$ cm-2)
Following the etching of ion tracks in 4% aqueous solution of hydrofluoric acid (HF) at room temperature, a precipitation of Zink was produced by chemical (CD) and electrochemical (ECD) methods at room temperature. Sn precipitated only by chemical method. Morphology of SiO2/Si structures' surface before and after precipitation was examined on SEM and AFM.

Pores are of conic form; during electrochemical precipitation, the filling of pores is quicker than during the chemical one. SEM and AFM investigations of the surface and cross section demonstrated filling of nanopores by ECD (Zn) and CD (Zn and Sn). Changes in luminescence as compared to non-precipitated samples were seen for Zn structures. Based on difference spectra we found that photoluminescence spectrum has weak peak at 352 nm and sharp peak at 492 nm. For ZnO, the former is related to emissive exciton annihilation [1], and the latter is related to oxygen vacancy [2]. Thus, it is safe to argue that ZnO forms in nanopores during the Zn deposition process. X-ray diffraction studies showed formation of ZnO nanocrystals with hexagonal primitive cells. The studies of electrical properties make it safe to argue the opportunity for creating p-n junction (ZnO-n type, Si substrate –p type).

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*Speaker

Luminescence of MgF2 ceramics activated by Wolfram

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We presents results of the research of ceramics based on MgF2., activated by wolfram ions. The samples were produced with the powerful electron beam used as a heater. The mixture consists of MgF2 powder with the addition of WO2 and LiOH with concentrations varying from 0.05 to 0.3%. The crucible with the mixture were heated during 1 s. by the electron beam with the electron energy of 1.4 MeV and power density of 18 kW/cm2 by the accelerator ELV-6. .After the interaction, the mixture hardened into the ceramic sample with the impurities ratio given in the mixture. SEM research showed that the surface has a complicated form, typical for the hardened melt. The injected impurities of wolfram and oxygen were nonuniformly distributed on the surface. The ratio of oxygen and wolfram ions changes significantly by 32 and 81% during the surface scanning. At the same time the ratio of magnesium and fluorine changed not more than by 7 %. Therefore, during the synthesis process the dissociation of the metal oxide happens and the entrance of activators into the matrix without the bound with the oxygen takes place. The luminescence spectrum of all samples showed the intensive line with the maximum at 480 nm. The intensity of the lines is higher in the crystals with the high concentration of the activator. The luminescence of the synthesized samples is excited by loght with shorter than 320 nm. In the range of 320-310 nm there is an increasing intensity of luminescence. In the range of 310-200 nm the luminescence intensity in the samples, where the activator was not purposely injected, does not depend on the wave length. In the samples contacting the activator, the increasing intensity of the luminescence can be noticed in the area between 230-200 nm with the growth of the length of the excitation light. Thus, the synthesis of MgF2 samples activated by polyvalent ions with luminescent properties is possible by powerful electron beam.

*Speaker

Luminescence of O- doped zinc tungstate crystals

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Injection of oxygen by ion bombardment with energy of 28 MeV fluence up to 1015cm-2 leads to decrease of effectiveness indicative of ZnWO4 luminescence for 2.6 eV and change of excitation spectrum's form. In the excitation spectrum of the bombarded crystal, in comparison with non-bombarded one, we can observe the same decrease for 3-4 times at the increase of quantum energy from 4 to 6.5 eV. Injection of oxygen by the means of thermal annealing in the oxygen atmosphere at temperature of 1173 K during 7-hour period also leads to change of the excitation spectrum. The changes in the excitation spectrum differs in such a way that in the range from 4 to 6.5 eV we can observe the decrease of luminescence's effectiveness along with the 5-times increase of the excitation quantum energy, whereas in the non-treated crystals – only for 30%. Significant decrease in luminescence's excitation effectiveness at the increase of the excitation photons' energy in the thermally treated crystal in comparison with crystal that have not been treated, is explained as follows. During diffusion injection, concentration of the entered oxygen decreases from the surface to the depths; concentration of the destroyed excitation complexes decreases as well. At the increase of excitation quantum energy in the range from 4 to 6.5 eV the characteristic depth of quantum run also decreases. It is suggested, that the destruction of the excitation complexes takes place at the depth correlating with the depth of penetration of the excitation photons. High-energy quanta are absorbed in the area of the crystal, where concentration of the destroyed centers is higher, thus the effectiveness of luminescence is lower. The evaluation of the oxygen's depth of penetration has been made; the characteristic depth of penetration equals 20 nm during 7-hour treatment of the crystal at 1173 K.

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Gamma and electron radiation effects in some hydrates of cement phases

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Nowadays, Portland cement based matrices are widely used for conditioning and embedding nuclear wastes. However, alternative matrices are required for some specific wastes. The matrices must be resistant to irradiation and produce the least possible hydrogen. The aim of this study is to compare the behaviour of several hydrates under irradiation taking into account both "real" cement pastes and synthetic hydrates. Two aspects are considered: the chemical damage (radiolytic H2 production) and the structural damage induced by irradiation.
Various cement pastes compositions and the corresponding pure calcium aluminate and calcium silicate hydrate phases were synthesized and characterized. Two types of irradiation experiments were performed: low dose gamma irradiation experiments within the range of that experienced during long term waste disposal with measurement of radiolytic yields, and medium dose electron irradiation experiments aimed at studying structural effects.

Low dose gamma irradiation: All the cement pastes and their constitutive hydrates were irradiated up to 600 kGy and up to 200 kGy in order to determine their hydrogen radiolytic yield. A new set of data on the H2 production of six types of hydrates under γ-irradiation was collected. The production of hydrogen depends on the nature of the hydrate. Gibbsite Al2H6O6 and Katoite Ca3Al2H12O12 are found producing less hydrogen under gamma irradiation than the other compounds.

Medium dose electron irradiation: two sets of hydrates were irradiated up to 100 MGy and up to 1 GGy using the LSI SIRIUS electron accelerator platform. XRD analysis was conducted before and after irradiation in order to study the impact of irradiation on their structure. No amorphization is observed for all the studied hydrates, illustrating their structural resistance in this flux range. Some structural evolution can be found in some specific cases to be discussed during this presentation.
This study highlights (i) the small structural impact of radiations and (ii) a strong dependence of the radiolytic hydrogen production on the composition of the hydrates.

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The Online Raman System at M3 GSI with first research results

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The first Version of the Online Raman System (M3 branch, GSI Darmstadt) which is used to investigate changes in crystal matter while irradiated with swift heavy ions has been tested successfully in beamtimes of the years 2014 and 2015 [1]. This version has already been used by several research groups and proofed itself as a reliable tool. During this beamtimes many experiences could be made. These experiences were used to create a new version of the Online-Raman System which was tested for the first time in June 2016 at the M-branch. Besides some modifications, some new features have been added to the system. For example, due to a 3-axis sample holder it is now possible to irradiate and measure several sample at a time. The contribution gives an introduction of the new system and shows some possible applications and new ideas.

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Domain formation during UO2 irradiation

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UO2 dioxide has been studied for more than 60 years, noticeably because it is the most used nuclear fuel in the world. Yet some questions still exist about its behavior under irradiation: what are the irradiation tracks due to Swift Heavy Ion irradiation made of [1], or what is the defect corresponding to the additional peaks observed by Raman spectroscopy on He irradiated UO2 [2]? New neutron diffraction results evidenced the existence of a local order in UO2 different from Fm3m, namely Pa-3 [3]. This new finding provides a new manner to interpret irradiation effects in UO2 that is related to the low symmetry domains that exist at the local scale. In this presentation a first attempt is made to evidence how such domains could influence UO2 behavior under irradiation either by their deformation or by their ordering.

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*Speaker

Characterization of latent track structure in polymer films

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The structure of latent tracks in polymer films is very important for understanding track formation mechanism, and fabricating micropores and nanopores. Previous research had shown that only small gas molecules could permeate through polymer film with latent tracks. Recently, highly selective ionic transport through sub-nanometer pores without chemical etching has been observed in polyethylene terephthalate(PET) films irradiated with heavy ions and subsequent UV radiation [1]. However, the structure of latent tracks in polymer films still remains unclear. In this work, small-angle X-rays scattering (SAXS), IR, UV-Vis spectrophotometry and XPS measurements were used to investigate the structure of latent tracks and sub-nanometer pores in polymer films. With SAXS measurements on the polymer films irradiated by 9.5 MeV/u Bi+ ions and UV radiation, a relatively lower density region along the latent track was observed and its diameter is in nanometer scales. After UV irradiation, the diameter changes because of photo oxidative degradation of polymer chains inside the tracks. FT-IR and UV-Vis spectrophotometry measurements on the polymer films under the same conditions reveals contents of functional groups such as C-O, C=O, and C=C changes when the dose of heavy ion irradiation and duration of UV irradiation varied. Furthermore, XPS was applied to investigate the transformation of specific chemical structures such as carbon chains in the PET film irradiated by lower-energy Si+ ions and UV radiation. The experimental results indicate that as the duration of UV irradiation is above a threshold value, the content of the polar group C=O starts to increase quickly till it reaches a level much greater than that in the untreated film. Based on the above experimental results and thermal spike theory, we proposed a primary model for the structure of latent tracks in PET films. [1] *Qi Wen et al., Advanced Functional Materials, 2016, 26(32): 5796-5803.*

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Nuclear track membrane-based plasmonic hierarchical nanostructures for ultrasensitive SERS analysis

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Surface enhanced Raman spectroscopy (SERS) is a label-free and non-destructive vibrational spectroscopy technique that allows for ultrasensitive and fast structural detection of trace-level molecules through the enhanced electromagnetic (EM) fields amplified by the excitation of localized surface plasmon Resonances (LSPR). Compared to conventional rigid SERS substrates, e.g. glass and silicon, flexible substrates provide flexibilities of configurable assembly which is critical to the applications such as on-line trace level detection. In addition, large-scale production is another concern for reducing cost. Here, we demonstrate a new type of double-sided, large-scale, and flexible metasurfaces for ultrasensitive, highly uniform, polarization-independent SERS detection. The SERS substrates are fabricated by simply sputtering densely packed gold nanoparticles on porous polycarbonate membranes which composed of conical pores created by asymmetric etching of ion tracks. Morphological characterizations reveal that the conical pores are uniformly distributed on both sides of membranes and uniform in shape and size. The porous polycarbonate membranes are covered with granular gold films which typically have sub-5 nm gaps among adjacent particles. Such metasurfaces show ultrasensitive SERS detection limit down to 10 pM which is comparable to the reported highest value (1 pM) for flexible substrates. The high uniformity is reflected by a low relative standard deviation (RSD) _˜10% over the entire wavenumber range (300-1800 cm-1). Numerical simulations disclose that the enhanced EM fields of granular gold films are further amplified by conical pores. Such hierarchical metasurfaces represent a step forward to low-cost, high performance, and reliable flexible platforms for ultrasensitive SERS detection.

*Speaker

Synthesis of silver nanoparticles by femtosecond pulsed laser ablation: fabrication of embedded nanoparticle multilayers and colloidal solutions

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In this work Femtosecond Pulsed Laser Ablation (fs-PLA) has been applied in vacuum and liquid environment to fabricate embedded silver nanoparticle multilayers and highly concentrated silver colloidal nanoparticle solution respectively.
In vacuum, deposits of exposed and embedded silver nanoparticles were grown on Si(100) and silica substrates by laser ablating high-purity silver and SiO2 targets using a femtosecond Ti:sapphire laser delivering 45 fs pulses at 804 nm and 1 kHz repetition rate. The effect of the laser fluence and irradiation time on the obtained nanostructures was investigated using several fluences between 650 mJ/cm2 and 3.2 J/cm2 and deposition times in the range of 1-20 minutes. Optical response of the deposits was characterized using optical absorption spectroscopy and the surface morphology was studied by scanning electron microscopy (SEM). Samples with the optimal optical response were obtained by depositing three successive Ag/SiO2 bilayers at the main laser wavelength (804 nm) under vacuum at substrate room temperature. They were composed of silver nanoparticles with an average diameter of 6 nm and a narrow size distribution; each layer of these nanoparticles was then separated by silica layers of approximately 100 nm. The laser fluence and deposition time for Ag (SiO2) were 650 mJ/cm2 (3.2 J/cm2) and 1 min (10 min), respectively.

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When applied in a liquid environment, fs-PLA is able to synthesize colloidal solutions of nanoparticles from the ablated material in a complex process [1]. Silver nanoparticle fabricated by femtosecond laser ablation was first reported in [2], where very low concentrated solutions were produced. We have used femtosecond laser ablation to generate highly concentrated silver colloidal nanoparticle solutions. When performed in pure water, such concentrations usually lead to a high level of agglomeration making the solutions nearly useless. To avoid this problem, we have employed two different organic stabilizers, namely hexadecyl-trimethyl-ammonium bromide (CTAB) and polyvinylpyrrolidone (PVP), and studied its effect on the size distribution, structural characteristics and concentration of the solutions by means of transmission electron microscopy and optical absorption spectroscopy. Our results show that the agglomeration can be considerably reduced or even completely eliminated with those stabilizers.

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Electrical control of NV centers in diamond by means of ion-beam-micromachined sub-superficial graphitic micro-electrodes

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The nitrogen vacancy complex (NV center) in diamond is an appealing system for applications in quantum optics and quantum sensing. The control of its charge state is important to ensure the stabilization of its opto-physical properties. In this work the electrical control of the relative population of the negative (NV–) and neutral (NV0) charge states of μm-deep NV centers was investigated. Pairs of sub-superficial (_˜3 μm deep) graphitic micro-electrodes with _˜10 μm spacing were fabricated into an "optical grade" single-crystal diamond substrate [1] using a 6 MeV C microbeam.

The current-voltage characteristics of the graphite-diamond-graphite junction displayed a ohmic conduction, associated with a moderate current injection at $<$ 350 V bias voltages (low-current regime). At higher voltages, an abrupt transition to a high-current regime dominated by the Poole-Frenkel conduction mechanism was observed, as well as the onset for electroluminescence (EL) emission from the inter-electrode gap. Ensemble photoluminescence (PL) spectra (532 nm laser excitation) acquired under electrical bias in the ohmic regime at increasing currents exhibited a linear increase in the NV– charge state at the expense of the NV0 population [2]. In high-current regime, PL emission was investigated together with the concurrent EL emission. The emission spectra exhibited the opposite trend at increasing bias voltages, where a steady decrease in the negative charge state component was observed.

A temperature-dependent electrical characterization of the device was performed to gain a deeper insight in the different electrical conduction regimes occurring in the device. Nitrogen-related defects were identified as the relevant trap/donors levels for the different conduction regimes. A _˜30% increase in the diamond dc dielectric constant was also determined by fitting the experimental data with the Poole-Frenkel conduction model.
Complementarily with respect to the strategies which are currently adopted to dynamically control charge-state conversion of diamond NV centers (i.e. p-i-n junctions [3] and chemical control

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of the surface termination [4]), buried graphitic electrodes enable the control and stabilization of the negative charge state of deep NV centers located at micrometric distances from the diamond surface, for which longer spin coherence times are expected [5].

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Figure: **a)** Optical micrograph of a graphite-diamond-graphite junction; **b)** Temperature-dependent current-voltage characteristics; **c)** Photoluminescence spectrum of the device under 532 nm laser excitation; relative variation of PL spectra under increasing bias voltage.

Characterizations of alkaline-earth borate crystals for radiation dosimetry

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There is a continuous growing interest in thermoluminescence (TL) and optically stimulated luminescence (OSL) materials for radiation dosimetry, especially in the fields of environmental, personal and medical applications. TL and OSL phenomenon are attributed to the recombination of electrons and holes at metastable levels in host material that is excited by thermally and optically stimulation. Various phosphors such as BaFBr:Eu, LiF:Mg, Cu, P and Al2O3:C are being used for these applications today, meanwhile the development of new TL and OSL materials having better light yield, sensitivity to neutron, X-ray and gamma-ray are demand. In recent study, the TL properties of borate crystalline phosphors have been reported because of their good tissue equivalence and excellent sensitivity to X-rays and gamma-rays. Among the phosphors, the use of MgB4O7 based crystalline phosphors has been investigated by several researchers due to its good tissue equivalent and excellent TL properties Therefore in this time, we investigate TL and OSL of alkaline-earth orthoborate crystals as well as optical and photoluminescence properties to examine the potential for radiation dosimetry. A crystal samples of Ca3B2O6 and Mg3B2O6 were prepared by using conventional Czochralski method. CaCO3 (4N), MgO (4N), and H3BO3 (4N) high purity powders were used as starting materials. As prepared samples were polished for the optical, photoluminescence, and dosimeter measurements. TL glow curves of the Ca3B2O6 and Mg3B2O6 crystals were recorded by a H11890-210 photon counting head (Hamamatsu) and a brass-plate-heater-connected programmable SCR-SHQ-A heat controller (Sakaguchi E.H VOC CORP.). The glow curve measurements were demonstrated in the temperature range from 310 to 650 K under heating rate of 0.5 K/s in air. An original X-ray generator (RIGAKU) equipped with a copper target was used as the X-ray irradiation source. A high voltage of 40 kV and current in the range 4–40 mA supplied the generator. In the glow curve of the crystals exposed to 1000 mGy dose X-ray, several glow peaks appeared at 368, 425, 503, and 542 K for Ca3B2O6 and, 377, 435, and 567 K for Mg3B2O6. By the result, it confirmed that the trapped electrons at anion centers due to X-ray irradiation were released by the heating, and then recombined with the holes through the intrinsic emission-centers.

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Thermal Behavior of Rare Gases in Implanted Uranium Dioxide

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The behavior of fission products in uranium dioxide has been widely studied by experimental and theoretical approaches. Significant quantities of xenon are produced under irradiation and the release of these fission gases induces an increase of the pressure inside the fuel pin and fuel swelling due to gas bubble formation. To prevent cladding failure and increase the fuel burn-up, a better understanding of the fission gas release process is essential. The purpose of this work is to get further insight into their diffusion mechanisms and their interaction with defects. To do this, separated effects studies coupling ion irradiations/implantations and fine characterizations using Thermal Desorption Spectrometry (TDS), Positon Annihilation Spectroscopy (PAS) and Transmission Electronic Microscopy (TEM) have been performed.
TDS available on the PIAGARA (Plateforme Interdisciplinaire pour l'Analyse des GAz Rares en Aquitaine) platform at CENBG in Bordeaux allows measurements of very low amount of gases in uranium dioxide. Experiments on UO2 discs implanted with various xenon amounts were performed to evaluate the thermal diffusion coefficient. From the gas release fraction, we determined a model of gas release taking into account the initial burst and diffusion in the bulk. The results show that xenon release decreases when the quantity of xenon implanted increases. This proves that fission gases are trapped in defects and the fraction of trapped gas is measured. Then for a low dose, where no trapping effect occurs in the material, diffusion coefficients are calculated as a function of temperature. This allows us to determine the Arrhenius law of xenon and krypton thermal diffusion in UO2.

UO2 discs implanted with various xenon concentrations are also characterized by PAS (Positron Annihilation Spectroscopy) which allows us to determine induced vacancy defects. The main defect present after irradiation seems to be the Schottky defect [1], [2]. But for a higher implantation dose, it seems that larger defect are produced like nano-cavities created by vacancies aggregation. This result will be completed by TEM observations.

The fraction of gas trapped determined by TDS measurements coupled to defect characterization in UO2 by PAS experiments allows us to make the assumption in which defects the gas is trapped. These coupled results will enable us to describe from the atomic scale the thermal

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behavior of rare gases in UO2 fuel.

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UV-Laser stimulated Fluorescence-Spectrometry of Ion-irradiated condensed matter

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UV-laser irradiation of ion tracks bearing calcite crystals stimulated a greenish fluorescence originated in the area of ion track occurrence. The ion tracks have been formed during irradiation of natural calcite crystals with swift heavy ions (238U, 1 x 1011 ions/cm2). The first investigations were performed by using a UV-laser-Raman system of Horiba (Labram HR Evolution with a 244 nm Argon-ion Laser) and a photoluminescence detector system (Symphony BI-UV). The intensity of the fluorescence varied according to the ion track density.These first results motivated to build a new UV-Laser (266 nm) stimulated fluorescence spectrometer to fully investigate the fluorescence caused by the volume density of ion tracks in condensed matter. The new system consists of a CryLas 266-200 UV laser with an energy of 200 μJ per puls at 20 Hz at 266 nm wavelength and an Ocean Optics USB 4000 UV/Vis spectrometer. Additionally, a new sample holder has been designed which fulfills the analytical requirements easy sample mounting, measuring, and monitoring. First experimental results using swift heavy ion irradiated calcite crystals (192Au, 238U) of varying ion track volume density proof the readiness of the system to perform UV-laser stimulated fluorescence experiments on selected matter. In the near future, the system will be adapted to determine online and in-situ the ion-induced change of matter at the experimental caves of the M-branch, the SIS18, and CRYRING.

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A multiscale model of wet chemical etching of swift heavy ions tracks in olivine

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Swift heavy ions (SHI, $M>$ 20a.m.u., $E>$ 1MeV/nucleon) transfer the most part of their energy ($>$ 95%) into the electronic subsystem of a target. Subsequent relaxation of this excitation may change chemical activity of a material at distances up to 1-2 μm from the projectile trajectory.
A model of reaction- and diffusion-controlled wet chemical etching of SHI tracks in olivine is presented. The model consists of blocks describing the track kinetics at different time scales. Monte-Carlo code (TREKIS, [1]) simulates the kinetics of the electron subsystem excited by an ion providing initial conditions for a Molecular Dynamics model describing excitation and relaxation kinetics of the atomic subsystem of a target [2]. Transition state theory [3] is used for estimation of a chemical activation level of an excited material in a track. Finally, these data are used in the model of wet etching of SHI tracks in olivine.

Controlled etching of olivine crystals from meteorites is used for searching of superheavy elements in the galactic cosmic rays spectrum [4,5] and the large database accumulated in these etching experiments can be used for testing of the presented model.

Application of the model reveals possibility of the diffusion-controlled etching of disordered material in nanometric vicinity of SHI trajectory. To take this effect into account, the original method was developed for the modelling of the reaction-controlled and diffusion-controlled wet chemical etching of SHI tracks as well as for the description of transitions between these two regimes.

Besides, an effect of impurites on etching of SHI tracks was investigated. Fe-bearing olivine ((MgxFe1-x)2 SiO4, x=0.89) was chosen as a system for this modeling. Neutralization of polyvalent Fe+ cations by spreading electrons generated in a track is assumed as the mechanism of chemical activation of this kind of olivine in the micrometer vicinity of SHI tracks. The comparison between the etching rates of SHI tracks in Fe-bearing olivine and Fe-free olivine (forsterite) was made.

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Morphology of un-etched and etched ion tracks in polymers studied by SAXS

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The interaction between swift heavy ions and materials, including polymers, is dominated by their inelastic collisions with the target electrons. The intense electronic excitation leads to the formation of "long cylindrical ion tracks" consisting of damaged material including broken bonds and loss of volatile radiation products. Ion track technology makes use of the preferential etching of the track damage and has attracted great interest for many applications, such as fabrication of nano-porous membranes for filter application, micro-capacitors, diodes and templates for nanowires fabrication for microelectronic devices and a large range of sensor applications. In this work, we present experimental results to better understand the morphology of ion tracks in aromatic polymers. Ion tracks were induced in polyethylene terephthalate (PET), polyimide (PI), polycarbonate (PC), polytetrafluoro-ethylene (PTFE), and poly-propylene (PP) using Au ions of 1.7 and 2.2 GeV kinetic energies of and fluences between 1×1010 and 1×1012 ions /cm2. For ion-track etching experiments on irradiated PC foils, the fluence of the 2.2-GeV Au ions was lower (5×1010 ions/cm2). Track etching was performed in 3M sodium hydroxide (NaOH) solutions at 55° C. Small-angle x-ray scattering (SAXS) was used to determine radii of etched and un-etched ion tracks. Structural changes in the polymers were characterised by Fourier-Transform Infrared Spectroscopy (FT-IR). The average radius of un-etched tracks was studied as a function of the irradiation fluence, indicating an increase in ion track radius from 2.6±0.02 to 3.4±0.3 nm with increasing fluence. Chemical etching of the ion tracks in PC leads to the formation of cylindrical pores with a radius linearly increasing with etching time, with a radial etching rate of 9.2 nm/min.

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Uptake of 226Ra Radiation by Micro- and Nanocomposites: Effect on Optical and Dielectric Properties

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The properties of versatile nanostructured materials can be exploited for sensing and neutralization of harmful agents in surrounding environment, one of the most critical of which is the harsh radiation. We present how the low dosage of the gamma radiation from 226Ra influences the optical and dielectric response of nanocomposite structures based on epoxy resin with the addition of different nanofillers.
A series of nanocomposite materials incorporating various nanofillers were prepared. Boron and boron nitride in the form of micro and nanoparticles were selected as nanomaterials of primary interest. Single-walled and multi-walled carbon nanotubes (CNTs) were also considered. Selected nanofillers were mixed with commercially available epoxy resin. Ultrasonic dispersion technique was applied and optical microscopy was used to monitor the distribution of the filler.

For each type of composite, samples with different concentration of nanofiller were fabricated. To observe the luminescence from nanocomposites as a function of dosage at the stage of mixing the epoxy with nanofiller the RH640 luminescent dye was added. A series of spectroscopic tests indicated the the most noticeable effect on luminescence is observed in case of the samples with the 2% concentration of boron nitride microsized particles (in particular, 50% drop in the intensity of the band at 470 nm was observed). Our studies also show that in samples with higher concentrations of reinforcing particles the influence of gamma rays on the emission properties is very weak.
Dielectric measurements have reflected changes in the impedance of the irradiated nanocomposite samples with respect to as-obtained samples. The detected variations of impedance of the samples might be due to the degradation of the polymer matrix itself as well as due to the interaction of gamma rays with nanoparticles/nanotubes.

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Effect of metal nano-clusters produced by ion implantation and subsequent high energy heavy ion irradiation on optical properties of transparent oxides

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Transparent oxides such as amorphous SiO2(quartz glass), and Al2O3 single crystal (sapphire) were implanted with 50-380 keV Ag ions at various fluences by using an ion-implanter of Takasaki Advanced Radiation Research Institute. After the ion implantation at room temperature, some samples were subsequently irradiated with 16MeV Au ions or were annealed at elevated temperatures. The effects of the implantation and the subsequent Au ion irradiation or the annealing on optical absorption spectra were studied by using UV-vis spectrometer. To investigate the microstructure of Ag-implanted samples, the transmission electron microscope was used.

The optical absorption measurements for Ag-implanted SiO2 show an absorption band around 400nm, corresponding to the well-known surface plasmon resonance of the Ag nanoparticles. The distribution of Ag spherical clusters with the diameter of 5-20nm was confirmed by TEM observation. With increasing the amount of implanted Ag ions, the intensity of 400 nm peak increases and another peak appears around 600nm. In the samples implanted with a large amount of Ag ions, Ag spherical clusters, the space density of which was much larger than for lower fluences, were observed by TEM. The absorption peaks around 600nm is, therefore, due to the interaction among Ag spherical clusters.

By the subsequent irradiation with 16MeV Au ions, the position of 400nm and 600nm peaks shifted to a lower wavelength side and their intensity remarkably decreased. As the TEM observation revealed an elongation of Ag clusters along the direction of 16MeV Au irradiation, the change in the position and the intensity of the optical absorption peaks should be attributed to the change in the shape of Ag clusters.

The result of the present study implies that the combination of metal ion implantation and the subsequent high energy ion irradiation can be used for the systematic control of optical

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absorption spectra for transparent oxides.

Kinetic Model of Color Center Formation in TiO2 Film by femtosecond laser irradiation

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Titanium dioxide (TiO2) has a wide range of potential applications in photocatalytic, optical coating, and solar cell materials. TiO2 is transparent in visible light because of the wide band gap energy greater than about 3.2 eV. Darkening of TiO2 film surfaces and reduction of their electrical resistance by femtosecond laser irradiation have been observed in experiments [1]. Darkening shows that a large number of color centers exist in TiO2 film surfaces It is believed that the reason for the darkening is oxygen deficiencies.
In this paper, we proposed a kinetic model to explain the formation of color centers or oxygen deficiencies by femtosecond laser irradiation. The kinetic model treats the formation of conduction band electrons and holes by the multiphoton absorption, self-trapped states from conduction band electrons and holes, and color centers. We introduce a coupling model of the rate equations base on the kinetic model and the laser propagation equation to investigate the darkening mechanism of TiO2 film surfaces by femtosecond laser irradiation.

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Formation and characterization of the near-surface radiation color centers in lithium fluoride

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Among alkali halides crystals, lithium fluoride occupies a special place because of its physical and optical properties. Color centers (radiation-induced defects) in this material were extensively investigated and found application in the realization of ionizing radiation dosimeters and broad-band emitting lasers and amplifiers in the optical domain operating at room temperature. In the present work it is shown that after γ-irradiation, near-surface (surface) color centers are formed in a near-surface layer and in areas with the broken crystal structure inside a lithium fluoride crystal. The experiments were performed with lithium fluoride nanocrystals and bulk crystals. Nanocrystals (with sizes d $\leq$ 1 μm) were obtained by mechanical fragmentation of a part of the single crystal. For prepared samples the developed surface and the high ratio of a surface to volume are characteristic. Absorption, luminescence and luminescence excitation spectra of such defects have been measured. We identified the following five types of near-surface color centers: FS2+, FS2– , FS2, FS3+ and FS3. These designations of surface color centers are similar to traditional designations of color centers in the bulk of the crystals. In our case, we added only the index s, which indicates that the centers belong to the surface centers. The measured photoluminescence and photoluminescence excitation spectra for surface color centers differ from the spectra for similar centers in the bulk of the crystal by positions of the maxima and values of the line widths. The photoluminescence excitation spectra of surface defects are characterized by the presence of several bands (two or three) with close intensities. Results of research of pre-irradiation annealing influence on efficiency of formation of the near-surface centers in lithium fluoride nanocrystals are presented. The increase in pre-irradiation annealing temperature from room to 250 oC leads to considerable reduction of such centers formation efficiency. At pre-irradiation annealing temperatures above 350 oC the near-surface color centers after gamma irradiation aren't found. It is established that adsorption of atmospheric gases on a surface of a crystal can't be considered as a necessary condition of radiation near-surface centers formation. To prove that fact, the radiation defects formation was studied in the bulk of lithium fluoride crystals with caverns fabricated by the pulsed radiation of Nd : YAG laser.

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Defect-Related Optical Properties of Gamma Irradiated Chalcogenide Glasses

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Ge-Ga-S/Se chalcogenide glasses have shown many advantages for potential applications in optical modulators or frequency converters, as efficient laser host materials and for fiber-optical amplifiers in the IR spectral region. Their structural and electronic modification by thermal annealing processes and/or irradiation results in changes of their functional properties.
The process of crystallization in 80GeSe2-20Ga2Se3 glasses influences their optical transmission spectra. Non-annealed glassy samples show maximum optical transmittance at the level of 65 %. Annealing at 380 ∘C decreases this transmittance and shifts optical transmission edge towards long-wave side. The appearance of growing of Ga2Se3 and GeGa4Se8 nanocrystals inside the glassy matrix induces light scattering at shorter wavelengths. Generally, this phenomenon shows the presence of large crystals that deteriorate optical transparency of the material rapidly, leading progressively to its complete opacity in the IR range.

The influence of gamma irradiation on optical properties of Ge-Ga-S/Se glasses was investigated using Co60 source. The dose of gamma-irradiation was near 0.8 MGy and the total duration of this procedure was 2 months.

The slight long-wavelength shift of the fundamental optical absorption edge and the decrease in transmission are observed in 80GeS2-20Ga2S3 glasses after irradiation. This indicates possible formation of additional defects in 80GeS2-20Ga2S3 glasses and their observed darkening. After irradiation, nanovoids with different size are created as intrinsic structural defects associated with topologically uncoordinated negative-charged centers. These defect centers form additional energy levels both near the bottom of the conduction band and in the vicinity of the valence band, as well as additional intrinsic electric fields. The mechanism of irradiation-induced darkening of 80GeS2-20Ga2S3 glasses is connected with oxidation processes most probably related with the appearance of GeS2 phase at the surface of the glasses.
Gamma irradiation practically does not alter the optical transmission spectra in the modified 80GeSe2-20Ga2Se3 glasses. The position of optical transmission edge and the spectra profiles in

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the saturation region coincide before and after irradiation. Such radiation stability of 80GeSe2-20Ga2Se3 glasses allows their use as radiation-stable optical sensors in the visible and IR spectral region.

Structure and optical properties of SiO2/Si with InAs nanoclusters irradiated with 167 MeV Xe ions

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The integration of III-V optoelectronic devices with Si electronics has attracted a great interest for decades. Ensembles of III-V quantum dots inside crystalline Si or amorphous SiO2 are of interest for applications in such optoelectronic devices as LEDs, photodetectors and lasers operating in the infrared range. High-fluence ion implantation followed with thermal treatment is the efficient technique for fabricating of III-V quantum dots. Modifying the regime of annealing or using the subsequent irradiation by swift heavy ions may provide a way to control the size, size distribution and crystalline quality of the formed precipitates. In this study, InAs nanoclusters were synthesized in SiO2 via high-fluence ion implantation with subsequent thermal treatment and/or irradiation by 167 MeV Xe ions with a fluence of 1 to 3×1014 cm-2. Wafers of n-Si (100) with 600 nm thermal SiO2 layers were implanted at room temperature first with As+ ions (170 keV, 3.2×1016 cm-2) and then with In+ ions (250 keV, 2.8×1016 cm-2). The second part of such wafers was implanted at room temperature in a multiple-energy regime to obtain 150 nm thick near-surface layer uniformly doped with In and As atoms up to equal concentrations ¸˜ 4.5×1020 cm-3. Then, a part of these two sets of samples was annealed at 900°C in argon for 30 min. Some annealed and some nontreated samples were afterwards irradiated with Xe ions. The RBS, TEM, XTEM, RS and PL techniques were used in this study. The Xe irradiation resulted in the ordering of InAs nanoclusters along the direction of the ion beam if the initial size of precipitates exceeds the diameter (calculated using the thermal spike model) of the molten SiO2 region around the trajectories of Xe ions. The round shape of larger precipitates become oval. The final diameter of nanoclusters did not exceed the diameter of the molten region. The effects of SiO2 matrix oversaturation with implanted species, annealing and Xe irradiation on RS and PL spectra as well as a nature of the registered RS and PL bands are discussed. The RS data show that irradiation with Xe ions resulted in the amorphization of a certain fraction of InAs nanocrystals and the formation of a large number of defects in crystalline clusters, damaging the surrounding SiO2 matrix.

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Ab Initio modeling of the Y, O solute interaction in iron matrix

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Oxide Dispersed Strengthened (ODS) steels are known for their high stability under irradiation conditions, which makes them a promising construction material for nuclear reactors. High irradiation damage resistance of ODS steels is a critical property for the future fusion reactors. Yttrium oxide is the most common dopant for the ODS steel production, introduced into the host material by mechanical alloying, followed by powder consolidation (e.g., by hot isostatic pressing). ODS particles of various size, shape and spatial distribution were observed experimentally. However, only a few theoretical studies discussed formation process of yttria nanoparticles. Atomic Tomography Probe experiments have shown presence of Y and O in the Fe lattice in a form of solutes.

Our atomistic investigation is focused on the comprehensive large scale calculations of pair-wise interactions between Y and O solutes as well as vacancies in the host *bcc* and *fcc* iron matrices. We present the results of *ab initio* modelling of Y, O and VFe defect complexes in both types of cubic Fe lattice. Large scale computer calculations were performed with the computer code VASP 5.3 in the 4×4×4 supercell. We show that vacancies play an essential role in Y stabilization and migration. We investigated vacancy cluster growth, interaction of this cluster with Y solute. Single Y solute migration in iron matrix was modelled in details. Pair-wise interactions of singe Y, O and VFe at many different relative distances were calculated. Various structural configurations for the complexes Y/O, Y/2O and 2Y/O were tested. Character of the Y-O chemical bonds in these complexes was analyzed. These results will be used in kinetic Monte Carlo simulations of the yttria nanoparticle growth.

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Ab initio simulations of interstitial oxygen migration in corundum crystals

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Due to technological, mineralogical and catalytic importance of corundum (α-Al2O3), its electronic structure, optical properties and radiation defects have been the subject of considerable experimental and theoretical studies. Radiation-induced changes in the structural and optical properties of corundum are mainly associated with primary Frenkel defects: neutral and charged interstitial oxygen atoms Oi, and oxygen vacancies (F-type color centers). Unlike the latter, the former are not well studied yet. Recent theoretical studies concluded that F-type defects in their highest charge states are more stable under most external conditions, but in some regimes neutral defects also exist.

In this study, we present the results of periodic *ab initio* simulations on basic properties and mobility of neutral and charged oxygen interstitials in corundum using DFT-LCAO method implemented in the CRYSTAL14 computer code. All defect calculations were performed using supercells 2×2×1 (120 atoms) and 3×3×1 (270 atoms). The defect geometries, migration paths and energies, as well as the Mulliken atomic charges, electron density distributions and vibrational frequencies for neutral and charged defects are compared. The octahedra center positions are shown to be unstable, both types of interstitials form oxygen O2-dumbbells with regular oxygen atoms. The O-O distances in dumbbells are 1.4 Å for a neutral defect and 1.84 Å for a charged one, respectively. The electronic density plots and the Mulliken population analysis do not reveal the covalent bonding within dumbbell with peroxide or superoxide ion formation. The dumbbells arise rather as the result of the Al-O bond formation. Migration energies were estimated as _˜1.3 eV for a neutral interstitial and _˜0.7 eV for single-charged interstitial. Obtained results were compared with available experimental data on kinetics of defect annealing in corundum.

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Aluminosilicate glass structure and behavior under electrons and ions irradiations

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The understanding of irradiation effects in oxide glasses is important in many fields (optical glasses, materials for space applications, nuclear waste conditioning...) and requires the evaluation of the role of the glass formers, mainly silicon, boron and aluminum, but also of the alkali and alkali-earth elements that can act either as modifier elements or charge compensators. In nuclear field, aluminoborosilicate glasses were highly studied and highlighted the role of boron coordination changes on structural evolution under irradiation. However, there are only few studies on aluminosilicate glasses and almost no information about the influence of aluminum and its charge compensators on the glassy network evolution under irradiation. The goal of this work is therefore to determine the effects of aluminum content and type of charge compensators (here, Na and Ca cations) on the glass structure evolution under irradiation.
To understand the different phenomena in complex oxide glasses, 13 simplified aluminosilicate glasses were elaborated, composed of SiO2, Al2O3, Na2O and CaO oxides, which were distributed in 3 series. Hence, the influence of Na2O/CaO, Al2O3/SiO2 ratios and Al2O3 content were investigated. To simulate alpha decays and compare electronic and ballistic damage, external irradiations at room temperature with 5 MeV He2+ and 7 MeV Au4+ were performed on glass pellets and powders. 2.5 MeV electron irradiations were also done to obtain bulk samples irradiated by electronic collisions at low stopping power. Structural evolutions induced by irradiations were investigated by micro-Raman and MAS NMR (23Na, 27Al and 29Si) spectroscopies. ToF-SIMS measurements on some irradiated samples were also done to probe any change of elementary composition with depth.

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From electrons and ions irradiations, it was observed that CaO improve the radiation stability of aluminosilicate glasses. Indeed, 27Al, 23Na and 29Si MAS NMR studies have shown little or no changes between pristine and irradiated glasses as CaO content increase. Moreover, the increase of the Al2O3/SiO2 ratio seems to stabilize glasses against irradiations too. From ions irradiations, observed structural effects were more important after gold ions irradiations than helium ions irradiations that seems to be due to nuclear energy deposition. Finally, micro-Raman spectra of electrons and He2+ irradiated glasses appear to be very close. The effect of electronic damage does not seem to depend on the stopping power value (higher for helium ions than for electrons) below ion tracks formation threshold.
Keywords: Aluminosilicate glass; Structure; Irradiation; Helium ion; Gold ion; Electron

Radiation modification and radiation hardness of microwave properties for some polymer nanocomposites under Co-60 gamma irradiation

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Research of composites made of polymers filled with conductive structured nano-additives (nanocomposites) showed that these materials can be prospective as broadband microwave absorbers. Starting from some critical concentration, variations of the fillers cannot provide further improvements of nanocomposite electromagnetic properties. We made assumption, that efficiency of the incorporation of nanofillers can be enhanced by radiation modification of a polymer matrix.

Nine nanocomposite materials based on epoxy resin filled with various kinds of graphite, fine artificial graphites, single-walled carbon nanotubes (SWCNT) and multi-walled carbon nanotubes (MWCNT) of concentration 1.0 wt.% along with composite materials based on polyethylene terephthalate (PET), polyvinyl acetate (PVAc), styrene-acrylic acid copolymer (SAC) filled with MWCNT of concentration 1.0 wt.% have been prepared and treated with gamma irradiation from Co-60 source up to absorption doses of 27 kGy, 115 kGy, 195 kGy, 420 kGy, step by step. Absorption doses were evaluated with film dosimeters FWT-60-00 placed near investigated nanocomposite samples. Irradiation dose rate was found as equal to 0.34 kGy/s. At each stage the electromagnetic properties (reflection, transmission, and absorption) of polymer nanocomposites have been measured. Measurements were performed using 2–408 network analyzer in the microwave frequency range of 26.0-37.5 GHz.

Microwave experiments revealed that electromagnetic properties of polymer nanocomposite based on PVAc filled with 1.0 wt.% MWCNT showed distinct improvement under Co-60 irradiation of about 90 kGy dose. Meanwhile was founded that electromagnetic properties of polymer nanocomposites based on epoxy resin, PET and SAC are tolerant to absorption dose of gamma-radiation up to 420 kGy.

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The preparation of Zn2SnO4 hollow nanostructures and its gas sensing properties

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Hollow and porous ZnO, SnO2 and Zn2SnO4 spheres were synthesized by the hydrothermal synthesis using carbonaceous spheres as templates in combination with calcination. The structure, morphology and gas sensing characteristics of the resultant product were investigated by X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray photoelectron spectroscopy (XPS), Brunauer–Emmett–Teller (BET) and gas-sensing measurement device, and the results showed that the variety of reaction parameters such as size of the template and different precursor materials have important effects on the formation of the shell structure. Compared with the solid counterparts, the hollow structures of the obtained samples were exploited as gas sensors and exhibited improved sensing performance to a series of gases (especially with regard to acetone). Moreover, sensitivity and response/recovery time of Zn2SnO4 hollow spheres to acetone were both higher than multilayered ZnO and SnO2 core-shell, and comparing the operating temperature (240oC) of zinc oxide and stannic oxide, zinc stannate had lower operating temperature (200oC). The formation mechanism and acetone sensing mechanism of Zn2SnO4 hollow spheres were also discussed in detail.

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*Speaker

Structural, electrophysical and optical properties of silicon dioxide with Zn nanoparticles: Effect of ion implantation and annealing

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Currently it is seen an increased interest in the silicon dioxide layers containing semiconductor or metallic nanoclusters. This is due to their potential applications in various fields, including data storage devices, optoelectronics and photovoltaics. In this study, thin layers of SiO2 (300 and 600 nm thick) were implanted at room and 500°C temperatures with 150 keV Zn+ ions in the fluence range of 2.5×1016 – 1×1017 cm-2. Afterwards, these samples were annealed at 700°C for 30 or 60 min in the air ambient. Co-implantation of Zn+ and O+ (50 keV) with equal fluences (2.5×1016 and 5×1016 cm-2) followed with the annealing in the above-mentioned regimes was performed also. The RBS, TEM, XTEM, RS and PL techniques as well as AC conductivity measurements in the temperature range from LNT to 373 K at frequencies in the range of 50 Hz to 5MHz were used in our examinations. Ion implantation at the elevated temperature (500°C) leads to the formation of an extended layer in the SiO2 matrix with Zn-containing nanoclusters of sizes up to 5 nm. SiO2 annealing results in an increase of cluster size (up to 10-12 nm) as well as their redistribution within the implanted layer. It should be noted that an extended layer of Zn nanoclusters also forms in as-implanted samples in the case of room temperature implantation with high fluences (1×1017 cm-2). The optical properties (RS and PL) of the implanted and annealed samples are discussed. Three activation energies of AC conductivity are registered. Strong frequency dependence of conductivity proves the electron hopping mechanism between the formed nanoparticles of different nature. The lowest activation energy (≈ 0.001 eV) corresponds to the electron hops between the zinc nanoparticles, the highest one (≈ 0.096 eV) – to the tunneling of electrons between the nanoparticles coated with zinc oxide and intermediate (≈ 0.025 eV) – to electron jumps from the coated to uncoated particles.

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RAMAN AND OPTICAL ABSORPTION STUDIES OF NEUTRON-IRRADIATED Gd3Ga5O12 SINGLE CRYSTALS

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Gd3Ga5O12 (GGG) garnets have a variety of technical applications such as solid-state laser media, phosphors, ionic conductors, and magneto-optic devices.
Atomic (i.e. vacancies and interstitials) and electronic (i.e. impurities) defects of various types produce many optical absorption bands in otherwise transparent crystals. Such point defects leading to a change in the color of the single crystals can be produced, in particular, by fast electron and neutron irradiation.

In this work we have performed comparative analysis of optical absorption (OA) and micro-Raman spectra for series of GGG single crystals irradiated with fast neutrons with doses from 1017 to 1020 n/cm2.

OA spectra have been measured at RT in the spectral range of 190 - 900 nm with resolution of 1.0 nm, while Micro-Raman scattering spectra were collected in back-scattering geometry using a Micro-Raman spectrometer (2400 grooves/mm grating), equipped with Ar laser (514 nm, 50 mW) and a Peltier-cooled CCD detector.

It was found that the OA spectra of non-irradiated Czochralski grown GGG consist of the relatively narrow lines in the UV spectral range related to the *4f* - *4f* transitions in Gd3+. Transitions from the *6S7/2* ground state to the *6P, 6J* and *6D* states in a Gd3+ cation are clearly detected. For a GGG crystal containing Ca impurity ions, additional OA band at 350 nm is observed and it is tentatively ascribed to oxygen vacancies associated with Ca impurities. Two more additional bands at 300 and 435 nm are observed in the OA spectra of fast neutron-irradiated Gd3Ga5O12 single crystals.

We have also found that fine structure (measured with 0.1 nm resolution) of the OA of gadolinium in the electronic transition region from *6S7/2* to the *6J* demonstrate clear changes with neutron dose.

Clear evolution of Raman spectra (514 nm Ar-laser) with neutron dose is also observed. In

*Speaker

particular, fine structure, observed between1350-1550 cm-1, is completely disappeared at high fluencies, while several significant changes and the emergence of new transitions have been ascertained in spectral range of 100-850 cm-1.
Finally, a study of the thermal isochronal annealing of defects in neutron-irradiated GGG crystals has been undertaken. The results indicate that the neutron-induced OA band at 300 nm could be annealed at temperatures above 700 K. The appropriate activation energy (1.4 eV) corresponds well to similar values obtained for other oxides.

Elongation of metallic nanoparticles at the interface of silica/silica, silica/silicon-nitride and silicon-nitride/silicon-nitride

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Dielectric materials containing embedded metallic nanostructures with a controlled anisotropy are of great interest due to their magnetic and plasmonic response. One method to fabricate such structures is by synthesis of nanoparticles (NPs) in a dielectric system followed by swift heavy-ion irradiation, which induces a shape transformation of the typically spherical NPs to well-aligned nano-rods. In this process, the energy deposited by swift heavy-ions can lead to the formation of so called "ion tracks", which in both silica and silicon-nitride comprise of an underdense core surrounded by an overdense shell. If the ion track and NP dimensions are comparable, elongation can be achieved from single events as it appears to be related to the ion track dimensions. As the plasmonic response of these systems depends on the dielectric function of the host matrix, it is highly desired to extend the approach developed predominantly for silica to other dielectric hosts. In this work we present experimental results of the shape transformation of Au NPs located at the interface of silica/silica, silicon-nitride/silicon-nitride and silica/silicon-nitride thin films upon irradiation with 185 MeV Au ions. After irradiation, the _˜16-18 nm diameter Au NPs transformed into continuous nano-rods with a strong dependence on the surrounding medium. For silica/silica we observed a high shape transformation efficiency with nano-rods over 100 nm long while keeping a width comparable to the ion track dimensions. On the other hand, for the silica/silicon-nitride configuration we observed an elongation process predominantly towards the silica region with a high aspect ratio as in the previous case. In contrast, elongation along the ion beam direction, yet with a faceted geometry was observed at the silicon-nitride/silicon-nitride interface with a mean length around 50 nm. We explain our results in terms of the difference in thermal conductivity (K) for silica and silicon nitride. If the thermal conductivity of the matrix is remarkably lower than that of most metals, it acts as a thermal insulator, resulting in complete NP melting. As K for silicon nitride lies in the intermediate region between silica and Au, the time-scale for ion track formation is much shorter than that of the NP melting process, limiting the NP expansion via longitudinal flow into the underdense core of the ion track.

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Radiation induced luminescence properties of Eu-doped SrO-Al2O3 single crystals

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Ionizing radiation detectors using inorganic luminescent materials are widely applied to various fields such as medical imaging, security, well-logging, environmental monitoring, high energy physics and personal dose monitoring. Luminescent materials for radiation detectors are generally insulators characterized by the wide band gap, and mainly classified into two types such as scintillators and dosimeters. Scintillators convert ionizing radiation into thousands of visible photons immediately, and dosimeters store and accumulate absorbed energy. In dosimeter materials, the absorbed energy is released and read out by optical (OSL; optically-stimulated luminescence) or thermal (TSL; thermally-stimulated luminescence) stimulations. Other than the application point of view, OSL and TSL are a useful tool to characterize material properties such charge trapping levels such as defects and impurities in solids. Strontium dialuminate (SrAl2O4) has been intensively studied particularly for long-lasting luminescence applications when co-doped with Eu and Dy; but we have recently shown that Eu-doped SrAl2O4 crystal shows notably high scintillation light yield. Therefore, to extend the study, the aim of this research to study radiation induced luminesence properties of other strontium aluminate crystal species such as SrAl4O7, SrAl12O19, and Sr3Al2O6. In this presentation, we prepared strontium aluminate crystals with various compositions by the floating zone method and investigated the radioluminescence and radiation induced storage luminescence properties such as TSL, OSL.

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Behavior under α auto-irradiation of a 241Am-doped glass ceramic

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In the French nuclear waste management strategy, minor actinides and fission products solutions are immobilized in the reference "R7T7" glass matrix. In this glass, the radioelements concentration remains below their solubility limit. The development of glass ceramic conditioning matrices is an interesting alternative strategy to increase the waste loading factor. The long term behavior evaluation of such glass ceramic material requires to study how radiation can affect the material structure and micro-structure. For that purpose a radioactive 241Am doped glass has been prepared above the solubility limit in the Atalante facility (CEA Marcoule) to induce the formation of a glass ceramic with apatite crystals Ca2.02La3.96Am4.02(SiO4)6O1.99 [1]. The evolution of these crystals has been followed until the total amorphization by X-ray diffraction, allowing to deduce a critical amorphization dose of 3.1018 α/g (2.1025 α/m3) for the apatite phase. Raman spectroscopy confirms the complete amorphization of crystals together with a modification of the local order around the SiO4 tetrahedral. This amorphization is also accompanied by a macroscopic swelling, observed by scanning electron microscopy. Nevertheless, this swelling did not induce any cracking in the glass matrix, contrary to the work of Weber [2] on a glass ceramic, who observed the formation of microcracking after similar α decay dose. This microcracking has been associated with the swelling of apatite phases during their amorphization. The absence of cracking in our study, where the size and the crystal density are smaller (until 100 μm of length and 20 μm of width) than in the work of Weber (until 200 μm of length and 70 μm of width), suggests that these two parameters have an impact on the formation of cracks within the glass matrix.

A mechanical simulation within a finite elements framework seems appropriated to reflect of the behavior of heterogeneous matrix according to the size and the density of crystals. A model will be developp to address this issue. The validation of this model will require the elaboration of new actinide doped glass ceramics in the Atalante facility.

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Nonlinear optical properties of Au nanoparticles in ion-implanted Nd:YAG crystal

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Noble metallic nanoparticles (NPs) embedded in rare-earth doped dielectrics have attracted tremendous attention due to their novel electrical, magneto-optics and optical properties for a wide range of scientific and technologic applications such as biological sensors and imaging, optical switching, and novel sub-wavelength optoelectronic devices [1]. In particular, Au NPs have been widely used for sensing due to their stability under the high temperature, biocompatibility, compatibility with surface functionalization, and ability to be tailored with uniform and different nano-size physical non-reactivity [2]. To fabricate the NPs in Nd:YAG crystal, several existing fabrication techniques have been employed including sol-gel methods, laser ablation, and ion implantation. As one of the simplest and most efficient techniques, ion implantation method exhibits many advantages of high stability, ability of multi-energy implants for complex profiles and offers the possibility of potential applications such as waveguides or other optical components associated with nonlinear optical effects. Particularly, the third-order nonlinear optical response, described by the $\chi(3)$ susceptibility, is responsible for effects such as third harmonic generation, self-focusing, Raman scattering, Brillouin scattering, phase conjugation, etc [3].

In the work, we report on the enhancement and modulation of nonlinear optical response in Au NPs embedded Nd:YAG laser crystal fabricated by ion implantation. The concentration depth of Au NPs is about 80 nm below the surface and the measured absorption band due to surface plasmon resonance (SPR) of Au NPs has the maximum around 588 nm, which has a redshift of 4% compared to the theoretical value. By using the Z-scan technique with femtosecond pulses at a wavelength of 515 nm, which is considered as an optical excitation within the SPR band, the nonlinear refraction index reaches as high as _˜10-12 cm2/W, enhanced by _˜4 orders of magnitude in comparison to that of un-implanted Nd:YAG (without Au NPs). In addition, it has been shown that embedded Au NPs in the Nd:YAG host reveal saturable absorption signifying the nonlinear responses, which exhibit the potential application as the saturable absorber for integrated pulsed laser.

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Effect of atom sizes in ionic compounds on ion channeling

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Ion channeling is a well-known radiation effect, important for understanding the passage of energetic ions and recoils in all crystalline materials. Its mechanisms have been examined by analytical theories as well as binary collision approximation and molecular dynamics computer simulations. However, there have been very few systematic studies of channeling in directions other than the principal low-index ones. Recently we developed a molecular dynamics-based approach to calculate ion channeling systematically over **all** crystal directions, providing ion 'channeling maps' that easily show in which directions channeling is expected [1]. The results show that channeling effects can be quite significant even at energies below 1 keV, and that in many cases, significant planar channeling occurs also in a wide range of crystal directions between the low-index principal ones. In all of the cases studied, a large fraction, 20 - 60%, of all crystal directions show channeling. A practical implication of this is that modern experiments on randomly oriented nanostructures will have a large probability of channeling. It also means that when ion irradiations are carried out on polycrystalline samples, channeling effects on the results cannot a priori be assumed to be negligible.

We also implemented channeling theory to give the fraction of channeling directions in a manner directly comparable to the simulations [1]. The comparison shows good qualitative agreement. In particular, channeling theory is very good at predicting which channels are active at a given energy. This is true down to sub-keV energies, provided the penetration depth is not too small.

As an extension of the previous work, which only considered pure elements [1], we consider here ion channeling in ionic compounds. To obtain a comprehensive understanding of the effect of varying atom sizes on ion channeling, we compare compounds with pure elements of the same crystal structure, where the atom mass of the element is about the average of that of the ions in the compound (for example comparing InP with Ge). The results show that the channeling effects in the compounds are different in some respects from those in the corresponding pure elements. The mechanisms behind the difference are analyzed.

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*Speaker

Impact of the outer-cladding on the radiation resistance of standard germanosilicate multimode optical fibers

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From the beginning of the 70's, research in optical fiber manufacturing technology has never been interrupted. At first optical fiber performs were manufactured in a single step but now the process consists of manufacturing a core preform rod (the primary perform), then outside the mandrel by a different technology manufacturing to increase the primary preform diameter in order to improve the production efficiency. The widely used processes include: OVD Clad, APVD (Advanced Plasma and vapor Deposition), and the RIT (Rod in Tube). RIT is the simplest cladding process and consist of cleaving the core rod with purchased high quality silica tube. This requires much less investments, in exchange of a more expensive material costs. In contrast APVD is a low cost proprietary process from Draka, consisting of depositing natural granulated silica crystal sand through a Plasma torch towards a core rod, and growing the glass layer by layer.
It is usually believed that outer-cladding affects mainly the cost of the fiber and has in principle no influence on the optical fiber performances such as transmission or radiation resistance. However, it has been shown that the outer cladding technology and its composition have a significant impact on the core structural relaxation (its fictive temperature) and thus on defects precursors and point defects. As a result outer cladding should impact significantly the radiation resistance of optical fibers. In particular APVD technology made of natural silica needs to be optimized for harsh environment applications.
In the present study, we introduced Na, K and Al in the outer-cladding of standard multimode fibers manufactured by PCVD process. In particular, we study small compositional variations of network former and modifiers (typ. 10-100 ppm) in the external part of the fiber in order to optimize the APVD outer cladding for harsh environmental applications. The study of these low losses MMF will include the investigation of defects centers generation under gammas radiation by means of optical absorption, photoluminescence and EPR in comparison to standard GeO2-SiO2 graded index multimode fiber with a RIT outer-cladding. Al-dopingshows negative impact on the RIA and high defects concentration namely AlOHC and AlE'. In contrast Na and K in then outer cladding can favors the core structural relaxation leading to a reduction of strained bonds and defects centers but they also increase the H2 sensitivity of fibers.

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Stopping of swift H+ and He+ ions in CaF2

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We have accurately measured the energy losses of 1H+ and 4He+ ions incident onto a CaF2 target over the ion velocity range, E _˜ (0.2 - 3.4) MeV/u in the labo system, using the indirect transmission method. The chemical composition and stœchiometry of the target were determined via usual Ion Beam Analysis techniques, notably RBS, EBS and NRA. The deduced stopping power experimental data were compared to sparse counterparts from the literature [1] and to values generated by the SRIM-2012 [2] and STAR [3] (ICRU-49 compilation) computer codes. Our S(E) data for alpha-particles, which are unique to our knowledge, show to be in excellent agreement with the ICRU-49 compilation [4] for projectile energies above 1.3 MeV. Besides, the measured S(E) data were analyzed within the framework of the modified Bethe–Bloch theory [5] assuming the validity of the Bragg-Kleeman additivity rule for compound targets [6], which allowed us to extract the mean excitation and ionization potential, I, as well as the Barkas-Andersen effect parameter, b, for the studied target. They were also confronted with the predictions of Sigmund-Schinner's binary collision theory [7] of electronic stopping using the PASS code [8]. The obtained results are reported and discussed with pointing out the effects of the electronic structures of both the projectiles and target material.
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Surface morhology and porosity induced by swift heavy ions of low and high stopping power in PMMA thin films

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We report on the surface modification of poly(methyl methacrylate) thin films induced by fast ions in a wide range of electronic stopping powers [14 keV/nm (2.2 GeV Bi), 2.2 keV/nm (17 MeV Au) and 0.019 keV/nm (2 MeV H)]. Thin films with initial thickness *close to* 100 nm were spun onto Si wafers with a native oxide layer. The topography of irradiated targets was characterized *ex situ* by scanning force microscopy. We observed marked differences on the effect of ion bombardment on the surface morphology, depending on the beam. The effect of the 2 MeV H beam was negligible: the surface of irradiated films remained flat and uniform even at high fluences, where chemical modification of the polymer is severe. For the heavier Bi and Au ions, strong morphological changes are seen on the surface, with development of porosity and other surface features in a broad range of spatial frequencies. For the swift heavy ions, surface changes develop in roughly two regimes: the single ion regime at low fluences, where most of the changes can be attributed to sputtering and mass transport in individual tracks; and the track overlap regime, where porosity emerge in a complex pattern of holes, with an areal density not directly related to the ion fluence. The various surface patterns observed for samples irradiated with 2.2 GeV Bi and 17 MeV Au in the track overlap regime are similar, but they appear at distinct values of the mean deposited energy density (the product of fluence and stopping power). A good correlation between the irradiation conditions and the changes in surface morphology was obtained when the product of fluence and (dE/dx)ˆ2 was used as the scaling factor. This indicates that the pattern production depends nonlinearly on (dE/dx), most probably because of the important role of electronic sputtering.

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Study on defects in borosilicate glasses with irradiations of electron and gamma ray

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Borosilicate glass has many applications in varied fields from the earth science to industry. With the characters of resistivity and viscosity, the borosilicate glass is expected as one of the candidates to vitrify the high level radioactive waste. The irradiation tolerance of borosilicate glass is important during radioactive waste disposal. The borosilicate glasses with different compositions were separately irradiated by electron and gamma rays with different absorbed doses. The irradiated borosilicate glasses were analyzed with ultraviolet and visible spectroscopy at room temperature. The color centers in the glasses were produced by the irradiation, which suggested the point defects were induced in the borosilicate glasses by irradiation. The parallel defects were identified with electron spin resonance spectroscopy at 77 K. The results from both ultraviolet and visible spectroscopy and electron spin resonance spectroscopy indicated that the densities of defects increased with the absorbed dose.Our result suggested the percent of sodium in borosilicate glasses might influence the formation of parallel defects.

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Hybrid organic-inorganic perovskites modified with ion irradiation

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Defects are usually seen as imperfections in materials that could significantly degrade their performance. However, at the nanoscale, defects could be extremely useful since they could be exploited to generate novel, innovative and useful materials and devices. Defect engineering is applied here to hybrid organic-inorganic perovskites (HOP) with 3D structures. HOP materials have become one of the most promising low-cost alternatives to traditional semiconductors in the field of photovoltaics and light emitting devices. A better knowledge of the electronic properties of such materials is obviously a prerequisite for their use and optimization in opto-electronic devices. We use here Helium ion irradiation at low energy, in the range 10-50 keV, as a tool for the introduction of point defects in a controlled way. At low fluences, mainly point defects are created that introduce defects energy levels and modify the electronic and light emitting properties of the materials. Contrary to usual semiconductors, like crystalline silicon for instance, where irradiation defects act as recombination centers for the electron-hole pairs and quench very efficiently the luminescence, we observe here an enhancement of the optical emission at low temperature. We can deduce from this observation that irradiation defects act here as active optical centers, essentially in the low-temperature orthorhombic phase as seen in the dependence of the total photoluminescence integrated intensity. Another effect of the ion irradiation directly observable is the suppression of the emission from the less tightly bound exciton. These behaviours are very intriguing and need further studies for a better understanding of the specificity of defects and their impact over opto-electronic properties in HOP materials.

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Comparative analysis and theoretical modeling of the annealing of EPR and optical absorption in neutron-irradiated MgO single crystal

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Detailed analysis of the thermal annealing of F-type centers in MgO single crystals irradiated by fast neutrons has been undertaken. Despite the fact that a detailed comparison of the annealing of single negative-ion vacancies in neutron-irradiated, electron-irradiated, and Mg-additively colored samples was performed earlier, the appropriate comparative analysis of *simultaneous* annealing of the F/F+ center optical absorption and the EPR signal corresponding to the paramagnetic oxygen dumbbell interstitials O2- so far was missing.
During the pulse annealing of the EPR signals of the F+ centers and oxygen interstitials O2- in MgO, it was observed that O2- centers decay in the relatively narrow temperature region, from 650 to 725 K, whereas the decay of F+ centres begins at 500 K and is not finished even at 800 K. This means that

(i) thermal annealing of the F-type centers is more complicated than it is usually assumed (a simple center-to-center F-type center annihilation by mobile interstitials).

(ii) thermal annealing of F -type centers measured by EPR and optical absorption looks very much similar.
Theoretical modelling of the annealing kinetics will be discussed. It gives the following migration energies: 0.23; 0.32 eV – based on the decay of the F/F+ optical absorption); 0.54 eV – from EPR of F+ centers; and 1.70-1.73 eV for migration energy of oxygen interstitials. Last energy values are in good agreement with the results of ab-initio calculations (1.6 eV).

*Speaker

Raman characterization of silica based optical fibers irradiated with heavy ions

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Abstract

Nowadays, silica-based Optical Fibers (OFs) are present as a part of several optic and photonic devices integrated in radiation environments, serving as sensors or for data transfer [1]. Several parameters that are related to harsh environments are known to influence the amplitude of radiation effects. Among them, the operating temperature and the nature of particles greatly affect the vulnerability of these devices. In this context, many previous studies were dedicated to ions implantation in bulk silica [2, 3]. In the present paper, we present a Raman characterization of heavy ions irradiation effects on silica-based OFs.

We investigated three OFs differently doped in their core (Ge, P) and in their cladding (F). The transverse cross sections of these fibers were exposed to heavy ion implantation in GANIL (Grand Accélérateur National d'Ions Lourds). The first irradiation was conducted with 92Mo at an energy of 7.8 MeV per nucleon (being _˜718 MeV in total) and with a fluence of 1.5 1012 ions/cm2, while 136Xe was used for the second run at an energy of 7.6 MeV per nucleon (being _˜1GeV in total) and with a fluence of 1012 ions/cm2. According to SRIM simulations, the projected range induced by both types of ions in silica is in the order of 70 μm.

First, based on the Raman spectrum measured by confocal microscopy, we can notice the impact of the incorporation of the dopants in the silica matrix of non-irradiated fibers. In the P-doped sample, for example, a new band is detected at _˜1330 cm-1 which is assigned to the P=O stretching mode. The presence of Ge is inferred by the band at _˜680 cm-1 associated with the presence of GeOSi bonds.

Regarding the ionic implantation impact, we followed the evolution of the D2 band area centered

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at _˜605 cm-1 and attributed to the three-membered ring structure of silica. Our results show an increase of the D2 band area after the ionic bombardment, regardless of the nature of the dopant or the used ion. The increase of the three-membered rings caused by the ionic implantation may lead to a densification of the material under exposure. Another type of ion (Ni) implantation will be discussed in the final contribution of the conference for a better comprehension of the observed effects.

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White light luminescence from annealed thin ALD-ZnO films implanted with Dy ions

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High-quality thin ZnO films grown by Atomic Layer Deposition were implanted with 150 keV Dy ions to fluencies 5E14,1E15 and 2E15 at/cm2. Implanted samples were subjected to two different kinds of annealing: rapid thermal annealing (RTA) and millisecond flash lamp annealing (FLA). In this study, the optical response to structural changes of Dy implanted and annealed ZnO films were evaluated by the photoluminescence (PL) spectroscopy and Channelling Rutherford Backscattering Spectrometry (RBS/c). Our results have shown, that independently of the used annealing technique, defects produced by ion implantation can be removed. Upon RTA performed at 800∘C a return of Zn atoms to their substitutional positions is accompanied by rejection of primarily substitutional Dy atoms to interstitial sites. Consequently, it leads to the out-diffusion and precipitation of Dy atoms on the surface and the degradation of the PL efficiency. As a result of the FLA treatment the single crystalline ZnO layer with substitutional Dy has been formed. The diffusion of implanted Pr during millisecond range FLA treatment is completely suppressed. The broadband luminescence (white luminescence) of the visible spectrum has been obtained after the heat treatment at 800∘C in oxygen. Moreover, the RBS/c results for as implanted layers revealed an intermediate defect band located between the surface and the damage peak. This defect band is produced by Zn enriched near surface layer and it is unstable for long time annealing at 800∘C in oxygen atmosphere. This leads to the conclusion that the mechanisms of the broadband PL could be explained by the native defects model and also with oxygen-bonding model on the porous surface ALD-ZnO.
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Keywords: Zinc oxide, Rare-earth, Ion implantation, rapid thermal annealing, flash lamp annealing, RBS, PL

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Using femtosecond laser pulses to control the assembly and welding of gold nanorods

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Direct assembly of gold nanorods using dithiolated molecular linkers is one of the most efficient methodologies for the morphologically controlled tip-to-tip assembly of this type of anisotropic nanocrystals but this process is characterized by difficulties in chain-growth control over nanoparticle oligomers. We have devised a light-controlled synthetic procedure where selective inhibition of the formation of gold nanorod trimers is attained by exciting the longitudinal localized surface plasmon resonance with 800 nm femtosecond laser pulses, allowing efficient trapping of the dimers by hot spot mediated photothermal decomposition of the interparticle molecular linkers. Laser irradiation at higher energies produces near-field enhancement at the interparticle gaps, which is large enough to melt gold nanorod tips, offering a new pathway toward tip-to-tip welding of gold nanorod oligomers. Optical and electron microscopy characterization indicates that plasmonic oligomers can be selectively trapped and welded, which has been analyzed in terms of a model that predicts with reasonable accuracy the relative concentrations of the main plasmonic species.
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Fabrication of Ion-Shaped Anisotropic Nanoparticles and their Orientational Imaging by Second- Harmonic Generation Microscopy

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In the last years, ion-shaping technique has been proposed as an innovative and powerful tool to sculpt the matter at the nanometer scale . Its importance relays in its unique capability to control both the morphology and the spatial orientation of metallic nanoparticles embedded within an amorphous host matrix. Consequently, ion-shaping technique can be seen as a novel route for downscaling the engineering of embedded NPs with a precision that is barely reachable with standard techniques
Here, we studied second harmonic generation (SHG) properties of arrays of spatially oriented ion-shaped nanonatennae. This is done by exciting the nanoantennae with a tightly focused polarized laser beam. A SHG is a nonlinear optical process, in which photons with the same frequency interacting with a nonlinear material are effectively "combined" to generate new photons with twice the energy. Ion-shaped nanostructures are first fabricated in different spatial orientations. Then, electron-energy-loss spectroscopy (EELS) is used to map their localized surface plasmon resonances (LSPR) and to choose nanoantennae whose aspect ratio allows to be efficiently coupled with the wavelength of our laser source (1060nm). The optimum samples are subsequently characterized using SHG microscopy with tightly focused linear (LP), radial (RP) and azimuthal (AP) polarizations.

We show that nanoantennae with different orientations give rise to distinct SHG features. These are due to the variations in the local state of polarization inside the focal volume. Our SHG imaging experiments are complemented by numerical modeling based on the frequency-domain boundary-element method (BEM). Owing to the precise control over the shape and orientation of the nanoparticles, this result pave the way towards the design of nanocomposites with distinct and tailorable linear and nonlinear optical properties such super-lenses and cloaking devices.
Slablab et al., Scientific Reports, 2016 Nov 24;6:37469

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Point defects and their optical properties in polyethylene chains

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Radiation damage in polymers can be initiated by a variety of mechanisms, according to the type of projectile. When dealing with insulating polymers, electronic excitations play a crucial triggering role. The theoretical understanding of defect formation and stability is however still poor. We consider here polyethylene (PE) for two reasons: first, it is a reasonably simple insulating model polymer; second, it is an important component of many cable insulators employed in a nuclear environment, where ageing under irradiation is a crucial issue. The formation and trapping of excitons in PE has been already discussed one decade ago [1] using Density Functional Theory (DFT). In the meanwhile, however, important progress has been made in methods that give a more accurate description of the electronic structure, like many body perturbation approaches based on the GW approximation and the Bethe-Salpeter equation (BSE), accounting for excitonic effects, or Time Dependent Density Functional Theory (TDDFT). The latter was recently used as a powerful tool to reveal ageing mechanisms of ancient paper [2].
Here we use DFT and the GW-BSE approach to study the optical absorption spectrum of PE containing carbonyl and vinyl defects; as a model for the polymer we rely both on alkane molecules of varying length and on periodic crystalline systems. For the structural relaxations we use a plane wave formalism using Quantum-Espresso and the SaX code [3] for the quasi-particle calculations of periodic systems. For isolated systems we take advantage of a recent localized basis set implementation of the GW-BSE formalism: the MOLGW program package [4]. We discuss convergence issues and some structural effects, which can be strong on the quasi-particle band structure, but tend to reduce on the excitonic spectra.

We discuss the excitonic structure and show that dark excitons are present in carbonyl defects. We compare our results to experimental results obtained by fluorescence. We also investigate the role of structural relaxations in the excited states and the possibility of self-trapping of excitons. Furthermore, we assess the thermodynamic stability of the above mentioned defects on the basis of our calculated formation energies, an approach currently applied to inorganic solids, but seldom encountered on polymers and soft matter in general.

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Atomistic simulations of swift heavy ion tracks in Al2O3

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The structure and formation threshold of swift heavy ion tracks in Al2O3 is studied using a combined modeling with original Monte-Carlo code TREKIS [1,2], describing the excitation of the electronic subsystem as well as energy and momentum transfer into the lattice, and classical molecular dynamics of excited lattice atoms. The advantages of the developed approach are the absence of free parameters, and accounting for collective effects of excitations of the electronic and ionic subsystems of a solid.
The data obtained for Xe 167 MeV ion impact onto Al2O3 demonstrate that the relaxation of the excess lattice energy results in formation of a cylinder-like discontinued disordered region of about 2 nm in diameter. It is consistent with the recent transmission electron microscope observations. The estimation of an SHI track formation threshold gives the value of _˜7 keV/nm, which is close to the experimental one (_˜9-10 keV/nm) [3]. The simulation of the X-ray diffraction patterns of irradiated material demonstrates that Al sublattice is damaged stronger than the oxygen sublattice in a track.

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Excitation of electronic system of subsurface layers of TiO2 and Al2O3 irradiated with swift heavy ions

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A swift heavy ion (SHI, E=1-10 MeV/nucl) penetrating through a solid deposits the largest part of its energy into the electronic subsystem of the target. Further kinetics of material excitation in the nanometric vicinity of the ion trajectory (ion track) crucially depends on achieved parameters of the disturbed electronic system. Exchanging energy and particles with an environment, a subsurface layer of the target can react unusually to the strong perturbation induced by an SHI, forming inhomogeneity in the parameters of excited electronic system along the ion trajectory.
The developed Monte Carlo model (TREKIS [1,2]) is applied to describe such surface effects of the excitation kinetics of the electron subsystem of Al2O3 and TiO2 film of 20 nm in thickness irradiated with swift heavy ions. The code uses cross sections taking into account collective response of the electron ensemble of a target that may be of principle importance under conditions of the extreme track kinetics.

Spatial redistribution of excited electrons near a sample surface, the temporal and radial distributions of the densities and energies of generated electrons and valence holes are calculated. In particular, propagation of a front of electronic excitation away from the ion trajectory is demonstrated. The temporal evolution of the excess energy accumulated in the lattice along the ion trajectory reveals decrease of its density within 5-6 nm from the surface.

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Temperature dependent Raman and luminescence spectroscopy of self-irradiated U, Th-bearing natural zircon

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Natural zircon (ZrSiO4) generally incorporates trace amounts of U (usually below 5000 ppm) and Th. Alpha-decay events cause self-irradiation with high-energy alpha particles (4.0-8.8 MeV) and heavy recoil nuclei (0.07-0.17 MeV) over geologic periods of time, eventually causing transition of the crystalline to a radiation-damaged state. Severely damaged zircon shows a nano-heterogeneous structure that consists of disordered crystalline remnants in an amorphous matrix.
The aim of the present study was to investigate the lattice dynamics and luminescence centers in the radiation-damaged zircon structure using T-dependent (T = 7–300 K) micro-Raman (633 nm excitation) and pulsed-laser-induced luminescence spectroscopy (263 nm excitation). Mildly to severely radiation-damaged, gem-quality zircon samples from Sri Lanka have been studied. The calculated self-irradiation doses of the samples are in the range of Dα = 0.6–9.2 ' 1018 a/g; however it should be noted that all Sri Lankan zircon has experienced partial annealing [1].

We have analyzed (i) the spectral position, width and line profile of Raman bands and (ii) the emission energy, width and relative intensity of laser-induced luminescence bands at 530 and 470 nm (- and B1-bands, respectively [2]). Our work aimed at an understanding of how these spectral parameters depend on temperature (T) and dose (Dα). The effect of T on Raman-band shifts (related to lattice thermal expansion and phonon interaction) is comparable in magnitude with that of Dα (causing structural strain in the crystalline remnants). In contrast, the effect of T on Raman-band broadening (associated with phonon interaction) is much smaller, compared to the Dα-induced broadening (associated presumably with phonon confinement, crystallite size distribution, point defects).

The mechanisms of optical-phonon decay via lattice vibrations were analyzed on the basis of T dependences of Raman parameters of samples with different degrees of radiation damage. Temperatures of luminescence quenching were estimated. Structural nano-heterogeneity of damaged zircon was taken into account in interpreting the results.

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Electronic excitation induced LSPR of Au nanoparticles in amorphous carbon matrix

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Nanocomposite thin films are of interest because they combine not only the properties of two materials but also provide the possibility of generation of new novel properties. Since one material is having atleast one dimension in nano meter regime, it gives the advantages of nanomaterials also. The optical and structural properties of these nanocomposite thin films can be tailored using energetic ion irradiation technique. With the help of swift heavy ion irradiation, nanosized ion tracks can be created into the target material and with-in these tracks, materials is modified due to the generation of very high temperature. The density of these track can be controlled just by changing the fluence of the beam. In the present work, nanoparticles of gold in carbon matrix are synthesized by co-sputtering of gold and graphite in high vacuum chamber using neutral Ar atom beam. Films are deposited on glass substrate, Si and carbon coated Cu TEM grids. These films are irradiated with 120 MeV Au ions at different fluences 1×1012, 5×1012, 1×1013 and 3×1013 ions/cm2 using Pelletron accelerator. The Au nanoparticles are found to be too small (1.5 ± 0.01 nm) to excite the plasmon resonance in the pristine film. With ion irradiation, a clear but broad SPR peak is seen at _˜ 526 nm for the film irradiated at a fluence of 1×1013 ions/cm2, which is slightly red shifted to _˜ 529 nm at a fluence of 3×1013 ions/cm2 with a broader width. The red shift is ascribed to the growth of the particles due to enhanced diffusion and ostwald ripening. The average particle size at 3×1013 ions/cm2 fluence is found to be 2.1 ± 0.03 nm.

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In Situ Measurement of Radiation Induced Polymerization Process Parameters Using Surface Plasmon Resonance Detector

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Proliferation of polymeric materials in different areas of science and industry creates a great challenge when properties of such materials have to be determined. Therefore the possibility to assess material properties in situ during its polymerization process is of great value. Radiation processing of materials is one of the most economically efficient methods of induced polymerization. It allows huge volumes of material to be processed in a relatively short period of time. The main drawback of this process is related to complicated methods for quality control in real time, mainly because of the high throughput volumes and strict requirements for accuracy of the measurements performed.[1] Similarly in the medical field accurate absorbed dose measurements are of high importance. Although in a lower dose range (up to 15 Gy) compared to industrial applications (tens of kGy), in situ dose measurement methods are either not sensitive enough, cumbersome to use and do not cover the required dose range completely.[2]

Proposed absorbed dose/degree of polymerization measurements method aims at evaluating the degree of polymerization of nPAG gels in situ during irradiation. The detector itself is based on the surface plasmon resonance phenomena, where a conductive base is covered with a sensing layer. In this particular case gold diffraction grating is used as a base and nPAG gel as the sensing layer on it.[3] Sensitivity of the detector depends on several factors, one of which is the thickness of the sensing layer which can be adjusted for different measurement conditions. Read out is performed by measuring the light absorption spectra of the detector. A spectral shift is observed when the degree of polymerization of the nPAG gel changes. Complete measurement setup including detector was placed within irradiation field of X-Ray therapy unit. Measurements were performed in situ irradiating dose gel covered detector up to 10 GY doses produced by high energy photon beam.

It was found that the spectral shift is dependent on the absorbed dose/level of polymerization in irradiated dose gels and might be measured in situ during radiation processing of polymeric gels.

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Velocity effect for creation of point defect halos of swift-heavy ion tracks in alkali-halides

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The dome-like shape of the dependence of the electronic stopping on the energy of a swift heavy ion (SHI) results in the so-called velocity effect when ions of different energies produce the same linear electronic energy losses in a target. Usually, the effect manifests itself in larger lattice damage produced by slower ions due to the smaller extension of the electron cascade and thus a larger initial local energy density deposited into the electron subsystem.
Parameters of the point defects halos (F-color centers) created via decays of self-trapped valence holes generated in the nanometric vicinities of the trajectories of gold ions of 275 MeV and 2187 MeV in LiF are estimated from absorption spectroscopy experiments. Such ions have approximately the same electronic stopping: 24.6 and 22.9 keV/nm, respectively. In spite that the slower ions produce higher deposited energy density, the defect halo reveals larger radii and larger defect concentrations for the higher ion velocity.

Peculiarities of spatial spreading of valence holes before their self-trapping result in these differences between the detected defect halos for the applied ions. Simulations with the Monte-Carlo code TREKIS [1] showed no significant difference in the initial spatial distributions of valence holes within the radii of the defect halos deduced from the experiments by the times of finishing of ionization cascades (_˜10 fs after the projectile passage). Using these distributions as initial conditions for spatial spreading of valence holes before their self-trapping, the diffusion coefficients of holes in tracks of 275 and 2187 MeV Au ions were estimated revealing about six times larger coefficient in tracks of the faster ion.

Possible mechanisms which may cause the detected effect are discussed: electromagnetic fields induced due to transient spatial separations of holes and electrons, and coupling of valence-holes

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Ab-initio modeling of lattice instability of Al2O3 after swift heavy ion impacts

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A swift heavy ion (SHI, M > 20 a.m.u., E > 1 MeV/nucl) loses the largest part of its energy on excitation of the electronic subsystem of a target in the nanometric vicinity of the trajectory (> 90%, 1–10 keV/nm). Extreme perturbation of the electronic subsystem followed by its relaxation stimulates unusual pathways of lattice excitations forming finally structure modified ion tracks. In particular, these electronic excitations may change the interatomic potential causing lattice instability in the closest vicinity of the ion trajectory.
Monte-Carlo code TREKIS [1,2] was applied to describe the excitation kinetics of the electronic subsystem of Al2O3 in SHI tracks up to 100 fs after the projectile passage. Spatial and temporal distributions of the densities and energies of excited electrons as well as of holes in the valence band and atomic shells are obtained in the nanometric vicinity of an ion trajectory.

Extracted parameters of the excited electronic subsystem were used as inputs in ab-initio simulations based on the density functional theory. These simulations gave us the transient changes of interatomic forces at different distances from the trajectories of different ions, which allow to estimate the effects of instability of Al2O3 lattice in SHI tracks.

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Effect of He+ ion implantation on Rb+-K+ exchange in KTiOPO4 optical waveguide formation

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We report on the effect of 500 keV He+ ion implantation with a fluence of 3×1016 ions/cm2 on Rb+-K+ exchange in KTiOPO4 optical waveguide formation. The process of implanted He+ ions into KTiOPO4 crystal was calculated by the stopping and ranges of ions in matter computer code. The dark mode spectra of the samples were measured by prism coupling method. The refractive index distribution after ion implantation, ion exchange, and ion implantation and subsequent ion exchange were reconstructed by reflectivity calculation method, inverse Wentzel–Kramers–Brillouin, and intensity calculation method, respectively. Field intensity distributions of the waveguides were simulated by Beam Propagation Method. The phase analysis of the samples has been measured by X-ray diffraction technique. Results indacate that effective refractive index changes due to the lattice damage. The damage layer formed in the depth of maximum nuclear energy deposition by ion implantation acts as a barrier to block the ions diffuse into the sample. The concentration of defects can modify the speed of ion exchange. Results exhibit that ion implantation and subsequent ion exchange is an effective means in optical waveguide formation.

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Strong optical activation of Eu+ ion implanted KTiOAsO4 at room temperature

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Eu attracts special attention for its intense emission around 612 nm originating from the 5D0®7F2 transition. Excellent optical activation of Eu3+ ions are caused by the formation of Eu-Oi complexes [1]. Potassium Titanyle Arsenate (KTiOAsO4, KTA) is an excellent nonlinear optical crystal with a band gap about 3.4 eV.
In this work 400 keV Eu ions were implanted into KTiOAsO4 crystals with an ion fluence of 5×1015 ions/cm2 at room temperature. After implantation annealing was performed in Ar atmosphere for 30 min at temperatures between 600 and 900∘C. Damage formation/annealing and optical emission were studied by Rutherford backscattering spectrometry in channelling mode (RBS/C) and by photoluminescence (PL).

The RBS/C spectrum of the pristine KTiOAsO4 crystals amounts to 5% of the random level indicating a good crystalline quality of the material. After implantation a damaged layer of 265 nm thickness formed which is much thicker than one would expect from the SRIM calculation which yields a mean projected range of the Eu ions of (110±30) nm. The aligned spectrum of the as-implanted material reaches the random level which may indicate the existence of an amorphous layer. After annealing at 600∘C this thickness of the damaged layer amounts to 110 nm only. This could be explained by an epitaxial recrystallisation of part of the as-implanted layer. It is found that the Eu atoms are redistributed towards the surface and almost no Eu occurs within the annealed part of the layer. This suggests that Eu atoms are pushed out of the material during the recrystallization.

The photoluminescence spectrum of the as-implanted KTiOAsO4 shows strong emission of light with wavelengths around 612 nm under 325 nm laser excitation at room temperature. Similar experiments were performed on KTiOPO4 and RbTiOPO4. However, in these cases almost no Eu-related emission could be detected at room temperature. From this results we assume that interaction of Eu with As supports Eu to be in the 3+ state. It is well known that Eu and As can form different crystalline phases [2]. Further RBS/C and PL investigations are in progress to understand ion-beam induced damage formation and annealing as well as the origin of the strong Eu emission in KTiOAsO4.

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Sub-band-gap optical response in Au-implanted silicon

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Recently it was suggested that Au doping in Si can be realized by ion implantation and pulsed laser melting. The sub-band-gap optoelectronic response is observed and increases with the implanted Au concentration [1]. In our work, Au implanted Si was fabricated by ion-implantation with three different fluences of 7×1014 cm-2, 1.4×1015 cm-2 and 2.1×1015 cm-2, followed by pulsed laser melting. The Raman spectrum results confirm the high-quality recrystallization of the Au implanted layer. And the Rutherford backscattering spectrometry / Channeling reveal that Au atoms diffused to the near surface region. In addition the detailed angular scans along Si [001] reveal that Au atoms are mostly in the interstitial lattice sites. From the transport measurements, a p-type conductivity and an increasing carrier concentration are observed in the implanted layer. Moreover, the transmission and reflection were measured using near infrared spectroscopy (NIR) to quantify the sub-band-gap absorptance in the hyperdoped silicon. In the Au implanted layer the spectral response extends to wavelengths as long as 3.2 μm. However, the sub-band-gap absorptance has no dependence on the Au fluence or the carrier concentration. [1] Mailoa, Jonathan P., et al., Nat. Commun. **5**, 3011 (2014)

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Hyperdoping silicon with tellurium for optoelectronics

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Chalcogen-hyperdoped silicon has been a topic of great interest due to its potential optoelectronic applications owing to the sub-band-gap absorption [1-3]. In our work, tellurium hyperdoped Si was fabricated by ion-implantation with different fluences ranging from 1.09×1015 to 1.25×1016 cm-2 followed by pulsed laser melting (PLM). The Rutherford backscattering spectrometry / Channeling (RBS/C) results reveal the high-quality recrystallization of tellurium implanted silicon by PLM. From the transport measurements, an insulator-to-metal transition is observed with increasing tellurium concentration. Moreover, the ellipsometry measurements show that the band gap narrows with increasing tellurium doping concentration. And the Fourier transform infrared (FTIR) spectroscopy show that tellurium hyperdoped Si has strong infrared absorption. This gives us a signal that hyperdoped silicon with tellurium could enable silicon-based optoelectronics in the infrared band.

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Surface-structure and photoluminescence properties of Ce:Lu2SiO5 crystals irradiated by carbon ions

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Recent decades have seen the development of scintillators served for medical and scientific imaging. As one of most popular scintillation crystal, Cerium doped lutetium oxyorthosilicate (Ce:Lu2SiO5, Ce:LSO) have been attract extensive attentions for its superior luminescence properties, and have been widely applied to detect gamma rays in many instrument such as computerized tomography (CT), positron emission tomography (PET) and high-energy physics (HEP). However, other optical properties of Ce:Lu2SiO5 crystals have rarely been reported. The optically polished 5 × 5 mm2 surfaces of Ce:Lu2SiO5 samples were subjected to 6MeV Carbon ion irradiation at temperature of 300 K varying ion fluences. The three samples are correspond to the specific irradiation conditions with beam fluences of 5e14 ions/cm-2, 1e15 ions/cm-2, 2e15 ions/cm-2, respectively. Optical waveguide structure was observed with the three samples. The damage behavior of Ce:Lu2SiO5 samples were characterized using techniques of X-ray diffraction (XRD) and Raman spectroscopy. The photoluminescence spectra of samples were measured at room temperature. Based on SRIM code, the nuclear and electronic energy loss profiles induced by 6.0 MeV carbon ions was simulated at an incident angle 7○ off surface normal. The optical-waveguide properties of Ce:Lu2SiO5 samples irradiated with energetic carbon ions were characterized using prism coupling and end-facing coupling techniques, and discussed through reflectivity calculation method (RCM) and finite difference beam propagation method (FD-BPM).

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Atomic simulations of amorphization of quartz under ion irradiation

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Quartz is a stable crystalline SiO2 material at room temperature. It draws a great deal of attention and interest due to its wide use in microelectronics, optoelectronics and other fields. Ion irradiation is a very useful method to modify properties of materials, which, at the same time, may lead to amorphization of crystalline structures. In this work, we use classical molecular dynamic (MD) methods to simulate the amorphization process of crystalline quartz under 50 keV Na ion irradiation. Then, Rutherford backscattering spectra (RBS) from the irradiated SiO2 structures were obtained by using the recently developed RBSADEC (RBS from an Arbitrary Defected Crystals) code [1] based on binary collision approximation. The simulation results show that RBS yields would increase as the irradiation doses. When the irradiation doses reach to about 8.0×10ˆ13 Na/cmˆ2 (equal to 3 eV/atom), the crystalline quartz would be fully amorphous, which is agreement with the experimental value 5.5×10ˆ13 Na/cmˆ2 (equal to 1.92 eV/atom) [2]. This simulation method is used for studying the amphorization process of other crystalline structures in future.

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Highly Selective and Ultrafast Alkali Metal Ionic Transport through Polymer Films with latent tracks

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Nanopores have great potential applications in separation or filtration of electrolyte ions due to their selective ion transport. Recently, polymer nanopores were fabricated in 12 μm thick polyethylene terephthalate (PET) films by irradiation with GeV heavy ions and subsequent 3 h exposure to UV radiation. These nanopores show ionic transport selectivity spanning more than 6 orders of magnitude: the order of the transport rate is Li+> Na+> K+> Cs+> > Mg2+> Ca2+> Ba2+, and heavy metal ions such as Cd2+ and anions are blocked. The transport can be switched off with a sharp transition by decreasing the pH value of the electrolyte. Structural measurements and molecular dynamics simulations suggest that the ionic transport is attributed to negatively charged nanopores and the selectivity is associated with the dehydration effect [1]. Moreover, after heating these PET films in the aqueous solution, the permeation rates were increased by about one order of magnitude and the alkali metal transport order is reversed as Cs+> K+ > Na+ > Li+. For 2 μm thick Mylar membranes without heat treatment, they also exhibit an excellent ionic selectivity of the alkali metal ion over the heavy metal ions, and an alkali metal transport order of Cs+> K+ > Na+> Li+. Notably, the transport rates of the alkali metal ions exceed a value of 10 mol/h×m2, which is much greater than those through the well-known graphene oxide membrane [2]. These ion-selective nanopore systems will have great potential in ultrafiltration, desalination, energy conversion, and many other applications.

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Effects of Ion Irradiation on Optical Property of Silicon Films

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As one of the most important semiconductor materials, silicon films have been considered as the most promising candidates for the fabrication of large area and low cost solar cells. Since the optical property of silicon films has great effects on the performance of the solar cells, modification of silicon films on optical property has attracted much attentions. In this work, amorphous and nano-crystalline silicon films have been irradiated at room temperature by Kr and Xe ions with the energies from several to hundreds MeV. The effects of ion irradiation on the optical property of silicon films have been studied. The obtained results show that the optical band-gap decreases at an exponentially rate as ion fluence increases. Combining the analysis of structural results, it has been considered that the irradiation induced reduction in optical band-gap of the samples is related with several aspects, including defect generation, amorphization and hydrogen release of the samples. The defects induced by the irradiation produce the defect energy levels in the forbidden band. These energy levels lead to the broadening of the valence and conduction band tails as well as the decrease of the optical band-gap. The amorphization of the nano-crystalline silicon films weakens the quantum size effect of the nano-sized crystallites and results in the decrease of the optical band-gap. Moreover, comparison of the results of hydrogenated and unhydrogenated silicon films indicates that the hydrogen release results in the decrease of short-range structural order, which also plays an important role on the reduction in optical band-gap.

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Damage characterization of displacement cascades in (U,Pu)O2 fuels by MD simulations

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Plutonium based MOX fuels (U,Pu)O2 are one of the most commonly used fuel in actual nuclear plants in France. However, little is known on its microscopic behaviour during irradiation. This is mainly resulting from the fact that experiments are difficult and expensive to set up with such compounds at such scales and conditions. Hence, atomistic simulations can bring valuable information and increase the scope of knowledge in this field. Molecular dynamics simulations have proved to be an excellent tool to study point defects creation, because of its intrinsic length and time scales. We present in this paper the insight brought by molecular dynamics simulations on primary damages in (U,Pu)O2 solid solution. The efficiency of four of the most recent rigid ions pair interactions for (U,Pu)O2 solid solution will be exhibited by comparing their thermo-mechanical and thermophysical properties at different temperatures and plutonium contents. Then, the primary damage state under irradiation will be discussed based on the analysis of the results of displacement cascades initiated with energies up to 500 keV and for different plutonium contents.

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Thermal diffusion of Mo and Cs in UO2: damage and chemical effects

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Determination of fission product thermal diffusion in Pressurised Water Reactor (PWR) nuclear fuel is necessary for source term modelling during normal and off-normal situations. We focused this study on caesium and molybdenum, two fission products with high fission yields and complex chemistry. In UO2, these elements are known to interact with each other to form the compound Cs2MoO4 [McFarlane1996]. This chemical effect has to be taken into account in the determination of diffusion coefficients.
Hence, the originality of the present paper is to perform the co-implantation of both Cs and Mo in UO2 in order to evaluate their possible chemical interactions. The ion implantation technique was used to introduce Mo and Cs, separately or together in UO2 pellets. It results in quasi-Gaussian distributions with a projected range (Rp) of about 100 nm for both Cs and Mo. The impact of atomic concentration was studied by implanting at two significantly different fluences: 2x1014 and 1016 at.cm-2. At the lowest fluence, the maximum concentration is about 0.02 at. % corresponding to a maximum damage close to 1 dpa (displacement per atom) for both elements. At the highest fluence, the maximum concentration is about 1 at. % leading to 65 dpa and 50 dpa for Cs and Mo respectively. PF diffusion is activated by annealing the samples in the 1400-1600∘C temperature range during 4 hours under reducing atmosphere in order to maintain the sample stoichiometry. The Secondary Ion Mass Spectrometry (SIMS) technique allowed following the evolution of Mo and Cs concentration profiles in UO2, before and after annealing treatments, using a device equipped with a rotating sample holder. Diffusion coefficients were deduced from the broadening of the Cs and Mo concentration profiles. The structural modification induced by temperature was followed by Raman spectroscopy.

In order to get insight in the diffusion mechanisms, a comparison of experimental data with dynamic molecular (DM) calculation using the Lammps code is also proposed.

MacFarlane1996

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Session XIII

Is there any evidence of amorphous to amorphous phase transformation due to radiation in oxide glasses?

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In amorphous material, the understanding of how the structure reacts with respect to radiation is still debated. Many studies have been performed on oxide silicate glasses using γ rays, electrons, ions, neutrons irradiations, radioactive decays of unstable isotopes incorporated in the glassy network, and molecular dynamic simulations of the damage induced by heavy ions. These studies have described the changes occurring in the glassy network, but there is still no unified theory to explain why such changes are observed according to the irradiation conditions. Because of the metastable character of the glassy state, an open question is related to its stability with respect to the excess of energy introduced by radiation into the material, particularly we still do not know if radiation can favor a more stable state and could induce crystallization or amorphous to amorphous transformations. In the current article we propose to compare how a specific sodium borosilicate glass reacts to various irradiation conditions, involving both electron energy loss (at low and high level) and nuclear energy loss, and therefore could help to go further into this discussion on the stability of the glassy state under irradiation. Mono beam irradiations will be compared to sequential double beam irradiations to describe the glass response as function of its initial glassy state.

*Speaker

Upconversion luminescence processes in rare earth doped fluorides and transparent oxyfluoride ceramics

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In the last decade, much attention has been paid to comprehensive research and application of upconversion processes in rare-earth doped materials, which involve optical absorption of multiple photons and subsequent emission of one photon of higher energy.
Upconversion effect could be used for different applications such as upconversion pump lasers, new materials for infrared visualization, next generation lighting or displays, biological nanolabels etc

In my talk, after presentation of some basics on

(a) *upconversion processes or* anti-Stokes emissions;

(b) different mechanisms of upconversion, either alone or in a combination, such as second harmonic generation, two-photon absorption, ground state followed by excited state absorption, energy transfer upconversion, and photon avalanche,

(c) distinction of the appropriate mechanism for a particular experiment,

(d) effects of the excitation power and the dopant concentration,

(e) requirement to host and dopants involved upconversion processes,

we will overview our recent results, namely

- site-selective spectroscopy of Er3+ in NaLaF4 and NaYF4

- excited state absorption and energy-transfer mechanisms of up-conversion luminescence in Er3+-doped oxyfluoride glass ceramics at different temperatures

- Upconversion luminescence of a transparent glass ceramics with hexagonal Na(Gd,Lu)F4 nanocrystals etc
Synchrotron VUV spectroscopy data obtained for rare-earth doped fluorides will be also analyzed.

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Comparison between the optical properties of defects induced by 2.5 MeV electrons and by neutrons in crystalline and amorphous SiO2.

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Optically active point defects in SiO2 are important in radiation-resistant or UV/high-power laser optical elements and optical fibers. While most applications use amorphous SiO2 (a-SiO2), many studies have focused on crystalline SiO2 form, α-quartz, since the ordered defect environment allows to extract more information. However, in spite of similar structures of corner-shared SiO4 tetrahedra, the defects in both materials are very different. In particular, dangling-bond type defects, which dominate optical absorption (OA) and photoluminescence (PL) properties of a-SiO2, are virtually absent in non-amorphized γ-irradiated α-quartz. Oxygen dangling bonds ("NBOHC's") in ordered and oriented crystalline environment were shown to exist in neutron –irradiated α-quartz [1] at the boundaries of amorphized tracks. In case of γ-irradiation (dose up to 50MGy) of α-quartz, NBOHC's are not induced, and Frenkel defects dominate [2].
This work reports the effect of 2.5MeV electron irradiation at up to 100 times higher doses than previously used [2] on PL and visible to vacuum-UV–range OA of high-purity α-quartz and a-SiO2. Results are compared to neutron irradiated α-quartz.

Large differences in defect formation between glass and crystal SiO2 persisted even at the highest dose, 4.5GGy (1.8×10ˆ19 e-/cm2). In comparison to glass, in crystals formation of oxygen and silicon dangling bonds (NBOHC and "E'-centers") and divalent Si centers ("SiODC(II)") was negligible. Dimerization of O interstitials to O2 molecules, characteristic to a-SiO2 and silicate glasses [1-3] was inefficient in α-quartz.

In contrast to electron - irradiation, glass-characteristic defects were present in neutron-irradiated (10ˆ19n/cm2) α-quartz. In addition to the previously reported [1] NBOHC and interstitial O2 defects, SiODC(II) was identified in quartz by its time-resolved PL bands at 4.1 and 2.55eV and characteristic long lifetime (
tau= 8.8ms) of the triplet PL at 2.55eV, which are close to those in a-SiO2 (4.3eV, 2.6eV, 10.2ms, respectively).

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Velocity correlated emission of nanocrystalline clusters in keV surface sputtering by a large polyatomic projectile

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Sputtering processes of solid surfaces by ion beams and sputtering related phenomena are of interest and importance in many fundamental and applied fields. These processes find increasing use in modification and analysis of surfaces at the nanoscale. Recent interest regarding fundamental mechanistic aspects is related with differences between the characteristics of sputtering induced by polyatomic/cluster projectiles as compared with that induced by atomic projectiles. For atomic ion projectiles, sputtering mechanisms are well studied. The underlying physics is described in terms of linear collision cascades or various thermal spike models. In contrast, mechanisms of particle emission following bombardment with large polyatomic ions are poorly understood.

We have recently found a new mechanism for the sputtering of solids by a large polyatomic projectile ion [1]. Emission of large cluster ions (TaC)n ; n = 1-10 and (Ag)n ; n=1-9 , with nearly the same velocity for all cluster sizes (n values) was observed following impact of a large polyatomic projectile (C60 anion at 14 keV kinetic energy) on Ta /TaC and Ag targets correspondingly . The TaC carbidic layers were pre-grown by exposure to the fullerene ion beam and were TEM characterized [1]. The measured kinetic energy distributions (KEDs) of the different clusters ejected by the C60 ion impact were found to behave oppositely to those observed using monoatomic projectile ions. We have rationalized our results in terms of a new surface sputtering mechanism where an outgoing, superhot, moving precursor (with some center of mass velocity), is the source of the emitted clusters. In agreement with a successful modelling of the KEDs by shifted Maxwellians . Here we will describe also recent additional observations and analysis with a focus on the impact induced emission of nanocrystalline carbidic cluster ions of the fifth group, (TaC)n ,(NbC)n , (VC)n, from the carbidic nanofilms. The general nature of the new mechanism will be discussed while comparing emission characteristics for the different types of carbidic nanoclusters within the same group.

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*Speaker

Session XIV

Optical detection of spin-dependent recombination for electron and hole defects induced by ionizing radiation in the wide-gap materials

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Optical detection of spin-dependent recombination will be applied for electron and hole defects induced by ionizing radiation in several types of wide-gap materials: garnet and fluorite crystals, semiconductors (ZnO, AlN, SiC, AgCl) and based nanostructures, superparamagnetics (gadolinium based garnets). Optically detected magnetic resonance (ODMR) techniques will be considered for characterization of electron and hole defects, bound excitons. In ODMR, the resonance conditions are created in the same way as in conventional EPR but instead of direct measurements of microwave absorption, microwave induced changes in the luminescence intensity are detected. This results in a giant increase in sensitivity up to recording of a single defect. It will be used recombination photoluminescence, tunneling afterglow and photostimulated luminescence (PSL).
One of the ODMR techniques is based on spin-dependent recombination detection via tunnelling afterglow and PSL which can be observed after x-ray or UV irradiation of crystals and in some cases persists for a long time after the irradiation. IR illumination of previously UV or x-ray irradiated samples leads to a considerable increase in the emission intensity - PSL. For the identification of radiation-induced defects conventional EPR study will be used along with ODMR.

It was found that in the irradiated rare-earth doped scintillator materials the energy released in the spin-dependent tunnelling recombination of electron–hole pairs and self-trapped excitons in the host crystal is directionally transferred to the rare-earth impurity-ions (e.g., Ce3+). To identify the origin of recombining electron and hole centres, their EPR spectra were detected by monitoring the tunnelling afterglow and PSL. The spin system of radiation induced defects in gadolinium based garnets was shown to accumulate significant energy which can be released in external magnetic field. This effect, which is caused by the huge local magnetic fields at the location of recombining defects, is suggested to be common for superparamagnetic materials.
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*Speaker

Radiation defect dynamics studied by pulsed ion beams

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The formation of stable radiation damage in crystalline solids often proceeds via complex dynamic annealing processes, involving migration and interaction of ballistically-generated point defects. Our current understanding of defect interaction dynamics is limited for most materials due to the lack of direct experimental methods to study them. We have developed a pulsed ion beam method to study defect interaction dynamics. This method allows us to measure effective time constants of defect interaction, defect interaction rates, and defect diffusion lengths. The strengths and limitations of the pulsed beam method will be illustrated with examples for SiC, Si, and Ge. This work was performed under the auspices of the US DOE by LLNL under contract DE-AC52-07NA27344.

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CREATION AND ANNEALING OF STRUCTURAL DEFECTS IN PARTICLE IRRADIATED MgAl2O4 SINGLE CRYSTALS AND CERAMICS

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Magnesium aluminum spinel exhibits high resistance against heavy irradiation, very little swelling even at high doses of fast neutron irradiation and can be exploited for various applications, incl. future fusion reactors. Radiation tolerance of MgAl2O4 is explained by the efficient interstitial-vacancy recombination during irradiation due to a huge concentration of as-grown vacancies and cation swapping between tetrahedral and octahedral sites resulting in the antisite defects and inverse spinel formation.

The present study deals with structural defects in MgAl2O4 single crystals induced by fast neutrons (> 1 MeV, ~60∘C, ~2.6e18 n/cm2). The damage was analyzed via induced optical absorption (IOA) at 1.4-9 eV and using X-band EPR spectrometer ELEXSYS E500. The annealing of IOA or the EPR signal of paramagnetic centers (total concentration 1.7e17 cm-3) was registered in a stepwise regime: the sample was heated in extra dry air to a certain Ti, kept there for 10 min and cooled down to 295 K, at which all spectra were measured. In addition, photoexcitation (5-10 eV) of different emissions was studied in virgin crystals and ceramics samples at 6 and 295 K. Inversion degree of lattice was estimated by XRD method.

The analysis of the EPR signal angular dependencies at different microwave power after each preheating to Ti allowed to reveal two novel radiation defects. These V1 and V2 centers with positive shift of the g-factor are ascribed to the holes localized at regular O2- nearby negatively charged defects (e.g., Al or Mg vacancies). The EPR signal of V1 contains up to 16 lines due to the superfine interaction with Al nuclei and is detectable at 200 mW, while the V2-spectrum has 2-3 broad lines saturating already at 10 mW. Notice that the EPR signals of two other V-type hole centers, known from the literature, were detected after the annealing of our neutron-irradiated crystal to 900 K and additional X-irradiation at 295 K. The annealing of V1 and V2 occurs at 360-520 and 450-770 K, respectively, via the delocalization of holes and their recombination with F-type centers. The changes of IOA within these temperature intervals were analyzed for the n-irradiated crystal and compared to those in MgAl2O4 optical ceramics irradiated with 0.23-GeV Xe ions or 100-keV protons. Irradiation strongly attenuates cathodo- and photoluminescence of spinel samples. The origin and microstructure of some radiation defects and luminescence centers in Mg-Al spinel is considered.

*Speaker

In situ Raman spectroscopy in hot cell of nuclear materials / comparison with ion beam irradiations

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Raman spectroscopy is a powerful technique for analyzing nuclear materials (fuels, claddings and containment matrices). For this purpose, the confocal Raman spectrometer of the Atalante facility (CEA/Marcoule), coupled to an optical microscope in a hot cell, is used to study the aging of these materials under service conditions (reactor, interim storage, waste disposal), subjected to complex scenarios of irradiation, temperature and interaction with the surrounding environment.
Analyses of UOx and MOx fuels have shown that the position of the T2g Raman-active band for the fluorite structure depends on the Pu content and oxidation state of the matrix [1]. These analyzes also show bands of defects as observed during ion beam irradiation [2]. Moreover, when subjected to water contact some studies have shown the appearance of secondary phases depending on the local redox conditions. Fuel claddings (Zircaloy-4) are surrounded by two oxide layers, at the water/cladding and the fuel/cladding interfaces. Raman analyzes highlight the presence of zirconia of different crystalline phases (monoclinic and tetragonal) and the presence of bands of defects also observed after ion beam irradiation and probably generated by ballistic collisions [3, 4]. Finally, the evolution by Raman spectroscopy of a borosilicate glass (ISG) doped with 244Cm has been compared to those irradiated with ion beam in nuclear or electronic regimes. The similar evolutions observed, reveal a depolymerisation of the borosilicate network and a decrease of the boron coordination number [5].

These analyzes show the interest to observe active materials having experienced the actual usage conditions, but also to continue studies on models materials irradiated by ion beams, to separate different parameters (electronic and nuclear energy losses, crystal orientations, temperature and influence of the surrounding environment).

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REI-19
VERSAILLES 2017

The 19th International Conference on Radiation Effects in Insulators, July 2-7, 2017, Versailles, France

Monday, July 3, 2017				Tuesday, July 4, 2017				Wednesday, July 5, 2017				Thursday, July 6, 2017				Friday, July 7, 2017			
	09:00	**Opening of Conference**		**Session V**	09:00	O'connell J.	**I-5**	**Session VIII**	09:00	Wucher A.	**I-8**	**Session X**	09:00	Yamaki T.	**I-9**	**Session XIII**	09:00	Popov A. I.	**I-12**
Session I	09:30	Jagielski J.	**I-1**		09:30	Lang M.	**O-13**		09:30	Liu S.	**O-24**		09:30	Kluth P.	**O-32**		09:30	Peuget S.	**O-43**
	10:00	Klaumünzer S.	**O-1**		09:50	Weber W.	**O-14**		09:50	Kalita P.	**O-25**		09:50	Papaleo R.	**O-33**		09:50	Skuja L.	**O-44**
	10:20	Uberuaga B.	**O-2**		10:10	Sall M.	**O-15**		10:10	Janse Van Vuuren A.	**O-26**		10:10	Tian J.	**O-34**		10:10	Kolodney E.	**O-45**
	10:40	**Coffee break**			10:30	**Coffee break with cakes**			10:30	**Coffee break**			10:30	**Coffee break**			10:30	**Coffee break**	
Session II	11:00	Tracy C.	**I-2**	**Poster session A**	10:30-12:30	**Poster session A**		**Session IX**	10:50	Simon P.	**O-27**	**Session XI**	10:50	Chen F.	**I-10**	**Session XIV**	10:50	Miro S.	**I-13**
	11:30	Bilgen S.	**O-3**						11:10	Haddad Y.	**O-28**		11:20	Forneris J.	**O-35**		11:20	Kucheyev S.	**O-46**
	11:50	Lian J.	**O-4**						11:30	Sarrasin L.	**O-29**		11:40	Fukuda K.	**O-36**		11:40	Baranov P.	**O-47**
	12:10	Yoshioka S.	**O-5**						11:50	Kotomin E.	**O-30**		12:00	Prada A.	**O-37**		12:00	Lushchik A.	**O-48**
									12:10	**Lunch**							12:20	Swainson I. (IAEA)	
	12:30	**Lunch**			12:30	**Lunch**							12:20	**Lunch**			12:30 - 13:00	**Closing of conference**	
																	13:00	**Lunch**	
Session III	13:30	Bolse W.	**I-3**	**Session VI**	13:30	Tripathi A.	**I-6**		13:15	**Departure for excursion**		**Session XII**	13:30	Murphy S.	**I-11**	**https://rei2017.sciencesconf.org**			
	14:00	Vazquez Muiños H.	**O-6**		14:00	Bröckers L.	**O-16**						14:00	Van Brutzel L.	**O-38**				
	14:20	Olivares J.	**O-7**		14:20	Skuratov V.	**O-17**						14:20	Fossati P.	**O-39**				
	14:40	Sellami N.	**O-8**		14:40	Hadley A.	**O-18**						14:40	Díaz Núñez P.	**O-40**				
	15:00	**Coffee break**			15:00	Volkov A.	**O-19**						15:00	Alessi A.	**O-41**				
Session IV	15:30	Toimil Molares M.E.	**I-4**		15:20	**Coffee break**							15:20	Mahfoudhi M.	**O-42**				
	15:50	Mota-Santiago P.	**O-9**	**Session VII**	15:50	Lorenz K.	**I-7**						15:40	**Coffee break with cakes**					
	16:20	Dhal S.	**O-10**		16:20	Sequeira M.	**O-20**		**14:00-18:15**	**Conference excursion**		**Poster session B**	15:40-17:40	**Poster session B**					
	16:40	Cesca T.	**O-11**		16:40	Djurabekova F.	**O-21**												
	17:00	Zhou S.	**O-12**		17:00	Wendler E.	**O-22**												
					17:20	Jozwik I.	**O-23**						**19:00 - 23:00**	**Conference dinner**					