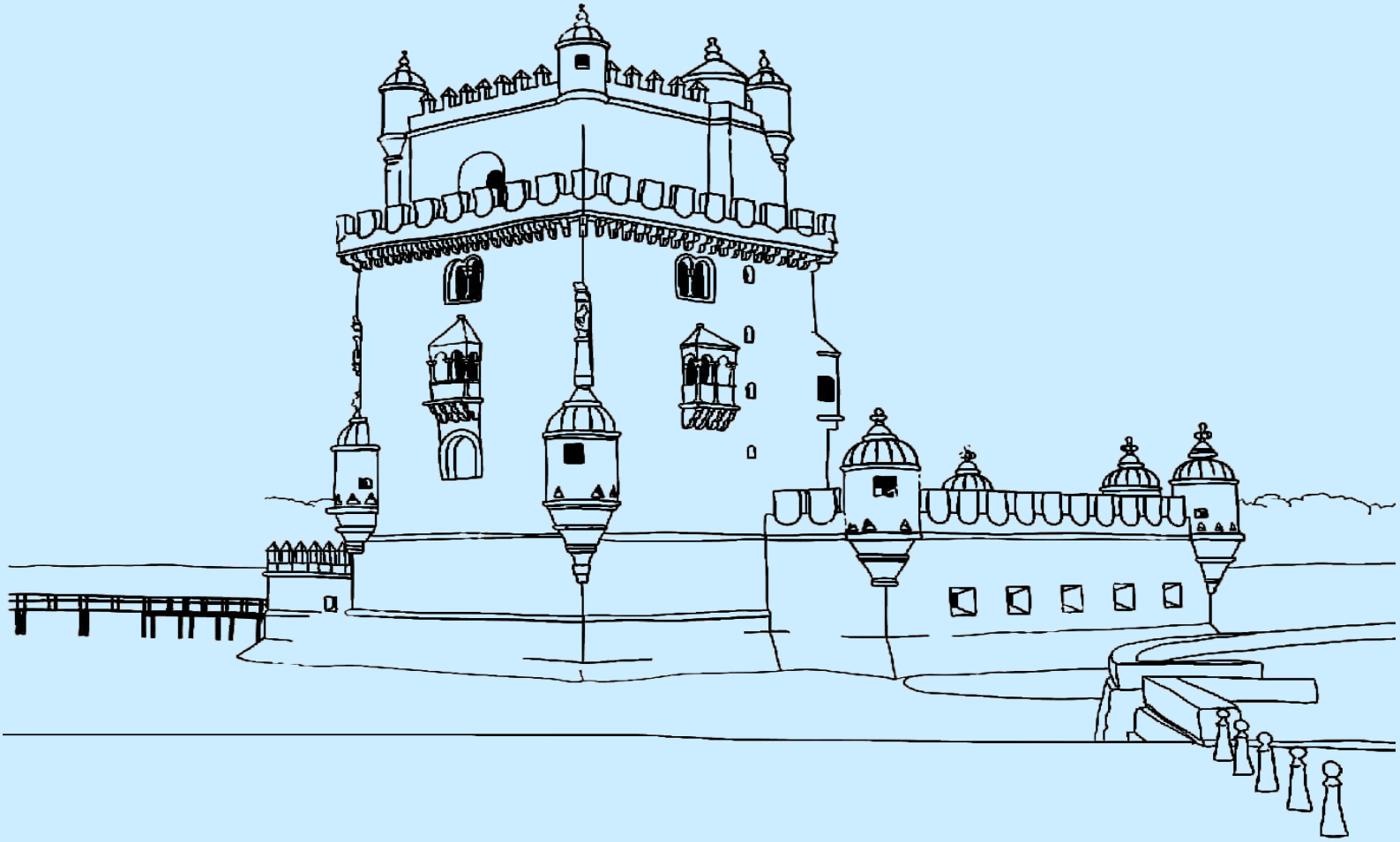
IBMM 22



BOOK OF ABSTRACTS

22th INTERNATIONAL CONFERENCE ON ION BEAM MODIFICATION OF MATERIALS

LISBON, 10-15 JULY 2022

Desktop Publishing/Design: Teresa Pires,

Editors: Katharina Lorenz, Eduardo Alves

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Date: 2022-07-05, Lisbon

PREFACE

On behalf of the Organizing Committee it is our great pleasure to welcome you to the 22nd International Conference on Ion Beam Modification of Materials (IBMM-2022). The Conference takes place at the beautiful city of Lisbon, an ancient settlement occupied by different cultures since the dawn of the first civilizations (VIII B.C.).

IBMM-2022 will last 6 days from July 10th to July 15th, 2022, and counts on 165 research participants from 6 continents. The conference gathers scientists in a friendly and relaxed atmosphere to exchange ideas and share new knowledge and future trends of ion beam technologies. It is always a rewarding feeling when, after all these years, we realize that ion beams are still playing an important role in the design of the new science and technology road map for the future. Major breakthroughs can be expected from the introduction of deterministic ion implantation on quantum technologies as well as testing and development of new materials to operate under extreme conditions.

Our speakers present and discuss the frontiers of ion beam research and highlight their major research achievements on ion beam modification of materials. The conference includes one plenary session, 12 Invited lectures and 46 specialized contributions on various topics related to *Basic Mechanisms and Irradiation Effects; Defect Engineering, Nano-science and Technology; Ion Beam Processing of Materials; Ion-Driven Self-organization and New Accelerator Systems and Single Ion Implantation*.

We wish to thank all those who helped us to organize IBMM-2022, and our sponsors for their contribution to the success of this conference.

Thank you for joining us for the 22nd International Conference on Ion Beam Modification of Materials which promises to be a memorable and outstanding meeting. You are the reason of our efforts and responsible for the coming back and success of our conference after the past and still continuing difficult times.

We are delighted that you made it to IBMM-2022. Thank you for your contribution to this enjoyable experience in Lisbon.

Katharina Lorenz, Eduardo Alves

Conference Chairs

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GENERAL INFORMATION

Venue

ESTeSL - Escola Superior de Tecnologias da Saúde de Lisboa
Av. D. João II, Lote 4.69.01
1990 - 096 Lisbon
GPS 38.776076º N / 9.097441º W

The conference will be held at ESTeSL (Escola Superior de Tecnologias da Saúde) Auditorium. The conference room is located at the School Campus at the Expo area of Lisbon by the majestic Tagus riverside. The Auditorium has excellent accessibility, either by underground, bus or train, several hotels and student university rooms are within 5-10 min. walking distance. The conference site will provide adjacent rooms to the lecture room, for posters, exhibitions, coffee-breaks, lunch and standard internet facilities (see google maps for address).

Address & Contacts

Campus Tecnológico e Nuclear
Instituto Superior Técnico, Universidade de Lisboa
Laboratório de Aceleradores e Tecnologias de Radiação
Estrada Nacional 10, 2695-066 Bobadela, Portugal
Tel: +351-21-994 6086 / 6088
Email: smmib2017@ctn.tecnico.ulisboa.pt
URL: www.ctn.tecnico.ulisboa.pt/SMMIB-2017

Emergency Number: 112

Dialling Code

International dialing code for all countries is 00. Dial 00 followed by the country code and phone number.

Registration / Information

The Registration Desk is situated at the Conference Hall for the whole duration of the Conference.

Opening hours

Sunday 10th: 17:00 - 20:00

Monday to Friday: During conference hours.

Attendance Certificate

The certificate of attendance will be provided upon demand.

Accomodation Organizer

Special prices will be available at a selection of hotels recommended by our partner: GeoStar. If you have any special request please contact directly Mrs.Manuela Samora: manuela.samora@geostar.pt. See on conference website the list of hotels.

INSTRUCTIONS TO PRESENTERS

Speakers

Technical support will be available every day throughout the conference.
Please bring your presentation on a memory stick and load it on the computer at de auditorium.

Instructions for Poster Presentes and Moderators

The Organization will provide boards and materials to fix your poster.
Presenters are requested to stand by their poster during the poster sessions and are invited to present their work and discuss it with the audience.

Poster sessions provide the opportunity for convivial scientific discussions and exchange. For further details, please refer to the list of Poster Sessions in the Scientific Programme.

WELCOME RECEPTION & REGISTRATION

Date: 10th july 2022 (17:00 – 20:00pm)
On Sunday afternoon come to ESTeSL (Escola Superior de Tecnologias de Saúde de Lisboa), to pick up your badge and conference material.

A full assortment of appetizers and drinks will be served. The reception is a great opportunity to meet old friends and make new ones.

POSTER SESSIONS

Dates: 12th july 2022 and 14th july 2022
A full assortment of appetizers and drinks will be served.

EXCURSION & DINNER

Date: 13rd july 2022

The West Coast
When the Sea invites the Land, magic happens.

Formerly known as Estremadura the Atlantic West is a fertile region. Thousands of hills with scattered whitewashed villages and the characteristic windmills that symbolize the West, dominate its landscapes full of color, varying with the seasons of the year.

It is bathed in intense sunlight and blessed with a gentle climate due to the Atlantic influence, creating a unique harmony between the coast and the countryside.

The passing of time left in the region of the West Coast is a remarkable track of Medieval Castles, Renaissance Palaces, Manor Houses, Churches and Convents that allow any visitor an encounter with the representations of bygone times.

Cabo da Roca is a wild and rugged headland that marks the westernmost point of mainland Europe. The windswept cliffs of Cabo da Roca were believed to be the edge of the world up until the late 14th century and the spectacular desolate scenery adds to the allure of the location.

The raging Atlantic Ocean waves pound the base of the massive jagged cliffs while challenging hiking trails follow the coastal paths.

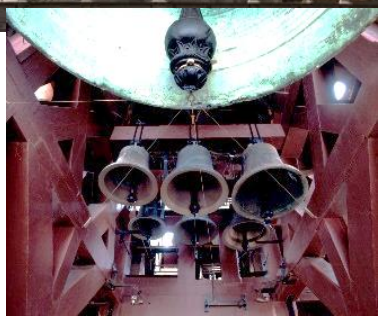
Convento de Mafra, built in the 18th century by order of King João V (1689-1750) in fulfilment of a vow he made, to be blessed with an heir from his marriage to Maria Ana of Austria, or be cured of a serious illness, the Royal Convent and Palace of Mafra is the most important baroque monument in Portugal.

All in limestone and marble from this region (Pêro Pinheiro and Sintra), the building covers an area of almost four hectares (37.790m2), including 1.200 rooms, more than 4.700 doors and windows, 156 stairways and 29 inner yards and courtyards.

The monument also contains one of the most important European libraries, with a precious collection of 36.000 volumes, a synthesis of 18th century encyclopedic knowledge.

Curiosities: The Royal Convent of Mafra has a set of two carillons, or rather a series of bells tuned to each other. There are actually ninety eight bells in all, which makes them the world's largest historic carillions. The story goes that the Marquis of Abrantes, upon the King's request, was informed that one carillon would cost him 400.000$00 *réis* – an astronomic price for a country as small as Portugal. Offended with such remark, King João V is said to have answered: "Well if it is that cheap, I'll have two".

The bells of the North tower carillon were wrought in Liège by Nicolau Levache, while those of the South tower were made in Antwerp by Willem Witlockx. Each bell tower had fifty eight bells, forty nine in each belonging to the carillon. Besides the carillon, there are eleven liturgical bells of Portuguese and Italian foundry, dating from 1730 to the late 19th century, an unique illustration of the liturgical use of bells.



Aldeia Típica de José Franco. Small town of Sobreiro, between Ericeira and Mafra, where one of the most recognized museum villages in the country is located. The history of the small village dates back to the birth of the potter José Franco, in 1920.

His father was a shoemaker and his mother, a pottery seller, selling clay from door to door, as well as through many fairs and markets in Extremadura. Since Sobreiro was an important pottery centre, José Franco was involved with the craft from an early age and, as a child, when he left primary school, he learned the craft with two local master potters, before working on his own, at the age of 17. At that time, he rehabilitated the pottery that had belonged to his grandfather, which had been inactive for a long time.

In the early 60s, José Franco gave wings to a dream of recreating an ethnographic village, where his childhood memories crystallized, a testament to the way of life of the local people, in homage to their land. His village would have two components: it would be a replica of the old workshops and shops, of the spaces lived, decorated and equipped with real objects, where the customs and work activities intrinsic to his childhood and to the peasant life of the Mafra region were reproduced. Today, the small world shaped by the hands of José Franco (who died in 2009) is visited annually by thousands of people. Enjoy yourself!

All this, together with an amazing gastronomy and a diversity of traditions and customs that were not lost despite its proximity to Lisbon, Mafra is a unique destination not to be missed!

In fairs, regular markets and shops, we can find products from this region such as handicraft, sweet pastries, great cheeses and fruits (lemons, strawberries and *rocha* pear).

Mafra is also known for its tasty bread (*Pão de Mafra*), along with delicacies from the Atlantic Ocean like our sardines.

Mafra has no shortage of wineries with solid signs of wine tourism and don't miss the secrets and flavours of the typical Portuguese convent pastry known as "*Fradinho*", traditional pie filled with sweetened white beans, almonds and egg cream.

DINNER (Casa Eermelinda de Freitas).

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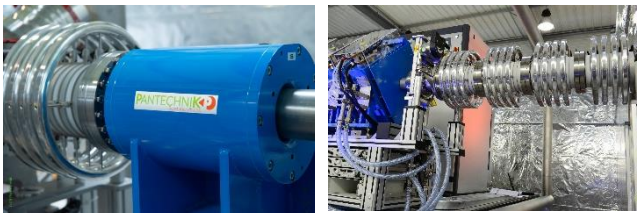
PANTECHNIK has been dedicated to proudly serve particle accelerators community for almost 30 years. Our customers are located all over the world, from big research facilities to regional physics lab, including industrial companies dedicated to health, analysis, safety… For this reason and many others, Pantechnik team is open-minded, passionate, committed, and convivial.

Our rules are simple:

- Find solutions together.
- With professional behaviour.
- No compromise on Quality (ISO 9001).



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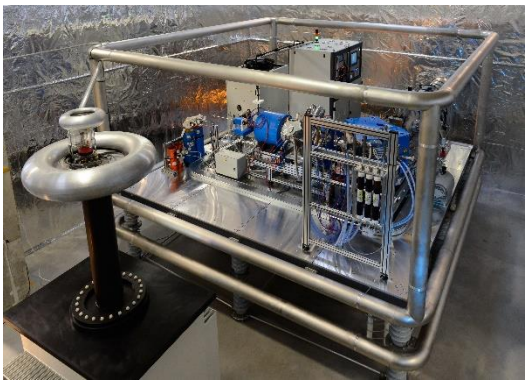
PANTECHNIK has decided to create an irradiation facility at its premises and rent the beam time to all users interested.

The beam facility LUTEX consists of our M1000 ion source, a system of ion acceleration up to 300 keV/u and an irradiation chamber with a substantial irradiation surface of 400 x 700 mm.

The distinguishing features of the facility are:

- Protons and any other ion.
- Energy up to 300keV.
- Available facility, open to all users.
- Large irradiation surface up to 400 x 700 mm.
- Fine-tunability of ion flux, energy, heat.
- Adjustable parameters within the same batch.
- Custom made test plan.
- High accuracy calibration
- On-line monitoring and recording of beam parameters.



The LUTEX irradiation facility is located in France, in the beautiful historical city Bayeux, 20 minutes from Caen and 2 hours 30 minutes' drive from Paris.

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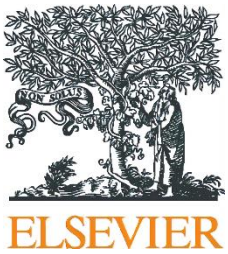
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SCIENTIFC PROGRAMME

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	Sunday, July 10
17:00 – 20:00	Registration + Welcome reception
	Monday, July 11
08:00 – 17:00	Registration
08:30 – 09:00	OPENING SESSION
09:00 – 09:40	**Plenary Lecture: David Jamieson** **Ion Beam Modification of Materials: from Earth to Space**
	SESSION: Basic Mechanisms and Irradiation Effects
	Chairs: William Weber & Michael Nastasi
09:40 – 10:10	**Invited Lecture: Steven Zinkle** **Fundamental Radiation Effects in Materials due to Ion Bombardment**
10:10 – 10:30	***Oral 01 – Stephen Donnelly*** Ion-irradiation-induced Grain Boundary Formation in Self-ion Irradiated Nickel
10:30 – 10:50	***Oral 02 – Mariana Timm*** Influence of dpa Rate on Carbide Precipitation and Ar Bubble Growth in AISI 316L Alloys Irradiated with Au and Ag Ions
10:50 – 11:10	***Oral 03 – Kai Nordlund*** Strong Crystal Grain Orientation Effects on Ion Sputtering
11:10 – 11:40	*Coffee-break*
11:40 – 12:00	***Oral 04 – Lin Shao*** A Quantitative Method to Determine the Region not Influenced by Injected Interstitial and Surface Effects in Ion-irradiated Metals
12:00 – 12:20	***Oral 05 – Parikshit Phadke*** Low Energy Ion Interactions with Transition Metal Films-ballistic and Diffusive Transport Processes
12:20 – 12:40	***Oral 06 – Claudia Montanari*** Stopping Power in Very Heavy Targets: from Lanthanides to Post-transition Metals
12:40 – 14:00	*Lunch*
	Chair: Robert Elliman
14:00 – 14:30	**Invited Lecture: Matheus Tunes (IBMM prize)** **The Solar System as a New Frontier for Materials at Extremes**
14:30 – 14:50	***Oral 07 – Weilin Jiang*** Microstructural Evolution and Deuterium Diffusion in γ-$LiAlO_2$ Irradiated with He^+ and D^+ Ions
14:50 – 15:10	***Oral 08 – Gihan Velisa*** Revealing the Onset of Unprecedented Transition from Synergistic to Competitive Effect in Defective $KTaO_3$
15:10 – 15:30	***Oral 09 – William Weber*** Inelastic Interactions of Ions with Disordered Oxide Perovskites
15:30 – 15:50	***Oral 10 – Marta Dias*** Synthesis and Irradiation Response of High Entropy Alloys with Transition and Refractory Metals for Operation at Extremes
15:50 – 16:20	*Coffee-break*
	Chair: Kai Nordlund
16:20 – 16:50	**Invited Lecture: Yanwen Zhang** **Ion Beams: Unique Tools to Study Radiation Effects in Complex Alloys**
16:50 – 17:10	***Oral 11 – Cyprian Mieszczynski*** Combining MD-LAMMPS and MC-McChasy 2.0 Codes for Dislocation Simulations of Ni-based Alloys
17:10 – 17:30	***Oral 12 – Mohamed El-Bakouri El-Haddaji*** Basic Study of the Relaxation Volume of Crystalline Defects in bcc Iron
17:30 – 17:50	***Oral 13 – Daniel Primetzhofer*** Electronic Excitations of keV Ions in Single-crystalline Self-supporting Targets
17:50 – 18:10	***Oral 14 – Joseph Graham*** Dynamics of Self-trapped Exciton Formation, Hopping, and Recombination within an Ion Track in Silica

	Tuesday, July 12
	SESSION: Ion Beam Processing of Materials
	Chair: Stephen Donnely
09:00 – 09:30	**Invited Lecture: Aurélie Gentils** **Ion Beam Synthesis of Nano-Oxides: Towards an Understanding of Precipitation in Oxide Dispersion Strengthened Steels**
09:30 – 09:50	***Oral 15 – Sérgio Magalhães*** Modelling the Strain Build-up in Nitrogen Implanted Tungsten Films on Silicon Substrates
09:50 – 10:10	***Oral 16 – Shengqiang Zhou*** Tailoring Oxide Thin Films by Ion Beams
10:10 – 10:30	***Oral 17 – Ovidio Peña Rodríguez*** Elongation Kinetics of Plasmonic Nanoparticles Studied *in situ* by Po-Larized Optical Absorption Spectroscopy9
10:30 – 11:00	*Coffee-break*
	Chair: Aurélie Gentils
11:00 – 11:30	**Invited Lecture: Marek Rubel** **Ion-induced Modification and Ion Beam Analysis of Diagnostic Components for Fusion Reactors**
11:30 – 11:50	***Oral 18 – Yongqiang Wang*** In-situ Positron Annihilation Spectroscopy for Materials Characterization Under Coupled Irradiation Extremes
11:50 – 12:10	***Oral 19 – Eduardo Pitthan*** Electronic Stopping Power of Pristine and Ion Irradiated Plasma Facing Materials for Light Ions
12:10 – 12:30	***Oral 20 – Zhongwen Yao*** Energetic Helium Ion Implantation to Emulate the In-reactor Neutron Damages in Ni Superalloy
12:30 – 14:00	*Lunch*
	Chair: David Jamieson
14:00 – 14:30	**Invited Lecture: Michal Bockowski** **Innovative Approach for Changing Electrical and Optical Properties of GaN**
14:30 – 14:50	***Oral 21 – Anna Mackova*** ZnO Nanorods with Au/Ag Nanoparticles Prepared by Ion Beam Implantation – Structural Modification and Optical Properties
14:50 – 15:10	***Oral 22 – José Cardoso*** Demonstration of Red Light-Emitting Devices Based on Europium-Implanted AlN p-n Junction Nanowires
15:10 – 15:30	***Oral 23 – Aurélien Debelle*** Effect of Energy Deposition on the Disordering Kinetics in Dual-beam Irradiated Single-crystalline Si, SiC and GaAs
15:30 – 16:00	SPONSORS: High Voltage Engineering (HVE) & Pantechnik
16:00 – 19:30	**POSTER SESSION + REFRESHMENTS**
19:30 – 23:00	**INTERNATIONAL COMMITTEE MEETING**

	Wednesday, July 13
	SESSION: Ion-driven Self-organization, Nanostructure Synthesis and Nanopatterning
	Chair: Jürgen Fassbender
08:30 – 09:00	**Invited Lecture: Stefan Facsko** **Emergence of Self-organized Surface Patterns under Ion Induced Non-equilibrium Conditions**
09:00 – 09:20	***Oral 24 – Jean Paul Allain*** Correlating Surface Nano Patterning and Compositional Changes Under Low-Energy Ion Beam Irradiation of Disordered Alloys
09:20 – 09:40	***Oral 25 – Andrés Redondo-Cubero*** Highly Ordered Silicide Ripple Patterns Induced by Medium-energy Ion Irradiation
09:40 – 10:00	***Oral 26 – Denise Erb*** In-situ Observation of Ion-induced Nanoscale Patterning on a Crystalline Ge(001) Surface
10:00 – 10:30	*Coffee-break*
	Chair: Andrés Redondo-Cubero
10:30 – 11:00	**Invited Lecture: Mukesh Ranjan** **Low Energy Ion Produced Nanostructuring for Surface Wettability and Sensing Applications in Healthcare**
11:00 – 11:20	***Oral 27 – Matteo Gardella*** Tailoring of Two-dimensional Semiconductors Optoelectronic Properties Via Ion Induced Nanopatterning
11:20 – 11:40	***Oral 28 – Karl Ludwig*** X-ray Photon Correlation Spectroscopy Study of Ion Beam Nanopatterning
11:40 – 12:00	***Oral 29 – Sukriti Hans*** Role of Ion Beam Parameters in the Evolution of Self-organized Nanoripple Superimposed by Triangular Features
12:00 – 12:20	***Oral 30 – Shiva Choupanian*** Low-energy Ion Channeling in Nanocubes
12:20 – 13:00	*Lunch*
13:00 – 23:00	**SOCIAL PROGRAMME + BANQUET**

	Thursday, July 14
	SESSION: Defect Engineering, Nano-science and Technology
	Chair: Christina Trautmann
09:00 – 09:30	**Invited Lecture: Flyura Djurabekova** **On Shaping Embedded Metal Nanoparticles by Swift Heavy Ion Irradiation**
09:30 – 09:50	***Oral 31 – Sjoerd Roorda*** Density Changes in Amorphous Silicon Provoked by Swift Heavy Ions
09:50 – 10:10	***Oral 32 – Miguel Sequeira*** Swift Heavy Ions Interaction with Group-III Nitride Layered Structures
10:10 – 10:30	***Oral 33 – Günther Dollinger*** Dosimetry of Heavy Ion Exposure to Human Cells Using Nanoscopic Imaging of Double Strand Break Repair Protein Clusters
10:30 – 11:00	*Coffee break*
	Chair: Sjoerd Roorda
11:00 – 11:30	**Invited Lecture: Christina Trautmann** **Material Science and Nanotechnology with GeV Ion Beams**
11:30 – 11:50	***Oral 34 – Caroline Bonafos*** Controlled Synthesis and Plasmonic Properties of Doped Si Nanocrystals Embedded in SiO_2
11:50 – 12:10	***Oral 35 – Przemyslaw Jozwik*** McChasy 1.0: Modeling of dislocations using Molecular Dynamics for Monte Carlo simulations of ion channeling
12:10 – 12:30	***Oral 36 – André Vantomme*** Towards an Ion-implanted Nuclear Clock
12:30 – 14:00	*Lunch*
	Chair: André Vantomme
14:00 – 14:30	**Invited Lecture: Aliz Simon** **Ion-beam Driven Materials Science and Quantum Technology Coordinated by the IAEA Physics Section**
14:30 – 14:50	***Oral 37 – Marco Peres*** Production of Microtubes and Nanomembranes of Ga_2O_3 by Ion Implantation
14:50 – 15:10	***Oral 38 – Martin Hafermann*** Fast Recovery of Ion-irradiation-induced Defects in $Ge_2Sb_2Te_5$ Thin Films at Room Temperature
15:10 – 15:30	***Oral 39 – Pedro Lopez*** Atomistic Modeling of the Acceptor Removal in p-type Si Induced by Neutron Irradiation
15:30 – 15:50	***Oral 40 – Susana Freitas*** MgO Thin Film Texture Control Using Low Energy Ion Beam Assisted Deposition
15:50 – 16:10	***Oral 41 – Lucas Colonel*** Pressurized Crack Gas Exchange in Ion Implanted Silicon
16:10 – 19:00	**POSTER SESSION + REFRESHMENTS**

	Friday, July 15
	SESSION: New Accelerator Systems and Single Ion Implantation
	Chairs: Katharina Lorenz & Roger Webb
09:00 – 09:30	**Invited Lecture: Kristian Stockbridge** **Single Ion Implantation by the Detection of Secondary Electrons**
09:30 – 09:50	***Oral 42 – Ulrich Wahl*** Fabrication of Diamond Quantum Colour Centres in "split-vacancy" Configuration Using Ion Implantation
09:50 – 10:10	***Oral 43 – Milan Vićentijević*** Detection of Single Low-Penetrating Ions in Diamond
10:10 – 10:30	***Oral 44 – Ella Schneider*** Isotopically Enriched ^{28}Si Substrates for Quantum Computers Using Ion Implantation Layer Exchange: Experimental Results
10:30 – 11:00	*Coffee-break*
11:00 – 11:20	***Oral 45 – Jonathan England*** Experiments and Modelling to Understand the Production of Isotopically Pure Si and Ge Layers by Implanted Layer Exchange for Quantum Computing
11:20 – 11:40	***Oral 46 – Paulo Fichtner*** Elastic Electron Scattering Experiments: an Alternative to Light Ion Irradiation
11:40 – 11:50	**AWARDS CEREMONY**
11:50– 12:00	CLOSING REMARKS
12:00-13:00	*Lunch*

2022-07-05

PLENARY / INVITED RESENTATIONS

NUMBER OF PLENARY & INVITED PRESENTATIONS: 13

ABS: 215. Ion beam modification of materials: from earth to space (PLENARY)

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My university is presently constructing a deep underground laboratory to shield sensitive dark matter detectors from radiation produced by ions from space. This is because cosmic rays, chiefly high energy light ions, induce many modifications to the state of electronic devices that obscure the signals from rare dark matter events. From the era of the first VLSI devices, the products of the first quantum revolution, radiation induced upsets required error correction strategies for reliable operation.

Ion beams also helped manufacture those classical devices that today have billions of transistors working together and are at the foundation of the global village. Now a second quantum revolution is emerging where the strange laws of quantum mechanics are exploited in engineered devices with the promise of revolutionary capabilities for the storage, processing and transmission of information.

We have developed the ultimate ion beam modification of materials technique to implant single donor qubits into prototype devices that show very long coherence times needed for future large-scale devices. However, there is some indication that the coherence time of quantum bits in quantum computers operating on the surface of the Earth will be degraded by the same radiation-induced effects seen in classical devices.

Our devices may one day occupy an adjacent cavern to the dark matter detector. This presentation will trace the development of ion beam modification of materials for device fabrication and operation and what the future holds.

ABS: 210. Fundamental radiation effects in materials due to ion bombardment

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Since 1975, the Norgett-Robinson-Torrens (NRT) model for defect production has served as an international standard for quantifying displacements per atom (dpa). However, it is widely recognized that the NRT model has several shortcomings including overestimating the defect production for energetic displacement cascade conditions. A group of international researchers recently proposed two modifications to the NRT model to apply athermal in-cascade recombination corrections (ARC-DPA) and to define a new parameter to quantify the magnitude of the atomic mixing "replacements per atom" (RPA) associated with collisions. These parameters do not include subsequent thermal-activated recombination and mixing processes within the remnant defects from primary knock-on collisions. A thermally stimulated "correlated recombination correction" to defect production (CRC-DPA) is proposed to quantify the surviving defect fraction that is relevant for irradiations performed where irradiation defects are mobile (typically at temperatures >30-100K). Modeling and experimental analyses will be summarized that indicate the CRC-DPA is ~20% of the NRT dpa value for temperatures where interstitials are mobile, and drops to ~10% of the NRT dpa if vacancies are also mobile, over a wide range of materials and knock-on energies. A second presentation topic is the impact of near-surface and implanted ion regions on the microstructure associated with ion irradiation. Processes such as amorphization at low temperatures and cavity swelling at high temperatures can be strongly affected by implanted ions. Temperature-dependent defect free zones near free surfaces can be used to experimentally determine fundamental parameters such as vacancy migration energies. Localized peak cavity swelling regions are frequently observed adjacent to the defect-free near-surface regions and are attributed to preferential loss of interstitials due to one-dimensional (1D) glide of interstitial clusters produced in displacement events. In general, this requires self-ion energies >5 MeV to obtain midrange "safe analysis zones" that are not affected by implanted ion or near-surface artifacts. Evidence for 1D gliding interstitial clusters during irradiation of Cu alloys as low as 40 K will be summarized. This indicates that radiation effects models based solely on 3D random walk migration of point defects may be inappropriate for evaluating irradiated materials. The final presentation topic will examine the stability of nanoscale precipitates during ion bombardment. Several important corrections to the historic Nelson-Hudson-Mazey (NHM) model of precipitate stability are shown to provide good quantitative agreement with experimental observations; in general, both the ballistic dissolution and radiation enhanced diffusion terms are larger than originally proposed in the NHM model. Experimental results on solid solution and aged Fe-Cr and Fe-Cu alloys ion irradiated over a wide range of temperatures, doses, dose rates and primary knock-on atom energies will be summarized and compared with model predictions.

ABS: 213. The solar system as a new frontier for materials at extremes (IBMM2022 Prize Award)

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The year of 2022 begins with two major accomplishments that holds a new dawn of scientific discoveries: the commissioning of two new space devices, the Parker Solar Probe (PSP) and the James Webb Space Telescope. While the latter is intended to unveil the secrets of the earlier Universe, shedding light on our own cosmic origins, the former is addressed to the study of thermonuclear instabilities occurring onto the Sun's corona, where an intense stream of Solar Energetic Particles (SEP) flows through the entire solar system up to the Heliopause, subjecting all astronomical objects within to an intense field of energetic particle irradiation. The PSP mission also encompass a complete characterization of the Sun's SEP spectrum considering ion species and energies with its onboard instrumentation. In addition, the PSP mission is intended to better understand the behavior of SEP under abnormal events known as Solar Flares: thermonuclear explosions on the coronal regions of the Sun, whose constitute the most energetic phenomenon occurring within the solar system, with energy release around of $10^{20\text{-}25}$ J. In this context, a new era for space exploration is now a reality. Space exploration is also expected to grow over the next years as a potential business model (e.g., space tourism), thus emphasizing the need for new materials and alloys for satellites, spacecrafts, spaceprobes, and derivatives. Either in normal or abnormal conditions, the intense field of energetic particles flowing from the Sun poses an immediate challenge to materials science regarding the design of space materials capable of resisting the impacts of highly-energetic solar particles. The study on the effects of radiation in solids has its roots at beginning of last century starting with the revolution in Physics that occurred upon the confirmation of the atomic nature of matter made by A. Einstein and L. Boltzmann [1]. N. Bohr and J.J. Thomson were the first scientists to formalize the ideas on the effects of electrified particles colliding with solids [2,3], whose can generate displacements in its periodic atomic structure through deposition of nuclear and electronic energies, causing radiation damage and degradation of properties. Since then, the development of these theories resulted in a century of accumulated knowledge within the engineering of nuclear materials [4] that now can be harvested to support new endeavors for the design of new space materials with high resistance to particle irradiation.

This seminar will be divided in three parts. Firstly, a state-of-the-art summary on Heliophysics and the radiation environment posed by the Sun will be reviewed. The materials challenges in the design of spacecrafts, probes and satellites will be thereafter introduced with focus in the mechanisms of materials degradation that are present in the solar system, including radiation damage and shielding needs, high-speed micrometeoroid impacts, thermal cycling, corrosion from monoatomic species in low-orbit conditions and plasma-interaction effects. Then, our current approach to materials design and radiation damage effects evaluation will take place considering the emergence of novel lightweight and nanocrystalline Al-based crossover alloys [5,6]. In this context, the use of ion beam technology for studies on modification of materials under the emulated radiation conditions found in our solar system will be shown. The focus of

the seminar will be to differentiate mechanisms of radiation damage that these materials can be subjected when under ion irradiation, considering their thermodynamic stability, inherent microstructural morphology, and formation of extended radiation-induced defects. A pathway for new space materials with higher radiation resistance will be given towards the development of novel lightweight and stable nanocrystalline terminal solid-solution alloys.

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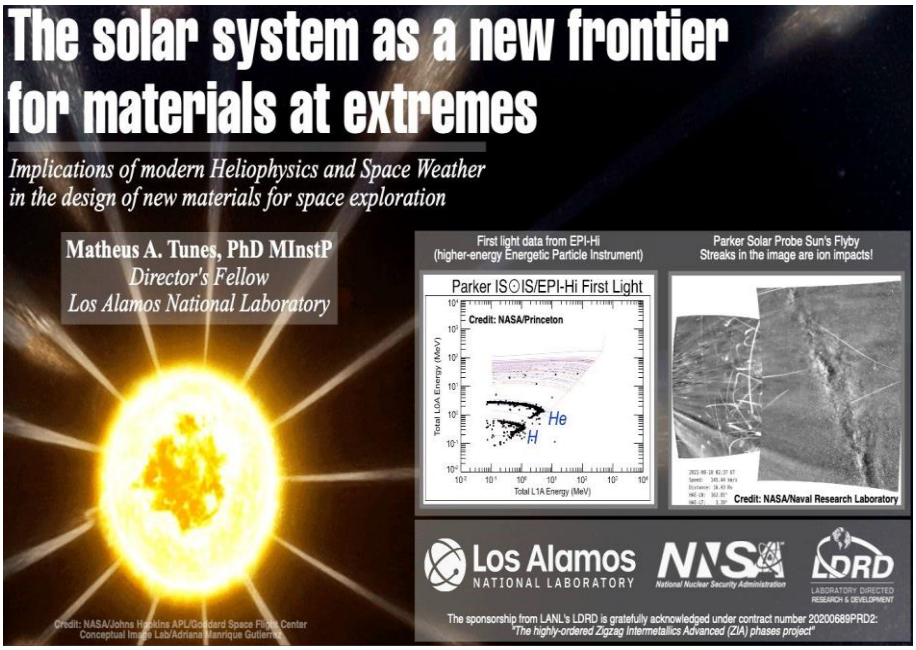

ABS: 217. Ion beams: unique tools to study radiation effects in complex alloys

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Concentrated solid solution alloys (CSAs), including high entropy alloys (HEAs), are formed near the centers of phase diagrams. CSAs are different from dilute alloys that appear near the corners of phase diagrams, in which minor concentrations of other elements are incorporated into pure metals. In CSAs, alloying elements interact with each other and result in distinctive properties [1-6]. At the level of electrons, disordered local chemical environments significantly enhance scattering processes and affect electrical and thermal conductivities. At the level of atoms, site-to-site lattice distortion and complex energy landscapes tailor defect migration and atomic transport.

Ion beams are used to create and measure displacement damages. Moreover, ion beams are also used as unique tools to understand coupled electronic and atomic effects, as the pronounced ionization effects alter atomic processes and modify defect dynamics [3,5,6]. Ionization effects in metals has been largely disregarded, as it is generally considered that the energy transferred to electrons is primarily dissipated by the highly conducting electronic subsystem, with minimal energy transferred to the lattice and little effect on the damage evolution. Defect formation and evolution in CSAs and some HEAs are investigated using energetic ions. Based on experiments and simulations, insights on the complex electronic and atomic correlations of energy deposition and dissipation on defect dynamics and structural stability are revealed. A pronounced ionization effect on strain relaxation and damage recovery, as well as grain growth, in complex alloys is attributed to both lower thermal conductivity and stronger electron-phonon coupling. This work highlights tunable chemical complexity in CSAs on controlling energy dissipation and defect dynamics, and provides a new design paradigm for enhanced radiation tolerance.

This work was supported as part of the Energy Dissipation to Defect Evolution (EDDE), an Energy Frontier Research Center funded by the US DOE/BES.

References:

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ABS: 76. Ion beam synthesis of nano-oxides: towards an understanding of precipitation in oxide dispersion strengthened steels

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Ferritic-martensitic steels reinforced by oxide dispersion, known as ODS steels, are being developed for high temperature applications and extreme conditions. The fine distribution of metallic oxide nanoparticles, generally composed of titanium and yttrium, considerably improves their resistance to creep and irradiation. Their conventional fabrication involves mechanical grinding of powders followed by consolidation at high temperatures. The optimization of their mechanical properties, in particular under irradiation, is dependent on the fine control of the nano-oxides characteristics, and therefore of the mechanisms involved during their nucleation and growth, not yet identified. In our study, ion beam synthesis was used to create metallic nano-oxides in a high purity Fe-10wt%Cr alloy in order to control different relevant parameters and decorrelate their influence on the precipitation. The nano-precipitates obtained for different sequences of ion implantations and subsequent thermal annealing temperatures, were characterized mainly by Transmission Electron Microscopy. The results show that the oxide that precipitates is not necessarily favored thermodynamically, but results from complex kinetic processes related to the interaction between implanted elements and defects created in the matrix [1]. For some ion implantation sequences, nano-oxides similar to those of conventional ODS steels are obtained, with typical characteristics such as a Cr-rich shell, or facets according to specific crystalline planes. Detailed crystallographic and elemental studies of the precipitates have provided key elements in understanding the early stages of precipitation.

References:

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ABS: 37. Ion-induced modification and ion beam analysis of diagnostic components for fusion reactors

Marek Rubel [1], Per Petersson [1], Sunwoo Moon [1], Laura Dittrich [1], Anna Widdowson [2], Norberto Catarino [3], Eduardo Alves [3]

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In fusion-related material research the role of ions is at least threefold: (i) modification of plasma-facing components by particle fluxes; (ii) ion beam analysis; (iii) simulation of neutron-induced damage.

This contribution is on metallic so-called first mirrors, i.e. essential components for optical plasma diagnostic in reactor-class controlled fusion devices. Two parallel programmes are carried out with Mo test mirrors: (a) exposure to plasma during campaigns in the Joint European Torus (JET); (b) irradiations of poly- and mono-crystals with 30 keV Mo, Zr, Nb and 2 keV H and He ions, to simulate the n-induced damage, transmutation effects and impact of charge exchange neutrals on the modification of optically active layer: 20 nm in Mo. The work is related to tests for ITER and DEMO. Surface characterisation is done by spectrophotometry, microscopy and IBA with ^{3}He-based NRA and ToF-HIERDA with a 36 MeV $^{127}I^{8+}$ beam. Special precautions are in handling JET samples containing Be and T. The test at JET for ITER was done for mirrors placed in pan-pipe cassettes in the main chamber and in the divertor. In the main chamber only mirrors located at the entrance to the cassette lost reflectivity (Be deposition from eroded limiters), while those in the channels were only lightly affected. All divertor mirrors were strongly degraded by deposition of Be, W and other species. Mirrors pre-damaged (2 & 20 dpa) by 1.4 MeV Mo+ were placed in JET to determine the impact of radiation of tritium retention in high-Z metals.

Work towards DEMO The stepwise irradiation up to 30 dpa by heavy ions caused only small changes in the optical performance. Stronger effects have been produced by He because of bubble formation which led to the reflectivity loss by over 20%. He retention studies revealed that only 7-9% of the implanted He was retained mainly in two types of bubbles. He residence time in Mo is long, as proven by analyses 1 day and 1 y after the irradiation.

ABS: 178. Innovative approach for changing electrical and optical properties of GaN

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It is well known that nitride semiconductors based on gallium nitride (GaN) and its cousins, indium nitride (InN) and aluminum nitide (AlN), are applied for building light emitting diodes, laser diodes as well as high-power and high-frequency transistors. These devices are used in many fields from general lighting, medicine through ecology up to defense. Although nitride-based devices show tremendous technological premise, their reliability and commercial success can still be improved by higher structural quality of crystallized material as well as more homogenious and precise dopining by donors and acceptors. One of the best methods for introducing dopants into semiconductors is ion implantation. The introduced structural damage can be removed by a proper annealing process. The high-temperature treatment enables also electrical and/or optical activation of the implanted dopants. In the case of GaN, annealing at high temperature (~1300°C - 1400°C) seems difficult. This coumpund loses its thermodynamic stability slightly above 800°C at atmospheric pressure. At higher temperature the crystal will decompose. One of the solutions is to anneal GaN at high nitrogen (N_2) pressure. Such technology is called ultra-high-pressure annealing (UHPA).

In this paper, application of UHPA for GaN crystals and layers implanted by different ions (acceptors and donors) will be presented. The latest results of the implantation with magnesium (Mg), beryllium (Be), zinc (Zn), and calcium (Ca) ions into GaN in order to obtain p-type conductivity will be discussed. Silicon (Si) implantation into GaN for n-type doping will also be analyzed. Structural, electrical and optical properties of implanted GaN after UHPA will be discussed in terms of application for GaN-based devices.

ABS: 211. Emergence of self-organized surface patterns under ion induced non-equilibrium conditions

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A plethora of nanoscale patterns emerges on surfaces which are irradiated by ion beams [1]. Depending on the irradiation conditions, hexagonally ordered dot or pit, checkerboard, or periodic ripple patterns are formed spontaneously due to the non-equilibrium conditions induced by ion irradiation.

On amorphous or amorphized surfaces, the formation of periodic patterns at high ion fluences results from the interplay of different roughening mechanisms, e.g., curvature dependent sputtering, ballistic mass redistribution, or altered surface stoichiometry on binary materials, and smoothing mechanisms, e.g., surface diffusion or viscous flow. The symmetry of these patters is determined by the ion beam direction, i.e., hexagonal near order at close to normal incidence and two-fold symmetry at off-normal incidence above ~45°. However, more intriguing patterns can also appear.

Above the recrystallization temperature, diffusion is affected by the Ehrlich-Schwoebel barrier on the crystalline surface: vacancies and ad-atoms are trapped on terraces and can nucleate to form pits or mounds, respectively. Patterns formed in this “reverse epitaxy” regime exhibit crystalline facets and the symmetry of the patterns is determined by the crystal structure of the surface [2]. However, ballistic effects can also play a role and shape the resulting morphology [3].

The fundamental understanding of the pattern formation is already quite advanced. Simulations based on atomistic methods, such as molecular dynamics (MD) and kinetic Monte-Carlo (kMC), or by continuum equations can describe in most cases the observations. However, theory has still not achieved predictive power in order to achieve full control of the ion-induced patterning process, for instance for special applications, where high ordering or special patterns are requested.

References:

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ABS: 13. Low energy ion produced nanostructuring for surface wettability and sensing applications in healthcare

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Interaction of low energy ions often leads to self-organized regular nanostructure on the surfaces. However, their arrangements, surface roughness depends largely on material properties, ion energy, ion angle of interaction with the surface and ion dose. In the recent time these artificially produced nanostructures have potentially been utilised for tailoring surface wettability, magnetism and optical properties of the bulk material. In the current work, we shall show how low energy ion can remarkably change surface wettability of PTFE polymer surface. Just in 10s of second exposure time, it becomes superhydrophobic due to the formation of freely standing Nanostructures [1]. Using the fast CCD camera we have investigated the bouncing dynamics of water droplets and effect of surface properties on the bouncing dynamics. Later the PTFE surface is tested for the self-cleaning applications [2]. In another application, we shall show that nanostructures produced on Si surfaces typically in the range of 30 nm produced by low energy ions can be used for making highly sensitive nanoparticles arrays [2-4]. Due to the compactness of the particles, such arrays are very good Raman active sensors and have been successfully shown detecting of Blood glucose level, cancer cells and various drugs. We will show that how the ions properties directly affects the sensitivity of the surface [2-4].

Reference:

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ABS: 126. On shaping embedded metal nanoparticles by swift heavy ion irradiation

Flyura Djurabekova [1], Aleksi Leino [1], Ville Jantunen [1], Spyridon Korkos [2], Timo Sajavaara [2], Kai Nordlund [1]

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Surface minimization principle limits any attempt to modify the shape of metal nanoparticles for developing new functionalities, e.g., for optical applications. One of the promising ways to enable controlled shape modification of nanoparticles is using energetic ions in the electronic stopping power regime while the metal nanoparticles are embedded in solids. Previously we showed that using the two-temperature model one can explain fairly well the elongation of nanoparticles along the ion track via material flow driven by thermal expansion. However, many assumptions in this early model remained to be clarified since the atomic interactions in energy barriers in the interface as well as a necessary recrystallization step prior the subsequent ion impact were overly simplified. In this talk, I will present our latest developments of the model that addresses the effect of energy barrier in the interface on the heat flow as well as corrected interaction of Au atoms with the surrounding silica matrix. Our simulations show importance of atomic dynamics before and after the silica matrix solidifies. We see that the nanoparticle continue growing even when no significant dynamics is observed for silicon and oxygen atoms. We also observe the active role of the matrix: the elongation does not proceed without addition stress imposed by nearby track developed in vicinity of nanoparticles. Moreover, we have recently demonstrated that energetic ions can be used not only for shape modification, but also for manipulation of nanorod orientation. This observation was made by imaging the same nanorods before and after swift heavy ion irradiation using transmission electron microscope. Our atomistic simulations were helpful to reveal a complex mechanism of nanorod re-orientation, which proceeded via incremental shape modification, however, eventually assuming the initial nanorod shape, but oriented along the ion track. The reorientation is found to be dependent of the nanorod size.

ABS: 219. Material science and nanotechnology with GeV ion beams

Christina Trautmann [1]

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The existing accelerators at GSI and the future facility FAIR (Facility for Antiproton and Ion Research) provide unique opportunities for material science and other interdisciplinary research disciplines. The interest in beams of such high energies is based on the large energy deposition and the severe modification of physical and chemical properties of materials.

The various research activities with GeV ion beams include the simulation of cosmic radiation to investigate astrochemical processes in space as well as irradiations of samples pressurized in diamond anvil cells to test how materials respond under extreme radiation and pressure conditions.

In the field of ion-track nanotechnology, membranes with parallel nanochannels are fabricated by irradiating polymer foils and subsequently convert ion tracks into open channels by chemical track etching. The density and orientation of the nanochannel as well as their diameter and shape are adjusted by the irradiation and etching conditions.

Electrodeposition in the channels results in nanowire arrays of various materials including metals, semimetals, and semiconductors. Various examples for applications of tailored nanochannels and nanowires will be discussed.

ABS: 221. Ion-beam driven materials science and quantum technology coordinated by the IAEA Physics Section

Aliz Simon [1]

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Ions from accelerators have a prominent role in testing and developing novel materials and devices due to their capability in introducing controlled damage based upon the possibility to define with high accuracy the ion fluence, determine the damage profile and localize the damaged region. Both immediate effects of radiation induced damage on material and device electrical properties and also the longer term accumulation of damage which can limit the useful lifetime can be characterised.

Direct experimental access to study the dynamics of radiation induced defects, from femto-seconds to seconds, makes it possible to design materials with tailored responses to radiation, from radiation hardness to the engineering of desired defects.

The IAEA coordinates a project to develop materials for quantum technologies (F11020). The CRP includes the development of new experimental techniques and the refinement of theoretical models, with an aim to understand radiation effects and ion interaction processes.

This paper will present some of the scientific results of the IAEA supported activities and projects in the above areas and an outlook for planned projects will be also given.

IAEA Accelerator Knowledge Portal: https://nucleus.iaea.org/sites/accelerators/

ABS: 212. Single ion implantation by the detection of secondary electrons

Kristian Stockbridge [1], David Cox [1], Gianfranco Aresta [2], Ian Brown [2], Steven Clowes [1], Ben Murdin [1], Roger Webb [1], Paul Blenkinsopp [2]

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Techniques for deterministic implantation of single ions are currently of high interest for quantum technology applications. Here we present single ion implant detection results from the first commercially produced single ion implanter designed specifically for rapid and precise positioning of deterministically single ions. This system uses a pulsed, low current beam of ions from a liquid metal or duoplasmatron source; Wein filter mass/charge filtering; and secondary electron detection to determine when an implantation event has occurred.

The waveform captured by the channel electron multiplier detectors show transient response(s) that each likely correspond to an ion impact. The distribution of integrated CEM signal for many implanted cites shows clustering corresponding to different numbers of ions in a pulse. This additional information will help quantify the success probability of implant jobs improving quality control.

ORAL PRESENTATIONS

NUMBER OF ORAL PRESENTATIONS: 46

ABS: 95. Ion-irradiation-induced grain boundary formation in self-ion irradiated Nickel

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[1]University of Huddersfield, UK, [2]School of Computing and Engineering, University of Huddersfield, UK.

In a "back to basics" attempt to understand the effects of temperature and displacing irradiation on metals without the influence of chemistry – i.e. with no implantation of foreign species and no segregation, precipitation or formation of new phases – we have conducted a series of experiments in which thin foils containing large polycrystals of Ni (single crystals from the perspective of Transmission Electron Microscopy (TEM)) have been irradiated with 300 keV Ni ions at various temperatures in order to re-examine the fundamentals of the build-up of extended defects in a "simple" system. Experiments were carried out using the MIAMI-2 facility in which the development of radiation damage is observed (and recorded) whilst irradiating in-situ in a TEM [1].

Surprisingly, all irradiations of the electrochemically-thinned foils of Ni resulted in the accumulation of dislocations to form low-angle grain boundaries such that single crystal material was converted into a series of grains, each typically less than 100 nm in width but more than 1 μm in length with the long axis approximately parallel to the edge of the foil.

An interpretation of this process of radiation-induced grain boundary formation will be presented in terms of the coupled effects of irradiation, temperature and stress induced by the radiation damage. The stress arises due to swelling in the irradiated thin region of the jet-polished specimens (with a wedge-shaped cross section) which is constrained by deeper-lying unirradiated material.

The early stages of damage formation are also consistent with molecular dynamics simulation of self-ion irradiated Ni [2].

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ABS: 49. Influence of dpa rate on carbide precipitation and Ar bubble growth in AISI 316L alloys irradiated with Au and Ag ions

Mariana Timm [1], Ítalo Oyarzabal [2], Gabriel Trindade [3], Erwan Oliviero [1], Paulo Fichtner [4]

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Solution-annealed AISI 316L complex alloys were implanted with Ar ions and annealed at 550 ºC to produce an array of Ar bubbles located in a 250 nm thick surface layer. Irradiation experiments with 5 MeV Au and 3.5 MeV Ag ions in samples kept at 550 ºC were performed at different beam fluxes to investigate the microstructure evolution under heavy ion irradiation to a damage level of about 20 and 40 displacements per atom (dpa). The results obtained via TEM and STEM-EDX investigations show the formation of metal-oxide and carbide precipitates and the growth of Ar bubbles. We demonstrate that the precipitate and bubble systems are susceptible to the ion species and the beam flux, rationalized in the produced dpa rate. At lower dpa rates, many different phases are present (G-phase, $M_{23}C_6$, MC, and Cr_2O_3), while at higher dpa rates, the $M_{23}C_6$ and Cr_2O_3 phases are predominant. The Ar bubbles' growth rate correlates with the dpa rate considering the effectiveness of the vacancy absorption process. The precipitation kinetics is discussed considering radiation-induced segregation (RIS) and radiation-enhanced diffusion (RED) mechanisms and collision cascade superposition effects.

ABS: 139. Strong crystal grain orientation effects on ion sputtering

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Sputtering is one of the most studied mechanisms of ion beam modification of material surfaces. Most sputtering models rely on the assumption of a sputtering yield independent of crystal grain orientation in polycrystalline materials. In a joint experimental-theoretical effort between IPP Garching, University of Helsinki and TU Wien, we have examined the effects of crystal grain orientation on sputtering yields in W. The results show for keV heavy ion irradiation of heavy metals, that the crystal direction of the surface normal can have a dramatic effect, of at least a factor of 5, on the sputtering yields. Since elemental metals are non-amophizable, during prolonged irradiation this leads to a major surface roughening. Moreover, the results show that there are no consistent sets of directions that would correspond to an amorphous material. A multiscale molecular dynamics simulation approach can reproduce the experimental results for all crystal directions without any fitting parameters. The simulation results show that the reason to the crystal direction dependence is that the sputtering yield follows well the energy deposition in the top surface layers, which in turn depends strongly on crystal orientation [1]. The reason to the strong dependence of energy deposition with crystal direction can in turn be understood mainly based on shadow cone effects [2].

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ABS: 152. A quantitative method to determine the region not influenced by injected interstitial and surface effects in ion-irradiated metals

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Accelerator-based ion irradiation has been widely used in nuclear engineering to emulate neutron irradiation, especially when considering the phenomenon of void swelling. However, ion-neutron equivalence is complicated by many issues. One major issue is the injected interstitial effect in which the implanted extra atoms act as interstitials and suppress void swelling. This effect is real, but how to define the region affected/unaffected by this reactor atypical effect has been a topic of great debate. The study concerns the credibility of accelerator irradiation in nuclear materials testing and also the reliability of the data extracted. We propose and demonstrate a microstructurally-based experimental method to quantitively determine the depth regions in self-ion-irradiated metals that are affected by the injected interstitial effect and various surface effects, focusing on the choice of safe analysis zones to minimize the impact of these phenomena. The goal is to define the depth ranges where extracted data can be confidently applied to ion-neutron correlations for reactor application. Since ion energies in the range of 1 to 5 MeV are most frequently employed by the radiation effects community, we conducted irradiations at four energies in this range. The experiment was conducted on relatively pure single crystal iron. It was shown that ion energies of ≤1 MeV did not yield a safe depth range, but irradiations at 2.5 MeV and above yielded useful safe zones with predicted swelling behavior becoming independent of ion energy. The surface-affected zone width was roughly twice that of the void-denuded zone width. The interstitial-affected region starts at about one-half of the projected range and does not show any “spreading” of influence in depth when the peak damage level increases from 50 to 100 displacements per atom (dpa). This study provides confidence that enhances the credibility of ion simulation when applied to void swelling in neutron environments.

ABS: 97. Low energy ion interactions with transition metal films-ballistic and diffusive transport processes

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Interactions of low energy ions (< 1000eV) with surfaces is of increasing importance to industries of semiconductor manufacturing, ion metrology and fusion. The nature of the interactions of ion species at high energies (>1000eV) can generally be classified as ballistic. As the energy decreases, approaching the so-called sputter threshold, the ion interactions are no longer purely ballistic. Adding to the complexity is the reactivity of certain ion-target combinations leading to dynamic changes in material surface properties. Here, we discuss the various processes of interactions between reactive ions of N_2 and O_2 with transition metal surfaces of industrial interest: Mo, Ru, Pd and W. Experimental studies by Angle Resolved X-Ray photoelectron spectroscopy (AR-XPS) shed light on the incorporation of implanted species and their distribution in depth. Corroborating with ballistic Monte-Carlo simulations we separate effects of ballistics from diffusion (bulk and radiation enhanced) and find that O_2 ions show an enhanced depth of implantation than predicted by ballistics near threshold. Further, while N_2 behaves as per ballistic mechanisms, the incorporation is unaffected by the ion energy. The interactions for similar mass species are widely different indicating a strong chemical effect near sputter thresholds and require more concerted efforts for understanding.

ABS: 23. Stopping power in very heavy targets: from lanthanides to post-transition metals

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The present state of the stopping data is discussed within the framework of the IAEA stopping database [1]. We focus on the need and importance of reliable values for very heavy targets, such as lanthanides, from lanthanum to lutetium, 6-period transition metals and post-transition metals. Full theoretical calculations are presented for the stopping power of protons in such atomic solids. The importance of relativistic radial orbitals and binding energies is discussed, not only for the deep but also for the outer shells. The electronic stopping power is described by combining three formalisms: i) the screened potential with cusp condition model [2] (SPCC), which is a non-linear binary formalism for the energy loss in the free electron gas (FEG); ii) the dielectric formalism [3] for the stopping in the FEG (in the energy region where plasmon excitations are important); iii) the shellwise local plasma approximation (SLPA) [4] for the bound electron contribution. The comparison with the well-known SRIM [5], DPASS [6] and CASP [7] results is presented and discussed. We consider that present results are a picture of the state of art of the stopping in lanthanides and post-lanthanides and also states doubts of some of the experimental data in the IAEA database [1] and employed in the SRIM [5] semi-empirical description.

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ABS: 117. Microstructural evolution and Deuterium diffusion in γ-$LiAlO_2$ irradiated with He^+ and D^+ ions

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Tritium (T) is a fuel for clean, sustainable fusion energy systems. As a tritium breeder, gamma-phase lithium aluminate (γ-$LiAlO_2$) has been investigated as a candidate material for fusion reactor blankets [1]. The material has an outstanding thermomechanical stability and low-swelling behavior under neutron irradiation. When isotope ^{6}Li captures a thermal neutron, it creates 2.73 MeV T and 2.05 MeV helium (He) particles from reaction ^{6}Li(n,He)T. Both particles will dissipate their kinetic energies through electronic and nuclear energy deposition processes, producing heat and initiating damage cascade collisions in the host material. It is important to understand microstructural evolution and its impact on T and Li diffusion and release in order to assess and predict material performance during neutron irradiation. Over the past years, we have performed emulation of damage accumulation, microstructural evolution, and tritium transport in γ-$LiAlO_2$ single crystals and polycrystalline pellets using sequential irradiation of He^+ and D^+ (a surrogate for T^+) ions at elevated temperatures [2-6]. This presentation will provide an overview of this work with new results from recent studies, and discuss ion irradiation effects in the material, including damage accumulation, amorphization, radiolysis, Li loss, second phase precipitation, isotope exchange, diffusion and release of gas species. A direct comparison of gas release data from ion and neutron irradiated γ-$LiAlO_2$ pellets will also be presented.

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ABS: 21. Revealing the onset of unprecedented transition from synergistic to competitive effect in defective $KTaO_3$

Gihan Velisa [1], Decebal Iancu [1], Eva Zarkadoula [2], Maria-Diana Mihai [1], Yanwen Zhang [2], William John Weber [3]

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Understanding how $KTaO_3$, with existing disorder induced by nuclear energy transfer (Sn), responds to subsequent electronic energy transfer (Se) may provide nonequilibrium pathways to tune the functional properties of this oxide. In this regard, pre-damaged $KTaO_3$ has been irradiated with several ion species (5 MeV C, 7 MeV Si and 12 MeV O ions) over an extended selection of ion fluences at 300 K. By exploring these processes in $KTaO_3$, the RBS/C clearly shows that, for Si ions, the synergistic effect is active and induces the formation of small ion tracks, which is well in line with the MD simulations. For C and O ions, RBS/C measurements reveal a spectacular transition from ionization-enhanced defect production to damage recovery process, not previously reported in $KTaO_3$. Thus, in this study, the transient synergistic effect is followed by the competitive effect. So far it is assumed, that the subsequent rapid quenching of this transient phase can leave unstable defect structures in a state that relax into an energetically more favorable configurations during further C or O ion irradiations (within or immediately following the inelastic thermal spike). Finally, based on the ion channeling results, the ion fluence of C and O ions may be applied as an effective ionization-induced processes manipulation knob to tune defect states, which may open new horizons for electronics and spintronics applications.

ABS: 26. Inelastic interactions of ions with disordered oxide perovskites

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Oxide perovskites exhibit fascinating properties that identify them as key materials for next generation of multifunctional devices, and ion-beam modification can be used to tune functionality. While it is well-established that atomic-level defects are created by elastic energy transfer, S_n, from ions to atomic nuclei, the effects of inelastic energy loss, S_e, to electrons is more complicated. High-energy ions with S_e values above a threshold interact synergistically with pre-existing disorder in $SrTiO_3$ and $KTaO_3$ to form amorphous nanotracks at 300 K. The nanotrack cross-sections increase with S_e and level of pre-existing disorder, and the inelastic energy loss threshold, S_{et}, decreases with increasing disorder. Application of the analytical thermal spike model suggests a decrease in melting temperature and increase in efficiency of track formation with increasing disorder. Molecular dynamics simulations combined with the inelastic thermal spike model confirm that the formation of these amorphous tracks is due to melt-quenching along the ion trajectory. While high energy ions contribute to damage production above S_{et}, the effects of inelastic energy loss on pre-existing disorder below S_{et} have not been studied in detail. To investigate this, pre-damaged $SrTiO_3$ has been irradiated with 2 MeV He, 1.2 MeV C, 5 MeV C and 12 MeV O ions. The results indicate two distinct regimes of ionization-induced recovery. While melt-quenching does not occur for these ions, the inelastic thermal spike for C and O ions, with S_e between 1.6 and 3 keV/nm, causes sufficient local heating via electron-phonon coupling to induce defect recovery, as confirmed by MD simulations. At lower values of S_e, the efficiency of defect recovery decreases by several orders magnitude for 2 MeV He ions and 200 keV electrons, and this recovery is attributed to local electronic excitations that enhance defect mobility.

ABS: 220. Synthesis and Irradiation response of high entropy alloys with transition and refractory metals for operation at extremes

Marta Dias [1], Ricardo Martins [1], Sérgio Magalhães [1], Rui Coelho da Silva [1], António Pereira Gonçalves [2], Patrícia Almeida Carvalho [3], José Brito Correia [4], Andrei Galatanu [5], Eduardo Alves [1]

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High-entropy alloys (HEAs) are a class of materials which have been intensely studied during the last years due to their innovative properties. However, their unconventional compositions and chemical structures hold promise for achieving unprecedented combinations of mechanical properties, microstrutures and irradiation resistance for the use in extreme environments. In this work results on two types of HEAs will be presented: based on transision metals (CuCrFeTiV) and refratory metals (CrNbTaVW). All the alloys were prepared by ball milling followed by consolidation by spark plasma sintering and then irradiated with Ar ions in order to check the adequacy for use as a thermal barrier in future nuclear fusion reactors. Structural changes were investigated by X-ray diffraction, and scanning electron microscopy and scanning transmission electron microscopy, both coupled with X-ray energy dispersive spectroscopy. Surface irradiation damage on CuCrFeTiV was detected for high fluences ($3x10^{18}$ Ar^{+}/cm^{2}) with formation of blisters of up to 1 μm in diameter. Cross-sectional scanning transmission electron microscopy showed the presence of intergranular cavities only in the sample irradiated with $3x10^{18}$ Ar^{+}/cm^{2}, while all irradiation experiments produced intragranular nanometric-sized bubbles with increased density for higher Ar^{+} fluence. Moreover, no severe superficial modifications were observed in the CrNbTaVW samples, after irradiation at different temperatures.

ABS: 52. Combining MD-LAMMPS and MC-McChasy 2.0 codes for dislocation simulations of Ni-based alloys

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The unique capability of the new, second version of the McChasy code is to provide the possibility to simulate Rutherford Backscattering Spectrometry in channeling direction (RBS/C) experimental spectra in large structures (ca.10^8 atoms). The virtual samples that can be investigated may originate from crystallographic data by using custom build-in McChasy procedures or external apps that provide positions of atoms in a structure of interest as an output e.g. ATOMSK [1] or LAMMPS [2] codes.

Ni-based alloys are nowadays one of the most investigated and promising materials that can be used in the power generation sector and in general for high-temperature applications because of their radiation resistance and immune response to harsh environmental conditions.

In this work, recent results of investigations regarding simulations of extended structural defects (edge dislocations and loops) developed in the directions typically observed in the fcc systems that are formed inside nickel-based single crystal alloys are presented. The extended defects models are created using ATOMSK and MD - LAMMPS thermalization process. The models are used then to create virtual samples and simulate experimental RBS/C spectra.

ABS: 143. Basic study of the relaxation volume of crystalline defects in bcc iron

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Crystalline defects, inevitably produced upon ion irradiation, generate long-range elastic distortions of the lattice that are subtle driving forces for the defects to migrate and cluster. It is usually at this stage of defect clustering that the changes in the material properties reach a climax. Modelling defect creation and subsequent evolution is a multi-scale approach that requires basic data characterics of those defects. Elastic properties such as the relaxation volumes (V_{rel}) are highly useful, as they can be the principal ingredients in estimating the strains and stresses on a macroscopic scale (at least to some extent), or they can also help exploiting X-ray diffraction experimental data related to irradiation-induced changes in the lattice parameters. In this work, V_{rel} of common crystalline defects in bcc iron (Fe), chosen as a test-case material, was determined from molecular dynamics simulation cells containing defects of varying size and/or concentration. We used both real and reciprocal space data: the former allowed to monitor the change in the MD cells volume, while the latter, obtained from computational X-ray diffraction of reciprocal space maps, were used to evaluate the change in the lattice parameter. We show that dumbbell SIAs have the largest V_{rel}, ~1.5 atomic volume (omega); ½ and interstitial dislocation loops exhibit a relaxation volume of ~0.905 omega and ~0.873 omega per interstitial, respectively. C15 clusters of size 12 and 48 atoms show a V_{rel} of ~0.91 omega and ~0.98 omega, respectively. Single vacancies are characterized by a negative V_{rel} (~ -0.11 omega) that exhibits increases to approach zero as vacancy clusters grow. Using these values, we predicted (with an error of maximum 2 %) the lattice strain in MD cells containing several types of defects, which indicates that the relaxation volume contributions can be summed up to estimate the change in the lattice parameter.

ABS: 163. Electronic excitations of keV ions in single-crystalline self-supporting targets

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Understanding energy deposition by energetic charged particles in matter is imperative for prediction of ion-induced materials modification, as in semiconductor doping or extreme environments, e.g. fusion devices. Such understanding also forms the basis for analytical tools based on ion beam and yields a well-defined test scenario for theoretical models, which aim to predict equilibrium [DFT] & non-equilibrium conditions [TD-DFT] in solids. The commonly employed description of energy deposition defines the specific energy loss per unit path length in a material as an average value along the ion trajectory despite its origin from discrete excitation events.

We present experiments using the Time-of-Flight Medium Energy Ion Scattering System at Uppsala University [1]. For measuring energy deposition, we employed self-supporting Si(100) & SiC(100) nanomembranes with thicknesses in the range from 50 – 200 nm & large-angle, position-sensitive detectors in backscattering and transmission geometries. Primary ion species from H to Ar in beams with fA current in the energy range of 5 – 200 keV were employed.

We compared spatial and energy distributions for axially channeled projectiles and particles transmitted off from low-index crystal axes as a function of projectile type and energy [2][3][4][5]. A clear energy dependence of energy loss ratios (channeling vs. random) is observed with characteristic behavior for different ion species. We analyze the origin of different energy loss contributions and their impact parameter dependence, e.g. due to formation of molecular orbitals and charge transfer inducing differences in the mean charge state for different trajectories as well as their relevance for applications.

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ABS: 129. Dynamics of self-trapped exciton formation, hopping, and recombination within an ion track in Silica

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Self-trapped excitons (STEs) play an important role in energy transfer and defect production in silica under ion irradiation and other forms of ionizing radiation. However, details of the formation, migration, and eventual recombination or disappearance of STEs in silica are poorly understood, especially considering the extreme range of electronic excitation densities, temperatures, and reaction rates that exist within an ion track. Cryo-ionoluminescence studies of the intrinsic emission of STEs in fused silica were performed at temperatures from 30-100 K using light and heavy ions (3 MeV H, 3.5 MeV He, 19 MeV Si, and 10 MeV Cl). The initial light yield of the intrinsic STE emission, its dependence on temperature, ion energy and mass, and its real-time kinetic evolution throughout the irradiation reveals a complex process of STE formation, migration, and recombination. A parameter-free model was developed that quantitatively reproduces the experimentally observed light yield. The model describes a competition between non-radiative Auger recombination, STE formation and dissociation, and carrier hopping with an activation energy of 0.12 eV. At lower electronic excitation densities, the light yield is essentially governed by an equilibrium established between STE formation and non-radiative Auger recombination. As the excitation density increases, the effects of the inelastic thermal spike become apparent and thermal dissociation of STEs into self-trapped holes and electrons shifts the equilibrium between radiative and non-radiative recombination channels.

ABS: 15. Modelling the strain build-up in nitrogen implanted tungsten films on silicon substrates

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A model of the strain accumulation in nitrogen implanted polycrystalline tungsten films deposited on 110 single-crystalline silicon substrates is presented. The films were implanted at room temperature, perpendicular to the sample surface with an energy of 60 keV N^{2+} and concentrations between $0.5x10^{17}/cm^2$ and $5x10^{17}/cm^2$. The proposed model is based on the simulations of the X-ray diffraction 2θ-ω in the vicinities of the ~500 nm thick 110 W most intense Bragg peak. Up to a fluence of $2x10^{17}/cm^2$, the increase of asymmetry towards lower angles of the 110 W peak is interpreted as a linear increase in strain affecting the entire implanted region. Then, the solubility of N in W saturates and phase transition to fcc β-W_2N is observed.
The phase transition occurs at the surface strain regions of the implanted crystal volume while the lowest strained regions are masked by the β-W_2N barrier and even evidence some relaxation. After $3x10^{17}/cm^2$, the strain deduced for the 111 and 200 planes of the fcc β-W_2N formed pseudo-layer increases at different rates. While the former comprises a maximum tensile deformation of 3.8 %, the latter is more resilient to nitrogen irradiation developing less than half of the strain magnitude (1.5 %).
After $4x10^{17}/cm^2$, Rutherford backscattering spectrometry measurements suggest partial sputtered N while X-ray diffraction indicates no strain-relief at the remaining surface fcc β-W_2N. The N concentration derived by the ion beam technique and the combined 110 W/ (111, 200) β-W_2N strain profiles as functions of depth agree with the Simulations of Ions and Radiation in Matter (SRIM) theoretical predictions.

ABS: 25. Tailoring oxide thin films by ion beams

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Complex oxides host a multitude of novel phenomena in condensed matter physics, such as various forms of multiferroicity, colossal magnetoresistance, quantum magnetism and superconductivity. Defect engineering via ion irradiation can be a useful knob to control these physical properties for future practical applications. Two prominent effects are disorder and uniaxial strain. Particularly, the uniaxial strain, manifesting as the elongation of the out-of-plane lattice spacing, is not limited to available substrates, the conventional and well-known strain engineering approach. In this talk, I will introduce the modification of oxide thin films by ion beams. Examples are the modification of magnetic and magneto-transport properties of $NiCo_2O_4$ [1] and $SrRuO_3$ [2, 3] and the attempt to enhance the ferroelectric properties of $BiFeO_3$ and KTN ($KTaNbO_3$) [4,5]. It is worth to note that ion beam technology has been well developed for microelectronics. Once the principle of concept is approved, the approach can be easily scaled up and integrated to the industry production line.

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ABS: 119. Elongation kinetics of plasmonic nanoparticles studied in situ by polarized optical absorption spectroscopy

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The elongation of metallic nanoparticles (NPs) embedded in a dielectric matrix after irradiation with swift heavy ions is a phenomenon that has been known for some years [1,2]. Nanorods obtained with this method have the larger axis aligned with the direction of the incident ion beam, which can be advantageous for many applications. However, the origin of the deformation is not yet fully understood, although this phe-nomenon has been extensively studied [1-5] and some theoretical models have been proposed [1,2,5]. One of the reasons that complicate this task is the lack of information during the intermediate stages of deformation. Here we report the continuation of our previous work [2], to exploit the strong dependence of the localized surface plasmon resonance on the nanorod's aspect ratio, to study in-situ the elongation kinetics. In a first step, spherical NPs were obtained by implanting 4 MeV Au ions in high-purity sili-ca and applying a subsequent thermal annealing. Then, NPs were transformed into nano-rods by means of a subsequent irradiation with 35 MeV bromine ions. Optical absorp-tion spectra were measured in-situ, using a polarizer, to obtain the signal only from the longitudinal plasmon mode of the nanorod. Then, the detailed deformation kinetics was calculated from a fit of these spectra. Use of polarized spectra allowed for a much more accurate analysis of the elongation kinetics, particularly useful in the first stages, where longitudinal and transversal modes overlap.

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ABS: 160. *In-situ* positron annihilation spectroscopy for materials characterization under coupled irradiation extremes

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Fast neutrons in advanced fission reactors and fusion devices produce not only atomic displacement damage but also incorporate none-soluble helium atoms in lattice structure through neutron induced nuclear reactions. Dual ion beam irradiation, concurrently from a heavy ion beam and a helium ion beam, have been used to study separate or synergistic effects of cascade damage and/or helium impact on materials microstructure, and thus to help establish scientific foundations for development of new concepts for improving the properties of existing alloys or designing new materials with exceptional radiation resistance.

While advanced in-situ characterization techniques such as transmission electron microscopy have been developed to measure defect formation and microstructural evolution during ion irradiation, an in-situ atomic scale defect probe, capable of detecting defect generation and propagation as well as defect-helium interactions on atomic scale during the early stages of radiation damage, is still missing.

To provide such capabilities, we developed an advanced positron beamline at the Ion Beam Materials Laboratory in Los Alamos National Laboratory that allows a range of in-situ atomic scale defect measurements under coupled dual-beam irradiations. In this presentation, I will describe the positron beamline development, challenges, advantages, and limitations. Examples of positron annihilation spectroscopy (PAS) measurements will be presented to demonstrate the unique capabilities.

ABS: 60. Electronic stopping power of pristine and ion irradiated plasma facing materials for light ions

Eduardo Pitthan [1], Marcos V. Moro [1], Jila Shams-Latifi [1], Philipp M. Wolf [1], Dmitrii Moldarev [1], Petter Ström [1], Primetzhofer Daniel [1]

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Sputtering and defect formation from plasma-wall interaction have been studied extensively since they are key processes to be understood in the operation of future fusion reactors with minimum maintenance. In these processes, electronic stopping powers for plasma species in wall materials is an important input variable for computer codes used to model erosion and implantation [1]. This quantity describes the energy deposited per unit path length in the electronic system of the target material by penetrating ions. Despite the importance, the number of experimental datasets of electronic stopping powers for ions in plasma facing materials is rather low. In addition, potential effects of defect formation by ion irradiation on the electronic stopping power of these materials are basically not known.

In this contribution, experimentally deduced electronic stopping power of candidates for plasma facing materials for next generation fusion devices (Fe, W and EUROFER) for impacting plasma species (H, D, and He) in pristine and irradiated materials will be presented. This information is extracted in the energy range of sub-keV to MeV based on the intensity of energy spectra recorded by backscattering spectrometry (BS) [2]. The presence of impurities on and in the samples is analyzed ex or in-situ prior to the analysis by means of time-of-flight-energy elastic recoil detection analysis (ToF-ERDA) and Auger electron spectrometry (AES). Ion irradiation experiments are carried out on the pristine samples which are additionally characterized by BS, ToF-ERDA, and X-ray diffraction analysis (XRD). Our results increase the amount of available electronic stopping power data and enhance the knowledge on e.g. how local details such as presence of defects caused by the ion-irradiation can influence fundamental quantities describing ion-solid interaction.

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ABS: 171. Energetic helium ion implantation to emulate the in-reactor neutron damages in Ni superalloy

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Inconel X-750 is an age-hardened Ni based superalloy extensively used in the cores of nuclear reactors, such as spacers in CANada Deuterium Uranium (CANDU) fuel channels. The recent mechanical tests on the ex-service Inconel X-750 spacers indicate significant embrittlement and reduced load carrying capacity compared to as installed condition. The primary degradation mechanism remains unclear, and thus provides the focus of this investigation. Helium ion implantation was employed as an emulator for neutron irradiation to explore the microstructural evolution and mechanical property degradation of X-750 Ni-based superalloy. The ion-irradiation has been conducted at different temperatures and up to different doses. In addition, the effect of helium impurities was investigated on microstructural changes. The discussion of the microstructural evolution is focused on characterization of irradiation-induced defects, including dislocation loops and cavities along with examination of the stability of strengthening phase γ'-precipitates. A major contribution of this work is to utilize a focused ion beam (FIB) and transmission electron microscopy (TEM) to perform precise defect characterization. In order to estimate the individual contribution of defects in radiation-induced hardening, three different obstacle-hardening models have been applied to fit TEM-obtained microstructural data. This approach is unique to the literature since it demonstrates both the individual and the combined effects of the microstructural features on mechanical behavior. Furthermore, the fracture behavior of the helium-implanted-material exhibited a mixed failure mode of inter-granular and trans-granular fracture. Eventually the importance of ion beam technique used in this study is discussed within current nuclear program.

ABS: 6. ZnO nanorods with Au/Ag nanoparticles prepared by ion beam implantation - structural modification and optical properties

Anna Mackova [1], Adela Jagerova [1], Ondrej Lalik [1], Petr Marvan [2], Zdenek Sofer [2], Vaclav Holy [3], Azarov Alexander [4], Ullrich Kentsch [5], Jan David Schutter [6], Augustinas Galeckas [4]

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ZnO exhibits wide direct bandgap, large exciton binding energy, high transparency and great photocatalytic properties [1]. The metallic NPs, consisting of two noble metals, can offer unique properties such as fine tuning of SPR position stability resulting from synergetic effect between two elements and final structure of NPs [2]. Core-shell NPs attract attention since the appropriate choice of shell atoms can enhance stability of NPs and core can increase photocatalytic activity [3]. ZnO nanorods of 380 nm in length deposited on Si wafer substrates were implanted with Au 400 keV and Ag 252 keV ions at various ion fluences from 2.5×10^{15} cm^{-2} to 1.0×10^{16} cm^{-2} and sub-sequently annealed at 600°C for 5 minutes. The Au/Ag nanoparticle coalescence in ZnO nanorods interplay with radiation damage was followed before and after annealing in connection to structure modification and optical properties. Rutherford backscattering spectrometry (RBS) was used to follow Au, Ag distribution in ZnO nanorods, X-ray diffraction analysis have shown the vertical and basal domain radii decreasing with the increased ion implantation fluence and partial recovery mainly in basal direction after the annealing in ZnO nanorods as well as observed by scanning electron microscopy (SEM). Photo-luminescence measurements have shown surface plasma resonance (SPR) response, developing progressively with the increasing Au, Ag-ion fluence and after the annealing in ZnO nanorods. Photocatalytic activity was tested on Au-implanted samples and discussed in connection to structure and optical properties.

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Acknowledgement:

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ABS: 147. Demonstration of red light-emitting devices based on Europium-implanted AlN p-n junction nanowires

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Red light-emitting diodes (LEDs) based on group III-nitrides (III-N) are essential for the monolithic integration of red-green-blue (RGB) emitters, enabling the development of efficient white LEDs and full-color displays. Colored III-N LEDs are obtained through bandgap engineering of InGaN/GaN multi-quantum well (MQW) structures. However, such an approach suffers from reduced external quantum efficiency (EQE) when high In-contents are required in the active region, i.e., for longer emission wavelengths. Indeed, their efficiency is known to decrease from about 85% (blue LEDs) to below 10% (red LEDs). Therefore, alternative approaches should be explored to improve the efficiency of red emitters based on III-N. One consists of doping III-N semiconductors with europium ions. When incorporated in III-N hosts, trivalent europium ions (Eu) lead to an intense red emission (620-625 nm) corresponding to the radiative recombination between the $^5D_0$ and $^7F_2$ multiplets. This strategy was already proven successful in realizing red LEDs. The state-of-the-art GaN:Eu (in-situ doping) LEDs exhibit EQE ~10%, exceeding those of InGaN-based red LEDs.

Recently, we reported an improvement of the luminescence properties of Eu in Eu-implanted AlGaN nanowires (NWs) for hosts with high Al-contents, including i) the luminescence intensity at low temperature (~5 K) increases and ii) the thermal quenching photoluminescence (PL) intensity of the Eu emission decreases. These results brought interest in Eu-implanted AlN NWs for developing red III-N LEDs with the possibility of surpassing the performance of GaN:Eu LEDs as long as the optical improvements compensate for the higher electrical resistivity of AlN. This work will present the recent achievement of red LEDs based on Eu-implanted AlN p-n junction NWs. To the best of our knowledge, this was the first LED obtained using rare-earth ion implantation into III-N hosts. The current challenges of this technology will be discussed as well.

ABS: 42. Effect of energy deposition on the disordering kinetics in dual-beam irradiated single-crystalline Si, SiC and GaAs

Aurélien Debelle [1], Gaelle Gutierrez [2], Alexandre Boulle [3], Isabelle Monnet [4], Frédérico Garrido [1], Lionel Thomé [1]

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[3]*Universié de Limoges, IRCER, Centre Européen de la Céramique, France,*
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During ion irradiation of materials, energy is transferred either to nuclei (nuclear energy-loss, here called Sn) or to electrons (electronic energy-loss, here called Se) of the target atoms. The energy partitioning between the electronic and atomic networks constitutes an important issue to address because synergistic effects can take place, the result of which being not necessarily the algebraic sum of the two energy-loss components. Coupled effects are here referred to as Sn&Se effects.

In the current work, we investigate the disordering kinetics in Si, SiC and GaAs under dual-beam irradiation experiments so that both Sn and Se components are present. For this purpose, we use 900 keV I ions (Sn) and 27 MeV Fe ions (Se) in combination with three characterization techniques: Rutherford backscattering spectrometry in channeling, Raman spectroscopy and X-ray diffraction; complementary transmission electron microscopy analyses allow imaging the crystals microstructures. We show that the three semiconductors irradiated under Sn conditions (at room-temperature) undergo an amorphous transition at a fraction of dpa. In contrast, when both Sn and Se ion beams are used simultaneously, amorphization is prevented, and when the flux ratio between Fe and I ion beams increases, the disordering rate decreases. Both the disorder and the elastic strain levels decrease under Sn&Se experiments. These results demonstrate that an efficient dynamic annealing takes place during the Sn&Se irradiation, due to a local increase in temperature related to a thermal spike effect induced by the Fe ions. Even though there is no spatial and time overlap between I and Fe ions, this annealing effect is shown to be much stronger under Sn&Se irradiations than it is for sequential (Sn+Se) irradiations. To finish, if the three materials behave similarly, their response to the electronic energy loss is not identical, GaAs being the most sensitive, followed by Si and SiC.

ABS: 138. Correlating surface nano patterning and compositional changes under low-energy ion beam irradiation of disordered alloys

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Bulk metallic glasses (BMGs) and high entropy alloys (HEAs) are two unique classes of emergent alloys with unique material properties [1]. For example, BMGs exhibit excellent corrosion resistance, enhanced mechanical properties and irradiation resistance. The use of low-energy ion beams between 0.1-1.0 keV at various fluences between 10^{15}-10^{19} cm^{-2} and at room temperature have led to self-organized surface nano patterning in compound semiconductors [2]. In this work we examine unique response of BMG and HEAs to irradiation to low-energy ion beams utilizing in-situ surface characterization. In particular, we study properties that have implications with unique surface-relevant properties in plasma-material interaction applications for nuclear fusion devices, bioactive response and enhanced optical properties.

In-situ X-ray photoelectron and low-energy ion scattering spectroscopies (XPS, LEISS) are used to characterize the compositional changes during ion-beam irradiation of two types of BMGs: $Zr_{52.5}Cu_{17.9}Ni_{14.5}Al_{10.0}Ti_{5.0}$ (Vit 105) and $Zr_{50}Cu_{40}Al_{10}$, and correlated to nano patterning and surface mechanical property variation under irradiation. Irradiation by Ar and Kr singly-charged ions at various fluence and incident angle conditions is used. Results indicate that highly-ordered patterns can be induced only if a controlled amount of additive metallic impurities exceeded a certain threshold. Patterning is associated with a number of stages: emergence of initial random dots, subsequent transition to ripples, and ordering of the ripple pattern through annihilation reactions of mobile defects, while the wavelength and amplitude remain invariant throughout the patterning.

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ABS: 86. Highly ordered silicide ripple patterns induced by medium-energy ion irradiation

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Self-organization mechanisms play an important role in the development of current low-dimensional structures. Ion beam irradiation is a well-studied process leading to patterns at the nanoscale such as dots and ripples. In the case of silicon substrates these patterns can be produced with the incorporation of metal impurities leading to both chemical and morphological patterns [1]. Interestingly, these structures can depict an enhanced order in comparison to some metal-free structures.

In this work we report the nanopatterning of silicon surfaces under 40 keV Ar irradiation with simultaneous Fe co-deposition [2]. The incidence angle was kept at 15º and fluences were varied from 1E17 to 1E19 cm^{-2}. Morphological and compositional analyses were performed by AFM (both in morphological and electrical modes), RBS, XPS, scanning Auger, as well as transmission and scanning electron microscopy.

The results show that, initially, nanodot structures randomly emerge, which, with increasing ion fluence, become progressively aligned along the perpendicular direction to the Fe flux. With increasing fluence, they coalesce, leading to a ripple pattern. The pattern dynamics and characteristics are faster and enhanced, respectively, as the distance to the metal source decreases (i.e., as the metal content increases).

Remarkably, the ripples can become rather large (up to 18 microns) and straighter, with few defects, and a pattern wavelength close to 500 nm. Furthermore, for a fixed ion fluence, the pattern order is improved for higher metal flux. In contrast, the pattern order enhancement rate with ion fluence does not depend on the metal flux. These experimental observations agree with the predictions and assumptions of current models [3].

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ABS: 2. In-situ observation of ion-induced nanoscale patterning on a crystalline Ge(001) surface

Denise Erb [1], Peco Myint [2], Kenneth Evans-Lutterodt [3], Karl Ludwig [4], Stefan Facsko [1]

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Ion-induced surface patterning has turned out to be a highly versatile technique for many applications where large areas of nanostructured surfaces or thin films are required. Both fundamental and applied research may benefit from in-situ studies revealing the kinetics of the patterning process, yielding further insight into the dominant mechanisms and thus enabling to gain precise process control. The surface-sensitive X-ray scattering technique of Grazing Incidence Small Angle X-Ray Scattering (GISAXS) is a well-suited method for such in-situ investigations, allowing for contact-less examination under various external conditions.

Here, we present a real-time in-situ GISAXS investigation of reverse epitaxy patterning in crystalline Ge(001). From the X-ray scattering pattern we deduce the significant morphological parameters of the surface, thus tracking the development of the surface morphology with time during ion irradiation.

These findings are compared with results from simulations based on a continuum equation of the local surface height. Good agreement of the simulation with both experiment and theory was only achieved when including in the continuum equation an additional term for regulating the pattern anisotropy. We then find that a continuum equation considering only diffusive effects reproduces the experimentally observed surface patterning kinetics well. Observing the kinetics of pattern formation in the non-linear regime, we find that the temporal evolutions of characteristic length and roughness conform to power laws, their exponents agreeing with scaling laws for conserved continuum equations with four-fold symmetry. Moreover, we find that the facet angle kinetics can be described by the Austin-Rickett equation for diffusion-controlled transformation processes, corroborating our assumption of a predominantly diffusive mechanism of pattern formation.

ABS: 140. Tailoring of two-dimensional semiconductors optoelectronic properties via ion induced nanopatterning

Matteo Gardella [1], Debasree Chowdhury [1], Mukul Bhatnagar [1], Maria Caterina Giordano [1], Francesco Buatier de Mongeot [1]

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Large area substrate nanostructuring in the subwavelength regime is an effective route for tailoring opto-electronic properties of ultrathin semiconductor layers [1]. In this field, two-dimensional Transition Metal Dichalcogenides (TMDs) are promising materials due to their high optical absorption coefficient combined with good electronic and mechanical properties. Being the effective absorption limited by the few nanometers thickness, light harvesting strategies are required in view of real-world applications [2].

We demonstrate that defocused Ion Beam Sputtering (IBS) can be employed to induce large area and self-organized nanostructuring of silica templates, exploiting the anisotropic nanowrinkling processes induced by ion irradiation [3]. MoS_2 layers conformally grown on top of this template show a polarization dependent optical response, induced by the extrinsic morphological anisotropy and by strain [1].

To boost light absorption in the TMD films, we reshape them forming periodic nanogratings fabricated via Laser Interference Lithography and Reactive Ion Etching. The subwavelength periodical corrugation of the MoS_2 layers promotes the launch of diffractive anomalies that lead to a light absorption enhancement up to 240% compared to reference flat films [2]. Our preliminary results also show that the nanograting height and morphology can be finely tailored by self-organized IBS at off normal angles, introducing asymmetric faceting with facet slope selected by ion dose and incidence.

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ABS: 33. X-ray photon correlation spectroscopy study of ion beam nanopatterning

Karl Ludwig [1], Peco Myint [2]

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While time-resolved x-ray scattering with a conventional non-coherent source has proven to be a powerful probe to investigate average surface evolution during ion beam nanopatterning, the coherent x-ray scattering technique of X-ray Photon Correlation Spectroscopy (XPCS) goes beyond the averaging inherent in use of a non-coherent source and enables the investigation of local fluctuation dynamics. Our recent work using XPCS to examine ion beam nanopatterning has shown rich structure in the development of the correlation dynamics as seen in the evolving correlation time and fluctuation relaxation exponent as a function of length scale. On length scales of the ripple structure, local structure becomes ever more long-lived as coarsening progresses. In addition, the correlation peak develops a peak on length scales corresponding to the ripple wavelength, a behavior reminiscent of de Gennes narrowing. As patterning progresses, correlation times become asymmetric between the positive and negative directions, suggesting the possibility of different dynamics on the slopes facing toward and away from the ion beam. Relaxation exponents show evolution from linear dynamics at early times to compressed exponential relaxation at low wave numbers, and stretched exponential relaxation at high wave numbers. Compressed exponential behavior is reminiscent of stress relaxation processes observed in glasses, though these general behaviors can be reproduced in simulations of a nonlinear model which does not explicitly include stress relaxation. Finally, it is shown that speckle motion during the surface evolution can be analyzed to determine spatial inhomogeneities in erosion rate and ripple velocity. This allows the direction and speed of ripple motion to be measured in a real time experiment.

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ABS: 11. Role of ion beam parameters in the evolution of self-organized nanoripple superimposed by triangular features

Sukriti Hans [1], Mukesh Ranjan [1]

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Ion beam sputtering can lead to formation of self-organized nanopatterns depending on different irradiation conditions and is applicable in different fields of materials research for e.g., optoelectronics, magnetic storage, and many technological applications. The evolution of ripple patterns has been progressively understood, but the formation of triangular features which superimpose them have been rarely studied experimentally. We present the triangular pattern formation on Si surface induced by low-energy by changing the beam energy, ion fluence, ion incidence angle and the substrate temperature. The dynamics of triangular patterns can be controlled and can be scaled to the sizes required for various applications. Experimentally, for the case of Si targets, several results are consistent with the modified AKS equation after the pioneering work given by Bradley and Harper. Using this equation, numerical simulations are done which shows dispersion is crucial for the formation of these patterns and also for producing highly ordered ripples [1]. Along with curvature-dependent sputtering, mass redistribution also plays significant role in erosion of the surface. To understand the effect of diffusion on these patterns, substrate temperature was varied experimentally and diffusion coefficient in modified AKS equation. The dynamics of these triangular patterns i.e., their lateral length and base angle were studied both experimentally and theoretically and it was observed that the temperature-induced effects are adequately replicated [2]. The performed simulations indicate that, the curvature-dependent sputtering seems to be the leading process during pattern formation along with dispersion which is essential for triangular features formation. The work presented here paves a way towards controlling the size of triangular features using various ion beam parameters.

ABS: 10. Low-energy ion channeling in nanocubes

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Focused ion beam (FIB) processing with low-energy ions has become a standard technique for the manipulation of nanostructures. Many underlying ion beam effects that deviate from conventional high-energy ion irradiation of bulk systems are considered today; however, ion channeling with its consequence of significant deeper penetration depth has been only theoretically investigated in this regime. We present here an experimental approach to determine the channeling of low-energy ions in crystalline nanoparticles by measuring the sputter yield derived from SEM images taken after irradiation under various incident ion angles. Channeling maps of 30 and 20 keV Ga^+ ions in Ag nanocubes have been identified and fit well with the theory. Indeed, channeling has a significant impact on the transport of energetic ions in crystals due to the large critical angle at low ion energies, thus being relevant for any FIB-application. Consequently, the obtained sputter yield clearly differs from amorphous materials; therefore, it is recommended not to rely only on, e.g., ion distribution depths predicted by standard Monte-Carlo (MC) algorithms for amorphous materials.

ABS: 18. Density changes in amorphous silicon provoked by swift heavy ions

Sjoerd Roorda [1], Codsi Stéphanie [1], Amélie Lacroix [1], Gabrielle Long [2], Fan Zhang [3], Steven Weigand [4], Christina Trautmann [5]

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Pure and gold-doped amorphous silicon membranes were irradiated with swift heavy ions (75 MeV Ag or 1.1 GeV Au ions) and studied by small angle X-ray scattering. The samples that were irradiated with 1.1 GeV Au ions produced a scattering pattern consistent with core-shell type ion tracks of 2.0 ± 0.1 nm (core) and 7.0 ± 0.3 nm (total) radius irrespective of gold doping and consistent with radii previously observed [Bierschenk et al., Phys. Rev. B 88, 174111 (2013)].

However, the core must be less dense than the original amorphous silicon, not more dense as argued in the same report, because its density is nearly 4 % different from that of the surrounding material. The compressive stress required to maintain the core 4 % more dense would exceed the yield strength of amorphous Si. The entire track (core + shell) is slightly less dense than the surrounding material, putting it under a lateral stress consistent with the macroscopic ”hammering” deformation seen when tracks overlap. No tracks were found in samples irradiated with 75 MeV Ag ions, and no signature specific to the gold impurity doping could be observed.

ABS: 201. Swift heavy ions interaction with Group-III nitride layered structures

Miguel Sequeira [1], Flyura Djurabekova [2], Kai Nordlund [2], Isabelle Monnet [3], Clara Grygiel [3], Patrick Kluth [4], Christian Wetzel [5], Eduardo Alves [6], Katharina Lorenz [7]

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Group-III nitrides have contributed immensely to modern semiconductor technologies and are still paving new ways to further scientific revolutions. In particular, their high resistance to radiation along with high thermal and chemical stability bring these materials to the fields of extreme radiation environments such as space and nuclear reactors. Both fields face an intense and renewed interest, requiring novel materials able to withstand harsh working conditions. However, the underlying physics behind their valuable properties is yet to be fully understood, in particular concerning their behaviour under strongly ionising radiation.

Here, we will inspect such behaviour using Swift Heavy Ions (SHI), specifically Xe, Au and Pb ions with energy losses in GaN between 15 and 46 keV/nm. Supported by our previous results on single SHI impacts in GaN thin films [1], we will focus now on more realistic cases. We will begin by understanding the effect of fluence on these thin films using large scale atomistic simulations and Rutherford Backscattering Spectrometry in Channelling condition. We then study the effects of SHI in InGaN, a compound used in conjunction with GaN to make Quantum Wells in LEDs. Two-Temperature Model - Molecular Simulations and Transmission Electron Microscopy suggest that InGaN thin layers buried inside GaN barriers are surprisingly resistant to radiation. In fact, these layers appear to reduce the damage formed by the SHI even in the adjacent GaN layers. In contrast, thin films of InGaN seem to be very susceptible to radiation.

The results presented here can lead to new radiation damage mitigation techniques, predict functional changes in the electronic devices under long radiation exposure, and ultimately improve device design.

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ABS: 22. Dosimetry of heavy ion exposure to human cells using nanoscopic imaging of double strand break repair protein clusters

Günther Dollinger [1], Benjamin Schwarz [1], Pavel Kundrat [1], Stefanie Girst [1], Matthias Sammer [1], Judith Reindl [1]

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The human body is constantly exposed to ionizing radiation of different qualities. DNA double strand breaks (DSB) or even DSB clusters are created as the most harmful irradiation effects in the human cells that are meant to be responsible for acute health effects at high doses and at least additional malignancy in humans at all dose levels. In particular, the exposure to high-LET (linear energy transfer) particles increases due to new tumor therapy methods using e.g. carbon ions. Furthermore, upon radiation accidents, a mixture of radiation of different quality is adding up to human radiation exposure with unknown distributions of LET and attributed dose levels. Finally, long-term space missions such as the mission to mars also pose great challenges to the dose assessment an astronaut was exposed to.

In this study, we developed a method where it is possible to count DSB which are separated by a distance of ~ 140 nm. For that, ee counted the number of ionizing radiation induced pDNA-PKcs (DNA-PKcs phosphorylated at T2609) foci (size = 140 nm ± 20 nm) called IRIF in human HeLa cells using STED super-resolution microscopy that has an intrinsic resolution of 100 nm. Irradiation was performed at the ion microprobe SNAKE using high-LET 20 MeV lithium (LET = 116 keV/µm) and 27 MeV carbon ions (LET = 500 keV/µm). Lithium ions produce (1.5 ± 0.1) IRIF/µm track length, for carbon ions (2.2 ± 0.2) IRIF/µm are counted [1]. These values are enhanced by a factor of 2–3 compared to conventional foci counting of high-LET tracks. Comparison of the measurements to PARTRAC simulation data proof the consistency of results. We used these data to develop a measure for dosimetry of high-LET or mixed particle radiation exposure directly in the biological sample. We show that proper dosimetry for radiation up to a LET of 240 keV/µm is possible.

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ABS: 164. Controlled synthesis and plasmonic properties of doped Si nanocrystals embedded in SiO_2

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Heavily doped semiconductor nanocrystals (NCs) with IR Localized Surface Plasmon Resonance (LSPR) tunable with doping concentration have recently received a lot of attention as an emerging new class of plasmonic nanomaterials [1]. In this work, highly phosphorus (P) doped small SiNCs were fabricated in a SiO_2 matrix that protects the NCs from aging RTA by sequential low energy ion implantation of Si and P and Rapid Thermal Annealing.
Dopants are incorporated in the SiNCs core at concentrations greater than their solubility in bulk Si, according to 3D mapping using Atom Probe Tomography. Increased P dose causes significant SiNC growth. We proposed a new mechanism to explain this growth enhancement based on the presence of Si supersaturation in the matrix caused by Si recoils generated during the P implantation process, which favors the increase of Si diffusivity and the feed of large SiNCs.
According to FTIR measurements, these massively doped SiNCs support LSPR that is tunable over the MIR region and stable over time. We developed numerical simulations that accurately described the experimental data, allowing us to calculate the active carrier density and electronic scattering time [2]. We demonstrate that LSPR can be supported with as few as ten active electrons per NC, revealing a very high optical confinement and probing the collective nature of plasmons. We discover a phenomenon that is unique to embedded NCs: the appearance of avoided crossing behavior caused by hybridization between the localized surface plasmon in the doped NCs and the silica matrix phonon modes. Finally, a careful examination of the scattering time dependence versus carrier density in the small size regime reveals the appearance of a new scattering process at high dopant concentration.

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ABS: 48. McChasy 1.0: modeling of dislocations using molecular dynamics for Monte Carlo simulations of ion channeling

Przemyslaw Jozwik [1], Cyprian Mieszczynski [1], Kazimierz Skrobas [1], Jacek Jagielski [1], Frederico Garrido [2], Eduardo Alves [3], Katharina Lorenz [3]

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[2]*IJCLab, Université Paris-Saclay-CNRS, France,*
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Ion channeling is a powerful technique for analyzing structural defects in single crystals. However, separation of convoluted signals coming from different kinds of defects is barely possible without computational methods, e.g., Monte Carlo simulations. One of the codes used for that purpose is called McChasy 1.0. It simulates trajectories of light ions in small structures (~10^2 atoms), which are deformed according to implemented defect models and given defect profiles to fit experimental channeling spectra. Its recent and unique achievements are the models of extended defects, namely dislocations and dislocation loops.The model of dislocations (based on the Peierls-Nabarro approach) assumes that the bending of atomic planes adjacent to an extra half-plane of a dislocation follows the arctan function. To date, coefficients of the function (also called geometrical parameters of dislocations) have been determined for several structures using high-resolution Transmission Electron Microscopy (TEM). It was shown that the parameters decrease with the distance from the dislocation[1]. However, since TEM analysis is destructive for samples, expensive, and time-consuming, there is a need to find the possibility of their determination differently. Here we present our recent study on the modeling of edge dislocations and dislocation loops using Molecular Dynamics (the LAMMPS code). As a case study, we consider nickel (Ni), a promising material (together with its supper-alloys) for a new generation of nuclear power plants. Ni structure was deformed by introducing extra half-planes/platelets of atoms at different orientations and relaxed until a stable defect was found. Bent planes were fitted using the arctan function to determine the function coefficients. Eventually, the parameters of dislocations were used in the McChasy 1.0 code to fit channeling spectra recorded for Ni-bombarded Ni single crystals.

Reference

[1] P. Jozwik *et al.,J.Appl.Phys.,* 126(19)195107, doi: 10.1063/1.5111619.

ABS: 107. Towards an ion-implanted nuclear clock

J. Moens [1], S. Kraemer [2], J.G. Correia 3, U. Wahl [3], G. Magchiels [1], S.M. Tunhuma [1], R. Villareal [1], L.M.C. Pereira[1], P. Van Duppen [2], A. Vantomme [1]

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The extremely low-energy ^{229}Th isomeric state (8.28 ± 0.17 eV [1]) can be used to construct a nuclear clock [2], expected to outperform current electronic-shell-based atomic clocks. This isomeric state has two possible decay channels towards the ground state: radiative decay and internal conversion (IC). Because of a calculated 109 difference in half-life, IC is dominant. Blocking the IC decay channel is critical for future high-precision measurements of the transition energy and for the realization of an efficient solid state nuclear clock based on fluorescence spectroscopy. According to density functional theory calculations, doping ^{229}Th atoms into a CaF_2 crystal can block the IC decay channel if the Th dopant takes its ground state configuration: Th^{4+} in a substitutional Ca site accompanied by two F^- interstitials for charge compensation [3]. In this work we experimentally assessed whether Th dopants occupy this ground state configuration in CaF_2 when introduced using radioactive ion implantation (at ISOLDE, CERN). Since 229Th is not implanted directly but via beta-decaying parent isotopes, we used the emission channeling technique to study the lattice location of both ^{231}Th (mimicking the end of the decay chain to ^{229}Th) and of ^{229}Ac (which decays to ^{229}Th). We have found that both ^{229}Ac and ^{231}Th primarily occupy Ca substitutional positions, agreeing with the ground state configuration that can block the IC decay channel, with minimal dependence on thermal annealing and (elevated) implantation temperatures. Dopant displacements provide information on which charge compensation mechanisms are present. In parallel experiments on these implanted crystals, the ^{229}Th radiative decay has been observed for the first time, which constitutes a major milestone towards a solid state nuclear clock.

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[2] E. Peik and C. Tamm, *EPL* 61 (2003) 181.

[3] P. Dessovic *et al., J. Phys.: Condens. Matter*. 26 (2014) 105402.

ABS: 207. Production of microtubes and nanomembranes of Ga_2O_3 by ion implantation

Marco Peres [1], Duarte Esteves [1], Daniela Pereira [1], Tiago Robalo [2],
Mário Rodrigues [2], Luis Santos [3], Luis Alves [4], Eduardo Alves [1], Katharina Lorenz [1]

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Ga_2O_3 is a semiconductor with a large bandgap (~4.9 eV at room temperature), high breakdown field (> 8 MV/cm), high transparency and controllable conductivity [1], with high potential for different types of electronic and optoelectronic applications [2]. In this work, we present an innovative process to produce and modify Ga_2O_3 microtubes and nanomembranes based on ion implantation of different ion species, e.g. W, Cr and Co. This process involves two main steps: in the first step, a commercial (100) bulk crystal of Ga_2O_3 is implanted at a specific energy, fluence, and flux in order to create a strain gradient that will induce and promote the formation of Ga_2O_3 microtubes. The second step consists of transferring and unrolling these tubes. It was observed that for tubes obtained with W, Cr and Co implantation, the unrolling is achieved by thermal treatment at temperatures lower than 700 ºC in air, forming nanomembranes with areas up to 1 mm^2 and thicknesses of hundreds of nm. Atomic Force Microscopy images of the produced microtubes and nanomembranes reveal a flat surface with the presence of some terraces with heights of a few nanometers as well as a direct relation between the nanomembrane and microtube wall thickness and the implantation energy.

Characterization by X-ray diffraction and Raman microscopy confirmed the presence of residual strain induced by the implantation defects in the unrolled membranes. Strain is completely removed after a thermal treatment at temperatures higher than 1000 ºC. These nanomembranes were transferred to SiO_2/Si substrates, Ti/Au and Cr/Au metal contacts were deposited by photolithography and characterized by I-V sweeps. It was observed that the resistivity of the nanomembranes can be tuned by a voltage applied to the SiO_2/Si substrate, working in this way as a conventional field effect transistor.

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[2] Higashiwaki and G. H. Jessen, *APL* 112 (2018) 060401.

ABS: 145. Fast recovery of ion-irradiation-induced defects in $Ge_2Sb_2Te_5$ thin films at room temperature

Martin Hafermann [1], Robin Schock [1], Chenghao Wan [2], Jura Rensberg [1], Mikhail A. Kats [2], Carsten Ronning [1]

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Chalcogenide-based phase-change materials, such as $Ge_2Sb_2Te_5$ (GST), can be fast and repeatedly switched by external stimuli between crystalline and amorphous states, typically accompanied by a tremendous difference of its electrical and optical properties. This is not only already been used in non-volatile electronic memory and optical data storage devices but is also of enormous interest for active optical metasurfaces. Other than applying a heat stimulus, such as thermally, optically, or electrically, to induce the change of state, we demonstrate that ion irradiation can directly be utilized to generate lattice defects, structural disorder, and ultimately amorphize GST to trigger the phase-change from crystalline to amorphous. As the amount of damage can be precisely controlled by adjusting the ion fluence, ion irradiation of GST enables gradually tailorable properties. By monitoring the optical reflectance and electrical resistance of thin GST films during the ion bombardment, we found that several transitions from crystalline to amorphous GST occur depending on the initial crystal structure – rock-salt or hexagonal. Furthermore, we observed different annealing behavior of defects for rock-salt and hexagonal GST. The higher amorphization threshold in hexagonal GST compared to rock-salt GST is caused by an increased defect-annealing rate, i.e., a higher resistance against ion-beam-induced disorder. Moreover, we used our in-situ method to show that the recovery of defects in GST is on the time scale of seconds or less at room temperature.

ABS: 88. Atomistic modeling of the acceptor removal in p-type Si induced by neutron irradiation

Pedro Lopez [1], Maria Aboy [1], Ivan Santos [1], Luis A. Marques [1], Miguel Ullan [2], Lourdes Pelaz [1]

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The effects of irradiation with energetic light particles in Si devices is a major concern in aerospatial and nuclear applications, as they compromise device performance and shorten its lifetime. Si radiation detectors built on p-type substrates show an enhanced radiation-hardness compared to their n-type predecessors, but they are still affected by irradiation. Displacement damage is considered responsible for the reduction of effective dopants upon irradiation, process known as acceptor removal. Experimental characterization of irradiated devices shows that the effective dopant concentration exponentially decays with fluence at low fluences and that, as the initial dopant concentration increases, larger irradiation fluences are required to achieve the same deactivation fraction. This behavior can be described by phenomenological models but they lack predictability and physical insight. To perform physics-based simulations of dopant deactivation by neutron irradiation, we have implemented a multi-scale modeling scheme: we first use the SPECTRA-PKA software to obtain the energy profile of primary knock-on atoms (PKA) resulting from 1 MeV neutrons; these PKAs produce collision cascades -defects- that are simulated with the binary collision approximation code Marlowe; finally, we model defect-dopant interactions with the kinetic Monte Carlo tool DADOS and extract dopant deactivation during the aging annealing of detectors. This approach provides a comprehensive description of the amount and distribution of irradiation-induced defects and their interactions with dopants. Our results contribute to clarify some of the most intriguing features of the acceptor removal process, such as the dependence of the removal efficiency on the initial dopant concentration. We also analyze the role of impurities (O, C) and explore strategies that could improve radiation-hardness in Si devices.

ABS: 64. MgO thin film texture control using low energy ion beam assisted deposition

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Ion Beam Assisted Deposition (IBAD) is known as an alternative to the more conventional Physical Vapor Deposition (PVD) as a method to produce crystalline films with tunable texture. Comparing with PVD, the plasma is generated far from the sample being deposited, thus limiting the damage of deposited film. Moreover, the energy of the ions and the number of ions are uncoupled parameters that can be controlled independently.

Despite the advantages of IBAD, PVD is still the deposition method producing high quality MgO/CoFeB spintronic devices, namely, magnetic tunnel junctions (MTJs).

For this work, MgO was deposited in a dual Ion Beam deposition system starting from an MgO ceramic target and using one of the ion beam guns to assist the deposition. The base deposition rate of MgO without an assist beam was changed between 0.01nm/s and 0.03nm/s, using different parameter sets for the deposition gun, and supported by a simple model of the ion beam gun phase diagram. Using large assist gun power the deposition rate during an Ion Beam Assisted Deposition decreases proportionally to the assisted gun ion beam power [I+ x V+]|, as expected with an ion beam competing with the deposition process.

The MgO layers deposited were characterized by x-ray diffraction, ellipsometry and RBS. The experimental results show that the texture of MgO can be enhanced by carefully choosing the parameters of the assist ion beam for each set of deposition parameters. Furthermore, the lattice constant of MgO can be tuned between 0.209nm and 0.212nm depending on the ratio between the deposition gun beam power and the assist gun beam power.

The impact of these structural modifications on the transport properties of MgO/CoFeB MTJ microfabricated devices will be assessed.

ABS: 90. Pressurized crack gas exchange in ion implanted Silicon

Lucas Colonel [1], Frederic Mazen [2], Didier Landru [3], Oleg Kononchuk [3], Nadia Ben-Mohamed [3], François Rieutord [3]

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The implantation of Hydrogen and Helium ions in Silicon substrates at doses in the 1e16 atoms/cm^2 range leads to the formation of a buried damaged layer, with point and extended defects made of vacancies and gas atoms. Upon annealing, these defects evolve to micrometer-scale cracks lying parallel to the surface, and a controlled fracture process occurs along the implanted layer [1,2]. The thin overlayer which splits above the fracture line can then be transferred onto a host substrate using direct wafer bonding. This concept gave rise to the SmartCutTM technology, enabling an industrial scale production of Silicon-On-Insulator (SOI) substrates [3]. However, the complete scenario of the underlying mechanisms, from atomic defects to macroscopic fracture, is still being investigated. In this work, we study the buried microcracks growth mechanisms based on imaging via in-situ confocal Infra-Red microscopy.
The *in-situ* analysis of crack growth upon annealing enables us to study individual crack evolution, and allows evidence of rapid intensity changes due to microcrack height variation events. These events, which involve at least two microcraks with heights evolving in opposite ways, are analysed with respect to mechanical crack theory. They are shown to be due to gas matter exchanges. This gas exchange mechanism, occurring all along the annealing and for different implantation processes, is then identified as being one of the most important phenomena which governing the crack population growth. It explains the emergence of major-size cracks in the populations while others cracks do not grow. A discussion about the exact exchange mechanism is proposed between gas percolating through porous cracked silicon or gas diffusion in silicon with respect to time and distance.

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ABS: 113. Fabrication of diamond quantum colour centres in "split-vacancy" configuration using ion implantation

Ulrich Wahl [1], A.R.G. Costa [2], G. Magchiels [2], J. Moens [2], S.M. Tunhuma [2], R. Villarreal [2], J.G. Correia [1], G. Andrini [3], V. Pugliese [4], E. Nieto Hernández [3]

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Diamond is a promising material for the development of emerging quantum technologies, since its optically active impurities, referred to as colour centres, are among the most appealing candidates for solid-state implementation of quantum information processing devices at room temperature. In this context, single-photon emitters (which can be synthesized by ion implantation) displaying desirable opto-physical properties, i.e., high emission rate and narrow linewidth, are widely investigated. A class of very promising colour centers are those that display the so-called "split-vacancy" configuration AV, which can be pictured as a foreign atom A centered inside a diamond double vacancy, hence, showing mirror symmetry and resulting in superior optical properties.

Previously we identified Sn in the SnV "split-vacancy" configuration using the emission channeling technique (EC) from radioactive ^{121}Sn [1]. Here we report on the creation of MgV centers using 30-100 keV ion implantation into single-crystalline CVD diamond and thermal annealing, and their identification by means of ^{27}Mg EC and photoluminescence microscopy (RT to 5 K) of their 558 nm zero phonon line (ZPL) [2] at the ensemble and single-photon emitter level. Possible configurations of Mg-related centers in diamond are discussed and compared to theoretical predictions [3]. The structural configurations of Mg-related centers are compared to the one of Sn, and common features and major differences regarding mechanisms and efficiency of formation are highlighted.

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ABS: 149. Detection of single low-penetrating ions in diamond

Milan Vićentijević[1], Georgios Provatas [1], Milko Jakšić[1], Tomislav Suligoj [2]

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[2]*Faculty of Electrical Engineering and Computing, University, Croatia*

Diamond, a wide bandgap semiconductor, is one of the most promising materials for future quantum devices. For example, nitrogen vacancy (NV) quantum center in diamond could serve as an error-correcting memory unit in large-scale quantum networks [1]. Development of such devices would require arrays of quantum centers to be created close to the diamond surface, with high yield. To determine whether it is possible to implant low-penetrating single ions in diamond with high efficiency we developed a diamond detector using commercially available diamond and front-end electronics. Ion microprobe and IBIC (ion beam induced charge) technique were used to map the spatial distribution of CCE (charge collection efficiency) of the detector, a crucial parameter for single ion detection. To determine the energy resolution of the detector, as well as to map the CCE distribution close to the surface, a series of irradiations was performed with ions ranging in energy from 100 keV to 1 MeV and penetration depth from 100 nm to 12.6 um, respectively. To achieve high energy resolution, necessary for detection of low-penetrating ions, we used state of the art XGLab CUBE PRE031 CMOS charge preamplifier. The measurements were done both at room temperature and at low temperatures (down to -30°C). The successful detection of 140 keV copper ions that penetrate on average around 100nm was demonstrated and the best achieved energy resolution was below 4 keV. The optimal position of implantation sites was also determined from the spatial distribution of CCE.

Reference:

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ABS: 108. Isotopically enriched ^{28}Si substrates for quantum computers using ion implantation layer exchange: experimental results

Ella Schneider [1], Jonathan England [1]

[1] *Surrey Ion Beam Centre, Advanced Technology Institute, Unive, United Kingdom*

Donor spin qubits hosted in silicon are attractive quantum computing architectures due to their long coherence times, scalability and compatibility with CMOS industrial manufacturing. An isotopically pure ^{28}Si layer is spin-free and therefore, when cryogenically cooled, can act as a "solid-state vacuum" - an ideal environment to isolate quantum qubit states for computational operations. Having a readily available source of ^{28}Si is essential to research and future mass production of quantum computers.

This presentation will first describe an "ILE" process to produce enriched ^{28}Si layers using ion implantation ("I") and layer exchange ("LE"). ILE involves depositing Al on a native oxide free silicon substrate, implanting the Al with ^{28}Si followed by a low temperature anneal to initiate layer exchange where the ^{28}Si diffuses through the Al to either nucleate at a grain boundary or epitaxially grow on the substrate. ILE allows high implantation energies to be used (where beam transmission is maximised), reduces required fluences compared to enrichment by direct implantation into Si, overcomes surface oxidation (negating the need for an implanter UHV endstation) and self-getters isobaric impurities. A major challenge is to achieve an acceptable residual Al concentration in the ^{28}Si layer.

The presentation will then describe the current levels of isotopic enrichment, crystal quality, Al contamination and layer uniformity achieved at Surrey using 30 keV isotopically pure $^{28}Si^{+}$ implants to fluences of $6.6x10^{17}$ ions/cm^2 into 100-200nm thick Al layers followed by an anneal at 500°C for 1 minute. The layers were analysed for enrichment by ToF-SIMS and for crystal quality and Al content by S/TEM-EDS. ILE cannot yet meet all the requirements of 'quantum-grade' silicon. Improvements, especially those to reduce residual Al retention and improve thickness uniformity will be discussed.

ABS: 96. Experiments and modelling to understand the production of isotopically pure Si and Ge layers by implanted layer exchange for quantum computing

Jonathan England [1], Ella Schneider [1]

[1] *University of Surrey, Guildford*

We are developing an implanted layer exchange (ILE) process [1-3] to produce isotopically pure Si and Ge layers for the manufacture of quantum computers. ILE uses standard implantation to implant ions of a single isotope into the surface of an Al film deposited on a substrate wafer. A post implant, layer exchange anneal causes the isotopically selected atoms to diffuse through the Al and grow on the substrate. The ultimate ILE process would produce non-defective, single crystal, isotopically pure, ^{28}Si or ^{74}Ge layers of uniform thickness containing no Al contamination. We believe a key route to achieving these goals is to ensure that ions implanted into the surface of an Al film rapidly diffuse during the anneal to epitaxially grow on a substrate rather than nucleate at grain boundaries in the Al. To develop this idea, we have compared ILE of Si after large area implants in a Danfysik beamline implanter to ILE of Ge after small area (100 micron^2) implants using a SIMPLE implanter [3]. Suppressing epitaxial growth during the anneal by damaging the substrate surface via implantation or by poor removal of native oxide before Al deposition did indeed lead to the formation of large poly crystals, observed using top down optical and secondary electron microscopy and cross sectional TEM. Interpretation of these observations has been underpinned by the use of TRIDYN [4] to model the implant profiles. A kinetic Monte Carlo model based on SPPARKS [5] is being developed to investigate the mechanisms that compete during the anneal part of the layer exchange process. We will present a selection of our observations and current understanding that identify the greatest challenges that will need to be overcome if we are to perfect our ILE method.

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[5] Plimpton et al https://spparks.github.io

ABS: 53. Elastic electron scattering experiments: an alternative to light ion irradiation

Paulo F. P. Fichtner [1], Barbara Konrad [2], Franciele S. M. de Oliveira [2],
Mauricio J. Nogueira [3], Zacarias E. Fabrim [3], Mariana M. Timm [4], Andre R. Muniz [5]

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[2]*Graduate Program in Materials Science, UFRGS, Brazil*
[3]*Institute of Physics, UFRGS, Brazil,* [4]*Université de Montpellier, CNRS, ENSCM, France*
[5]*Department of Chemical Engineering, UFRGS, Brazil*

The properties of surface located atoms affect a myriad of size-dependent physical properties P of nanoscopic objects. This includes, for example, cohesion energy, melting temperature, surface diffusion energy, surface binding energy, heat capacity, and Young modulus. Their size-dependent values ΔP/Po (scaling as ΔPi/Poi≈ΔPj/Poj, where Po is a fiducial state value) allow predicting all Pj variations if Pi and Poi are known. This work reports on the use of elastic electron scattering processes to modify the size/shape of nanoscopic objects and determine: the atomic surface binding energy of Si and N atoms in silicon nitride thin films;1 the binding energy of Ag atoms in Ag nanoparticles,2 and the surface migration energies of Au atoms in Au thin films.3 The electron irradiations are performed at distinct energies (80-200 keV) in a 200 kV transmission electron microscope allowing for direct observations of object size or shape modifications. The electron beam parameters (energy and current density) are fine-tuned to avoid sample heating and promote displacements only from surface atoms. The results are compared with He^+ and Ne^+ irradiation experiments. The discussions comprise model calculations accounting for size-dependent properties for Ag and Au nano-objects. Recent molecular dynamic analyses for the elastic electron collisions in Au nano-objects suggest that the surface migration of Au atoms is rate controlled by atoms located at specific positions along the film edges.

References:

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[3] F. S. M. de Oliveira, M. J. Nogueira, Z. E. Fabrim and P. F. P. Fichtner, *J. Mater Sci: Mater Electron* 32 (2021) 13291-13304.
[4] F. S. M. de Oliveira, M. J. Nogueira, A. R. Muniz and P. F. P. Fichtner, work in progress.

POSTER PRESENTATIONS

NUMBER OF POSTERS PRESENTATIONS: 107

POSTERS SESSION #1

TOPIC: Basic mechanisms and irradiation effects

ID	FirstName	LastName	ShortTitle
24	Claudia	Montanari	Systematic study of the stopping power in Lanthanides
28	Mariana	Timm	Modification of thermal and electrical properties of amorphous $CrSi_2$ thin films by Ne and Al ion implantation
31	Norberto	Catarino	Codeposit *vs.* ion implantation for D retention on beryllium-based plasma-facing materials
48	Przemyslaw	Jozwik	McChasy 1.0: modeling of dislocations using molecular dynamics for Monte Carlo simulations of ion channeling
62	Rodrigo	Mateus	Deuterium retention in W and W-Ta coatings
68	Nathalie	Moncoffre	The French Research Federation of Accelerators for Irradiation and Analysis of Molecules and Materials
70	Alma	Dauletbekova	Luminescence of zirconium dioxide ceramic compacts irradiated with swift heavy ions
72	Agata	Zaborowska	High *vs* low energy ion implantation impact on alumina coatings properties
73	Damjan	Ivekovic	Raman measurements of ion irradiation induced damage in HOPG
75	Katarzyna	Mulewska	Ion irradiation effects on hardening mechanisms of crystalline iron: nanoindentation experiments and multiscale modeling
79	Patrick	Kirscht	Improvement of light element analysis by external proton beam
80	Frederico	Garrido	Alpha-decay damage in natural apatite: buildup and recovery mechanisms for thermochronological applications
83	Alma	Dauletbekova	Luminescence and tracks in BaFBr crystals irradiated with fast Kr ions
94	Lehlohonolo	Lisema	Synthesis and modification of Boron Nitride nanotubes using ion implantation
98	Magdalena	Gaweda	Surface and in-depth structural changes in various graphitic materials irradiated with noble gases described with Raman imaging
99	Mamour	Sall	Point defect creation in AlN: coupled effects of oxygen impurities and ion energy deposition mechanisms
100	Pavo	Dubcek	Lowering the threshold for high energy heavy ion irradiation damage in Al_2O_3, MgO and CaF_2
103	Matej	Kubiš	Multi-energy high fluence he ion implantation for micromechanical testing of materials
104	Daniel	Kiphart	Magnetic domains without domain walls in Tb/Co layered system after patterning by Ga^+ focused ion beam
112	Malgorzata	Frelek-Kozak	Investigation of mechanical and structural properties of nickel-based alloys submitted to high energy ion irradiation
116	Weilin	Jiang	Ion Irradiation study of lithium silicates for fusion blanket applications
120	Md Shadab	Anwar	Irradiation-induced magnetostructural transition in $Fe_{60}V_{40}$ Alloy Thin Films
123	Serhii	Sorokin	Transport properties of FeAl under ion irradiation
131	Miguel	Crespillo	Non-radiative decay kinetics of self-trapped excitons in strontium titanate under energetic heavy-ion irradiation
132	Miguel	Crespillo	Ionoluminescence as a real-time sensor of damage to the anion sublattice of ion irradiated strontium titanate
133	Miguel	Crespillo	The ionoluminescence kinetics of amorphous silica at cryogenic temperatures — competition and interplay between emitting centers
137	Iván Santos	Tejido	Atomistic study of damage generated from low energy collective collisions in SiC

ID	FirstName	LastName	ShortTitle
144	Eli	Kolodney	Velocity correlated emission of secondary clusters in fullerene - solid impact : probing extreme subsurface spike conditions
146	Chase	Hargrove	Helium induced bubble formation in dispersion strengthened tungsten alloys for fusion applications
151	Lin	Shao	Irradiation response and mechanical property changes of conventionally and additively manufactured 316L stainless steels
153	Zoltan	Szaraz	The effect of lead ion irradiation on microstructure and micromechanical properties of T91 steel
154	Ashrakat	Saefan	Effects of helium implantation on mechanical properties at the tungsten-carbide interfaces using nano-indentation technique
157	Graeme	Greaves	Irradiation effects in 3C silicon carbide
159	Fabian	Naab	Michigan Ion Beam Laboratory For The Study of Radiation Effects
162	François	Robert	A magnesium mass independent isotopic fractionation revealed by NanoSims analyses of micrometer grains condensed in plasma.
167	João	Gaspar	Degradation and recovery of proton-irradiated Cu(In,Ga)Se_2 Solar Cells
169	Nikolay	Cherkashin	Most stable surface-emerging defects in ion implanted Si annealed at extreme temperature
170	Tiago	Pardal Fernandes	Proton Irradiation effects on hexagonal boron nitride crystals
172	Cláudia	Figueiredo	Effect of swift heavy ions in AlGaN compound semiconductors
181	Alexis	Dujarrier	Influence of the microstructure of additively manufactured Ni-20Cr microstructure on aging under irradiation
182	Eduardo	Alves	Irradiation of bulk W at the PF-1000U device with deuterium plasma discharges
183	Nuria	Gordillo	An approach to amorphous topological superconductors by ion beam irradiation
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39	Andreas	Kling	Creation of gold nanoparticles in langasite
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61	Felix	Linß	Manipulation of silicon etching with surfactant sputtering
66	Mateusz	Kowacz	Strong asymmetric modification of interfaces in Ir/Co/Pt layered system induced by low energy Ga^+ ion bombardment
106	Oleksandr	Romanenko	Comparison of PMMA shrinkage in ion beam lithography: PMMA on glass substrate vs free standing PMMA film
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20	Felix	Junge	Doping of 2D materials by ultra-low energy ion implantation
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34	Sunmog	Yeo	Hydrogen gas detection using ion beam irradiated graphene
89	Alena	Nikolskaia	Modification of Ga_2O_3 by ion implantation
91	Alena	Nikolskaia	Light-emitting 9R hexagonal silicon phase synthesized by ion implantation
93	Matthew	Sharpe	Time of flight elastic recoil detection and rutherford backscattering spectrometry analysis of reRAM devices
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109	Daniela	Pereira	Incorporation of modified MoO_3 crystals and pseudo-layers into Field Effect Transistors
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130	Joseph	Graham	Fabrication of novel plasmonic nanostructures in silica using ion irradiation, etching, and nanoparticle deposition
134	Alexandre W.	Lussier	Towards relaxation and stress micro-mapping in amorphous silicon by raman spectroscopy
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142	Dmitrii	Moldarev	Modification of photochromic properties of oxygen-containing yttrium hydride films by irradiation using keV ions
148	Xing	Wang	Role of carbide-tungsten interfaces on improving resistance to helium ion irradiation of dispersion-strengthened tungsten
150	Duarte	Magalhães Esteves	Sensitising the Cr^{3+} luminescence by irradiation-induced defects in β-Ga_2O_3
156	Esther	Enríquez	High energy ion irradiation of MgF_2 for improving the physical properties for FUV applications
158	Joao	Salgado Cabaco	Properties of Cr_2AlC thin films disordered by ion-irradiation
165	Gabriel	Marques	Luminescent properties in CVD grown diamond single crystal modified by laser irradiation and ion implantation
177	Afonso	Caçador	Defect and strain profiles caused by ion implantation in gallium nitride
198	Yadong	Wei	Multiple phases and electronic structures of silicon monoxide
200	Petter	Ström	3D ferromagnetic microstructures produced in paramagnetic thin films by ion implantation through masks
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TOPIC: Ion Beam processing of materials

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9	Abdalla	Zaki	Effects of helium on the structural evolution and migration behavior of silver and strontium implanted into polycrystalline SiC
17	David	Jamieson	Ion beam modified silicon: both 28-Si enrichment and donor doping for quantum devices
29	Xuhui	Yao	Effective Li dendrite penetration reduction in solid-state batteries through Xe ion created surface compressive stress
30	Claudia	Montanari	Twenty years of electronic stopping power of ions in matter: tendencies, areas of interest and lack of data
44	Jiranat	Techarang	Low-energy heavy-ion beam capable of simultaneous induction of multiple chromosomal aberrations for rice mutation
45	Jiranat	Techarang	Low-energy ion beam induced brown-planthopper resistant thai jasmine rice mutants
56	Mariapompea	Cutroneo	Overview of polyethylene terephthalate foils patterned using low energy ions for the realization of micromembranes
57	Jarmila	Degmova	The effect of oxide dispersoids on the helium bubble formation in advanced structural materials for nuclear applications
58	Filip	Ferencik	Ion beam synthesis of high oxidation state palladium and copper oxides
65	Marta	Dias	Behavior of Cu-Y_2O_3 and CuCrZr-Y_2O_3 composites as thermal barriers for nuclear fusion applications
69	Ricardo	Martins	Irradiation damage on CrNbTaVWx high entropy alloys
71	Abdirash	Akilbekov	Radiation resistance of aluminum-magnesium spinel: optical effects of high-energy ion irradiation
74	Erik	Rohkamm	Characterization of a RF-excited broad ion beam source relevant for the machining of surfaces used for optical applications
77	Aurelie	Gentils	Overview of the JANNuS-SCALP facility at Orsay: ion beams for synthesis, modification and analysis of materials
78	Darina	Manova	In-situ X-ray diffraction for elucidating the initial formation of expanded austenite during ion nitriding
81	Jill	Kessler	Phase control of multivalent vanadium oxides by ion-beam sputter-deposition
84	Martin	Becker	Capabilities of ion-beam processing with radio-frequency ion sources
85	Claudia	Montanari	Machine learning modeling of the stopping power experimental data
101	Marko	Barac	Optimization of MeV TOF SIMS technique for inorganic targets in the low primary ion beam energy mode
115	Ulrich	Wahl	Fluence and doping dependence of lattice location of ion implanted Mg in GaN
135	Karolina	Pagowska	Selected aspects of GaN doping by Si^+ ion implantation and subsequent activation annealing
141	Matteo	Gardella	Maskless ion beam sputtering deposition of two-dimensional transition metal dichalcogenides Van Der Waals heterostructures
155	Miguel	Crespillo	Processing of Al_2O_3 with High-energy heavy-ion irradiation and pulsed laser irradiation for optical waveguides fabrication
174	Kacper	Sierakowski	Investigation of zinc diffusion for various crystallographic directions in GaN grown by HVPE
175	Kacper	Sierakowski	Investigation of beryllium diffusion for various crystallographic directions in GaN grown by HVPE

TOPIC: Ion Beam processing of materials

ID	FirstName	LastName	ShortTitle
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TOPIC: New accelerator systems and single ion implantation

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102	Pavol	Noga	Recent developments in the CAMBO Ion Beam Laboratory
118	Le	Xiaoyun	Influence of magnetic field of magnetically insulated diode on emission behavior of intense pulsed ion beam
223	João	Cruz	Nitrogen targets production and characterization for 14N(p,γ)^{15}O reaction measurement at LUNA-MV
224	Mason	Adshead	Isotopic resolution in a novel pulsed focused ion beam system

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ABS: 24. Systematic study of the stopping power in Lanthanides

Claudia Montanari [1], Jesica Peralta [1], Alejandra Mendez [1]

[1] *Institute of Astronomy and Space Physics, CONICET and Univer, Argentina*

The knowledge of electronic stopping is important in many fields, from basic physics to technology and medicine [1]. We focused on lanthanides due to its electronic complexity (open 4f-subshell, need of relativistic description [2]); the importance of rare-earth oxides [3], and discrepancies among experimental data. In this work we perform a systematic study of the stopping cross sections from Ce (Z=58) to Lu (Z=71). Fully relativistic atomic structure calculations were developed for the atomic wave functions and binding energies. These values are the only inputs of our full theoretical calculations for bound electrons using the shellwise local plasma approximation [4]. Our results cover an extended energy region by considering separately the free electron gas (FEG) and the bound electrons as in [4]. For Gd the present results describe nicely the latest experimental data around the stopping maximum [5]. For others such as La, Dy, Lu, Tb we note disagreements with old data [6]. We will show that the systematic study of all the lanthanides states some doubts about the SRIM predictions [7] for this type of targets.

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ABS: 28. Modification of thermal and electrical properties of amorphous $CrSi_2$ thin films by Ne and Al ion implantation

Mariana Timm [1], Erwan Oliviero [1], Weanxiang Sun [2], Severine Gomes [2], Georges Hamaoui [3], Paulo Fichtner [4], Nicole Fréty [1]

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[2]*CNRS, INSA Lyon, CETHIL, Univ Lyon, UMR5008, 69621 Villeurba, France,*
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$CrSi_2$ (chromium disilicide) is a potential thermoelectric material that has attracted attention in the last few years due to its semiconductor properties and high thermal stability. In this sense, the ion implantation technique can be used to tailor the physical properties of different materials and enhance their semiconductor and/or thermoelectric performance. This work investigates the influence of different ion species and implantation conditions on the microstructure, electrical resistivity, and thermal conductivity behaviors in amorphous $CrSi_2$ thin films. ~ 260-nm-thick $CrSi_2$ films were produced by magnetron sputtering and deposited onto a SiO_2/Si substrate. Samples were implanted at room temperature and at 250 ºC either with Ne or Al ions to form a concentration-depth plateau reaching a concentration of 1.0 at.% (Ne), or 0.008 at.% (Al).

TEM and STEM-EDX were used to characterize the samples' microstructure and elemental distribution observed in cross-sectional TEM species. The electrical resistivity was measured by the van der Pauw method, and the thermal conductivity measurements were obtained with SThM.

The results obtained show that room temperature Al and Ne implantations cause the reduction of the electrical resistivity as compared to the non-implanted film. In contrast, the electrical resistivity values are significantly higher for Ne and Al implantations in heated substrates. For all implanted samples, the thermal conductivity is reduced concerning the non-implanted film value. The electric and thermal behaviors are discussed considering radiation-induced damage and the formation of nanocrystallites and nanocavities (or bubbles) observed by TEM.

ABS: 31. Codeposit vs. ion implantation for D retention on beryllium-based plasma-facing materials

Norberto Catarino [1], Rodrigo Mateus [1], Corneliu Porosnicu [2], Cristian Langu [2],
vko Siketić; [3], Ivančica Bogdanović; Radović [3], Antti Hakola [4], Eduardo Alves [1]

[1]*Instituto de Plasmas e Fusão Nuclear, Instituto Superior Téc, Portugal,* [2]*National Institute for Lasers, Plasma and Radiation Physics, Romania,*
[3]*Ruder Bošković; Institute, Croatia,*
[4]*VTT Technical Research Centre of Finland, Finland*

Beryllium tiles will be use in the next generation of fusion reactors. Tiles will cover chamber walls and will be subjected to extreme operating conditions such as erosion, radiation damage, and fuel trapping. One method for studying retention processes is to manufacture various types of Be coatings in a laboratory.

We present results obtained on 400 nm Be-C-O-D films deposited on both Si and W plates and compared to D implanted films. The efficiency of the two methods for incorporating D into the films is compared, as well as the role of the interlayers between the films and the substrates in the retained contents.

At room temperature, implanted films were prepared using 15 keV D ion beams. To avoid major morphological changes that could enhance gas release, the fluence was limited to 2 x 10^{17} ion/cm^2.

Samples were analyzed with ion beam techniques namely, elastic backscattering spectroscopy (EBS), Rutherford backscattering spectroscopy (RBS) and nuclear reaction analysis (NRA) making use of 1600 keV ^{1}H, 2000 keV ^{4}H and 1000 keV ^{3}He$^+$ incident beams, respectively.

To ascertain the aging effects on the samples, some months after implantation, the coatings were analyzed by time of flight elastic recoil detection (TOF-ERDA) to evaluate D release. The results point to ion implantation as an alternative to in-situ loading for deuterium incorporation into thin layers, with retained contents close to 3 at.% of D easily obtained for the used ion fluence. The depth profiles of Be, C, O, and D in thin layers evaluated by EBS/RBS/NRA or TOF-ERDA are compatible. The release of D in aged samples also agrees with previous findings.

For the case of thick coatings (5-10 μm), the limited ion implantation to thin layer imposes a saturation concentration of 2 x 10^{17} ion/cm^2, the amounts of D obtained by co-deposition, on the other hand, are independent of thickness but are dependent on defect density and C incorporation.

ABS: 48. McChasy 1.0: modeling of dislocations using molecular dynamics for Monte Carlo simulations of ion channeling

Przemyslaw Jozwik [1], Cyprian Mieszczynski [1], Kazimierz Skrobas [1], Jacek Jagielski [1], Frederico Garrido [2], Eduardo Alves [3], Katharina Lorenz [3]

[1]*National Centre for Nuclear Research, Poland,*
[2]*IJCLab, Université Paris-Saclay-CNRS, France,*
[3]*IPFN, IST-CTN, Universidade de Lisboa, Portugal*

Ion channeling is a powerful technique for analyzing structural defects in single crystals. However, separation of convoluted signals coming from different kinds of defects is barely possible without computational methods, e.g., Monte Carlo simulations. One of the codes used for that purpose is called McChasy 1.0. It simulates trajectories of light ions in small structures (~10^2 atoms), which are deformed according to implemented defect models and given defect profiles to fit experimental channeling spectra. Its recent and unique achievements are the models of extended defects, namely dislocations and dislocation loops.The model of dislocations (based on the Peierls-Nabarro approach) assumes that the bending of atomic planes adjacent to an extra half-plane of a dislocation follows the arctan function. To date, coefficients of the function (also called geometrical parameters of dislocations) have been determined for several structures using high-resolution Transmission Electron Microscopy (TEM). It was shown that the parameters decrease with the distance from the dislocation[1]. However, since TEM analysis is destructive for samples, expensive, and time-consuming, there is a need to find the possibility of their determination differently. Here we present our recent study on the modeling of edge dislocations and dislocation loops using Molecular Dynamics (the LAMMPS code). As a case study, we consider nickel (Ni), a promising material (together with its supper-alloys) for a new generation of nuclear power plants. Ni structure was deformed by introducing extra half-planes/platelets of atoms at different orientations and relaxed until a stable defect was found. Bent planes were fitted using the arctan function to determine the function coefficients. Eventually, the parameters of dislocations were used in the McChasy 1.0 code to fit channeling spectra recorded for Ni-bombarded Ni single crystals.

Reference

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ABS: 62. Deuterium retention in W and W-Ta coatings

Rodrigo Mateus [1], Norberto Catarino [1], Marta Dias [1], Luís Cerqueira Alves [2], Zdravko Siketić; [3], Iva Bogdanovic Radovic [3], Antti Hakola [4], Eduard Grigore [5], Eduardo Alves [1]

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Tungsten is the main plasma facing material for nuclear fusion applications. Nevertheless, it has a high ductile-to-brittle temperature, which results in intense thermal stress under periodic and operative plasma discharges. Like W, Ta has low neutron activation but has higher ductility, toughness, radiation resistance and higher hydrogen diffusivity, leading to lower retention rates for hydrogen isotopes. Therefore, the development of W-Ta alloys to improve the behaviour of W-based materials under irradiation is attractive for fusion applications.

In this experiment, W and W-Ta(5 at.%) coatings were produced via high power impulse magnetron sputtering (HiPIMS). Afterwards, they were irradiated at room temperature with a single deuterium implantation (30 keV $^{2}H_{2+}$ ion beam) or a dual deuterium plus helium implantation (a first implantation with a 30 keV $^{2}H^{2+}$ beam, followed by a second implantation using a 30 keV $^{4}He^{+}$ beam). All the individual deuterium and helium fluences were of 5×10^{17} ion/cm². A homogeneous distribution of Ta in the W matrix was observed by proton induced X-ray emission with a nuclear microprobe (μ-PIXE) and Ta quantification was precisely accessed with a broad proton beam by PIXE. Additional techniques used for elemental characterization were elastic backscattering spectrometry (EBS) to measure the coatings' thickness, time-of-flight elastic recoil detection (ToF-ERDA) to better characterize light element contents in the implantation zone and nuclear reaction analysis (NRA) to quantify the retained deuterium. Any modification imposed by surface irradiation became visible during scanning electron microscopy (SEM) observations. Despite high retention rates for deuterium after high energetic ion irradiation, the experimental results are promising, while they always reveal retained amounts in W-Ta significantly lower than those observed in W after single (deuterium) but also dual (deuterium plus helium) irradiations.

Acknowledgments

The present IPFN/IST activity received financial support from Fundação para a Ciência e a Tecnologia, Portugal, through projects UID/FIS/50010/2020 and PTDC/FIS-PLA/31629/2017. Particularly, the analytical work made use of a detection system developed for deuterium quantification under the scope of the PTDC/FIS-PLA/31629/2017 project.

ABS: 68. The French research federation of accelerators for irradiation and analysis of molecules and materials

Nathalie Moncoffre [1]

[1]*CNRS/IP2I and Lyon 1 university, France*

This contribution aims at presenting the French EMIR&A network (Federation of Accelerators for Irradiation and Analysis of Molecules and Materials). It is built around several structuring and innovative facilities, that are shared to provide access to ion and electron beams to the largest scientific community at the national and international scale. The facilities are complementary by the nature and energies of the accelerated particles, the associated Ion beam Analysis and in situ material characterization instrumentation such as Transmission Electron Microscopy (TEM), Raman spectroscopy, X-Ray Diffraction (XRD), infrared spectroscopy, or optical absorption.

Once a year, this set of accelerators and instrumentations is made available to users everywhere in the world, after evaluation by an international scientific committee. It is a recent step towards an overall national structure for ion and electron beam science and applications such as those which nearby countries have implemented (e.g. the UK National Ion Beam Centre, Surrey, or the Helmholtz-Zentrum at Dresden-Rossendorf in Germany). It aims at connecting the scientific communities that study condensed matter with ion or electron accelerators, to establish new collaborations through the pooling of these instruments and the associated expertise.

EMIR&A includes a total of 15 ion and electron accelerators installed on 11 platforms distributed over six sites, mainly in the northern half of France (Caen, Orléans) and in the Paris region (Paris, Palaiseau, Orsay, Saclay). Those facilities are owned by many Higher

Education institutions, CNRS (National Scientific Research Centre), Universities, Grandes Ecoles and CEA (French Alternative Energies and Atomic Energy Commission), making this structure a worldwide unique portal for such research.

More information about the facilities and contact persons can be found at https://emira.in2p3.fr/

ABS: 70. Luminescence of zirconium dioxide ceramic compacts irradiated with swift heavy ions

Alma Dauletbekova [1], Sergei Nikiforov [2], Sergei Zvonarev [2], Darya Ananchenko [2], Amangeldi Zhunusbekov [1], Zein Baimukhanov [1], Gulzhanat Akhmetova-Abdik [1]

[1]*L. N. Gumilyov Eurasian National University, Kazakhstan,* [2]*Ural Federal University, Russia*

Phosphors based on ZrO_2 are used for the manufacture of oxygen sensors, biological sensors, laser technology devices, optoelectronic devices, UV and ionizing radiation dosimeters, scintillators, high-energy radiation visualization devices, etc. For these applications, an important task is to ensure the stability of the luminescent properties of the material when exposed to various types of radiation. This problem is especially relevant when using ZrO_2-based devices in the nuclear industry and space technologies.

In present work ZrO_2 compacts were studied. Ceramic compacts were formed by cold uniaxial pressing of nanostructured zirconium dioxide powder produced by the plasmochemical method. The samples were irradiated with 200 MeV Xe and 4.8 MeV N ions in fluence range (10^{10}- 10^{14}) cm^{-2} at cyclotron DC-60 (Nur-Sultan, Kazakhstan).

Photoluminescence(PL)spectra were observed under excitation light with wavelength 230 nm.Tthere is one intense band with a maximum 480 nm in the fl spectrum The dependence of the PL intensity on the fluence is established. Thermoluminescence (TL) was measured in the linear heating mode at a rate of 2 K/s in the spectral range of 200-600 nm. TL curves of the virgin and irradiated compacts showed two TL peaks at 330-430 K and 430-550 K. The peak at 430-550 K is most intense in the nonirradiated sample. The greatest change in the TL intensity of this peak occurs in the sample irradiated with N ions: Three times the intensity decreases The kinetic parameters of the TL peak at 430-550 K (kinetic order b, activation energy E, and frequency factor S) were determined from the analysis of the TL curves. Also, XRD studies have shown changes in the structure of irradiated ceramics. Analysis of the results showed a complex nature of changes in the properties of ceramics irradiated by SHI.

ABS: 72. High *vs* low energy ion implantation impact on alumina coatings properties

Agata Zaborowska [1], Łukasz Kurpaska [1], Fabio Di Fonzo [2], Alexander Azarov [3], Marcin Turek [4], Małgorzata Frelek-Kozak [1], Jacek Jagielski [1]

[1]*National Center for Nuclear Research, Poland,* [2]*Istituto Italiano di Tecnologia, Italy,* [3]*University of Oslo, Norway,* [4]*Maria Curie Skłodowska University, Poland*

It is well known that ion irradiation can be successfully used to reproduce microstructural features triggered by neutron irradiation. Although the implantation process brings many benefits, it is also associated with several drawbacks. For example, the penetration depth of the ion beam in the material is very limited. Consequently, extracting information exclusively from the modified volume may be challenging, and therefore extreme caution must be taken when interpreting obtained data.

Our work aims to compare the findings of nanomechanical studies conducted on implanted thin amorphous ceramic coatings to different depths. In our experiment, 1 µm thick Al_2O_3 films deposited on 316L SS by Pulsed Laser Deposition (PLD) were ion irradiated at room temperature with 250 keV and 1,2 MeV Au^+ ions up to the dose of 25 dpa. Afterward, we studied the influence of ion irradiation on nanomechanical properties of virgin and ion irradiated specimens by using the nanoindentation technique.

It was found that irradiation led to the slight softening of the investigated coating. Interestingly, although the data on low energy irradiated material was affected by several effects, the qualitative relationship between nanohardness and irradiation damage level appears to be very similar for both experimental energies. Structural analysis revealed that the coating possesses a fully amorphous structure that does not evolve under irradiation conditions. These findings indicate that alumina coating remains amorphous and maintains its structural integrity under RT ion irradiation over the whole range of tested doses. Additionally, obtained results suggest that quantitative assessment of the mechanical changes using nanoindentation may be feasible even for very shallow implantation depths.

ABS: 73. Raman measurements of ion irradiation induced damage in HOPG

Damjan Ivekovic [1], Andreja Gajovic [1], Marko Karlusic [1]

[1] *Ruder Boskovic Institute, Croatia*

Irradiation by high energy ion beams is among the most important tools for modification of materials at the nanometer scale. Therefore, it is of crucial interest to understand the underlying phenomena resulting in the ion induced damage. In this study, we have applied Raman spectroscopy for estimation of damage done in HOPG (Highly Ordered Pyrolytic Graphite) by high energy beams (oxygen, silicon, copper and iodine beams in the energy range between 1–23 MeV).

As it is widely known, G peak measures sp2 vibrations of the pristine graphite structure and D peak is measure of emergent carbon modes due to the defected structure. The ratio of these two peak intensities (ID/IG) is generally considered as an indication of level of damage. We observed an increase of ID/IG ratio with increasing ion fluence.

With the presented experimental data from different ion beam irradiations, it is possible to estimate the relative efficiency of electronic and nuclear stopping induced damage in HOPG.

ABS: 75. Ion irradiation effects on hardening mechanisms of crystalline iron: nanoindentation experiments and multiscale modeling

Katarzyna Mulewska [1], Francisco Javier Dominguez-Gutierrez [1], Fabrizio Rovaris [1], Łukasz Kurpaska [1], Amirhossein Naghdi [1], Anna Kosińska [1], Iwona Jóźwik [1], Witold Chromiński [1], Stefanos Papanikolaou [1], Mikko Alava [1]

[1] *NOMATEN CoE, National Centre for Nuclear Research, Poland*

Ferritic/martensitic steels are structural materials with several promising mechanical properties used as the core components of future generations for fission and fusion reactors [1]. To better understand the behavior of these steels in extreme working conditions, experimental work has to be supported by numerical modeling [2]. This study investigates the mechanical properties of pristine and ion-modified specimens experimentally by nanoindentation and Electron Backscatter Diffraction (EBSD) [3] and computationally by molecular dynamics (MD) simulations and discrete dislocation dynamics (DDD) combined with finite element method. We observed the elastic to plastic transition in pristine and irradiated polycrystalline iron in both methods. The sample was irradiated at 300ºC with 5 MeV Fe ions up to a dose of 2.4 dpa at the peak damage. We noticed the appearance of a sudden displacement burst during the loading process in the experimental measurements. This phenomenon is connected with increased shear stress in a small subsurface volume until it reaches a critical value at which dislocation slip is activated, either by mobilization of pre-existing dislocations or by dislocation nucleation, which is visible as a pop-in. Modeled dislocation nucleation mechanisms by MD/DDD at different crystal orientations provide an insight to the mechanical response of the material and its plastic instability. Described events allow us to understand better the behavior of the model material submitted to ion irradiation for applications in extreme operating conditions.

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ABS: 79. Improvement of light element analysis by external proton beam

Patrick Kirscht [1], Felix Junge [1], Hans Hofsaess [1]

[1] *Georg-August-Universitaet, Germany*

We present new developments for ion beam analysis (IBA) using an external proton beam with an energy range of 2.0-2.5 MeV for simultaneous NRA, RBS, PIXE and C-ERDA measurements [1]
The primary objective is the detection of light elements, such as hydrogen and lithium in free standing foils or thin films.
We will show that the concentrations of light elements (H, Li, N, C, O, F) of materials can be determined outside of vacuum chambers which is essential for porous or humid samples. Furthermore, the destructive influence of the proton beam to the samples during the measurement is shown.
As a further upgrade, we are working on an extension that allows rotation of the sample and thus counteracts unwanted effects such as channeling. This provides the possibility to compare the data with simulations, which will be done, with the new SDTrimSp/ImintDyn [2] software.
With present results for the detection limit for hydrogen, lithium and flourine. The setup for Li detection will be further improved by upgrading the detectors for the U+2077 Li(p,U+03B1) U+2074 He reaction.

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ABS: 80. Alpha-decay damage in natural apatite: buildup and recovery mechanisms for thermochronological applications

Dee Jay Cerico [1], Frederico Garrido [1], Cécile Gautheron [2], Aurélie Gentils [1], Stéphanie Jublot-Leclerc [1], Florian Pallier [1], Przemyslaw Jozwik [3], Cyprian Mieszczynski [3], Lech Nowicki [3], Cyril Bachelet [1]

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Thermochronology is an earth science discipline involved in the reconstruction and timing of past geological processes. In this field, accessory minerals such as apatite are collected from rocks to determine Helium (He) ages used in modeling rock thermal histories. As alpha-decay damage in apatite affects thermochronological modeling, the kinetics and mechanism of two physical processes linked with alpha decay events are studied in this research using ion beam techniques and microscopy: (1) ballistic, radiation damage buildup separately-induced by the recoil nuclei and alpha particles and (2) the athermal, ionization-induced recovery of pre-existing defects attributed to the electronic energy loss of alpha particles. The results of this study strongly suggest that the buildup of radiation damage in apatite could be described as a two-step kinetic process, and that each step could be characterized by the presence of specific main types of irradiation-induced defects. The first step is a transformation from a near perfect crystalline structure to a partially-damaged one, while the second step results in a further structural transformation leading to a highly-damaged state. Amorphization due to alpha recoil irradiation and helium bubble formation due to alpha particle irradiation are the two physical mechanisms that led to rapid apatite crystal destabilization in the second step. With regard to ionization recovery, experimental results suggest that only certain types of defects such as amorphous clusters could be efficiently recovered by alpha particles, and that point defects are likely less sensitive to this recovery effect. This means that alpha-particle induced recovery of pre-existing defects does not occur or is likely insignificant for natural apatites with very low U and Th concentrations (few hundreds of ppm).

ABS: 83. Luminescence and tracks in BaFBr crystals irradiated with fast Kr ions

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In this work using photoluminescence (PL), optical luminescence induced by X-Ray (XEOL), optical absorption (OA), Raman spectroscopy (RS) and atomic force microscopy (AFM) the radiation damage and degradation of BaFBr crystals irradiated with 147 MeV ^{84}Kr ions to fluences (10^{10}-10^{14}) ion/cm^2 were investigated. The effect of the oxygen impurity, which is present in the studied crystals, is also considered. In the spectra of PL and XEOL detected bands associated with oxygen impurity placing the halide sites. In the XEOL spectrum, the luminescence band of a self-trapped exciton is also observed.

The quenching and shift of the PL and REOL maximum with increasing fluence is due to the overlapping of tracks and aggregation of defects.

Electronic and hole aggregate color centers arise mainly in the bromide sublattice. High irradiation doses lead to crystal degradation.

ABS: 94. Synthesis and modification of boron nitride nanotubes using ion implantation

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Boron Nitride (BN) nanotubes were grown on Silicon (Si) substrates using chemical vapor deposition (CVD) at temperatures ranging from 900 to 1100 ºC. Ion implantations were carried out with boron (B) ions at energies of 150 keV and fluences of $1x10^{14}$ and $5x10^{14}$ ions/cm^2. Raman analysis revealed a peak at 1367/cm, which is an indication of the sp^2 hybridized BN planar bonding attributed to the high frequency mode for the hexagonal BN peak, but which is more clearly characterized at 1100 ºC. The glancing incidence X-ray diffraction (GIXRD) analysis revealed a well-defined peak at angles of 51-57º, indicating the hBN (004) peak.
Scanning electron microscopy (SEM) images show BN nanotubes and BN nano particles of various shapes and sizes.

ABS: 98. Surface and in-depth structural changes in various graphitic materials irradiated with noble gases described with Raman imaging

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Malgorzata Frelek-Kozak [1], Lukasz Kurpaska [1], Iwona Jozwik [1], Jacek Jagielski [1]

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Raman spectroscopy is a technique based on incoherent light scattering. The difference between the energy of the monochromatic output beam and the scattered light indicates the energy of particular vibrational levels present in the molecules and functional groups of the analysed substance. The set of the energy values constitutes a so-called fingerprint spectrum allowing identification of the examined compound but is not limited to that. Due to its sensitivity, with Raman spectroscopy, one can describe subtle structural changes such as the crystallites' evolution, their occurrence or types of defects, and internal stress. Recent advancements in the hardware enable point-by-point and in-depth analyses of the materials – the so-called Raman imaging.

In this study, the complete performances of the WITec alpha 300R Raman spectrometer were taken for detailed examination of the structure of graphitic materials (IG-110, NBG-17 and laboratory's in-home material). Studied specimens were irradiation with Ar and He-ions up to fluencies in between 1e12 and 2e17 ion/cm^2. The importance of the obtained results is indicated by the application of graphite in high-temperature gas-cooled reactors (HTGR) as both constructive material and moderator. Thus, irradiation was performed to simulate the working conditions of the material. It is known that the efficiency of a material's performance is strongly dependent on the physicochemical properties being the result of structure. Therefore, establishing the degree of order is a crucial factor. The performed evaluation showed stronger disordering of the material with heavier Ar-ions than with lighter ones - He. The chemometric K-means cluster analysis depicted a lack of perfect homogeneity in the pristine material, which was transferred into the irradiated samples. Moreover, the general observations of emerging structural changes based on the average Raman spectra did not appear gradually but abruptly with a specific fluency value.

ABS: 99. Point defect creation in AlN: coupled effects of oxygen impurities and ion energy deposition mechanisms

Mamour Sall [1], Clara Grygiel [1], Ons Yahyaoui [1], Hoda Alassaad [1], Florian Aubrit [1], Yvette Ngono-Ravache [1], Mathieu Lalande [1], Stéphane Guillous [1], Emmanuel Balanzat [1], Isabelle Monnet [1]

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Among the family of nitride semiconductors, AlN, a wide bandgap material, is used as a native material substrate for optoelectronic devices operating in the deep UV range [1]. Particular attention is paid to the UV-absorbing defect such as Al-vacancy and oxygen complex defects that could limit the development of applications [2]. These defects generally created during the material growth due to contamination by impurities such as oxygen, could also be generated under ion irradiation. We demonstrated that a positive synergy between electronic excitations (Se) and nuclear collisions (Sn) is responsible for the creation of the defect absorbing at 4.7 eV in AlN under Swift Heavy Ion (SHI) irradiation [3].

To study possible coupled effects of the Se/Sn synergy for point defect creation and SHI induced impurity introduction/diffusion into the AlN layer, we have performed SHI irradiation in different controlled atmospheres (vacuum, oxygen, helium or argon partial pressure). While the noble gas atmospheres inhibit the creation of the optical defect, O_2 atmosphere in comparison to vacuum hugely enhances defect creation. At the same Se, the Se/Sn synergy parameter [3] is increased by up to two orders of magnitude with irradiation under O_2 compared to irradiation under vacuum. The synergy parameter considered so far solely dependent on Se, must also be linked to the presence of oxygen during irradiation either in the irradiation chamber atmosphere or (and) in the AlN sample prior to irradiation. We will discuss the mechanism of this new-coupled effect (Se/Sn synergy and oxygen content) and the effect of other impurity types on the synergy.

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ABS: 100. Lowering the threshold for high energy heavy ion irradiation damage in Al_2O_3, MgO and CaF_2

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Irradiation of a material by high energy heavy ions results in permanent damage when the density of deposited energy surpasses the threshold value for the given material. This threshold can be lowered due to presence of defects in the target material, or in the vicinity of the surface. In the present study, we established significantly lowered thresholds values for Al_2O_3, MgO and CaF_2 in case of sequential and grazing incidence irradiation.

We show that ion beams like 3 MeV O and 5 MeV Si can easily modify structure of investigated materials despite low density of deposited energy along the ion trajectory, which was confirmed by means of atomic force microscopy and Rutherford backscattering spectrometry in channelling mode. The obtained results also show how the unexpected damage build-up can result in structural breakdown, which is relevant for radiation hardness studies.

ABS: 103. Multi-energy high fluence he ion implantation for micromechanical testing of materials

Matej Kubiš [1], Zoltán Száraz [1], Filip Ferenčík [1], Vladimír Kršjak [1], Pavol Noga [1]

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Materials in new generation nuclear reactors, fission as well as fusion, have to cope with high transmutation helium production. Hence their testing requires either a powerful source of fast neutrons or, as a suitable surrogate, high fluence irradiation generating or implanting sufficient amounts of helium to investigate its effect on the material. Most studies concentrate on basic phenomena such as defect evolution, void swelling, etc., thus radiation effects at the nanoscale, whereas the investigation of engineering relevant properties, bulk properties is underrepresented.

High fluence multi-energy ion irradiations modifying several tens of micrometers of the analyzed substrate might fill this gap. We irradiate selected structural steels designed for harsh radiation environments using a helium ion-beam with energies from 17 MeV down to 500 keV in reasonably small steps to achieve a homogeneous 1000 appm helium „box-profile“ that corresponds to 5E17 at/cm² fluence.

This work was co-funded by the European Regional Development Fund under contract Nº ITMS2014+: 313011W085.

ABS: 104. Magnetic domains without domain walls in Tb/Co layered system after patterning by Ga^+ focused ion beam

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Recently it has been shown that ion bombardment (IB) can be used to modify the properties of ferrimagnetic (FIM) rare-earth/transition metal (RE/TM) multilayers primarily due to preferential oxidation of RE after bombardment [1]. This process was used to locally change the compensation point and other magnetic properties by reducing the relative contribution of the RE sublattice to the properties of the RE/TM system. This magnetic patterning was performed by 10keV-He^+ IB through a photoresist mask and allows to fabricate TM^+ regions dominated by TM (TM^+) embedded in a matrix dominated by RE (RE^+) for films that were RE^+ prior to bombardment. It was shown that this pattern can exhibit magnetic domains without a domain wall. This brings a new interesting spin texture, which opens a way to fabricate domains in a smaller scale than what is currently possible. A promising method to follow this idea is to use a focused ion beam (FIB), because it can be focused below 10 nm. Therefore, in this work, we used 30keV Ga^+ FIB to investigate the magnetic properties of Tb/Co multilayers after IB. We found that compensation point and therefore, the coercive field and magnetization saturation can be tuned in the IB area by appropriate choice of fluence, as for He^+ ions. Based on these results, a series of 2D square lattices consisting of TM^+ areas (with size varying from 0.1-50μm) embedded in a RE^+ matrix were patterned with 4 different fluences from $7x10^{13}$-$12x10^{13}$ ions/cm². This pattern allows us to show that magnetic domains without domain walls can be achieved in a FIM layer after ion bombardment. The magnetic stability of that spin texture depends not only on the size of the square but also magnetization saturation inside the squares, which can be tailored by ion fluence. This study was supported by OPUS National Science Centre Poland: UMO-2020/39/B/ST5/01915.

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ABS: 112. Investigation of mechanical and structural properties of nickel-based alloys submitted to high energy ion irradiation

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Nickel-based superalloys display set of outstanding properties such as excellent creep strength, remarkable fracture toughness parameters as well as superior oxidation and corrosion resistance. This spectacular combination of properties allows Ni-based materials to be considered as materials dedicated for IV. gen of nuclear reactors. Although these materials seem to be resistant to high fluxes of neutron radiation, their radiation resistance is still not fully understood and was not subjected to careful evaluation.

Our work focuses on verifying the structural and mechanical properties of two types of Ni-based alloys submitted to ion irradiation. This technique is a standard methodology that introduces radiation defects into microstructure without activation of the specimen. Therefore, implementation of this procedure allows the evaluation of the material's behavior in the simulated nuclear environment in a very safe and quick manner.

In this work, we investigated two commercially available nickel-based alloys (Hastelloy X and Haynes 230), produced by Haynes International Co. Structural and mechanical properties have been investigated by means of SEM/EBSD observations, X-ray diffraction analysis, nanoindentation tests, tensile and micro-hardness tests. Radiation damage effects were introduced to the microstructure of materials by ion irradiation using Ar+ ions with energy 320keV with two fluences: 1E15, 1E16 ions/cm^2 at 400ºC. This corresponds to damage of 1.7 dpa and 17 dpa, accordingly. Obtained results have revealed hardening effects for both levels of damage (1.7 and 17dpa). However, more intensive effects were observed for Hastelloy X. Recorded phenomena are related to the increment of density and complexity of occurring structural defects and the mechanism of their interaction with the matrix.

ABS: 116. Ion Irradiation Study of Lithium Silicates for Fusion Blanket Applications

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9In order to achieve optimum performance for fusion blanket applications, tritium breeding materials should have a good structural stability, rapid tritium release, and low lithium volatility under fusion extreme conditions, including high irradiation flux and high temperature. Lithium silicates are selected for this study due to a high Li/O ratio to increase tritium production and enhance tritium diffusion. Lithium silicate pellets were fabricated by hot pressing of powders with mixed phases of Li_4SiO_4 and Li_2SiO_3. Sequential irradiation with Si^+, He^+ and D^+ ions was performed to emulate high-energy neutron irradiation damage and gas contents in the pellets. The irradiation conditions from this study produce 30.6 dpa and 2.2 at.% He and D at the depth of 500 nm, corresponding to one-year burnup of ^6Li (5.0 at.%) in $^6Li_4SiO_4$ in layer 5 of SlimCS DEMO [1]. The irradiated pellets have been characterized using a number of methods, including GIXRD, ToF-SIMS, and STEM. The results indicate that there are three crystalline phases of monoclinic Li_4SiO_4, orthorhombic Li_2SiO_3, and monoclinic Li_2CO_3 (due to C contamination from graphite tooling) in the pellets. Both high-temperature irradiation data and post-irradiation thermal annealing data suggest that the pellets have an outstanding property of efficient D (and T by inference) diffusion and release. A significant Li loss in the near-surface region was observed during ion irradiation at 500 °C. Li_2SiO_3 appears to be more resistant to irradiation-induced amorphization than Li_4SiO_4. Amorphization of Li_2SiO_3 was observed to initiate from the surface, instead of the damage peak, due to a combination of FIB damage and radiolysis from ion irradiation.

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[1] S. Sato, *et al., Fusion Engineering Design* 87 (2012) 680.

ABS: 120. Irradiation-induced magnetostructural transition in $Fe_{60}V_{40}$ alloy thin films

Md Shadab Anwar [1], Hamza Cansever [1], Boehm Benny [2], Rodolfo Gallardo [3],
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Tuning and control of intrinsic magnetic properties, such as saturation magnetization (Ms) and Gilbert damping provides a pathway for modulating magnetic functionality on the nanoscale. One way to achieve such modulations is by inducing phase transitions. A well stablished method of achieving phase transition in a systematic way is ion-irradiation. In certain binary alloys such as B2 $Fe_{60}Al_{40}$ [1] and B2 $Fe_{50}Rh_{50}$ [2], the ion-irradiation causes chemical disorder in the crystal structure and consequently the Ms can be tuned. Here we explore irradiation induced ordering in $Fe_{60}V_{40}$ alloy thin films, from a short-range ordered (SRO) to a bcc structure.

$Fe_{60}V_{40}$ thin films (~ 40 nm) were grown onto SiO_2/Si substrate. The as-grown films are weakly ferromagnetic with low Ms of 17 kA/m; whereas irradiation with 25 keV Ne^+-ions at fluences of ~ 5 x 10^{15} ions/cm^2 leads to an increase of Ms to ~ 750 kA/m. X-ray diffraction as well as transmission electron microscopy reveal a structural short-range order in the as-grown films, that transform to A2 Fe60V40 with increasing Ne^+-fluence. The dynamic magnetic properties e.g. low value of Gilbert damping (~ 0.002) has been obtained from the frequency dependence of the resonance line width. These results and optimized broad beam irradiation parameters leads to further investigations on nanomagnets embedded within $Fe_{60}V_{40}$ thin films by using focused ion beam irradiation. The structures were produced in form of stripes with varying aspect ratio, which shows a variation in domain pattern from single to multidomain. Tunable crystal structure, low damping and high Ms provide a pathway for the rapid patterning of magnetic and microwave device elements.

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ABS: 123. Transport properties of FeAl under ion irradiation

Serhii Sorokin [1], Gregor Hlawacek [1], Shadab Anwar [1], João Salgado Cabaço [1], Richard Boucher [1], Kay Potzger [1], Jürgen Fassbender [1], Jürgen Lindner [1], Rantej Bali [1]

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Applications such as magnetic data storage as well as magnetic sensors and spin-transport devices require a precise control of intrinsic magnetic properties at the nano- and meso-scales [1]. In $Fe_{60}Al_{40}$ [2] ion irradiation can be used to control the saturation magnetization (Ms) due to the gradual transition from paramagnetic (ordered B2-phase) to ferromagnetic (disordered A2-phase) as a function of ion fluence. The corresponding changes to the transport properties occurring during these phase transition are lesser known. Here we track the variation of electronic transport properties in parallel with gradual ion irradiation. Transport behavior is measured on a Hall bar of dimensions 5×200 μm^2 patterned onto 40 nm thick B2 Fe60Al40 films. The Hall bar is inserted into a He/Ne-ion microscope and contacted with feedthrough probes to enable step-wise measurements during Ne^+-irradiation. A permanent magnet is placed in proximity of the Hall bar, to provide a magnetic field aligned perpendicular to the film plane. The variation of the resistance and the Hall voltage are tracked as a function of the Ne^+-fluence, as the ordered B2 structure transforms into a disordered A2 structure. Peaks in the electrical resistance and the Hall voltage are observed corresponding to the existence of a partial B2/A2 state, thereby hinting at the important role of the induced ferromagnetic clusters and their distribution on the transport properties. The state of disorder in the Hall bar is reversible by annealing with higher electric current and can be converted to an electrical signal, thereby showing potential for sensing applications.

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ABS: 131. Non-radiative decay kinetics of self-trapped excitons in strontium titanate under energetic heavy-ion irradiation

Miguel Crespillo [1], Joseph Graham [2], Fernando Agulló-López[1], Yanwen Zhang [3], William Weber [4]

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Strontium titanate is an advanced oxide perovskite with a number of remarkable optical and electrical properties at low temperatures. The kinetics of the 2.5 eV luminescence emission of strontium titanate under energetic heavy-ion irradiation and their dependence on temperature and electronic excitation were studied. Trends seen in the experimental observations can be understood using a novel model which describes the non-radiative decay of self-trapped excitons (STEs). For all temperatures studied, the initial light yield grows rapidly and reaches a quasi-steady-state level, after which it decays in response to the accumulation of non-radiative recombination sites from radiation-induced structural disorder.

The intensity of the quasi-steady-state luminescence yield depends linearly on the excitation density, suggesting a constant STEs formation efficiency. The variation of the light yield with temperature follows Arrhenius behavior with an activation energy of 55 meV. This energy is in good agreement with experimental values measured for non-radiative STE decay under nanosecond pulsed laser excitation, and reasonably consistent with density functional theory predictions of the migration energy of a small-polaron adiabatically hopping.

A new non-radiative mechanism is discussed involving self-trapped hole (STH) migration through thermally activated hopping and annihilation with the STE-electron. Luminescence kinetics associated with the annihilation of Cr^{3+} centers through recombination with migrating STHs support this model.

ABS: 132. Ionoluminescence as a real-time sensor of damage to the anion sublattice of ion irradiated strontium titanate

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Structural damage to the cation sublattice of ion irradiated dielectric materials is often investigated through ion channeling measurements. Ion channeling, however, provides poor sensitivity to damage on the anion sublattice. We describe the use of ionoluminescence (IL) as a means of measuring damage to the anion sublattice of strontium titanate (STO). Previous IL experiments on STO have resolved the emission spectra into a 2.0 eV component, associated to electron-polaron Ti^{3+} states trapped at oxygen vacancies, a 2.5 eV component due to self-trapped excitons (STEs), and a 2.8 eV component, recently attributed to transitions from conduction band states to the STE ground state. In this work, luminescence experiments were performed under irradiation with H (3 MeV), O (8 Me), Si (15 MeV), Cl (18 MeV) and Ti (18 MeV) ions at several temperatures (100 K, 170 K and 300 K). They cover a broad range of ion masses and energies and represent differing degrees of electronic and nuclear energy loss. The emission spectra can be decomposed into nearly Gaussian bands at 2.0 eV, 2.5 eV and 2.8 eV. The 2.0 eV and 2.5 eV bands evolve in parallel, through a rapid initial growth stage corresponding to electronic excitation of the relatively undamaged crystal, followed by a slower decay stage associated with amorphization. The parallel evolution of the Ti^{3+} (2.0 eV) and STE (2.5 eV) bands supports a previous theoretical treatment. A phenomenological model based on the Avrami formalism is used to describe the evolution of the oxygen vacancy concentration during the irradiation. The results obtained through IL for the anion sublattice have been discussed in relation to those previously reported for the cation sublattice. They appear consistent and clearly illustrate the potential of IL as a unique tool to analyze, in situ and in real time, the damage evolution on the anion sublattice.

ABS: 133. The ionoluminescence kinetics of amorphous silica at cryogenic temperatures - competition and interplay between emitting centers

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Controversies regarding the origin of luminescence emissions in silica have been resolved using cryo-ionoluminescence. Measurements were carried out on fused silica specimens using energetic light and heavy ions from 30 K to room temperature. The initial spectral evolution at low temperatures enables the deconvolution of heavily overlapping and asymmetric emission bands centered at 1.9 eV, 2.2 eV, and 2.7 eV. Based on their kinetic behavior with respect to temperature, electronic energy loss, and nuclear energy loss, the identity of those previously ambiguous emissions can now be definitely associated with Non-Bridged Oxygen Hole Centers (NBOHCs, 1.9 eV), intrinsic recombination of Self-Trapped Excitons (STEs, 2.2 eV), and Oxygen Deficient Centers (ODCs, 2.7 eV). It has been ascertained that following the initial ion-solid interaction, an equilibrium is established between the ionization rate and the STE lifetime. STEs slowly migrate to preexisting lattice defects such as silanol groups (yielding NBOHCs at 1.9 eV), as well as to oxygen vacancies generated by nuclear elastic collisions (ODCs at 2.7 eV). The lowest temperature light ion irradiations reveal rapid kinetics of the 2.2 eV emission uncorrelated with nuclear energy loss or ion fluence, and hence point to the intrinsic recombination of STEs. The generation of NBOHCs and ODCs follow different routes. Electronic excitation processes are mainly responsible for the generation of the NBOHCs, whereas the ODCs mostly result from ion-atom collisions. A detailed analysis has confirmed, through comparison of the results with SRIM simulations, that the intensity of the 2.7 eV emission is, indeed, well correlated to the predicted oxygen vacancy production rate and therefore attributed to the ODC.

ABS: 137. Atomistic study of damage generated from low energy collective collisions in SiC

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SiC has proven excellent performance for power devices (^{4}H-SiC polytype) and radiation-hard detectors (^{3}C-SiC polytype). Device fabrication using ion implantation and operation in radiation environments entails damage generation in the lattice, which must be understood to optimize devices. Previous theoretical studies focused on the evaluation of threshold displacement energies and on the statistical description of damage generated by keV cascades, but many issues remain elusive. In this work, we used Classical Molecular Dynamics (CMD) with different empirical potentials [1-3] to generate damage by recoils that simultaneously strike a group of atoms – from 1 to 8 atoms – with energies bellow the displacement threshold, and ab-initio methods to characterize specific defects. Among all defects, we payed particular attention to neighboring antisite-pair (NAP) defects, which were assigned a key role on amorphization [4] and were associated to the DI photoluminescence center [5]. Nevertheless, this correlation is in question because this defect was considered unstable and unlikely to form by other authors [6,7]. We found that Tersoff and Erhart-Albe potentials predict that NAP defects are directly generated through collective collisions, and they are stable even at high temperatures. We confirmed the energetics and stability of NAP defects by ab-initio molecular dynamics simulations. Our work revives the relevance of the NAP defects in SiC for damage accumulation and photoluminiscence.

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ABS: 144. Velocity correlated emission of secondary clusters in fullerene - solid impact: probing extreme subsurface spike conditions

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An important aspect of keV ion-solid collisions is the impact induced emission of large secondary clusters from the target. The emission dynamics can be well characterized by measuring kinetic energy distributions (KEDs) of all the outgoing secondary cluster ions emitted from a given target. Here we describe our recent observations and analysis of a new mechanism where following a single impact of a large polyatomic projectile anion (C60), all the large clusters (e.g. Aun cation clusters up to n=15 emitted from a gold target) are emitted in a velocity correlated mode (moving with nearly the same most probable velocity) [1-4]. This behavior is found to be in sharp contrast to that reported earlier for KEDs of cluster ions emitted following impact of a heavy monoatomic ion. The effect is driven by the exceptionally high subsurface energy density induced by the C60 anion impact [2]. The measured KEDs are shown to uniquely reflect the buildup of the extreme subsurface conditions at the early subpicosecond phase of the thermal spike [2,4].

The velocity correlated cluster emission effect was measured so far for six different targets (following 14 keV C60 anion impact) thus demonstrating its general nature. We will describe our recent progress in studying and characterizing the effect.The measurements are supported by modelling and molecular dynamics (MD) simulations [2,4].

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ABS: 146. Helium induced bubble formation in dispersion strengthened tungsten alloys for fusion applications

Chase Hargrove [1], Evan Lambert [1], Ashrakat Saefan [1], Eric Lang [2], Xing Wang [1], Jonathan Hinks [3], Jean Paul Allain [1]

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Tungsten (W) is a promising candidate as a plasma-facing component (PFC) in the divertor region of fusion tokamak reactors. Tungsten exhibits excellent thermomechanical properties such as a high melting point (3422°C) and modulus, and low coefficient of thermal expansion (4.5C-1). However, these desirable qualities can be significantly altered under He irradiation. The addition of transition metal (Ti, Ta, Zr) carbide dispersoids into a tungsten matrix has been shown to suppress grain growth and increase hardness with no detrimental effects on D retention [2]. The Radiation Surface Science and Engineering Laboratory (RSSEL) has been developing transition metal carbide dispersoid-strengthened alloys (DS-W) in the range of 1-10 wt% fabricated via spark-plasma sintering as PFCs. In this study, the effects of 2keV He ions on a W-TiC sample is investigated via a transmission electron microscope. Samples were heated to 950°C and held at this temperature throughout irradiation. Previous work has shown He^+ induced bubble formation at temperatures ranging from 12-100K. The bubble density was observed to increase with fluence, but the bubble size is suppressed in TiC particles.[3] Agarwal et al revealed gas release resulting from near-surface blistering of He clusters in ZrC.[4] The microstructural evolution as a function of helium fluence is shown qualitatively; attention is shown to the carbide-matrix interface, which has shown no bubble evolution in previous works with W-TaC[5]. Suppression of both bubble size and density as a function of fluence is observed in the W-TiC sample.

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ABS: 151. Irradiation response and mechanical property changes of conventionally and additively manufactured 316L stainless steels

Lin Shao [1]

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Additive manufacturing (AM) has attracted intensive interest from the nuclear industry for its low cost and flexibility in producing components of complicated geometry. A combination of accelerator ion irradiation, atomic-scale characterization, and micromechanical testing was used to evaluate materials' performance of AM 316L stainless steels prepared by the direct energy deposition method. Our major findings include: (1) printing-introduced large pores have amorphous cores, which are silicon and oxygen-rich. The pore edges develop shell-like structures enriched in Cr and Mn; (2) residual stress introduced by AM processing makes materials harder. However, the residual stress can be effectively removed by applying a post-printing relaxation annealing; (3) proton irradiation induces complicated dislocation networks and short-range ordering around dislocations, which is featured by Ni and Si segregation over a range of a few nanometers; (4) different from wrought counterparts which deform through dislocation gliding, AM variants have a transition from dislocation gliding to a mixture of dislocation gliding + twinning, and twinning only as a function of damage levels; (5) the deformation mechanism change is caused by irradiation hardening which allows the yielding stress high enough to exceed the required shear stress to initialize dissociation of perfect dislocation; (6) twinning benefits the homogeneity in plasticity flow; (7) both high angle grain boundaries and cell walls exhibit defect sink property, but high angle grain boundaries are more efficient; (8) the irradiation-induced swelling in AM variants is less than the wrought counterpart. In summary, AM alloys show unique (and better) irradiation responses and mechanical properties. The study provides useful knowledge in quality control, optimization, safety analysis, design, and further improvements for AM alloys in reactor applications.

ABS: 153. The effect of lead ion irradiation on microstructure and micromechanical properties of T91 steel

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In this study 9% chromium ferritic-martensitic steel T91 was investigated. At present high chromium ferritic-martensitic steels are considered as one of the most promising construction material candidates for the core structures of generation IV nuclear reactors. Sub-sized flat tensile specimens were cut from the 15mm hot rolled plate. The dog bone shaped specimens, with a total length of 30 mm, have a gauge length of 5.6 mm and a cross-section of 1.5x2 mm². One set of specimens was ion irradiated at room temperature with Pb ions at two irradiation conditions: four specimens at ion energies of 250 keV to total fluence of $6.5x10^{14}$ ions/cm², and four at 500keV to total fluence of $1x10^{15}$ ions/cm². Two opposite flat sides of each specimen were irradiated under the same conditions. The depth profile of injected Pb atom concentrations has been measured with Ion Beam Analysis techniques and compared to theoretical calculations with SRIM/TRIDIM. One specimen per condition was heat treated at 450°C for 100h and the diffusion profile of Pb measured. The microstructure of irradiated and irradiated + heat-treated specimens was investigated with transmission electron microscopy. Nanoindentaion, using a Berkovich indenter, was applied to measure the depth dependence of the hardness in irradiated specimens and unirradiated reference. Relationship between the depth-resolved radiation damage and indentation response are considered.

ABS: 154. Effects of helium implantation on mechanical properties at the tungsten-carbide interfaces using nano-indentation technique

Ashrakat Saefan [1], Xing Wang [2], Eric Lang [3], Jean Paul Allain [1]

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Tungsten (W) is a candidate plasma-facing material of future fusion reactors because of its high melting point, low sputtering yield, and high thermal conductivity. Exposure to helium (He) ions from the plasma edge and transmutation reactions in W leads to surface morphology changes and degrades the mechanical properties. Adding second phase dispersoids is a promising approach to improve the material radiation tolerance since phase boundaries can act as defect sinks to promote recombination of point defects. In this work we focus on the effects of He irradiation on mechanical properties at the interfaces between the dispersion-strengthened W (DS-W) matrix and carbide particles. Three types of DS-W samples with 5 wt.% added TiC, ZrC, and TaC dispersoids and average W grain sizes of 2.1, 4-.5, and 4-.5μm respectively, were fabricated using spark plasma sintering. To simulate neutron-induced He production and facilitate the investigation of He effects on mechanical properties, the samples were irradiated by 2 MeV He^+ to the fluence of 5×10^{16} cm^{-2} at room temperature using the NEC Pelletron Accelerator at UIUC [1]. The radiation damage peak was about 2.7 μm below the sample surface. We will use the Berkovich indenter to measure the hardness and elastic modulus at different indentation depths near tungsten-carbide interfaces. We expect a reduction in hardness at the interfaces due to the He bubbles packed at the interfaces. These bubbles or cavities could decrease the activation barrier for the plasticity threshold via the interface's mediation of dislocation nucleation [2].

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ABS: 157. Irradiation Effects in 3C Silicon Carbide

Graeme Greaves [1], Benjamin Clay [1]

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Silicon carbide is one of many candidate materials for next generation fission and fusion reactors, where the materials are expected to be exposed to higher temperatures and radiation doses than in current reactors. With excellent thermal, neutronic and oxidation properties SiC is being considered for various applications such as fuel cladding or in the case of fusion as a plasma facing material. However, more data is still required on SiC performance whilst under irradiation in these extreme environments. In this work the MIAMI facility which combines ion irradiation with TEM has been utilised enabling the observation of the irradiation at the nanoscale in real time. Presented here will be the results of helium ion irradiation of 3C SiC *in-situ* at various temperatures from 400ºC up to 1200ºC [1], showing the developing microstructure with increasing dose, with nanobubbles forming at the lower temperatures moving to platelets at the higher temperatures.

Also presented will be preliminary results on ion irradiation of SiC in a aqueous environment undertaken at the Michigan Ion Beam Laboratory. Where the SiC underwent enhanced erosion when compared with regions not exposed to the ion beam.

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ABS: 159. Michigan Ion Beam Laboratory for the study of radiation effects

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The Michigan Ion Beam Laboratory (MIBL) is a user facility in the University of Michigan built to study the radiation effects on material used for different applications.
The research in MIBL focuses in understanding the radiation damage in structural materials in nuclear reactors using ion irradiations. Ion irradiation has been used for many years to understand the basic elements of radiation damage in materials, and in recent years, ion irradiation has been considered as a surrogate for neutron irradiation with the goal of substituting for neutron irradiations in determining how materials will respond in reactor. Ion irradiation has the potential to emulate the full suite of radiation effects in a reactor environment, thus greatly speeding the development of new materials to enable both the introduction of advanced reactor concepts and the extension of the current LWR fleet.
This presentation will discuss the capabilities of the Michigan Ion Beam Laboratory to conduct single, dual and triple ion beam irradiations, creep irradiations, in-situ single and dual ion beam irradiations with direct TEM observation, and irradiation accelerated corrosion.

ABS: 162. A magnesium mass independent isotopic fractionation revealed by NanoSims analyses of micrometer grains condensed in plasma

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In microwave plasma, the molecules are dissociated by electron impact producing highly reactive radicals. Vapor pressures of Pentanol and $MgCl_2$ were injected into a gas vector (N_2) and pass through a cylinder glass tube (Ø = 1 cm, l = 10 cm) where the microwave discharge is initiated. The pressure in the plasma is maintained at 1 Torr by dynamical pumping. The purpose of the introduction of Pentanol along with a Mg gaseous carrier, is to produce carbonaceous CxHy• radicals that can react with the activated complexes $[Mg_2Cl_2]$* formed by the reaction Mg + $MgCl_2$ [1]. Magnesium-rich hydrocarbon solids are deposited in a silicon wafer located after the discharge and directly analyzed with the Nanosims without any other preparation.

Extremely large variations in the magnesium isotopic ratios $^{25}Mg/^{24}Mg$ and $^{26}Mg/^{24}Mg$ are observed (ranging from -40 to +100% relative to the initial composition of $MgCl_2$). In NanoSims imaging, isotope effects appear as 100-200 nanometer size hotspots embedded in a carbonaceous matrix. This effect is referred to as the Mass Independent Isotopic Fractionation (MIF) originally discovered in ozone by [2]. The present results suggest that the MIF effect characterizes the plasma chemistry [3]. We interpret this effect as a consequence of a difference in the reaction probabilities between the activated complex isotopomers which are formed by dist- or by indistinguishable isotopes [4, 5].

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ABS: 167. Degradation and recovery of proton-irradiated Cu(In,Ga)Se_2 solar cells

João Gaspar [1], Norberto Catarino [2], Luís Alves [1], Victoria Corregidor [1], João Barbosa [3], Jennifer Teixeira [3], Pedro Salomé [3], Joaquim Leitão [4], José Marques [1], Eduardo Alves [2]

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Cu(In,Ga)Se_2 solar cells are a promising power source in harsh radiation environments. In this study, the effects of 1 MeV proton irradiation on the performance of Cu(In,Ga)Se_2 cells were first evaluated by monitoring the evolution of the dark J-V characteristics with several irradiation fluences, and subsequently by monitoring the post-irradiation J-V behavior over time in dark conditions. The interpretation of the J-V characteristics was based on the single diode model, which relates the performance of a solar cell to its carrier recombination mechanisms and parasitic resistances [1].

Irradiation with fluences up to 10^{12} H^+/cm^2 reveals only a moderate degradation of the cell performance, while for larger fluences the rate of degradation grows rapidly, as suggested by the increase of the saturation current and the ideality factor. In particular, the increase of the ideality factor from ~1.7 to values larger than 2.3 could be related to enhanced recombination at the p-n interface due to radiation defects. Partial recovery in dark conditions was observed in the month following the irradiation, as evidenced by the decrease of the saturation current from 3.5×10^{-7} to 1.5×10^{-7} A/cm^2.

Furthermore, the impact of light soaking on the recovery of irradiated Cu(In,Ga)Se_2 devices was studied, by comparing the dark J-V evolution of an unirradiated and an irradiated cell after being subjected to similar periods of intense light exposure. While the metastable changes in the unirradiated cell were found to be reversible after a period of 3 days in the dark, in the case of the irradiated cell a significant long-term reduction of both saturation current and ideality factor was observed, which suggests that a partial recovery of recombination-inducing defects was achieved with the soaking treatment.

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ABS: 169. Most stable surface-emerging defects in ion implanted Si annealed at extreme temperature

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Ion implantation followed by thermal annealing allows for a targeted modification of the materials. This process spans a considerable part of physics and has boosted the developments of silicon technologies over the past decades. Fabrication of ultra-shallow junctions in Si via doping and silicon-on-insulator (SOI) substrates via material fracture are only a few of the examples. The basic physical processes behind the manufacturing are linked to the thermally triggered interaction of implanted species with self-interstitials and vacancies formed due to matrix damaging. The presence of a wafer surface has an impact on their further evolution. Depending on its chemical reactivity with the environment, the surface can be either a source or an effective recombination sink for point defects. When annealing is performed in a neutral environment, it is generally believed that an extremely high temperature would ensure complete dissolution of defects since the system tends towards the least possible energy state which is defect-free. In this work, we questioned such a hypothesis and identified a novel class of most stable surface-emerging defects formed after H^+ ions implantation in Si, moderate temperature annealing, oxidation and eventually extreme temperature annealing. Such a defect was characterized using diverse electron microscopy techniques (SEM, HR-TEM, electron holography). It's called a "tent-like defect" for its long (µm) length and shallow "V" shaped structure. It's made up of four {111} stacking faults and five stair-rod Lomer-Cotrell partial dislocations. We elucidated its precursor to be an elongated (rod-like) extrinsic type dislocation loop (DL) truncated by the surface. We will present and discuss a complete scenario for the formation of tent-like defects, starting with the defects precipitation in the as-implanted state and progressing through their growth and transformation that occur during various annealing processes.

ABS: 170. Proton irradiation effects on hexagonal boron nitride crystals

Tiago Pardal Fernandes [1], Duarte Magalhães Esteves [2], Luís Cerqueira Alves [3], Luís Santos [4], Ana Luísa Rodrigues [3], Maria Isabel Dias [5], Norberto Catarino [6], Marco Peres [2], Katharina Lorenz [2]

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Hexagonal boron nitride (h-BN) is a semiconductor with a very large bandgap of almost 6 eV at room temperature (RT) with exceptional properties like a very high thermal stability and conductivity, resistance to oxidation and mechanical strength, and a high breakdown field, making it very attractive for dielectric applications. Due to its layered structure, thin nanomembranes can be easily exfoliated from bulk crystals, which can be used in nanoelectronic devices. h-BN has also raised interest recently due to the discovery of single photon emitters associated to its defects, which are required for several quantum technologies.

We used proton beams of up to 2 MeV to irradiate and generate defects on high purity h-BN crystals. In order to study the effects of proton irradiation we performed in situ characterization during the irradiation through ionoluminescence (IL) at RT, which allows the evolution of the luminescence to be monitored and to be related to the formation of defects in the crystal. The effect of thermal annealing at different temperatures on the recovery of the induced defects was also analyzed. The IL spectra are characterized by a broad unstructured ultraviolet (UV)/blue emission peaked at ~3.7 eV, with a clear dependence with the fluence. In particular, a quenching of 75% of the UV/blue emission was observed after a fluence of 1×10^{16} protons/cm². The nature of the defects was further studied by thermoluminescence measurements and the structural characterization of the crystal lattice was made by X-ray diffraction and Raman spectroscopy.

ABS: 172. Effect of swift heavy ions in AlGaN compound semiconductors

Cláudia Figueiredo [1], Miguel Sequeira [2], Isabelle Monnet [3], Clara Grygiel [3], Marco Peres [1], Katharina Lorenz [1], Florent Moisy [3], Mamour Sall [3]

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III-nitride semiconductors are regarded as promising alternatives to silicon power devices. GaN has found use in high power electronics and has shown high energy efficiency and radiation resistance. Because of their even wider bandgap, AlGaN compounds have been considered for space applications and power electronics, primarily HEMTs. However, the effect of high energy heavy ions on their crystal structure is yet to be fully understood. Commercial samples of GaN, $Al_xGa_{1-x}N$ (x=0.189 and x=0.77) and AlN were used for this study.

The GaN samples were grown on sapphire substrates by MOCVD and the AlGaN and AlN samples were grown by HVPE. These samples were irradiated at GANIL with 0.9 GeV Uranium-238 ion beams with fluences of (0.5, 1, 5, 10) $\times 10^{11}$ ions/cm^2. The samples were studied using Optical Spectroscopy, X-Ray Diffraction and Transmission Electron Microscopy. It was found that the lattice parameter c increases for higher fluences for GaN but it decreases in the case of AlN. For $Al_xGa_{1-x}N$, the results vary for different compositions. The $Al_xGa_{1-x}N$ samples with lower AlN content had similar results to GaN and show an increase of the lattice parameter c for higher fluences. The opposite happens for the samples with higher AlN content. These show a decrease of the lattice parameter c for higher fluences – the same result obtained for AlN.

These results might be explained by the differences in resistance towards amorphous track formation. High energy ions induce amorphous track formation in GaN with subsequent track recrystallization [1][2] while AlN shows extraordinary track formation resistance [2].

In agreement with the XRD results, TEM images suggest a strong track formation resistance for $Al_xGa_{1-x}N$, likely related to its AlN content.

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ABS: 181. Influence of the microstructure of additively manufactured Ni-20Cr microstructure on aging under irradiation

Alexis Dujarrier [1], Mamour Sall [2], Isabelle Monnet [2], Eric Hug [1]

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The additive manufacturing (AM) is a fast growing process. This method presents many advantages such as the quick design of intricate parts and it is already employed in industrial sectors like aeronautic. For this reason, its use is considered in the nuclear field, for example for easy replacement of outdated parts. Due to their interesting properties such as irradiation and oxidation resistance or their stability under high temperature [1], Ni-based superalloys are considered as candidate materials for the next generation nuclear reactors. AM Ni-20Cr alloy can be considered as a material model for these complex alloys.

The microstructure of AM parts is very different from that of wrought parts. For example, the formation of precipitates or a structural anisotropy due to columnar grain growth are often observed [2]. This can strongly affect the properties and their response to irradiation. We have studied the defects induced by irradiation in both wrought and AM Ni-20Cr alloys, mainly by Transmission Electron Microscopy (TEM). Conventional TEM observations highlight that irradiation mainly induce the formation of Frank type dislocation loops. The irradiation damage build-up and the effect of the AM material anisotropy are studied with particular attention on the density and the size of dislocation loops. In this presentation, we will compare the behaviour under irradiation of AM and wrought alloy to determine if the use of AM Ni-20Cr in next gen reactor is conceivable.

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ABS: 182. Irradiation of bulk W at the PF-1000U device with deuterium plasma discharges

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The radiation resistance of plasma facing materials (PFM) in magnetic plasma confinement (MPC) devices is tested in tokamaks or linear plasma accelerators where plasma durations range from hundreds of μ-seconds to seconds. The mechanical, structural or elemental modifications imposed by irradiation are characterized by electron microscopy and ion beam analysis (IBA), among others techniques. In opposition, studies of radiation damage imposed to PFMs in inertial plasma confinement (IPC) experiments, using dense and short discharges of tens of nanoseconds, are scarce and most of the published work relates the mechanical behaviour of the materials. However, worst irradiation effects are probably presented by fast ion streams in both MPC and IPC.

Plasma Focus (PF) units generate hot plasma flows and fast ion streams that mimic IPC environments. Fast deuterons in the discharges of the PF-1000U device have a mean energy of ~100 keV, promoting their implantation in the target materials. The present work points the advantages of IBA techniques to characterize irradiation effects in PF experiments.

Mirror quality W plates (99.6 %) were irradiated with 1, 3 and 5 plasma discharges in PF-1000U using distinct average power flux densities and deuterium or a deuterium-helium mixture as background gas. Nuclear reaction analysis (NRA), Rutherford backscattering spectroscopy (RBS), Proton induced X-ray emission (PIXE) and Energy dispersive X-Ray spectroscopy (EDS) led to the quantification of retained deuterium down to depth ranges of ~4 μm. Copper (PF electrodes) was found thinly deposited at the surface of the irradiated surfaces. Retained deuterium mainly increase from 1 to 3 discharges, by adding helium to the background gas and by increasing the distance from the target to the plasma pinch (12 to 24 cm). Surface morphologies were followed by scanning electron microscopy (SEM) and relate with deuterium amounts (maximum of ~6×10^{15} at/cm^2).

ABS: 183. An approach to amorphous topological superconductors by ion beam irradiation

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In this work, we study the possibility of amorphizing a buried layer of bismuth-antimony (Bi-Sb) alloys by swift heavy ions, carried out at CMAM. The goal of these experiments is to fabricate regions of amorphous Bi or Bi-Sb inside the crystalline alloys, which could remain robust enough at room temperature. If the created structures remain amorphous and avoid recrystallization, they should exhibit superconductivity at helium temperatures and would have the potential to behave as promising Amorphous Topological Superconductors (ATS) [1].

We have performed Monte Carlo simulations (SRIM code [2]) to determine the proper ion range and fluences to create about 10-40% of vacancies. Afterwards, samples of pure Bi and Bi_xSb_{100-x} alloys were irradiated simultaneously, either with self-ions or with H^+ beams at wide energy ranges to create the amorphous buried layer few microns under the surface. Fluences around $10^{12}-10^{13}$ ions/cm^2 (for Bi ions) or $10^{16}-10^{17}$ ions/cm^2 (for protons) were respectively used. The irradiation effects can produce isolated amorphized regions and it is therefore possible to create a fully-amorphized buried layer [3,4]. Our hypothesis is that the recrystallization could be prevented by the "internal pressure" exerted by the Bi matrix when the amorphized layer tries to transform into a crystal, in principle, due to the lower mass density of the latter.

These studies will help to define future strategies and methodologies to keep the irradiated films in the metastable amorphous state at ambient conditions in these materials.

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ABS: 205. Silicon amorphization studies by synergistic MeV proton implantation and femtosecond laser irradiation

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Silicon is a material of great industrial interest in fields such as electronics or photonics, but also a very relevant material for understanding the dynamics of material melting and solidification when subjected to intense irradiations. Among triggered phenomena, it is of interest the selective amorphization processes induced by femtosecond (fs) laser pulses. Due to the different optical properties of the two phases and their transparency in the telecommunication wavelength regime, the control (spatial and axial) of the amorphization process could enable the fabrication of optical waveguides, a milestone on silicon photonics. Therefore, there is a clear motivation to investigate novel strategies in which the amorphization limits can be understood and overpassed.

In this work, we present the first results on the influence on silicon amorphization of the synergistic effects of MeV ion implantation and fs-laser irradiation. Firstly, silicon samples were implanted with a proton beam with energy range from 0.6 to 2 MeV and fluences of 10^{13} and 10^{15} ions/cm^2. On the ion-implanted regions no optical or structural changes were detected. Secondly, fs-laser (120 fs and 800 nm wavelength) irradiations were performed. After laser irradiation, the ion implantation areas was revealed by an increase on surface reflectivity and changes on the micro-Raman spectra, but limited to samples with high implantation levels. Those changes are associated to the formation of amorphous silicon whose layer thickness exceeds the generated by only irradiating with fs-laser pulses. In this work will be summarized how the different parameters of proton irradiation (energy and fluence), laser irradiation (fluence and number of pulses) and crystallographic orientation favor the formation of a thick amorphous silicon layer. Furthermore, by comparing with simulations, we will demonstrate that the density of vacants is a critical parameter for ion-laser synergetic effects.

ABS: 209. Damage in InGaN/GaN layers upon Xe and Pb swift heavy ions irradiation

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InGaN/GaN 350 nm and 550 nm thick layers were irradiated with different energies (from ~82 to ~38 MeV) of xenon (Xe) ions and different fluences of 1.2 GeV lead (Pb) ions. The radiation effects of the swift heavy ions (SHIs) bombardment were investigated using X-Ray Diffraction (XRD) and Rutherford Backscattering Spectrometry in Channeling mode (RBS/C). To assess damage profiles, the RBS/C analysis was followed by Monte Carlo simulations using the McChasy code, revealing that InGaN is more susceptible to irradiation damage than GaN. Moreover, the simulations suggest that both randomly displaced atoms (possibly due to partial amorphization) and dislocation loops are formed. The elastic response to radiation was estimated by measuring the expansion of the c-lattice parameter. XRD revealed a homogenous strain even in low fluence samples where only a small fraction of the sample volume suffered direct SHI impacts. As a driving force of the lattice expansion, we point out the Poisson effect resulting from the pressure exerted by the SHI tracks on the surrounding undamaged crystal structure.

ABS: 218. Measurement of of $^{9}Be(^{3}He,p_i)^{11}B$ (i =0−9) nuclear reaction cross sections at the energy range 1.0–2.5 MeV

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The interaction between the plasma and the wall materials in a fusion reactor is the key factor in determining the useful life of the wall components. This interaction includes the erosion and redeposition of material in the plasma-facing wall, accompanied by the formation of alloys from the different materials present. These processes are critical for the retention of hydrogen isotopes by the wall materials.

Determining the amount and depth profile of ^{9}Be and other elements is crucial for understanding those phenomena. The spectra of fusion-related samples can be complex and peak superposition can occur. Nuclear Reaction Analysis (NRA) using ^{3}He is an important IBA technique to overcome these limitations, making the knowledge of the nuclear differential cross section for reactions induced by ^{3}He essential for ion beam analysis of these systems.

In this work, we determined the $^{9}Be(^{3}He,p_i)^{11}B$ (i=0−9) cross sections, obtained using a thin beryllium film target at the backscattering angles between 110º and 165º with a 5º step and in the energy range between 1.0 and 2.5 MeV, which is the typical energy range for the ion beam techniques. The results were compared with the two previous studies in the same energy range and differing by a factor of 1.4. The results are in very good agreement with one of these studies and were benchmarked with the measurement of thick target reaction yields from a pure beryllium target at 2.0 MeV for 135º.

ABS: 225. SRIM2022 - A new Installation for SRIM

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The SRIM code has been largely updated and re-written so that it is much easier to install and update. The new version should look and feel very much like the older 2013 version. We will describe this new beta release and ask people to try it and feed back their experiences so that we can gradually improve the software for the community at large. We aim to eventually release the source code as open source once the beta release has stabilized.

ABS: 38. Ion incidence angle dependent pattern formation at AZ® 4562 photoresist by (reactive) ion beam erosion

Tom Rüdiger [1], Martin Mitzschke [1], Andrea Prager [1], Ying Liu [2], Bernd Abel [1], Agnes Schulze [1], Frank Frost [1]

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Polymers are part of our daily life and the morphology, roughness as well as the chemical composition of their surfaces are decisive for their properties. Depending on the intended use, e.g., in food packaging, clothing or as a photoresist, these properties need to be adjusted. Plasma etching is a powerful method to influence the morphology as well as the chemical composition of the surface/near-surface area of a material. The drawback of this method is the limitation to perpendicular incidence angle. In contrast, ion beam etching offers the opportunity to change the ion incidence angle and can thus lead to different surface morphologies. This can cause a modification of properties and may allow the tailoring of properties.

In recent studies, a wide range angle-dependent (0° – 75°) pattern formation on the commercially available photo resist AZ® 4562 was investigated by utilizing Ar^{+}- as well as O_2/CHF^{3-} ion beams with a Kaufman-type ion source. To study the morphology of the surfaces atomic force microscopy (AFM) and scanning electron microscopy (SEM) was used. These studies reveal a multitude of patterns (holes, ripples, facets) that are formed in dependence of the ion incidence angle. The sequence of patterns resembles the known sequences of inorganic materials. A peculiarity is found at an incidence angle of 70°, where facets and a high etch rate are observed, but the roughness is much lower than for samples with comparably high ion incidence angles. In addition, the temporal evolution of these nanopatterns was observed for both types of ion beams. An altered chemical composition in form of a C-rich layer on the polymer could be detected by X-ray photoelectron spectroscopy (XPS) and ellipsometry [1].

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ABS: 39. Creation of Gold Nanoparticles in Langasite

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Langasite ($La_3Ga_5SiO_{14}$) is a material with interesting ferroelectric and optical properties for applications in environments with high temperature and/or high ionizing radiation level. The formation of metallic nanoclusters in transparent materials is, due to their unique nonlinear-optical properties, of high technological interest. The present paper aims at the investigation of the formation and removal of implantation-induced radiation damage as well as the production of Au-nanoparticles. Langasite single crystals were implanted with Au^+ ions at an energy of 150 keV and a fluence of 1.0×10^{16} cm^{-2}. The thickness of the damaged layer and the implantation profile agreed with the predictions by the SRIM code. The implanted samples were subjected to annealing in air at temperatures between 600 °C and 1000 °C. Optical absorption measurements showed that in the Au-implanted samples stable nanoparticles formed for temperatures of 800 °C and above. RBS/channeling studies showed that also a complete recovery of the crystal structure without takes place and that the Au implantation profile stays unaltered. On the other hand, samples treated at 600 °C showed whether nanoparticle formation nor measurable lattice recovery.

ABS: 59. Plasmonic Au nanoparticles by ion implantation

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The potential of gold nanoparticles as biosensors was being studied in a variety of fields including biology, medicine, chemistry, and physics. In this work, it was used ion implantation technology to control the formation of Au-nanoparticles in TiO_2 dielectric layers deposited in different substrates, silicon, and glass. Two different energies of 50 keV and 150 keV were used to achieve a wider Au distribution in depth, with fluences ranging from 1×10^{16} to 2×10^{17} ions/cm². After the Au ion implantation process, the samples were subjected to heat treatment for 15 min at a 500˚C to induce the precipitation of the Au ions. Before and after annealing, the depth profiles were examined using Rutherford backscattering spectrometry and the microstructure evolution was observed by scanning electron microscopy.

The results have shown that there are no significant changes in the Au profile after annealing. X-ray diffraction analysis revealed the presence of the (111) Au diffraction peak in both substrates and the microstructure of these samples confirm the presence of nanoparticles. The presence of an optical transmission band around 580 nm also confirms the presence of Au plasmonic nanoparticles. In particular, for the glass samples innovative and promising results were obtained, it was observed that Au is mobile enough to agglomerate in nanoparticles uniformly across the surface of the sample, but not mobile enough to form large clusters as observed in silicon samples.

ABS: 61. Manipulation of silicon etching with surfactant sputtering

Felix Linß [1], Frank Frost [1]

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Ion beam etching has gained increasingly attention due to the ability to machine ultraprecise surfaces and surface modifications. One main field in application is the optics fabrication, where ultra-smooth surfaces are necessary. Previous investigations showed that co-deposition of metals during silicon etching or sputtering supports the formation of nanoscale surface structures or patterns. These can increase surface roughness. A variety of metal species have been analysed to that effect. Eminent for the formation of such structures is the ability to from silicide compounds. To evaluate these effects in an industry relevant setup for future optic fabrication is the aim of this work.
The used experimental setup exists of a substrate holder for a silicon wafer, on which a target (co-deposition source) can be mounted with an angle of 45° to the substrate. With this setup parallel sputtering of the substrate and the target was provided. A broad beam RF ion beam source was used in the experiments. Which was operated with Argon and the following parameters: 220W RF power, 700V Beam Voltage, 100mA Ion current. A silicon removal on the wafer of 3µm was aimed for all experiments. Measurements with AFM & SEM were made to investigate the effect on the surface topography and the removal rate. Furthermore, characteristic dependencies for pattern formation shall be evaluated.
It could be shown that known silicide formers enable the formation of structures on the substrate. The removal rate varies with the co-deposition material. The main dependence for the alteration in roughness and removal is the surfactant species, as silicide formers strongly increase the removal. Hofsäß postulated a correlation between surfactant species and sputtering yields of the substrate material [1]. This could be verified with our results.

The work is financed by the EU, the BMBF & the Carl Zeiss SMT company.

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ABS: 66. Strong asymmetric modification of interfaces in Ir/Co/Pt layered system induced by low energy Ga^+ ion bombardment

Mateusz Kowacz [1], Marek Schmidt [1], Feliks Stobiecki [1], Piotr Kuświk 1

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In magnetic thin-film systems, a crucial role plays effects induced by the interfaces, which are the source of many important magnetic properties [1-2] (e.g. the perpendicular magnetic anisotropy (PMA), the Dzyaloshinskii-Moriya interaction). These properties can be controlled by the appropriate selection of ferromagnetic layer and its surrounding as well as by the quality of ferromagnet interfaces. In that systems, the interface-induced properties originate independently from both interfaces. Therefore it is important to tailor the interfaces in a controlled way, which can be performed by ion bombardment.

In this work, the bombardment of the perpendicularly magnetized Ti/Au/Ir/Co/Pt films with Ga^+ ions was performed in the energy range $5 \leq E \leq 30$ keV and dose range $10^{12} \leq D \leq 10^{15}$ Ga^+/cm^2. Polar magneto-optical Kerr effect measurements reveal that for low energy the spin reorientation transition from PMA to easy plane anisotropy occurs for higher doses than for higher E. This suggests that for lower E the efficiency of the ballistic mixing is weaker. Indeed the Monte-Carlo simulations (TRIDYN code) show that for low E the interfaces are less modified than for higher E, however with stronger asymmetry between the bottom and upper interface. From the analysis of this asymmetry and the correlation between the PMA and the number of displaced atoms at each interface, we found that the PMA in the Ir/Co/Pt system is more strongly related to the lower, i.e., Ir/Co interface. This indicates, that appropriately selected ion bombardment parameters enable stronger modification of the upper interface, which can be used to more effectively tailor magnetic properties induced by the upper interface.

This study was supported by National Science Centre Poland: OPUS (UMO-2019/33/B/ST5/02013).

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ABS: 106. Comparison of PMMA shrinkage in ion beam lithography: PMMA on glass substrate vs free standing PMMA film

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One of the prominent feature of the Poly(methyl methacrylate) (PMMA) is shrinkage under ion beam irradiation. It has been shown that this property of PMMA can be used to create 3D microstructures without any additional processing. Optical transparency, easy handling and low cost make this polymer advantageous for the manufacturing of optical elements. Our previous work has proven that diffraction grating can be produced by ion beam lithography exploiting shrinkage of PMMA caused by irradiation [1]. We discovered that the value of shrinking is different for the free standing film and the film deposited on a substrate despite the same film thickness and irradiation condition. In present work we focus on this phenomenon. We prepared 2 sets of samples: the first set consists of free standing PMMA films of four different thickness, and the second set – PMMA films of the same thickness as in the first set, but deposited on the glass substrate. The thickness of the films was 13, 20, 30 and 40 μm. Ion beam irradiation was performed as ion beam lithography with 2 MeV protons focused to 1.0×3.7 μm^2 with a beam current of 190 pA. The scan pattern for lithography represents parallel lines 1 μm thick and 1 mm long, spaced 10 μm apart. The fluence was 2.5×10^{14} protons/cm^2. Analysis of the PMMA shrinkage was performed by atomic force microscopy. It revealed that the shrinkage of the free standing film increases proportionally to its thickness, while the film on the substrate does not have a pronounce dependence. Comparing the shrinkage of free standing films with films on the substrate, it was fond that under the same irradiation conditions, the film on the substrate shrinks more and in the studied thicknesses the difference reaches 6 times.

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ABS: 161. Focused ion beam modification using gas and liquid metal alloy ion sources

Nico Klingner [1], Karl-Heinz Heinig [1], David Tucholski [1], Wolfhard Möller [1], René Hübner [1], Lothar Bischoff [1], Wolfgang Pilz [2], Gregor Hlawacek [1], Stefan Facsko [1]

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Broad ion beams have shown their wide applications for materials modification. Focused ion beams can be used in a similar way while simultaneously providing process monitoring. Here, we demonstrate this on a new kind of ion-induced structural evolution.

Sub-micrometer Sn spheres were irradiated in a helium ion microscope with a subnm beam of 30 keV He ions. Above a fluence of ~10^{17}/cm², Sn extrusions appeared on the surface of the spheres, which were imaged using the secondary electron signal. Initially, small, pyramid-like faceted extrusions form at the equator of the spheres (north pole pointing to the ion source). Later, each sphere becomes completely covered by the extrusions.

A model was developed that assumes that each He ion generate ~70 Frenkel pairs. The implanted helium atoms, interstitials, and vacancies will be confined by the oxide skin of the spheres. Some He atoms will occupy vacancies, which partially prevent their recombination with interstitials. Furthermore, the ion irradiation leads to erosion and opening of the SnO skin. The interstitials can now escape from the interior of the Sn sphere and form an epitaxial regular Sn lattice on the exterior. Transmission electron microscopy, Auger electron spectroscopy as well as TRI3DYN [1] and 3D kinetic lattice Monte Carlo [2] simulations support these findings.

In addition, we provide a perspective on focused ion beams from our in-house development and production of liquid metal alloy ion sources, which can be used for applications from self-organized patterning, over altering magnetic or electrical properties, to quantum photonics and computation [3].

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ABS: 3. Controlling the thermal properties of graphene by defect engineering

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Two dimensional (2D) materials such as graphene have attracted considerable scientific and technological interest in recent years due to their unique structure, extraordinary physical and chemical properties and emerging applications. Significantly, many critical properties (e.g. mechanical, thermal, electronic, magnetic and chemical) depend on the crystallinity of the 2D material and can be modified by structural defects. This raises the possibility of using defect engineering to enhance, functionalise or tailor materials for specific applications. While this can be achieved using a range of methods, energetic ion-irradiation offers a particularly practical and flexible approach. Here we present an overview of our recent studies of defect engineering in graphene, with particular emphasis on understanding how the concentration and defect type depend on the irradiation conditions and how these defects affect the material's thermal properties.

Supported and suspended graphene films are irradiated with 30 keV H-, C-, Li-, Si- and Geions to fluences in the range 10^{10}–10^{16} ions/cm^2 and the resulting defects characterised by Raman spectroscopy. Defect concentrations are determined from the intensity of the Raman D peak using the phenomenological model of Lucchese *et. al.* [1] and are shown to scale with the displacement cross-section of the ions. The nature of the defects is determined from the intensity ratios of Raman D and D' peaks using a model by Eckmann et. al. [2] and shown to depend only on the total defect density. The thermal conductivities of the irradiated films is then determined using Raman thermometry [3]. Details of these measurements and their implications are discussed as part of this presentation.

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ABS: 20. Doping of 2D materials by ultra-low energy ion implantation

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The ongoing development and current status of ultra-low energy ion implantation for the doping of graphene and transition metal dichalcogenides (TMDs) is described. For successful implantation in 2D materials, the ions are decelerated as low as 10 eV before impinging on the target. A new deceleration unit ensures that only part of the sample is irradiated by electrostatic masking, and thus a concentration gradient can be implanted without the need of a physical mask to ensure surface integrity [1]. For demonstration purposes, ion optical simulations were made and compared with experiments of 25 eV Mn on ta-C. With the help of RBS measurements, it is shown how the masking influences the amount of introduced Mn. In addition, an ion source combining a hot filament hollow cathode source with a sputter source was developed to provide ion beams of a wider range for the implantation [2]. An advantage of this source is that ion beams can be generated from low vapor pressure elements such as Mo. By test implantation with ultra-low energy (20 eV) in ta-C, we observe that these elements are suitable for implantation in 2D materials. After implantation, the elements were verified by RBS and PIXE measurements. As a first step towards an implanted pn-junction in graphene, laterally controlled implantation was used to implant B with 20 eV and a fluence of up to 5e14 B/cm². Subsequently, the surface potential was determined along the sample by scanning kelvin probe microscopy to investigate the transition region.

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ABS: 32. Coarsening of Embedded Ag nanoparticles under Ne^+ ion irradiation

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Silver nanoparticles (NPs) at the surface or embedded into dielectric thin films present interesting properties for biosensors, energy, information, and telecommunications technologies. The behavior of such NPs arrays is dependent on the NP size, shape, and distribution. This work explores the effects of Ne^+ and electron irradiations on the array characteristics of Ag NPs embedded in Si_3N_4 produced via magnetron sputtering. We performed room-temperature ion irradiations with 200 keV Ne^+ ions tilted 30° to the sample normal inside a medium energy ion scattering (MEIS) system. A 200 keV Ne^+ beam was used to characterize the microstructure. The corresponding MEIS measurements demonstrate that, upon a total irradiation fluence of $\Phi \approx 4x10^{15}$ Ne cm^{-2}, the initially oblate NPs (mean semiaxis values R = 4.1 nm and r = 3.69 nm) follow a coarsening process and evolve into structures containing an Ag core (c) and an Ag enriched Si_3N_4 shell (s) presenting mean dimensions R_c = 7.96 nm, r_c = 4.25 nm and R_s = 12.74 nm, r_s = 9.2 nm. In contrast, 160 and 200 keV electron irradiations under transmission geometry rendered NP spheroidization followed by its radius decrease [1]. The reduction of the NPs radius promoted by the electron irradiation is size-dependent and correlates with the reduction of the binding energy of surface located atoms. The microstructure evolutions observed by these irradiation experiments (electrons and Ne^+ ions) are discussed concerning the irradiation geometries and atomic displacement behaviors of Ag, Si, and N atoms.

Acknowledgment

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ABS: 34. Hydrogen gas detection using ion beam irradiated graphene

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Hydrogen gas detection is getting more important due to the hydrogen production, storage, and transportation as well as the development of hydrogen fuel cell vehicle. Thus, many materials and methods are being developed to meet various circumstances. Among the materials, graphene is also important candidate materials because it has a perfect 2-D nature and can be easily functionalized by a chemical manner or by a physical manner. However, graphene itself hardly detects hydrogen gas due to the low adsorption energy between H_2 and carbon dangling bonds. In order to function as hydrogen detector, pristine graphene can be customized by introducing heteroatom doping, inserting metal (or metal oxide) nano-sized domain, and converting to graphene oxide. In this research, we present that simple defect formation on graphene works as a hydrogen detector. Defects on graphene are generated by ion beam irradiation. Interestingly, the hydrogen detection efficiency increases with increasing the number of defects. In addition, DFT calculation reveals that defective graphene has higher adsorption energy. We discuss the hydrogen detection based on the simple resistance measurements with the defective graphene gas sensor.

ABS: 89. Modification of Ga_2O_3 by ion implantation

Alena Nikolskaia [1], Dmitry Korolev [1], Alexey Mikhaylov [1], Alexey Belov [1],
Elena Pitirimova [1], Dmitry Pavlov [1], Vladimir Trushin [1], Ruslan Krykov [1],
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Broad interest to gallium oxide is stimulated by the unique properties of this material. Monoclinic beta-Ga_2O_3 is a wide-bandgap (4.4-4.9 eV) semiconductor promising for applications in high-power electronics and solar-blind photodetectors. Its advantages also include high chemical resistance, multifunctionality, and the ability to grow large diameter ingots. However, new approaches are required to control the structure and defect-impurity composition of Ga_2O_3, including doping type and charge carriers concentration, which determine the main parameters for electronic applications. In order to solve this problem, we propose to use nonequilibrium methods, such as ion implantation, to control the introduction of defects and impurities of a required type and a given concentration into the material. In this work, we have studied the effect of irradiation with Si^+ ions on the structural, optical, and electrical properties of beta-Ga_2O_3 single crystals with different surface orientations: (-201) and (010). The dependence of structural perfection on the surface orientation is established. It is shown that electrical properties of the implanted beta-Ga_2O_3 layers are determined by the competing effect of radiation defects and the activation of implanted impurity. The highest degree of electrical activity of Si takes place for the (-201) orientation and reaches ~100% at a dose of 4×10^{14} cm^{-2} and annealing temperature of 950 degrees Celsius. For the (-201) orientation, a transition of the irradiated layer to the p-type is found at annealing temperature of 600 degrees Celsius. The creation of p-type is one of the main and most difficult tasks in Ga_2O_3 technology!
The results are discussed taking into account the anisotropy of the beta-Ga_2O_3 structure and its effect on the diffusion and drift of mobile radiation defects.

The work was supported by the RFBR (No. 19-57-80011).

ABS: 91. Light-emitting 9R hexagonal silicon phase synthesized by ion implantation

Alena Nikolskaia [1], Dmitry Korolev [1], Alexey Mikhaylov [1], Alexey Belov [1], Anton Konakov [1], Artem Sushkov [1], Dmitry Pavlov [1], David Tetelbaum [1]

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Silicon optoelectronics is a rapidly developing field of research due to the demand for increased speed of signal transmission in integrated circuits. The main problem of creating such optoelectronic silicon-based circuits is the insufficient luminescence efficiency of originally cubic silicon (c-Si). To resolve this problem, hexagonal modifications of silicon can be used. Previously, we have established the appearance of a photoluminescence (PL) peak at ~1240 nm when the SiO_2/Si system is irradiated with Kr^+ ions, which is associated with the formation of the 9R-Si hexagonal phase at the film-substrate interface [1]. It is assumed that the formation of 9R-Si phase is associated with the relaxation of elastic stresses arising in the interface Si layer under the action of a stressed SiO_2 film containing implanted atoms, as well as recoil atoms penetrating from the film to the substrate.

In this work, various factors affecting the formation, structure, and optical properties of the 9R-Si hexagonal phase synthesized upon ion implantation of the SiO_2/Si system are considered. It is revealed that the formation and properties of this phase are significantly influenced by the thickness of the SiO_2 film, the conductivity type and orientation of the Si substrate, the type of implanted ions, and also the parameters of post-implantation annealing. An interpretation of the obtained results is given.

The work was supported partly by the RFBR (No. 20-32-90204), Grant of the President of Russian Federation (MK-4092.2021.1.2) and by the support of the federal academic leadership program "Priority 2030" of the Ministry of Science and Higher Education of the Russian Federation.

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ABS: 93. Time of flight elastic recoil detection and rutherford backscattering spectrometry analysis of ReRAM devices

Matthew Sharpe [1], Mikko Laitinen [2], Pierre Couture [1], Jeevan Dulai [1], Horatio Cox [3], Wing Ng [4], Anthony Kenyon [4], Timo Sajavaara [2], Jonathan England [1]

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Redox-based resistive random access memory (ReRAM) devices have potential use in next generation non-volatile memories [1]. They offer low programming energy per bit, rapid switching and effortless integration [2]. Intrinsic resistance switching metal-insulator-metal structures, with two electrodes sandwiching a high resistance thin SiO_x layer, have been studied in particular for ReRAM devices [1]. Investigating O movement within the material is crucial, along with measuring amount of H, C and N present which affect the conductivity of the SiO_x.

Using Ion Beam Analysis techniques was expected to give accurate compositional information along with identifying the lighter elements. The structures studied were 25-40nm SiO_x on 70-200nm Mo, atop 1μm thermally grown SiO_2 on p-type Si wafer. The SiO_x was deposited via various techniques including reactive sputtering, atomic layer deposition and hydrogen silsesquioxane spin coating.

The time-of-flight elastic recoil detection (TOF-ERD) system at University of Jyväskylä [3], in preparation for Surrey Ion Beam Centre receiving their own setup, was used to measure various SiO_x/Mo structures. TOF-ERD, using 10.2MeV Cl^{5+}, was able to analyse all elements present in sample individually with no overlap, enabling each layer to be fully characterised to obtain layer compositions and thicknesses. The Mo, while heavier than the beam, was characterised using the scattered incident Cl beam, with Mo having sufficient separation from other elements. A 2MeV He^+ Rutherford Backscattering Spectrometry (RBS) measurement was taken for each sample to compare layer compositions and thicknesses, especially for thicker Mo layer samples. Both techniques showed good agreement, as well as information on the O reservoir-like behaviour of Mo.

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ABS: 105. Kinetics and PL quenching evaluation of optically active centres in β-Ga_2O_3

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The monoclinic β-Ga_2O_3 is a promising ultrawide-bandgap (UWBG) semiconductor that is attracting great attention in the scientific community due to its wide bandgap energy (~4.9 eV at room temperature) and high breakdown field (8 MV/cm), which are important properties for many applications including power electronics and solar-blind photodetectors. Defects play a crucial role in the electrical and optical properties of UWBG semiconductors. Hence, identifying the location of their energy levels within the gap, as well as understanding the behaviour of the optically active centres is critical to the development of optical device applications. Within the forbidden energy band of b-Ga_2O_3, several electronic states originating from defects are frequently encountered, with many of them not fully comprehended yet. Typically, under band-to-band excitation, undoped samples exhibit broad bands in the ultraviolet (~370 nm/3.35 eV) and blue (~420 nm/2.95 eV) spectral regions, associated with the recombination of self-trapped excitons and/or vacancy related defects. The incorporation of ions into the lattice, such as Cr^{3+}, gives rise to a red emission and the observation of narrow R-lines (~690 nm/1.8 eV) superimposed on a broad band with a maximum at ~730 nm/1.7 eV. The present work investigates those optically active defects on β-Ga_2O_3, in particular, the effect of ion irradiation on these optically active defects will be discussed, using steady-state and transient photoluminescence (PL), with excitation below and above bandgap, aiming to clarify the nature of the defects and establish recombination models.

ABS: 109. Incorporation of modified MoO_3 crystals and pseudo-layers into field effect transistors

Daniela Pereira [1], Chamseddine Bouhafs [1], Sónia Pereira [2], Carlos Díaz-Guerra [3], Marco Peres [1], António Fernandes [2], Bohdan Kulyk [2], Florinda Costa [2], Maria Rosário Correia [2], Eduardo Alves [4]

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Orthorhombic molybdenum oxide (α-MoO_3) is a wide band gap semiconductor with promising electrical and structural properties for several applications such as biosensors, gas sensors, solar cells and lithium ion batteries. Due to its lamellar structure, α-MoO_3 can be easily exfoliated in 2D flakes, promoting the transduction process. Additionally, its electrical properties can be efficiently tuned from insulating to metallic behavior, by controlling the oxygen stoichiometry of MoO_x (with x between 3 and 2).[1,2]

In this work, α-MoO_3 thin exfoliated crystals and pseudo-layers are obtained by a mechanical exfoliation process using adhesive tape and by the Pulsed Laser Ablation in Liquid technique, respectively. These materials are incorporated into field effect transistor (FETs) using two different processing strategies. Both FET devices show a modulation of the channel resistance with gate bias. A decrease of channel resistance with increasing gate voltage is observed, which agrees with the characteristic n-type behavior of α-MoO_3. Complementary, structural, morphological and optical characterization of MoO_3 pseudo-layers by Raman spectroscopy, Scanning Electron Microscopy, UV/Vis absorbance and X-ray diffraction will be discussed. As the α-MoO_3 is intrinsically insulating, it is necessary to modify its electrical properties to work in a FET device. In this way, ion implantation will be presented as a technique to increase the conductivity of this material. Indeed, an increase of conductance of about four orders of magnitude is observed for higher oxygen fluences, which is attributed to the formation of extended defects and new suboxide minority phases.[3,4]

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ABS: 110. IBIC: ion beam induced charge, nanobeam mapping photodiode and response of a diamond-based microdosimeter devices assessing charge

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Ion beam induced charge collection (IBIC) was developed mainly to analyse microelectronic devices, semiconductors, semi-insulating materials and light emitting diodes [1] with the capability to map leakage current effects [2]. This analysis technique measures the amount of induced charge collected from an ionisation event in the depletion layer of a junction [3]. The ionisation is caused by an incident ion beam in the MeV range [2]. This approach can be used to image material defects/damage and analyse the efficiency of charge detection [4].
In this study, a 2.5 MeV H^+ beam with a diameter of 0.5µm was used to analyse the features and induced damage in a Hamamatsu photodiode. Spectra were collected with an applied reverse bias of 10V. Beam damage caused reduced contrast on the map due to increased recombination, reducing the measured pulse height [5]. A diamond-based microdosimeter was exposed to 1.5 MeV He^+ to assess the detector responsiveness. IBIC maps showed the uniformity of the disperse charge across the detectors. Whereas for the photodiode charge efficiency varied significantly in time due to the exposure to an intense ion beam resulting in diffusion of the spectral peak towards lower energy, the microdosimeter was much less affected by the exposure. Incomplete charge collection was observed within a 2µm thick region surrounding the sensitive volume. The ability to detect such thin region with good accuracy, highlighted the excellent spatial resolution (smaller 1µm) achieved with IBIC.
This study leads to an investigation of cancer therapy detector.

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ABS: 111. Radio-frequency magnetron sputtering and annealing of Ga_2O_3 thin films

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Gallium oxide is an emerging semiconductor which shows great promise due to its ultra-wide bandgap (around 4.8 eV). Its applications range from high power electronics to solar-blind UV detectors. For this study, gallium oxide was deposited using radio-frequency magnetron sputtering at room temperature, allowing for low-cost, wafer-scale film growth on different substrates. All samples were prepared using the same deposition time of 30 min. Different substrates were considered (sapphire, quartz, and silicon) as well as different deposition parameters (argon flow and magnetron power). It was found by X-ray diffraction that the as-deposited films were mostly amorphous. Increasing the magnetron power from 20 W to 80 W increases the film thickness from ~60 nm to ~300 nm while the argon flow has negligible influence on the deposition rate, as suggested by Rutherford Backscattering Spectrometry.

After 1-hour annealing at 1000 °C in air, the films start to crystallise. For the case of quartz and silicon substrates, the films show polycrystalline characteristics with a preferential orientation. Interestingly, the films grown on c-plane sapphire reveal an epitaxial crystallisation and grow with a (-201) surface orientation. Furthermore, the thermal annealing leads to an interdiffusion at the interface and the formation of an $Al_xGa_{2-x}O_3$ compound. The Al-concentration can be tuned by varying the annealing time.

ABS: 114. Influence of proton irradiation damage on GaN core-shell p-n junction microwire radiation detectors

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Gallium nitride (GaN) nano- and microwires have gained increasing interest due to their unique geometry and flexibility, and have already been successfully applied in optoelectronics. One important advantage is their superior crystalline quality in comparison to their thin-film counterparts. Beside this, GaN is also known for its high radiation hardness, owed to the large displacement energy of the atoms in its crystal lattice and efficient dynamic annealing properties.

In this work, single GaN core-shell p-n junction microwires have been processed into radiation detectors and it was already shown that these are capable of sensing UV light and ionizing radiation [1]. However, it is relevant to quantify precisely what the impact of the ionizing radiation on the electrical properties of the sensors is, namely compared to their silicon counterparts. Therefore, the detectors were irradiated using 2 MeV protons up to different fluences, more specifically in the range of $5x10^{13}$ protons/cm² to $2x10^{16}$ protons/cm² , while measuring the dark, photo- and ionocurrent in-situ. Furthermore, the photoconductivity before and after irradiation is compared.

The results show that for fluences up to $1x10^{15}$ protons/cm² there is no significant modification of any of the parameters. For fluences above $5x10^{14}$ protons/cm² the photo- and ionocurrent start to decrease and the reverse bias leakage current starts to increase, reducing the signal-to-dark current ratio significantly and indicating introduction of defects in the crystal lattice of the microwires. Nonetheless, only when the fluence exceeds $1x10^{16}$ proton/cm², the detectors start to show serious deterioration, eventually leading to breakdown of the p-n junction properties. Additionally, EBIC measurements performed on irradiated samples show that a reduction of the space-charge region occurs as a consequence of the irradiation damage.

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ABS: 130. Fabrication of novel plasmonic nanostructures in silica using ion irradiation, etching, and nanoparticle deposition

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Plasmonic nanomaterials are expected to be a key technology that will unify electronics, electromechanical devices, and photonics. A novel route for manufacturing plasmonic metamaterials on the surface of crystalline and amorphous silica is presented. Silica substrates were irradiated with 20 MeV Ni ions and 40 MeV I ions at fluences below the overlapping track regime. The irradiated substrates were subsequently dry etched in hydrofluoric acid vapor to create nanowells with a variety of sizes and morphologies. Nanowell depth, anisotropy, and aspect ratio can be controlled by altering the etching time and etchant concentration. After etching, a colloidal suspension of gold nanoparticles (AuNPs) was deposited onto the substrates. Scanning electron microscopy and atomic force microscopy reveal that the AuNPs preferentially migrate to and agglomerate in the nanowells. Linear growth in the Raman scattering intensity as a function of AuNP concentration was found at low AuNP concentrations indicating that plasmonic hot spots in the interparticle spaces enhance the plasmon-phonon coupling to the quartz crystal. As much as a 200-fold enhancement was observed in the first micron of the material. At higher AuNP concentrations, however, a decrease in the enhancement factor following the Beer-Lambert Law was attributed to absorption by the deposited gold layer. Finally, ellipsometry measurements reveal changes in the effective dielectric function of the surface layer. This work presents a new route for functionalizing the surface of silica and producing thin metamaterial layers, the properties of which can be tuned through the choice of ion energy, fluence, beam angle, etching conditions, and nanoparticle deposition.

ABS: 134. Towards relaxation and stress micro-mapping in amorphous silicon by Raman spectroscopy

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Local variations of the stress and relaxation state at the nano- or microscale are of great interest in the field of functional coatings as they affect the mechanical and optical properties of these materials. Here, we propose a method to map these properties in amorphous films. We analyze local variations of the Raman spectra of amorphous silicon (a-Si) samples produced by self-implantation in Si(100). In this material, structural relaxation leads to a narrowing of the Raman TO peak and a small peak position change [1,2], whereas stress can be deduced from the TO peak position variation on a uniformly relaxed sample [3]. A self-implanted a-Si layer relaxed by annealing at 500˚C, and featuring a 3 µm-thick photoresist micro-pattern of lines and squares (1-20 µm), is self-re-implanted.

Mapping with a scanning micro-beam (µ-Raman) shows local zones of peak amplitude changes, position shifts (~10 cm^{-1}) and widening (~8 cm^{-1}) of the TO peak, corresponding to unrelaxed amorphous silicon zones. A Hyperspectral Raman Image shows local zones of similar shape but less precise amplitude changes and position shifts. Its higher spatial resolution (130 nm compared to 1 µm by µ-Raman) enables to resolve features at the interface between relaxed and unrelaxed a-Si. After correction of peak shifts due to relaxation, these measurements indicate that a local stress down to 70 MPa could be mapped by µ-Raman in amorphous films.

We note, however, that the µ-Raman method suffers from a trade-off between sample heating and laser power, which limits the statistics and leads to long acquisition times.

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ABS: 136. Formation of crystalline $Si_{1-x}Ge_x$ top layers by ion implantation in crystalline Si

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Si and Ge nanocrystals incorporated in a dielectric film offer new possibilities for optoelectronic devices such as photovoltaic tandem cells, where it could be used to exceed the Shockley-Queisser theoretical conversion limit. However, the charges generated in a dielectric film are hard to collect so it would be better if the charges were generated in a semiconductor matrix such as Si, which has better conductivity. Implanted Ge atoms have poor mobility in a Si matrix and thus Ge nanocrystals formation is not likely but it would still be interesting to form crystalline $Si_{1-x}Ge_x$ alloys.

In this work, 36 keV, 110 keV, and 350 keV Ge ions were implanted in crystalline Si, with fluences ranging from 5×10^{15} to 4×10^{17} Ge/cm² at temperatures up to 600 °C. Rutherford Backscattering Spectrometry (RBS), Raman Spectroscopy (RS), and Transmission Electron Microscopy (TEM) were used to investigate the $Si_{1-x}Ge_x$ alloys.

RBS spectra in channeling mode (RBS-c) show that Ge is mostly incorporated in substitutional sites for samples implanted at room temperature (RT) after 30 minutes annealing at 800 °C under N_2 atmosphere. XRD, RS, and TEM confirm that the $Si_{1-x}Ge_x$ layer on top of the c-Si substrate is monocrystalline with the possible presence of nanostructures and extended defects. Implantation was also carried out at temperatures up to 600 °C. RBS shows that the Ge profile is more extended in depth for the samples implanted at 600 °C, indicating that Ge diffuses in depth during implantation at 600 °C. However, RBS-c shows that the minimal yield is higher for implantations at 600 °C, indicating a high concentration of interstitials or that crystallinity is deteriorated, as confirmed by TEM.

ABS: 142. Modification of photochromic properties of oxygen-containing yttrium hydride films by irradiation using keV ions

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Oxygen-containing yttrium hydride (YHO) reversibly changes its optical absorption under illumination with UV and visible light, which is referred to as photochromic effect. A uniform decrease of the transmittance in the range of visible wavelengths makes this material a promising candidate for a plethora of applications, e.g. in smart windows and sensors. Some parameters of the photochromic response can be tuned via altering the chemical composition of YHO films. For example, faster bleaching speed can be achieved by increasing the O:H ratio [1]. However, higher oxygen concentration in the film leads to a larger band gap and thereby the material becomes photo-sensitive to a smaller range of wavelength in the visible regime [2]. Alternatively, photochromic properties can be changed by controlling the defect structure of YHO films. An effect of thermal annealing on photochromic behavior has been reported [3], while the effect of radiation damage remains so far unexplored.

We present a study of photochromic properties of oxygen-containing yttrium hydride after irradiation with keV ions. Films are exposed to different fluxes and fluences of ion beams with primary particle energies of a few hundred keV and characterized with respect to their optical properties. Possible changes in chemical composition due to ion irradiation/implantation are assessed employing Rutherford Backscattering Spectrometry and time-of-flight-energy elastic recoil detection analysis. Additionally, x-ray diffraction was conducted to reveal ion-induced modification of crystalline structure.

Our results on irradiation-induced modification of photochromic properties pave the way for tailor designed YHO-based devices as well as help complementing models for the photochromic behavior in YHO.

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ABS: 148. Role of carbide-tungsten interfaces on improving resistance to helium ion irradiation of dispersion-strengthened tungsten

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Because of its excellent thermal properties and sputtering resistance, tungsten (W) is chosen as the plasma-facing material for tokamak divertors. The high flux of helium (He) ions in the divertor region is a major threat to W since the generated He bubbles and ensuing fuzz formation can significantly modify the surface and thermomechanical properties of W. We showed that adding small concentrations of carbide dispersoids provided a promising approach to manage the excess He and improve the material resistance to He irradiation. The dispersion strengthened-W (DS-W) was fabricated using spark plasma sintering with 1 to 10 wt.% carbide, including ZrC, TiC, and TaC [1]. Irradiation of DS-W samples using 250 eV He ions at 800°C to the fluence of 1E20 cm^{-2} led to obvious nanostructuring (e.g., ripples and pores formation) on W surfaces, but less or even no morphology change of carbide surfaces. Transmission electron microscopy (TEM) analysis of cross-section samples found that a high density of He bubbles appeared in the W matrix, but no bubbles formed at the carbide-W interfaces [2]. Similar phenomena were also observed in DS-W samples irradiated by 2 keV He ions at 950°C.

Two mechanisms were proposed to explain the suppressed bubble formation at the interface, i.e., i) the interface acts as a fast diffusion path for He to reach other defect sinks like sample surfaces, and ii) efficient Frenkel pair recombination at the interface results in a low vacancy concentration for bubble growth. *In-situ* TEM analysis at elevated temperatures is conducted to identify the governing mechanism for carbide-tungsten interfaces to control bubble formation.

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ABS: 150. Sensitising the Cr^{3+} Luminescence by irradiation-induced defects in β-Ga_2O_3

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β-Ga_2O_3 is an emerging wide bandgap semiconductor with promising exciting applications. It is a good host material for optically active centres in the spectral region spanning from the infrared (IR) to the ultraviolet (UV) due to its high transparency (wide bandgap of ~4.9 eV at room temperature). In addition to the intrinsic UV/blue luminescence of undoped β-Ga_2O_3, Cr doping provides an efficient red/IR emission due to Cr^{3+} intraionic transitions. In this work, we studied the modification of the optical properties of β-Ga_2O_3 single-crystals doped with Cr or with Cr and Mg (Cr, Mg-doped) upon ion irradiation. The iono- and photoluminescence spectra of pristine Cr-doped samples were observed to be dominated by the intrinsic UV/blue luminescence; however, during ion irradiation, this emission was progressively quenched, while the Cr^{3+} luminescence was enhanced. On the contrary, for Cr, Mg-doped samples, the Cr^{3+} emission yield was already high in pristine samples, and no further increase occurred during ion irradiation. The same distinct behaviour of the two sets of samples was also observed by thermoluminescence (TL) measurements, monitored at the Cr^{3+} emission wavelengths: while pristine Cr, Mg-doped samples showed strong TL signals, Cr-doped samples revealed no such signal prior to the ion irradiation. TL was activated after ion irradiation and quenched after thermal annealing at 650 °C. X-ray absorption near edge structure measurements suggest that the Cr charge state was not altered by the ion irradiation, invalidating the hypothesis that the enhancement of the Cr^{3+} emission is due to a change in the Cr charge state. Alternative mechanisms, including charge/energy transfer paths involving defect levels, will be discussed. This study thus contributes to a better understanding of the sensitisation of the Cr^{3+} luminescence by defect levels in β-Ga_2O_3 and unveils the potential of Cr-doped β-Ga_2O_3 for optically detecting ionising radiation, either in- or ex-situ.

ABS: 156. High energy ion irradiation of MgF_2 for improving the physical properties for FUV applications

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The far ultraviolet (FUV, wavelengths shorter than 200 nm) spectral range contains fundamental spectral lines for astrophysics and solar physics communities, who require efficient optics and coatings tuned at such wavelengths. Multilayers (MLs) based on two fluorides are the only available coatings to provide narrowband FUV reflectors. The most common materials to make these MLs alternate either AlF_3 or MgF_2 with LaF_3 [1,2]. MLs based on these materials are proposed for LUMOS (LUVOIR Ultraviolet Multi-object Spectrograph) instrument and we are collaborating with the Laboratory for Atmospheric and Space Physics of the Colorado University in Boulder to develop stable, high-performance MLs based on these fluorides for LUMOS. Ion irradiation is a well known method to modify most of the physical properties of the near surface region of materials. This can be addressed using both, high energies (several MeVs, i.e. using the electronic damage), or lower energies (i.e. using the nuclear damage).

We have studied for this work the physical and optical changes induced in MgF_2 (both in bulk samples and in ultrathin evaporated films) irradiated with a broad set of ions (He, C, F, Si, I), energies (1-50 MeV) and fluences. We have performed in-situ optical measurements for obtaining a detailed kinetics of the damage creation and accumulation. RBS/C has been performed to obtained in-depth damage profiles. Raman spectroscopy has been used for water content and strain/stress assessment.

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ABS: 158. Properties of Cr_2AlC thin films disordered by ion-irradiation

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MAX phases are nano-lamellar composite materials of the form Mn+1AXn, where n is 1, 2 or 3; M an early transition metal; A is an A-group element (mostly groups 13-14) and X is C/N [1,2]. An interesting combination of metallic and ceramic properties as well as potential applications in spintronics [1,3] led to significant research interest in MAX phases. Disorder can be introduced in the crystal structure by using ion beams at different energies/fluences of irradiation. Here we observe the magneto-transport properties and attempt to separate the contributions of structural changes due to the irradiation and magnetic effects due to the doping on the magneto-transport. A prototype material is Cr_2AlC, formed from a unit cell of Cr_2C sandwiched between atomic planes of Al. In this work, we study 50 nm and 500 nm thin films of Cr_2AlC grown on Si (111) by sputtering and subsequent annealing. Structural characterization with XRD shows a visible MAX phase, confirmed by the occurrence of the 002 superlattice reflection. The films were irradiated with Co+ at 450(50) keV for the 500(50) nm thick films. The Co^+ fluence varied between 10^{12}-10^{15} ions.cm^{-2}. The Co^+ irradiation led to a gradual suppression of the 002 superlattice reflection, while preserving the fundamental peaks, implying the intermixing of the nano-laminar MAX phase structure. Magnetic properties are characterized using VSM at low temperatures, showing an increasing paramagnetic behavior as the Co^+ fluence increases. In comparison, magneto-resistance measurements show that for the 500 nm film thickness, the magnetoresistance reaches up to 3%(10 T) for 100 K, at Co^+-fluence of 5×10^{13} ions.cm^{-2}. The results suggest that in the low-fluence regime, the irradiation-induced disorder remains sufficiently low to obtain pronounced magneto-resistance values. Understanding the defect state in the optimized MAX phase films will shed light on the magneto-transport mechanisms in these nano-laminated materials.

ABS: 165. Luminescent properties in CVD grown diamond single crystal modified by laser irradiation and ion implantation

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Presently, quantum technologies are being widely studied, especially for information and sensors. The nitrogen-vacancy (NV^0 and NV^-) are among the most studied optical centres in diamond, with particular interest for quantum information processing applications, as it is possible to study the properties of single NV^- centres, assessing each state of the qubit by optical pumping and read-out the final state by optical spectroscopy. There are several methods to generate these centres that can be summarized in three main steps that account for 1) the presence of N impurities, 2) lattice vacancies, and 3) thermal annealing treatments. In this work, commercial single-crystalline diamond samples grown by chemical vapour deposition were subjected to two different approaches to modify/generate new optical centres: (i) room temperature ion implantation with europium (Eu) ions, using fluences of 1×10^{13} Eu/cm^2 and 1×10^{14} Eu/cm^2 with an energy of 300 keV, followed by thermal annealing; and (ii) laser modification, focusing a laser beam of 355 nm with a frequency of 30 kHz and power that varied from ~1.2 W to 5W during different times (up to 5 min) on a sample immersed in distilled water. The latter were conducted with and without the presence of Eu ions in the liquid medium. All samples were analyzed by Fourier-transform infrared, Raman and photoluminescence (PL) spectroscopies. On the samples implanted with Eu, the PL spectra show no significant differences in the optically active centres present, however, the Raman data revealed new bands peaked at 1147 and 1397 cm^{-1} near the 1333 cm^{-1} vibrational mode, likely due to radiation damage induced during the implantation process. The samples subjected to laser radiation show a meaningful increase in the PL intensity of the H3 and NV^0 centres (both already present in the as-grown sample), which can be related to irradiation and heating processes and so, to the creation of additional defects.

ABS: 177. Defect and strain profiles caused by ion implantation in gallium nitride

Afonso Caçador [1], Przemysław Jozwik [2], Sérgio Magalhães [3], Eduardo Alves [3], José Marques [4], Paul Kutza [5], Elke Wendle [5], Michal Bockowski [6], Katharina Lorenz [7]

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Gallium Nitride (GaN) is a wide bandgap semiconductor, belonging to the III-nitrides family, along with AlN, InN and their ternary and quaternary alloys. It possesses properties, such as high electron mobility, bandgap, and electric breakdown field, which allow it to operate under high voltage, high temperature and high-frequency regimes without sacrificing its characteristics. This makes GaN an ideal candidate as the next generation replacement of the common Si devices, namely in the field of power electronics. In order to manipulate some of the crystals' properties, ion implantation is often performed. Despite its advantages, this technique creates a lot of defects and strain in the materials, which may hamper proper device operation and reduce its efficiency. In this work, GaN samples were implanted with heavy low energy Europium (Eu) ions and light high energy Silicon (Si) ions using several different fluences. Experimental techniques, such as Rutherford Backscattering Spectrometry in Channeling mode (RBS/C) and X-Ray Diffraction (XRD) are employed in order to find the defect and strain profiles for the implanted samples. In the case of the GaN:Si samples, in-situ measurements of the samples' bending were carried out to obtain the evolution of the induced stress with the fluence. The defect profiles were extracted from RBS/C using analytical models and Monte Carlo simulations. These profiles agree well, and are consistent with the strain profiles extracted from XRD. The profiles' evolution with fluence suggests that defect transformations occur, namely from point defects to more complex defect structures. This process leads to stress/strain relaxation, observed both in the strain profiles and in the results of the bending experiments. A model for the evolution of stress, based on the results from the profiles, was built and describes well the obtained experimental curve.

ABS: 198. Multiple phases and electronic structures of silicon monoxide

Yadong Wei [1], Kaijuan Pang [1], Ku Ruiqi [1], Ming Sha [1], Hongxi Huang [1], Jianqun Yang [1], Xingji Li [1], Weiqi Li [1]

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The properties of silicon-based electronic device are noticeably affected by the electronic states and characteristic of defects at the interface of Si/SiO_2. Recently, people discovered that the assembly of O-deficient localized structures made up of the 1:1 ratio of silicon and oxygen are visible near the interfaces under specific process conditions. Although the potential applications in anode material of high-power lithium battery are explored, the difficulty to catch the localized structural information by experiment limited the study of reliable physical mechanisms of interface properties.

In this work, via the highly efficient structure-searching algorithm named after particle swarm optimization (PSO), we discovered nine possible phases of silicon monoxide with lowest formation energy, and systematically studied their electronic properties. Most thermodynamically stable phase structures have metal band gaps, while there are two phases with band gaps of 0.12 eV and 2.71 eV respectively.

The diversity of electronic band gaps endows silicon oxide with rich electronic characteristics and provides local energy levels for interface trapping of carriers. This study reveals the local electronic characteristics of unconventional stoichiometry in the interface structure, and provides a theoretical reference for studying its influence on the interface electronic characteristics, and then designing the interface heterojunction structure with radiation resistance and high electron mobility.

ABS: 200. 3D ferromagnetic microstructures produced in paramagnetic thin films by ion implantation through masks

Petter Ström [1], Tuan Tran [1], Daniel Primetzhofer [1]

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Palladium, an element which is paramagnetic on its own, can constitute the majority component in a ferromagnetic alloy if mixed with minute quantities of e.g. iron or cobalt. The effect as such is well known and has been studied in both thin films and bulk materials for over half a century. In a recent publication, we investigated ion implantation as a method for introducing the alloying element [1]. It was shown that knowledge of the composition depth profile in the resulting material can be used to calculate its macroscopic magnetic properties.

Quantities like Curie temperature, coercivity and saturation moment vary based on the local minority element concentration. Variation in these quantities can thus be engineered by controlling the amount of the minority element that is introduced at different positions in a sample. Ion implantation enables control of the depth distribution of implanted species, while the addition of a mask makes lateral patterning possible. The possibility to engineer 3D magnetic micro- or nanostructures is thus provided.

In this contribution we present basic theory and results for the magnetic properties of polycrystalline Pd films, implanted with a laterally homogenous distribution of singly charged Fe-56 ions at the Uppsala Tandem Laboratory [2]. We also show data obtained after implantations through masks, comparing contrasts in (a) the abundance of the minority element measured by scanning electron microscopy and ion microbeam analysis, and (b) magnetic properties probed with Kerr effect microscopy. A brief discussion on applications is given, with focus on size constraints and limits for properties obtainable with the investigated methods.

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ABS: 208. Electrical contacts in cleaved and exfoliated Ga_2O_3 crystals

V. Martins Miguel [1], Pereira Daniela R. [1], Duarte M. Esteves [1], Verheij Dirkjan [1], Bouhafs Chamseddine [1], Peres Marco [1], Freitas Susana [2], Lorenz Katharina [1]

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Gallium oxide has a very wide band gap of 4.6-4.9 eV [1,2] and a high breakdown field of around 8 MV/cm [1,2] making it an appealing semiconductor for both sensing and power applications. Additionally, its monoclinic phase (the most thermally stable) can be exfoliated and easily cleaved along the planes (100) and (001) [2], making it easy and fast to obtain high quality quasi-2D crystals in a laboratory setting. Electrical contacts deposited on cleaved and mechanically exfoliated crystals were studied in order to find what metals, deposition methods and annealing steps lead to ohmic and Schottky contacts.

For example, for sputtered Cr/Au contacts, the electrical characteristic is initially ohmic, but begins to show rectifying behaviour after annealing in Ar at 300 ºC. Given the high work functions of Au and Cr, the Schottky barrier should be high. The ohmic response is probably due to the defect states created by the sputtering process, which might lower the Schottky barrier. Inversely, for Ti/Al/Ni/Au deposited through ion beam deposition, an ohmic response is obtained only after annealing in Ar.

These thin crystals, obtained by exfoliation, were also used as channels in field effect transistors, with emphasis on sensing applications.

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ABS: 4. The effect of nano-sized helium bubbles on the migration behaviour of selenium implanted into polycrystalline silicon carbide

Zaki Abdalla [1], Mahjoub Ismail [1], Hesham Abdelbagi [1], Eric Njoroge [1], Johan Malherbe [1], Thulani Hlatshwayo [1]

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The migration behaviour of selenium (Se) implanted into polycrystalline silicon carbide (SiC) in the presence of helium (He) was investigated. SiC wafers were first implanted with Se ions of 200 keV to a fluence of 1×10^{16} cm^{-2} at room temperature (RT), 350 °C. Some of the implanted wafers were then implanted with 17 keV He with a fluence of $1x10^{17}$ cm^{-2} at RT. The implanted samples were then annealed at 1000 °C for 10 h under vacuum. Structural and morphological characterization of the samples was performed before and after annealing by Raman spectroscopy and scanning electron microscopy (SEM). Rutherford backscattering spectroscopy (RBS), elastic recoil detection analysis (ERDA) and Transmission electron microscopy (TEM) were used to analyze the migration of implanted ions. The results were qualitatively compared with the published results obtained after implantation of SiC with Se only.

The formation of He bubbles were clearly observed in Se&He-SiC after implantation near the ion projected range. Annealing the Se&He–SiC at 1000 °C led to the appearance of a network of cavities and pores. Migration of Se towards the surface was observed in the Se & He-SiC implanted sample at this temperature. In contrast, migration was observed in Se-SiC sample, indicating that helium assisted the migration of ions as suggested by Se & He-SiC results.

ABS: 9. Effects of helium on the structural evolution and migration behavior of silver and strontium implanted into polycrystalline SiC

Zaki Abdalla [1], Gcobani Ntshobeni [1], Johan Malherbe [1], Thulani Hlatshwayo [1]

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The effect of He on the migration behavior of silver (Ag), and strontium (Sr) co-implanted into polycrystalline silicon carbide (SiC) was investigated. Ag ions of 360 keV were first implanted into polycrystalline SiC to a fluence of 2×10^{16} cm^{-2} at 600 ºC, followed by implantation of Sr ions of 280 keV to a fluence of 2×10^{16} cm^{-2} also at 600 oC. Some of the co-implanted samples were then implanted with 17 keV He ions to a fluence of 1×10^{17} cm^{-2} at 350 ºC. The dual (Ag&Sr-SiC) and triple (Ag&Sr&He-SiC) implanted samples were isochronal annealed at temperatures ranging from 1000 ºC to 1300 ºC in steps of 100 ºC for 5 hours. The as-implanted and annealed samples were then characterized using Raman spectroscopy, scanning electron microscopy (SEM), atomic force microscopy (AFM), elastic recoil detection analysis (ERDA), and Rutherford backscattering spectroscopy (RBS). Both dual and triple implantation resulted in the reduction of Raman peaks intensity accompanied by broadening indicating accumulation of defects without amorphation of SiC structure. Triple implantation also resulted in the appearance of blisters and holes indicating He bubbles and cavities in the implanted layer. Progressive annealing of defects as a function of temperature was observed in both annealed samples. Implantation of Sr caused pre-implanted Ag to form precipitates indicating some limited migration while implantation of He in caused some migration of both pre-implanted Ag and Sr. No migration of Ag and Sr was observed in the dual implanted SiC, however annealing the triple implanted SiC at 1000 ºC caused some migration towards the bulk and surface resulting in the formation of double peak profiles indicating the trapping of the implants by cavities. Hence, He bubbles do have a role in the migration of implanted Ag and Sr and cavities limit the migration.

ABS: 17. Ion beam modified silicon: both 28-Si enrichment and donor doping for quantum devices

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The features of group-V-donor spins implanted in isotopically enriched 28-Si crystal make them attractive qubits for large-scale quantum computer devices. Useful attributes include the long spin lifetimes of 31-P, hyperfine clock transitions in 209-Bi or electrically controllable 123-Sb nuclear spins [1]. Practical architectures require deterministic fabrication of arrays of individual near-surface dopant atoms placed with high yield. Using one-for-one ion sputtering from high-fluence 45 keV 28-Si ion implantation we demonstrated depletion of the non-zero nuclear spin isotope 29-Si to 250 ppm [2] and electron spin resonance measurements of near-surface 31-P donors with depletion of 3000 ppm produced a T2-Hahn electron coherence time of 285 μs commensurate with previous work. The resonance amplitude as a function of time showed a single component exponential decay without the need for a third order term imposed by dipole interactions with residual 29-Si. For implanting donor atoms, we employ on-chip electrodes with optimised charge-sensitive electronics to demonstrate the near room temperature implantation of single 14 keV 31-P ions with an unprecedented >99.8% detection confidence for near-surface implants [3].

These methods are potentially compatible with localised enrichment zones to house donor qubits in larger n-Si wafers by employing 28-Si^{++} beams produced by focused ion beam systems. Wafer-scale enrichment is also possible in an industrial fab which could potentially allow both 29-Si depletion and qubit donor array construction in the same ion implantation system for mass production.

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ABS: 29. Effective Li dendrite penetration reduction in solid-state batteries through Xe ion created surface compressive stress

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The high energy density solid-state batteries (SSBs) with Li metal anode is a promising solution for the carbon-neutral future. Still, the short-circuit failure caused by the Li dendrite penetration needs to be addressed first.[1] Recently we demonstrated a clear improved performance of SSB by introducing surface compressive stress in garnet-type $Li_{6.4}La_3Zr_{1.4}Ta_{0.6}O_{12}$ (LLZTO) electrolyte through multiple energy Xe ion implantation.[2]

This presentation will evaluate the impact of stress on solid-state electrolytes and the design of a rational experimental modification route. A sequential multiple energy Xe ion-implanted LLZTO solid-state electrolyte is used to build Li-metal cells, with implanted Xe ions distributed in a range of 160-600 Å from the surface. The cell with a volume concentration of 10^{19} Xe/cm^3 exhibits stable Li stripping/plating cycles and significantly extended lifespan, while lower concentrations of 10^{18} Xe/cm^3 or higher concentrations of 10^{20} Xe/cm^3 are still facing cell failures. This improvement is attributed to the ion implantation with an appropriate Xe concentration inducing sufficient surface compressive stress balanced over grains. We have confirmed this by thorough grazing incidence X-ray diffraction studies. Other supporting experimental observations will also be presented.

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ABS: 30. Twenty years of electronic stopping power of ions in matter: tendencies, areas of interest and lack of data

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Stopping powers are relevant to a wide range of applications, spanning materials sciences, cultural heritage, medical applications, fission and fusion technologies and space applications. They are directly used in experimental techniques such as ion beam analysis, deposition ranges, ion implantation, and studies of radiation damage, to name a few. Reliable values of stopping powers are also needed in isotope production and detector development for basic and applied research. In this work we give an overview of the last twenty years of experimental effort, identify the trends in recent measurements [1-5], and discuss the emerging data needs. Our analysis is based on the comprehensive experimental electronic stopping power database of the International Atomic Energy Agency [6,7], and on selected semi-empirical and theoretical descriptions. We also present the recent effort to modernize the IAEA stopping power database and create a versatile tool adaptable to the needs of a continuously developing user community.

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ABS: 44. Low-energy heavy-ion beam capable of simultaneous induction of multiple chromosomal aberrations for rice mutation

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We reveal that applying low-energy heavy ion beam (LEHIB) has a special advantage in simultaneous induction of multiple chromosomal aberrations for crop mutation breeding. Rice is an example in this study. Seeds of Thai jasmine rice KDML105 were bombarded using tens-keV nitrogen-ion beam only once and subsequent screening enabled us to obtain simultaneously multiple mutations in offspring generations which possessed improved traits including high yielding, photoperiod insensitivity, dwarf or tall stature, early mature, dark color grains, high resistance to blast disease, prolonged seed storability, drought tolerance, brown planthopper resistance, etc.

Molecular biology analyses for genetics responsible for the phenotypic changes demonstrated that all 12 chromosomes of the rice genome corresponding to the trait changes were modified.

Physics involved in the simultaneous modification of the chromosomes caused by LEHIB is discussed to illustrate the advantage in comparison with high-energy ion beam.

ABS: 45. Low-energy ion beam induced brown-planthopper resistant thai jasmine rice mutants

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Brown planthoppers (BPHs) constitute one of the most devastating annual threats to Thai jasmine rice, which is BPH-susceptible. To fight against BPHs with a novel manner, we applied low-energy nitrogen-ion beam to irradiate the rice seeds for screening of BPH resistance. Three rice mutants were obtained exhibiting moderate resistance to BPH demonstrated by analyses of antixenosis, antibiosis and catalase activity after infestation tests.

Genomic sequence analysis of catalase genes in one of the mutants, which exhibited the highest catalase activity after the BPH infestation, revealed a number of point mutations in the non-coding region of catalase gene CATALASE ISOZYME A (CATA), as compared with its wild-type.

ABS: 56. Overview of polyethylene terephthalate foils patterned using low energy ions for the realization of micromembranes

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Polymer membranes are conventionally prepared by high-energy particles from radioactive decay or by bombardment of hundreds MeVs energy ions. In both two circumstances, tracks of damage are produced by particles/ions passing through the polymer, and successively, the damaged material is removed by chemical etching to create long and narrow pores. These processes ensure the achievement of well controlled pore-diameter but also random placement of pores leading to not uniform local pore density and low membrane porosity to reduce their overlapping.

On the contrary, the use of low energy ions (lower than tens of MeV) for the realization of micromembranes leads to several advantages: membrane's production can be not limited to the use of huge ion accelerators, the ion irradiation cost can be significantly reduced, membranes with high density pores without overlapping and customized pore positions can be fabricated.

Since membranes are typically made from polyethylene terephthalate (PET) or polycarbonate (PC), the present study is focused on the use of PET foils with different thickness, irradiated by 10.0 MeV carbon ions easily available at ordinary ion accelerators. The ion irradiation conditions, the etching conditions and the etching time were monitored to obtain high aspect-ratio pores in PET. The effectiveness of low energy ions to produce tailored micromembranes of PET was explored. The quality of the pores generated in the micromembranes have been analysed by Scanning Transmission Ion Microscopy for possible application for cells culture and filtration technology.

ABS: 57. The effect of oxide dispersoids on the helium bubble formation in advanced structural materials for nuclear applications

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The present contribution discusses the early stage of the ageing process introduced into f/m steels due to exposure to harsh radiation environments. Fusion applications or spallation neutron sources, i.e., radiation environments with high transmutation helium production rates, cause substantial radiation embrittlement of structural materials accompanied by helium bubble formation. The slow positron beam spectroscopy is employed to characterize the nucleation and growth of nano-scale helium bubbles and to reveal the differences in the radiation tolerance of Fe_9Cr steel and its variant strengthened by thermodynamically stable nano-oxide dispersoids (ODS Fe_9Cr). The harsh radiation environment is simulated by irradiation with 500 keV He^+ ions with a fluence of 10^{22} m^{-2}. The irradiation is conducted using a 500 kV open-air implanter at a slightly higher than ambient temperature. The study is complemented with transmission electron microscopy analyses (TEM). Combining the two techniques enables us to characterize a wide range of helium-vacancy agglomerations i.e., the evolution of helium bubbles from small clusters of radiation-induced vacancies to large cavities well resolvable by TEM. Superior radiation resistance of oxide-dispersion strengthened steels dominates only in the early stages of bubble evolution, where positron lifetime measurements provide a missing piece of the microstructural puzzle conventionally constructed by TEM.

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ABS: 58. Ion beam synthesis of high oxidation state palladium and copper oxides

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High oxidation states of several transition metals are virtually missing on the stoichiometric map of transition metal oxides. We have efficiently obtained stable PdO thin films with RF sputtering of a Palladium wire. To achieve and stabilize the higher oxidation state, in this case to obtain Pd(IV)O_2, we employ Plasma immersion ion implantation (PIII) of Oxygen as well as ion implantation using ion accelerators to obtain the 1:2 ratio between Pd and O in the layer. Synthesis of the PdO_2; phase was successfully reported only once [1], while all other works report PdO_2 stabilised by other metal oxide phases. The experiment [1] as well as DFT calculations [2] indicate its structure being rutile type with lattice parameters very close to TiO_2. Another experiment will use TiO_2 monocrystalline substrates to facilitate epitaxial growth as well as elevated temperatures to increase the oxidation rate. Another system being explored is CuO_2 where the synthesis seems easier than in the case of PdO_2. Base films for ion implantation of oxygen were prepared by DC magnetron sputtering, synthetizing CuO, the phase with highest oxygen to Cu ratio of all stable and obtainable CuO_x phases, followed by ion implantation. Both Palladium and Copper oxides will be analysed by transmission electron microscopy, selected area electron diffraction as well as grazing angle x-ray diffraction and hard x-ray photoelectron spectroscopy (HAXPES).

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ABS: 65. Behavior of Cu-Y_2O_3 and CuCrZr-Y_2O_3 composites as thermal barriers for nuclear fusion applications

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The Cu-Y_2O_3 and CuCrZr-Y_2O_3 composites have been proposed as interlayers between W and CuCrZr to act as a thermal barrier in the divertor part of the nuclear fusion reactor. These composites were prepared in a glovebox to avoid the oxidation of the metals with different volume fractions of Y_2O_3 (1, 5, 10, and 15). The materials were then consolidated by spark plasma sintering between 775-800 ºC under pressures of ~57 MPa with a holding time of 5-8 min.

All consolidated materials show densifications between 90 and 99 % of the theoretical values with decreasing densities upon increasing of the Y_2O_3 %. The microstructure of the consolidated samples revealed dispersions of Y_2O_3 regions in the Cu matrix or in the CuCrZr and the formation of Y_2O_3 agglomerates. After the analysis of the results, only two samples (Cu- 5%Y_2O_3 and CuCrZr- 5% Y_2O_3 with higher densification) were chosen to perform some relevant studies for this application as: thermal diffusivity, mechanical properties and irradiation resistance. The thermal diffusivity of the samples Cu5%Y_2O_3 and CuCrZr- 5% Y_2O_3 is similar, and the values are lower than pure CuCrZr and Cu, but higher than W. Ductile behaviour was observed in whole temperature range and the CuCrZr-based samples exhibited a rupture strength six times higher than in the Cu-based material, although this difference was decreasing as the temperature increased.

No significant changes in the microstructure of the samples irradiated with Ar were observed, which is a good indication of the materials irradiation resistance.

ABS: 69. Irradiation damage on $CrNbTaVW_x$ high entropy alloys

Ricardo Martins [1], José Correia [2], Piotr Czarkowski [3], Ryszard Miklaszewski [3], Artur Malaquias [1], Rodrigo Mateus [1], Eduardo Alves [1], Marta Dias [1]

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$CrNbTaVW_x$ high entropy alloys have been devised for thermal barriers between the plasma-facing tungsten tiles and the copper-based heat sink in the first wall of fusion nuclear reactors. $CrNbTaVW_x$ (x =1, 1.7) were prepared by ball milling and consolidated by Upgrade Field Assisted Sintering Technology at 1600 °C and under 90 MPa of pressure. The samples with different compositions were then irradiated with deuterium plasmas in the PF-1000U facility with 1, 3, and 5 discharges. Typical parameters of the energies discharge in PF-1000U are of order around 600-1000 kJ, individual ions have average energy close to 100 keV and a fluence of $7.5x10^{15}$ ions/cm^2 by discharge for the fast ion streams. Structural changes prior to and after the irradiation were investigated by scanning electron microscopy, coupled with energy-dispersive and X-ray spectroscopy. Particle induced X-ray emission and Rutherford backscattering spectrometry spectra were collected with 2300 and 1750 keV $^1H^+$ ion beams, respectively, to identify possible contaminants in the irradiated samples, while nuclear reaction analysis was carried out with 2300 and 1000 keV $^3He^+$ ion beams to evaluate the profile and amount of retained deuterium in the irradiated samples. After irradiation, both samples revealed swelling and in the case of $CrNbTaVW_{1.7}$ partial melting. The damage on the microstructure after irradiation was more severe for sample $CrNbTaVW_{1.7}$ when compared with the CrNbTaVW. Moreover, the D retention increased for both compositions as well as the number of shots, and the CrNbTaVW evidenced high retentions when compared with $CrNbTaVW_{1.7}$ considering the same number of shots.

ABS: 71. Radiation resistance of aluminum-magnesium spinel: optical effects of high-energy ion irradiation

Abdirash Akilbekov [1], Meruert Mamatova [2], Vladimir Skuratov [3], Nikita Kirilkin [4], Andrze Olejniczak [5], Alexander Mazanik [6], Nikolai Kazuchits [6], Alma Dauletbekova [1], Sholpan Giniyatova [1]

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Nowadays, special attention is paid to the aluminum-magnesium spinel $MgAl_2O_4$, which exhibits exceptional radiation resistance. It is especially important that $MgAl_2O_4$ was chosen as a matrix for transmutation of actinides by capturing neutrons in nuclear reactors, as a matrix for storing radioactive waste. Also, the intensive development of photonics and electronics requires the development of new functional materials with high radiation resistance, transparency in a wide spectral range, and thermal stability.

The work presents of optical effects induced in crystals of $MgAl_2O_4$ by irradiation with high-energy heavy ions, simulating the impact of fission products of nuclear fuel.

The samples were irradiated by 46 MeV Ar, 107 MeV Kr, 150 MeV Xe and 710 MeV Bi ions in the fluence range of 10^{10}-10^{13} cm^{-2} (IC-100, U-400 cyclotrons FLNR JINR, Dubna, DC-60 Nur-Sultan). The PL measurements were performed in two experimental geometries: standard (λexc. = 355 nm) and confocal (λexc. = 355 nm, 445 nm, 473 nm and 532 nm) at RT.

The PL spectra of unirradiated $MgAl_2O_4$ contain emission bands of Cr^{3+} (1.8 eV) and Mn^{2+} (2.4 and 1.6 eV) impurities. Irradiation induce a broad luminescence band at 2.48–3.1 eV (standard geometry) with a three-peak structure, which is similar to MgO crystals. The PL spectra (confocal geometry) showed an intense non-elementary bands around 1.55-3.1 eV under excitation light with wavelengths 355 nm, 445 nm, 473 nm and 532 nm. Intensities of these bands increase with the ion fluence up to 10^{12} cm^{-2}.

The analysis of the PL spectra obtained in standard geometry allowed us to assume that the radiation-induced defects created in the track region are surrounded predominantly by Mg and O ions. In confocal geometry, upon different energy of excitation, the PL spectra of samples have been demonstrated the similar spectral shapes (emission bands), which have been tentatively ascribed to some of impurity centers in different charge states.

ABS: 74. Characterization of a RF-excited broad ion beam source relevant for the machining of surfaces used for optical applications

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The manufacturing and engineering of high-precision and functional optical surfaces have gained even more importance in the last years. In this context, broad beam ion etching technologies are used for the manufacturing of optical elements for semiconductor lithography processes or telescope mirrors. The increasing importance of large surface machining and, thus, long process times, can be encountered by using RF-excited broad beam ion sources with a high ion current density and a low maintenance period. Additionally, to achieve a surface roughness in the sub-nm range and gather a higher understanding of the long-term behavior of the ion beam source, a systematical characterization of the ion beam concerning the energy distribution and composition, especially for reactive species, in dependence of the process parameters is essential.

The ion energy distributions and ion current density distributions were investigated for a commercially available broad ion beam source operating with Ar, recorded with an energy-selective mass spectrometer and a Faraday-cup array [1]. For a variation of the applied RF-power, the formation and the shift of a bimodal structure of the ion energy distribution was shown. The evaluation of the ion current density distributions shows a deformation of the ion beam profile, as well as a big influence of resonant charge exchange processes outside the ion beam source.

Recent studies examined the variation of the distance between the ion beam source and the analytical devices. It can be seen that for a variation of the measuring distance, i.e. the processing distance, influences on the ion energy distribution, as well as the ion current density have to be considered.

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ABS: 77. Overview of the JANNuS-SCALP facility at Orsay: ion beams for synthesis, modification and analysis of materials

Aurelie Gentils [1], Cyril Bachelet [1], Cedric Baumier [1], Philippe Benoit-Lamaitrie [1], Jerome Bourcois [1], Laurent Delbecq [1], Silvin Herve [1], Christine Oriol [1], Florian Pallier [1], Sandrine Picard [1]

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JANNuS-SCALP is an interdisciplinary research platform supporting many scientific fields ranging from materials science to astrophysics, including geology and nuclear physics. The domains of application are varied: nuclear (fusion / fission) and solar energy, microelectronics, production of isotopes for the medical sector. The platform consists of different equipment for ion irradiation / implantation (ARAMIS 2 MV ion accelerator, IRMA 190 kV ion implanter and 40 kV SIDONIE isotope separator) and analysis (RBS, PIXE, PIGE, ERDA, and TEM, SEM, AFM, …) [1].
The coupling of a Transmission Electron Microscope with ARAMIS and IRMA is unique in the world due to the diversity of elements that can be accelerated inside the microscope in a wide range of energies, with a well-controlled dosimetry, making it possible to characterize in situ at the nanometric scale the evolution of structural and chemical modifications of materials subjected to one or two ion beams. The diversity of sample-holders for ex/in situ ion implantations and irradiations allows experiments at low or high temperatures, or large series of materials for fluence-dependent studies. A brief description of the various equipment and selected related examples will be given in this presentation.

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ABS: 78. *In-situ* X-ray diffraction for elucidating the initial formation of expanded austenite during ion nitriding

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Expanded austenite, formed by inserting colossal amounts of nitrogen into austenitic stainless steel, is characterised by 25 – 40 at.% nitrogen in solid solution leading to a lattice expansion of 5 – 12%. While the upper limit of the nitrogen content appears to be given by thermochemical considerations, no detailed investigations for a potential lower limit are known. At the same time, the correlation between nitrogen insertion, concentration and enhanced diffusion complicate such investigations while tribological applications necessitate thick layers produced within a short period.

Using low current ion implantation at moderate energies near 1 keV in combination with in-situ x-ray diffraction (XRD) allows us to follow the initial phase formation with a sufficient time and depth resolution. While the depth resolution is given by the information depth of the x-rays, this limitation can be overcome using sputter etching with energetic ions (of noble gases, e.g. Ar) at moderate temperatures, at which no diffusion or phase transformation processes are active.

Hence, it is shown that during the initial phase, a step-like transition from a low expansion towards a high expansion phase occurs without any accompanying changes in the local nitrogen concentration or the nitrogen diffusivity. At 400 °C, this transition occurs at an incident flux less than 10^18 (superscript) nitrogen atoms/cm², corresponding to a layer thickness near 700 nm and a surface concentration of about 14 at.%. Interestingly, the transition in the lattice expansion of the whole modified layer appears to be nearly instantaneous within less than 10 minutes, despite an ion range of 5 – 10 nm which is much smaller than the region of interest.

ABS: 81. Phase control of multivalent vanadium oxides by ion-beam sputter-deposition

Jill Kessler [1], Martin Becker [1], Florian Kuhl [1], Limei Chen [1], Angelika Polity [1], Peter J. Klar [1], Sangam Chatterjee [1]

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Ion-beam sputter-deposition is a versatile tool for controlled deposition of different phase-pure vanadium oxide thin films. Tuning parameters like substrate temperature and oxygen flux allows to select the desired oxidation states of the vanadium.

Specifically, we use a metallic vanadium target and adjust the stoichiometry of VO_x by controlling the oxygen flux in the gas mixture of argon and oxygen, the oxygen flux is set between 1-9 sccm. The substrate heater temperature is varied from 25 to 600 °C. Within this parameter space, we identify unique settings for six vanadium oxides (V_2O_3, δ-V_2O_5, α- V_2O_5, V_6O_{13}, VO_2 and V_3O_7) and several mixed phases. X-ray diffraction and Raman spectroscopy provide structural and compositional analysis and scanning electron microscopy reveals the surfaces morphology. UV/Vis/NIR spectroscopy served as a tool to measure the transmittance dependence on temperature and wavelength.

ABS: 84. Capabilities of ion-beam processing with radio-frequency ion sources

Martin Becker [1], Sebastian L. Benz [1], Jill Kessler [1], Angelika Polity [1], Peter J. Klar [1], Sangam Chatterjee [1]

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The sputter deposition of (poly-)crystalline binary oxides seems allegedly simple. However, this is not entirely true, since there exist binaries which being crystalline only exhibit one stoichiometry and one crystal structure, those which possess different polytypes and those which feature crystalline phases at different stoichiometries. The material's properties and phase will strongly depend on the distinct synthesis parameters, e.g., substrate, growth temperature, gas fluxes, etc.

We present the immense capabilities of ion-beam bombardment for processing, especially for thin-film deposition by ion-beam sputtering. Here, combining several ion sources allows an additional fine-tuning of the material's properties and enables material screening. The versatileness of ion-beam techniques in the synthesis of thin films and multilayer structures is highlighted by giving several examples on metal oxides.

In this context we emphasize a novel approach to coat substrates simultaneously from both sides avoiding strain effects.

ABS: 85. Machine learning modeling of the stopping power experimental data

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The International Atomic Energy Agency (IAEA) stopping power database [1] is a valuable public resource, which is continuously updated [2], making available compilations of the experimental measurements published over the last nine decades [3] to the global scientific community. The purpose of this work is to apply machine learning methods to predict the electronic stopping power cross section based on this important compilation of data. The experimental data compiled from published articles by diverse authors is not standardized. The data is presented in distinct units and formats, including the mix of stopping cross sections per atom, per molecule, per mass and also energy loss per unit path length. We devoted a significant effort in the reorganization of the database, unifying units, and arranging the data in a standard (csv) format, enabling to obtain the information easily and quickly. Considering that the database contains several dozen of thousands input values, purging manually this data requires also a considerable amount of work.

To this purpose, we developed a machine learning method to clean up the existing compilation of experimental data, based on an unsupervised clustering technique (DBSCAN) which identifies outlier values, and determines which data to keep in cases of overlapping, taking into account the year of production. The refined data is used to train a deep neural network, able to accurately reproduce the input experimental results, and to predict new results in cases which have never been seen in the training procedure (the test set). In this opportunity, the code ESPNN (Electronic Stopping Power with Neural Network), performing all these tasks will be presented, and the results discussed.

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ABS: 101. Optimization of MeV TOF SIMS technique for inorganic targets in the low primary ion beam energy mode

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MeV TOF SIMS is a variation of a conventional TOF SIMS using a primary ion beam produced in an MV particle accelerator instead of keV ions, achieving energies of a few to tens of MeV. Hence, electronic stopping is much more prevalent than nuclear stopping, and energy is transferred fast, leading to rapid heating and causing higher molecular secondary ion yields and lower fragmentation compared to keV SIMS. MeV SIMS is mainly used to detect organic molecular ions and finds applications in biomedical research, forensics, cultural heritage, etc.

This work investigates the idea of low energy range (100 keV – 5 MeV) primary ion beam mode in MeV SIMS and its potential in exploiting the capabilities of both conventional keV SIMS and MeV SIMS simultaneously – the analysis of inorganic species, while still being able to sputter and analyze larger biomolecules. This energy mode was named LE (Low Energy) MeV SIMS. Secondary ion yield dependence on the primary ion energy of leucine and various inorganic targets was studied. Next, imaging of a hybrid organic/inorganic target made of Cr and leucine was performed showing that the contrast between the organic and inorganic area is almost completely diminished when lowering the primary ion beam energy. LE MeV SIMS depth profiling of a dual-layer Cr-ITO sample in a dual-beam mode was also explored and the obtained depth profile was compared against well-established keV SIMS. Depth profiles demonstrated solid chemical sensitivity to inorganic secondary ions and satisfactory depth resolution, given that a simple low-cost sputter source was used for etching.

Systematic investigation of MeV TOF SIMS in the low energy regime opens up new possibilities in both the fundamental understanding of the impact of the primary ion stopping power on the detection of secondary ions of organic and inorganic species and expanding the application of MeV SIMS to analysis, imaging and depth profiling of inorganic species with increased efficiency.

ABS: 115. Fluence and doping dependence of lattice location of ion implanted Mg in GaN

Ulrich Wahl [1], João Guilherme Correia [1], Ângelo R.G. Costa [2], Eric David-Bosne [3], Menno J. Kappers [4], Manuel R. da Silva [3], Gertjan Lippertz [2], Tiago A.L. Lima [2], Renan Villarreal [2], André Vantomme [2]

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GaN devices are about to replace Si power electronics on a massive scale [1]. With the aim of improving device performance, this has greatly renewed interest in ion implantation into GaN [2] which allows precise transverse and lateral control of dopant concentrations, also at levels exceeding those achievable by doping during growth. However, efficient electrical activation for the only feasible p-type dopant Mg, remains a challenge, particularly at fluences >1E14 cm^{-2}. Novel approaches, such as high-temperature implantation [3] are deemed crucial.

Using β emission channeling, we investigated the lattice location of ^{27}Mg in GaN of different doping types as a function of implantation temperature and fluence [4]. We elucidate the amphoteric nature of Mg, i.e. the concurrent occupation of substitutional Ga and interstitial sites: while low fluence implantations at RT lead to significant fractions of interstitial Mg, implantations >400 ºC convert interstitial ^{27}Mg to substitutional Ga sites due to the onset of Mg interstitial migration and combination with Ga vacancies. Interstitial Mg is also progressively reduced with increasing fluence, due to the accumulation of Ga vacancies. Thus, implantations >1E14 cm^{-2} achieve >95% substitutional Mg. Our findings show that ion implantation is a very efficient method to introduce Mg into substitutional Ga sites, i.e. that the challenges towards high electrical activation of implanted Mg are not related to the lack of substitutional incorporation.

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ABS: 135. Selected aspects of GaN doping by Si^+ ion implantation and subsequent activation annealing

Karolina Pagowska [1], Maciej Kozubal [1], Andrzej Taube [1] Iwona Sankowska [1] Renata Kruszka [1]
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Ion implantation is efficient method of selective doping of gallium nitride for fabrication of various electronics and optoelectronics devices. To obtain high net doping and electron concentration, high implantation fluences are required (up to 1×10^{16} cm^{-2}). However this can lead to introduction of a high concentration of different types of defects to GaN, which should be, at least partially, removed during activation annealing at high temperatures over 1000°C.

This work explore the influence of some technological process parameters on the properties of implanted GaN layers and investigated the formation of very low-resistance ohmic contacts to GaN using the retarding layer. The defect formation in GaN during Si ion implantation and its transformation after subsequent activation annealing were studied. We investigated different encapsulation layers and activation annealing temperatures, as well as the ion implantation fluence. To achieve a quasi-uniform Si profile with just one implantation, implantations were done through a SiO_2 retarding layer. We characterized GaN samples after Si doping by electrical and structural methods, the latter supported by depth profiles of point and extended defects, calculated by McChasy simulation code based on measured Rutherford Backscattering/channeling spectra.

We have shown that increasing the Si ion fluence led to far better electrical results, but the point and extended defect concentration also increased. To overcome this we employed the sequential doping scheme (implantation/recrystallization cycles), developed by us previously. For the 250 keV Si^+ implantation to the effective fluence of 1.1×10^{16} cm^{-2}, we achieved excellent electrical results: sheet resistivity RSH $\lesssim$ 50 Ω/sq., specific contact resistance RC $\lesssim$ 0.1 Ω·mm and ρC ≈ 2×10-7 Ω·cm^2.

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ABS: 141. Maskless ion beam sputtering deposition of two-dimensional transition metal dichalcogenides Van Der Waals heterostructures

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Transition Metal Dichalcogenides (TMDs) are two-dimensional semiconductors featuring high optical absorption coefficient combined with good transport and mechanical properties. A peculiarity of 2D-TMDs is the possibility to stack them forming van der Waals heterostructures, paving the way to new applications exploiting the coupling of different band structures.

Although mechanically exfoliated TMD flakes ensure the best opto-electronic properties, homogeneous large area growth techniques are mandatory for real world applications [1,2]. Light harvesting strategies are also required in opto-electronics to enhance the poor effective optical absorption caused by the few nanometers thickness. In our previous works, we have demonstrated that periodic modulation of MoS_2 layers on large area nanostructured samples offers an effective solution to the absorption problem [3,4].

Here, we propose Ion Beam Sputtering (IBS) deposition as a promising route for large area deposition of vertically stacked 2D-TMD van der Waals heterostructures, using bulk TMD targets as material sources. Our custom prototype allows sequential deposition of large area arrays of TMD nanostructures exploiting nanogrooved silica substrates as growth templates. Lateral confinement of TMD nanostripes on one side of the silica grating is obtained in a single maskless step by IBS sputtering at glancing angles.

Preliminary results show that van der Waals heterostructures, formed by stacking in sequence a continuous MoS_2 layer over WS_2 nanostripes, can effectively engineer and amplify the periodic modulation of refractive index, boosting light extinction in the heterostructure. These results show the potential impact of large area 2D heterostructures in the field of nanophotonics and light conversion applications.

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ABS: 155. Processing of Al_2O_3 with high-energy heavy-ion irradiation and pulsed laser irradiation for optical waveguides fabrication

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Sapphire (crystalline Al_2O_3) is a technologically attractive material with excellent physicochemical properties. Ti:Al_2O_3 has allowed developing the technology of ultrashort pulsed lasers. There is a general need for developing miniature, integrated lasers using optical waveguides structures. However, it is challenging to process sapphire for fabricating such demanded optical waveguides by light ion implantation [1]. Some studies have reported latent track formation and amorphization, after track overlapping, under swift heavy ion irradiation [2-4]. The generation of surface amorphous layers was reached with Xe ions, with high electronic stopping power (10-12 keV/nm), at moderate accumulated fluences (1E14 cm^{-2}).

Here, we have addressed the fabrication and characterization of amorphous/disordered layers, placed buried a few microns underneath the surface, having the appropriate refractive index change to allow the formation of optical waveguides. Three methods have been investigated, using 1) the electronic and/or the nuclear damage alone; 2) the synergistic coupling between nuclear and electronic damage; and, 3) the synergistic coupling of the ion damage (electronic or nuclear) with pulsed (ns and fs) laser irradiation.

Systematic irradiations with heavy ions (C-I) of 10-50 MeV energy in a broad fluence range (E12-E16 cm^{-2}) were conducted. The successful fabricated waveguides were characterized by the prism-coupling modal spectroscopy allowing a detailed in-depth damage profile. The optical properties were characterized by in-situ reflectance and transmittance measurements. RBS/C, for structural characterization, and DC electrical measurements have also been performed [2,5].

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ABS: 174. Investigation of zinc diffusion for various crystallographic directions in GaN grown by HVPE

Kacper Sierakowski [1], Rafal Jakiela [2], Tomasz Sochacki [1], Malgorzata Iwinska [1], Piotr Jaroszynski [1], Michal Fijalkowski [1], Marcin Turek [3], Michal Bockowski [1]

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Ion implantation (I/I) seems to be nowadays one of the most important techniques for manufacturing gallium nitride (GaN) based semiconductor devices. High-energy ions might be implanted into crystals in order to create doped regions. To achieve the required conduction in the implanted layer, p-type or n-type, one must anneal the structure to activate the dopant. Temperature treatment is also required to remove the I/I-induced structural damage.

In the case of GaN high-temperature annealing is difficult due to thermodynamics of GaN (thermal decomposition above 800°C in atmospheric pressure). Ultra-high-pressure annealing (UHPA), which involves high pressure of nitrogen, allows to avoid the decomposition of GaN samples. The most popular p-type dopant in GaN is magnesium (Mg). However, other elements are also investigated.

One of other possible candidates for p-type doping is zinc (Zn) [1]. In the presented work GaN doping by Zn implantation was investigated. HVPE-GaN layers were grown on ammonothermal seeds of three polarities: (0001), (10-10), and (11-20). Zn I/I was performed with the energy of 230 keV and fluence of 10^{16} cm^{-2}. The samples were then treated with UHPA in the temperature range 1250°C–1450°C for 30 and 240 minutes. A constant nitrogen pressure of 1 GPa was applied for all the annealing runs. X-ray diffraction measurements were employed to assess the success of structural damage removal by annealing. The depth profiles of Zn and atmospheric impurities were determined by secondary ion mass spectrometry (SIMS). This allowed to study the diffusion of the implanted element in GaN. An anisotropy of diffusion was observed for the different crystallographic directions.

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ABS: 175. Investigation of beryllium diffusion for various crystallographic directions in GaN grown by HVPE

Kacper Sierakowski [1], Rafal Jakiela [2], Tomasz Sochacki [1], Malgorzata Iwinska [1], Piotr Jaroszynski [1], Michal Fijalkowski [1], Marcin Turek [3], Michal Bockowski [1]

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Gallium nitride (GaN) is nowadays considered to be one of the most significant materials for fabrication of electronic and optoelectronic devices. A very convenient method for selective area doping is ion implantation. In order to obtain p-type the implanted acceptors have to be activated. Additionally, post-implantation damage in the crystallographic structure has to be removed. Both can be accomplished by high-temperature annealing of a sample. However, such treatment also results in the diffusion of the implanted element. In this work diffusion of Be was investigated for the main crystallographic directions in GaN: [0001], [10-10], and [11-20].

GaN layers were grown by halide vapor phase epitaxy (HVPE) in the mentioned above polar and non-polar directions on ammonothermal GaN seeds of the highest structural quality. Beryllium was implanted into the samples at room temperature with a dose of 2.9×10^{15} cm^{-2} and energy of 200 keV. Ultra-high-pressure annealing (UHPA) was performed to repair the post-implantation damage and activate the dopants [1]. Depth profiles of Be and atmospheric impurities (oxygen, hydrogen, and carbon) were measured by secondary ion mass spectrometry. A significant anisotropy of Be diffusion was measured for different crystallographic directions. The correlation between the maximum Be solubility and oxygen concentration in the samples was observed. The diffusion coefficients were calculated and summarized in an Arrhenius plot: D(1/T). From this relation values of the pre-exponential factor D0 and the activation energy were calculated.

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ABS: 176. Implantation of steel samples with boron ions

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A classic problem of engineering is to increase the surface stability of materials without changing their bulk properties. Accordingly, the effect of applied methods should be confined to the near-surface layer. Some methods change the crystal structure of the near-surface layer (annealing), while others insert additional materials into the surface layer causing a structural change in it (alloying). Surface alloys can improve not only the mechanical properties of steel samples, but also their chemical resistance. With application of a lead-free soldering technology, the degradation mechanism of industrial soldering tools is intensively accelerated inducing significant reduction of lifetime. Boriding of steel surfaces seems to be a good solution for this problem, since iron soldering tools covered with an iron-boride layer have strong chemical resistance to lead-free solders and very good wettability for solders which is also very important in technology. Chemically, two phases of borides can be formed on iron surfaces, FeB and Fe_2B. Although the desired technological requirement can be achieved by both phases, their crystal structures are incompatible with each other and they form an unstable layer together. The problem can be avoided by creating a sole Fe_2B layer. The realization of this solution is not possible by classical surface diffusion process because the presence of FeB is unavoidable in addition to Fe_2B phase. The aim of our research is to implant the iron surfaces by boron ions in depth of a few hundred nanometres in order that finally let the composition of this thin layer form Fe_2B. We hope that using this method the formation of a harmful alloy layer at the iron surface can be avoided.
The results we have achieved so far will be presented.

ABS: 54. An ultralow-energy ion implantation set-up at the Tandem Laboratory, Uppsala University

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Due to the decreasing size of devices, low-energy ions are becoming more frequently employed for near-surface modification of materials. For instance, to manufacture the ultra-shallow junctions required for advancing MOSFETs, ultralow-energy ion implantation of dopants like boron in silicon is a feasible method [1]. Moreover, low-energy ion implantation of hydrogen in silicon solar cells affects surface passivation and enhances conversion efficiency [2]. High-flux low-energy ion irradiations are capable of simulating the effect of the fusion plasma on structural components of future fusion devices [3]. Furthermore, the electronic properties of 2D materials can be tailored by utilizing ultralow-energy ions to replace individual target atoms with dopants [4,5].

The 10 keV ion implanter, presented in this contribution, is a new setup at Uppsala University's Tandem Laboratory to initiate studies on the above-mentioned topics and provide the capability to perform ultralow/low-energy ion implantations for users. Its lowest delivered beam energy, produced from gas/solid sources to the sample position, ca. 1.3 m away from the ion source, is expected to be 25 eV using a decelerator unit. The goal is to achieve up to 20 μA target current in focused mode enabling a fluence of up to 10^{23} particles/m² for gaseous species. Samples with a diameter up to 50 mm will fit on the sample holder and can be annealed up to 500°C.

We will present the first benchmarking experiments implanting hydrogen and boron primary ions primarily into silicon which have been characterized using different ion beam analytical methods such as elastic recoil detection analysis and nuclear reaction analysis.

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ABS: 102. Recent developments in the CAMBO Ion Beam Laboratory

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Recently, significant upgrades were done and are progressing at the 6 MV-Tandetron tandem accelerator at the CAMBO ion beam laboratory in Trnava [1]. The first part of these upgrades ensures an increase of ion beam currents and reliability of operation. An upgrade of the HVEE 358 duoplasmatron ion source was performed, which now reliably delivers 4-5 µA He^- ion currents. Additionally, an NEC TORVIS together with the corresponding injector beamline was added to the system, which is expected to deliver up to 100 µA H^- and up to 10 µA He^- to serve high-fluence experiments as well as ensure redundancy to minimize accelerator down-times. Together, these upgrades will support the scientific programme moving towards the development and testing of radiation tolerant materials for nuclear energy and space applications. Moreover, the reliable operation of a recently commissioned end-station dedicated to high-energy ion implantation services is secured. In combination with modification of the original HVEE ion implantation end-station, high-energy ion implantations/irradiations with 1E16 at/cm² to 1E18 at/cm² fluences are feasible in reasonable times. Another beamline, which is under construction, will have a time-of-flight Elastic Recoil Detection Analysis end-station based on the Jyväskylä design [2].

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ABS: 118. Influence of magnetic field of magnetically insulated diode on emission behavior of intense pulsed ion beam

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As a novel material modification technology, intense pulse ion beam (IPIB) has been widely used for surface hardening, surface mixing, film deposition and improvement of wear and corrosion resistance. In this study, we investigated influence of magnetic field between the anode-cathode gap (A-K gap) of magnetically insulated diode (MID) on the emission behavior of IPIB. The experiments were carried out on the pulsed ion beam accelerator BIPPAB-450. High voltage divider and Faraday Cylinder were used to record the acceleration voltage and ion beam density by changing of magnetic field intensity. The magnetic induction intensity B varied within the range of B/Bcrit less than 1.5. Here, Bcrit is the critical magnetic field which prevents direct electron loss to the anode. It is found that the breakthrough time and breakdown voltage in the A-K gap increased with the growth of magnitude of magnetic field. Besides, ion beam density rose monotonically with the magnetic induction intensity. With average magnetic induction intensity in the A-K gap up to 1.1 T, the ion beam density reached 130 A/cm^2. The distribution of the magnetic field in the A-K gap of diode was further analyzed by finite element method. It is revealed that the distribution and the intensity of the magnetic field of the A-K gap significantly affected the electron sheath formation, the generation and expansion of anode plasma and the space uniformity of the ion emission. The calculation results explain the phenomenon of more serious depletion of anode outer ring than other area. This work provides guidance for improving beam generation efficiency and enhancing the service life of anode.

ABS: 223. Nitrogen targets production and characterization for $^{14}N(p,\gamma)^{15}O$ reaction measurement at LUNA-MV

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The LUNA (Laboratory for Underground Nuclear Astrophysics) collaboration aims to measure nuclear reactions of astrophysical interest near stellar burning energies. Probing these processes involves measuring cross sections with extremely low counting rates. This is made possible primarly by the suppression of the cosmic rays component of the background enabled by the deep underground location of the experiment in the Gran Sasso National Laboratories (LNGS), Italy. For the last 20 years a 400 kV accelerator provided stable ion beams with high beam intensity at LNGS. Currently, a new 3.5 MV machine, that will allow to study the advanced phases of helium and carbon burning, is under installation. As a pilot project for the new facility, the $^{14}N(p,\gamma)^{15}O$ reaction will be measured over a wide energy range. This reaction is the bottleneck of the CNO cycle and therefore it controls the speed at which it proceeds, directly influencing the predicted CNO solar neutrino rates and the lifetime of massive stars. In this work we describe the production and characterization of solid nitrogen targets through ^{14}N implantation on Tantalum, performed at the Ion Beam Laboratory of Istituto Técnico Superior (IST), in Lisbon, and through Titanium and Tantalum nitride thin film deposition using Reactive Magnetron Sputtering at the Legnaro National Laboratories (LNL), in Italy. The targets are characterized with RBS and NRRA techniques and tested for contaminants and stability under high-current irradiation at the 2 MV Tandetron accelerator at Atomki and at the LUNA-400 facility at LNGS.

ABS: 224. Isotopic resolution in a novel pulsed focused ion beam system

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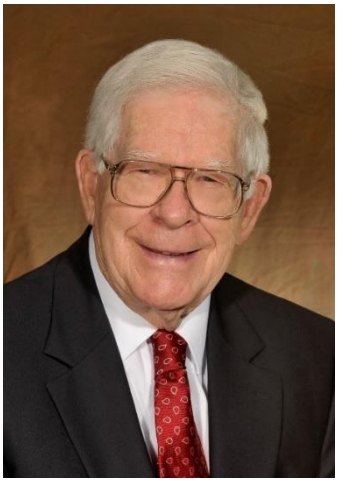
The Platform for Nanoscale Advanced Materials Engineering (P-NAME) tool is a pulsed ion implantation system with co-incident scanning electron microscope capabilities which enables high resolution implantation with accurate and non-destructive sample localisation. The tool is capable of high and low dose implantation work (down to single ion implantation). Recent developments of the system have improved the mass resolution of the Wien filter to provide isotopic resolution of a range of liquid metal alloy ion sources. This enables a significant and diverse range of applications, including spintronics and quantum information devices, whilst maintaining functionality in versatile applications such as high dose implantation (up to 10^{20} ions cm^{-2}) for alloying, enrichment, and ion beam lithography. The work presented here is a demonstration of the Wien filter isotopic resolution for a variety of species, along with the use of a verified analytical model to predict the mass resolution of new sources that are currently in development with our collaborators. Also included are the results of secondary ion mass spectroscopy (via nanoSIMS) of silicon moderately doped with germanium-70 (^{70}Ge).

IN MEMORIAM

Professor Carl J. McHargue



Professor Carl J. McHargue, age 96 of Knoxville, TN (USA), passed away at his home on February 27, 2022.

He was Professor Emeritus at the University of Tennessee-Knoxville and long-time, active member of the ion-beam modification, ion-beam analysis and radiation effects communities both domestically and internationally. Many of us knew him as a mentor, research colleague and gifted orator.

A native of Corbin, Kentucky, Carl served in the U.S. Army during World War II. Following his discharge in 1946, he entered the University of Kentucky, receiving a Bachelor of Science in metallurgical engineering (with honors) in 1949, and a Master of Science in metallurgical engineering in 1951.

Carl joined the staff of the Oak Ridge National Laboratory (ORNL) in 1953 where he developed one of the largest programs in basic materials research in the United States and made major contributions to the understanding of irradiation effects in solids. He also initiated the materials development program in support of the Fusion Energy Program, as well as programs to support other advanced energy systems. In 1954, Carl was appointed to dual positions with the Oak Ridge National Laboratory and as professor of Materials Science and Engineering at the University of Tennessee-Knoxville where he played a major role on the Accreditation Board for Engineering and Technology (ABET), the organization that accredits college and university programs in various disciplines. He was recognized as a Fellow of ABET in 2008. His work in international engineering education led to honorary membership in the Order of Engineers (Portugal).

The excellence and dimension of his work can be found and will remain in scientific journals and institutions where he served or collaborated. We miss him.

Professor Joseph Gyulai

On February 12, 2021, Professor Joseph Gyulai passed away at the age of 88.

He was, professor emeritus both of the Institute for Technical Physics and Materials Science (MFA) and of Budapest University of Technology and Economics. He was very active and known worldwide by his peers as an originally thinking, bright researcher maintaining good, even friendly relations with colleagues. Not only in the field of physics or materials characterization, but e.g. in the world of music, as well.

A turning point in his career happened when Professor Joseph Gyulai got a one-year scholarship to work with Jim Mayer at Caltech, USA, whose work on detectors was known to Joseph.

In the Communist Hungary, behind the iron curtain during the cold war it was a dream to get a chance like that. When at the end of 1969 Joseph arrived at Pasadena, Jim Mayer's group was switching to ion implantation and Rutherford Backscattering Spectrometry (RBS). He was immediately noticed when he extracted the depth profile from the RBS spectra of compound layers using an appropriate energy-to-depth conversion procedure. Just a few weeks after his arrival he already published a first-authored paper on Si-SiO_2 composition analysis.

The dimension of his scientific record can be found and will stay forever spread in the journals and institutions where he worked or collaborated. We miss him.

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IBMM-2022 Hotels

Stars identify hotels:

(1) Hotel Eurostars Universal Lisboa

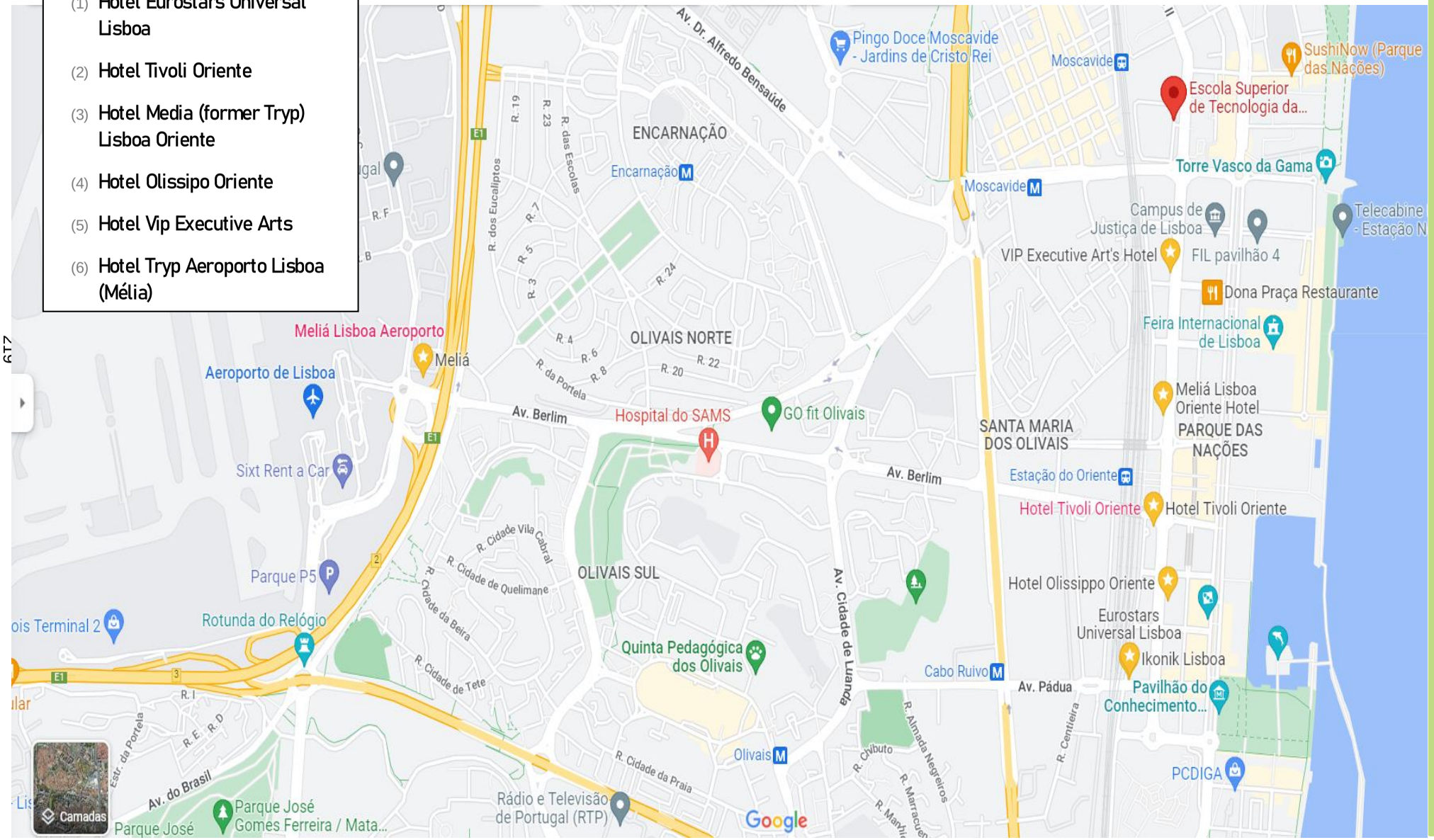
(2) Hotel Tivoli Oriente

(3) Hotel Media (former Tryp) Lisboa Oriente

(4) Hotel Olissipo Oriente

(5) Hotel Vip Executive Arts

(6) Hotel Tryp Aeroporto Lisboa (Mélia)

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