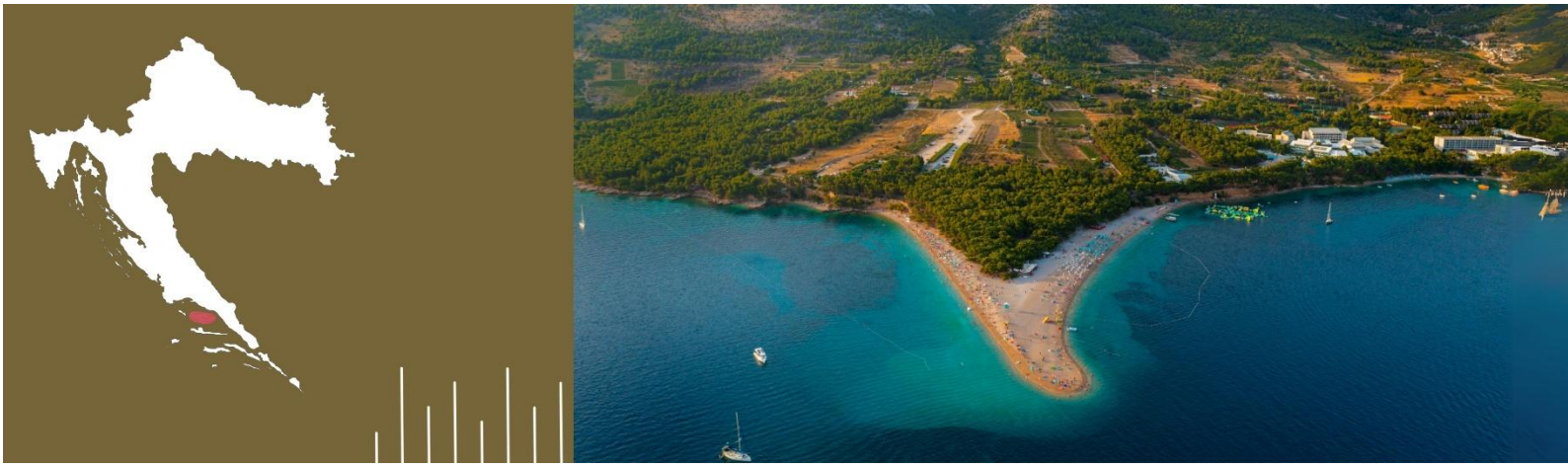


31st International Conference on Atomic Collisions in Solids (ICACS)

13th International Symposium on Swift Heavy Ions in Matter (SHIM)

ICACS & SHIM 2026: Book of Abstracts

27th September – 2nd October, 2026

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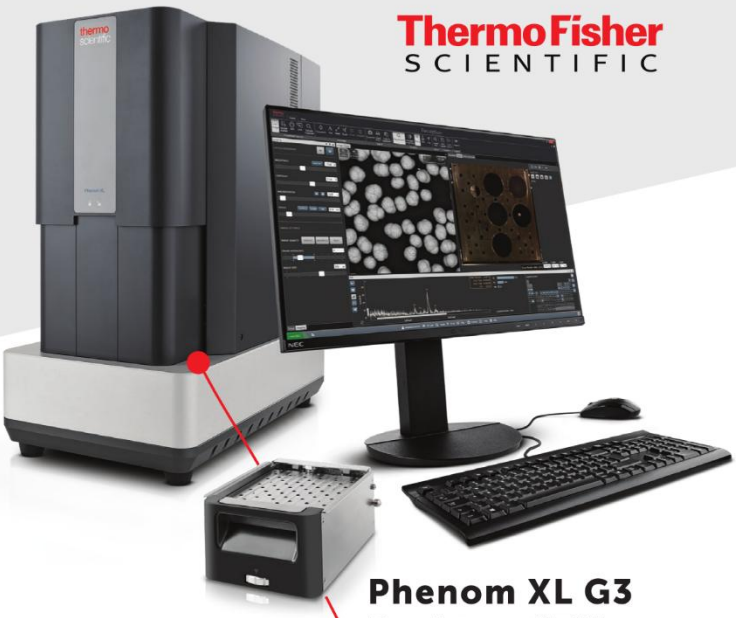
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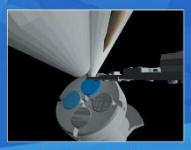
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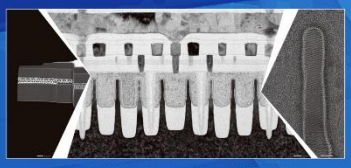




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Abstracts (Oral contributions) **20**

Abstracts (Poster contributions) **81**

Welcome to ICACS & SHIM 2026

Dear Colleagues,

On behalf of the Local Organizing Committee, it is our privilege to present this Book of Abstracts for the joint 31st International Conference on Atomic Collisions in Solids (ICACS) and 13th International Symposium on Swift Heavy Ions in Matter (SHIM), convened at the Bluesun Hotel Elaphusa, Bol, on the island of Brač, Croatia, from 27 September to 2 October 2026.

The ICACS series, established in Aarhus, Denmark, in 1965, and the SHIM series, established in Caen, France, in 1989, together constitute one of the longest-standing forums for the study of particle–solid interactions. Over the decades, ICACS and SHIM have drawn together specialists working mainly with energetic heavy ions from a wide range of fields. With an emphasis on both fundamental and applied research, conferences have played a key role in linking theoretical understanding with experimental practice across various areas. Following the first joint meeting of the two series in Kyoto in 2012, subsequent joint conferences were held in Caen (2018), Helsinki (2022), and Canberra (2024). The present volume documents the continuation of this collaboration in Croatia.

The contributions collected herein address atomic collisions in solids and swift heavy ion–matter interactions, radiation-induced material modification and chemical and biological effects, applications of ion beams in research and industrial contexts, and the development of experimental and computational methodologies. They represent the work of invited speakers and contributing authors from across the international community, including a significant number of early-career researchers.

The Local Organizing Committee wishes to record its gratitude to the International Program Committee, the invited and contributing authors, and the sponsoring institutions, whose collective efforts have made both the conference and this compilation of abstracts possible. It is our hope that this volume will serve not only as a record of the scientific proceedings but also as a lasting reference for the continued advancement of the field.

Zagreb, 21st September 2026

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ICACS-31 & SHIM-13
Conference Programme

27 September-2 October 2026 | Bluesun Hotel Elaphusa, Bol, Island of Brač, Croatia

Sunday, 27 September 2026

16:00-18:00	**Registration**
18:00-18:15	**Opening ceremony**
18:15-19:00	**Christina Trautmann	Lindhard Lecture (LL)** GSI Helmholtz Centre for Heavy Ion Research, Germany *Experimental and simulation challenges in swift heavy ion track formation.*
19:00-20:30	**Welcome reception at Bluesun Hotel Elaphusa**

Monday, 28 September 2026

08:00-09:00	**Registration**
SESSION 1	**chair: Zhiguang Wang**
09:00-09:30	**Mamour Sall | I1 Invited talk** Center for Research on Ions, Materials and Photonics, Caen, France *Inducing Uniaxial Magnetic Anisotropy in $La_{0.7}Sr_{0.3}MnO_3$ by Means of Surface Nanostructuration with Low and High Energy Ion Irradiation*
09:30-09:50	**Mandla Msimanga | O1 Contributed talk** Mulungushi University, Zambia and Tshwane University of Technology, South Africa *Defect-Engineered Charge Transport in ITO/PANI-Graphene/Al Schottky Diodes via Swift Heavy Ion Irradiation*
09:50-10:10	**Milko Jakšić | O2 Contributed talk** Ruđer Bošković Institute, Croatia *IBIC characterisation of the charge transport using heavy ions*
10:10-10:30	**Ricardo Papaleo | O3 Contributed talk** Pontifical Catholic University of Rio Grande do Sul, Brazil *Thickness dependence of bond-breaking cross sections in PMMA thin films: new insights from in situ spectroscopic investigations with 9 MeV/u C ions*
10:30-11:00	**Coffee break**
SESSION 2	**chair: Friedrich Aumayr**
11:00-11:30	**Cíntia Aparecida Pires da Costa | I2 Invited talk** Physics Department - University of Trento, Italy and Aix-Marseille University, France *O_2 plasma-induced modifications in the surface of space-technology polymers*
11:30-11:50	**Hermann Rothard | O4 Contributed talk** CNRS CIMAP, France *Swift Ion irradiation of ices containing organic molecules at GANIL*
11:50-12:10	**Michael Dürr | O5 Contributed talk** Justus Liebig University Giessen, Germany *Highly site-selective fragmentation of peptides induced by swift heavy ion impact*
12:10-12:30	**Lars Breuer | O6 Contributed talk** University of Duisburg-Essen, Germany *Velocity-resolved SNMS as a probe of electronically driven sputtering under swift-heavy-ion irradiation*
12:30-12:38	**Sponsor presentation (SCAN)**
12:40-14:00	**Lunch break**

Monday, 28 September 2026 (continued)

SESSION 3	**chair: Stefan Facsko**
14:00-14:30	**Anna Niggas | I3 Invited talk** TU Wien, Austria *Identifying electronic doorway states in secondary electron emission*
14:30-14:50	**Chad Sosolik | O7 Contributed talk** Clemson University, USA *X-ray emissions from slow multiply-charged ions on Si and Nb targets*
14:50-15:10	**Eliezer Kolodney | O8 Contributed talk** Technion - Israel Institute of Technology, Israel *Recent progress in studying the velocity correlated cluster emission (VCCE) effect in surface impact of keV C_{60}^- ions*
15:10-15:30	**Richard Wilhelm | O9 Contributed talk** TU Wien, Austria *Chirality switching in 1T-TaS_2 with Slow Highly Charged Ions*
15:30-16:00	**Coffee break**
SESSION 4	**chair: Flyura Djurabekova**
16:00-16:30	**Toma Susi | I4 Invited talk** University of Vienna, Austria *Atom and ion irradiation of graphene: disentangling inelastic from elastic scattering and the role of phonons*
16:30-16:50	**Milena Majkić | O10 Contributed talk** University of Pristina - Kosovska Mitrovica, Serbia *Two-velocity regimes in nanostructure formation on metal surfaces induced by slow highly charged ions*
16:50-17:10	**Sabrina Gouasmia Boussahoul | O11 Contributed talk** Ruđer Bošković Institute, Croatia *Modeling of Sputtering from Solid Surfaces Under Argon Cluster and Ion Bombardments: Comparison with Experimental and Simulated Data.*
17:10-17:30	**Alexander Redl | O12 Contributed talk** TU Wien, Austria *Picosecond Ion Pulses from Laser-Stimulated Desorption at Tungsten Nanotips for Time-Resolved Ion-Solid Interaction Studies*

Tuesday, 29 September 2026

SESSION 5	**chair: Christina Trautmann**
09:00-09:30	**Hongwei Cheng | I5 Invited talk** Institute of Modern Physics and School of Nuclear Science and Technology, University of Chinese Academy of Sciences, China *Reactivate the rule of "smaller and stronger": breaking the small size limit of mechanical metamaterials by swift heavy ions*
09:30-09:50	**Xiang Lian | O13 Contributed talk** Australian National University, Australia *Osmotic Energy Conversion using Ion Track Etched Conical Nanopores in SiO_2*
09:50-10:10	**Mohan Li | O14 Contributed talk** GSI Helmholtz Centre for Heavy Ion Research, Germany *Electrodeposition-Based Fabrication of Hierarchical Nanoporous Au Nanowire Networks with Tunable Electrochemical Functionality*
10:10-10:30	**Shankar Dutt | O15 Contributed talk** Australian National University, Australia *Ion Track-Etched Silicon Dioxide Nanopores: A Swift Heavy Ion Route to Single-Molecule Biosensing*
10:30-11:00	**Coffee break**
SESSION 6	**chair: Maik Lang**
11:00-11:30	**Alexander Azarov | I6 Invited talk** University of Oslo, Norway *Irradiation-induced phase transformations in Ga_2O_3 polymorphs*
11:30-11:50	**Azat Abdullaev | O16 Contributed talk** Nazarbayev University and National Laboratory Astana, Kazakhstan *Polymorphism-Driven Thermal Conductivity Degradation in Swift Heavy Ion Irradiated β-Ga_2O_3*
11:50-12:10	**Flyura Djurabekova | O17 Contributed talk** University of Helsinki, Finland *Amorphization versus defective spinel phase evolution in gallium oxide subjected to different ion beam irradiation conditions*
12:10-12:22	**Sponsor presentation (ITR-LAB)**
12:25-14:00	**Lunch break**

Tuesday, 29 September 2026 (continued)

SESSION 7	chair: Devesh Avasthi
14:00-14:30	**Amirthapandian Sankarakumar | I7 Invited talk** Indira Gandhi Centre for Atomic Research (IGCAR), India *In-situ investigation of ion beam induced dissolution, displacement and deformation of particles using i4-FESEM facility*
14:30-14:50	**Friedrich Aumayr | O18 Contributed talk** TU Wien, Austria *How boronization alters tungsten erosion: Insights from ion-beam studies of W-B mixed layers*
14:50-15:10	**Andreja Gajović | O19 Contributed talk** Ruđer Bošković Institute, Croatia *Study of the WTaVCr high entropy alloy for fusion application by irradiation with Cu and He ions in DiFU*
15:10-15:30	**Jean-Marc Layet | O20 Contributed talk** Aix-Marseille University, CNRS, France *Production of negative ions at surfaces exposed to a low-pressure deuterium plasma: comparison between boron- and phosphorus-doped diamond, graphite and gadolinium*
15:30-17:30	**Poster session and coffee break**
17:30-19:30	**ISC meeting**

Wednesday, 30 September 2026

08:30-15:00	**Boat Excursion with lunch**
SESSION 8	**chair: Pedro Grande**
15:30-16:00	**Nikita Medvedev | I8 Invited talk** Institute of Physics, Czech Academy of Sciences, Czechia *Heating mechanisms in SHI tracks: nonthermal effects*
16:00-16:20	**Alexei Zverev | O21 Contributed talk** University of Helsinki, Finland *First-Principles Modeling of Swift Heavy Ion Track Formation*
16:20-16:40	**Raquel Giulian | O22 Contributed talk** Federal University of Rio Grande do Sul, Brazil *Simulation of InSb Nanofoams Induced by Ion Irradiation using the Cellular Potts Model*
16:40-17:00	**Ruslan Rymzhanov | O23 Contributed talk** Joint Institute for Nuclear Research, Russia and Institute of Nuclear Physics, Kazakhstan *Non-radial Recovery Kinetics in Swift Heavy Ion Tracks in Monoclinic Zirconia*
17:00-19:00	**Poster session and coffee break**

Thursday, 1 October 2026

SESSION 9	**chair: Norito Ishikawa**
09:00-09:30	**Ina Schubert | I9 Invited talk** GSI Helmholtz Centre for Heavy Ion Research, Germany *Size-dependent swift heavy ion irradiation effects in nanostructures*
09:30-09:50	**Jacques O'Connell | O24 Contributed talk** CHRTEM, Nelson Mandela University, South Africa *Combined S/TEM-MD study on the nanostructure of ion tracks in $MgAl_2O_4$ spinel*
09:50-10:10	**Hiro Amekura | O25 Contributed talk** National Institute for Material Science (NIMS), Japan *Fluence dependent ion-track formation and transition to self-organized nanodots in Si under 9 MeV C_{60} ion irradiation*
10:10-10:40	**Coffee break**
SESSION 10	**chair: Patrick Kluth**
10:40-11:10	**John Hirtz | I10 Invited talk** University of Tennessee, USA *Advances in Neutron Scattering Characterization of Swift Heavy Ion Irradiated Nuclear Ceramics*
11:10-11:30	**Ayman El-Said | O26 Contributed talk** King Fahd University of Petroleum and Minerals (KFUPM), Saudi Arabia *Tailoring Optical Properties of GaP Single Crystals by Irradiation with Energetic Heavy Ions*
11:30-11:50	**Christopher Schröck | O27 Contributed talk** GSI Helmholtz Centre for Heavy Ion Research, Germany *Investigating Nanomaterials Under High-Pressure and Swift Heavy Ion Irradiation*
11:50-12:10	**Norito Ishikawa | O28 Contributed talk** Japan Atomic Energy Agency, Japan *Track morphology in quartz irradiated with swift heavy ions: Thickness and edge effects*
12:10-14:00	**Lunch break**

Thursday, 1 October 2026 (continued)

SESSION 11	**chair: Daniel Primetzhofer**
14:00-14:30	**Kevin Vomschee | I11 Invited talk** Uppsala University, Sweden *Atomic collisions in solids - what can we learn from exit charge states, photon emission and their correlation?*
14:30-14:50	**Hidetsugu Tsuchida | O29 Contributed talk** Kyoto University, Japan *Stopping power measurement of liquid water for heavy ions*
14:50-15:10	**Karoly Tokesi | O30 Contributed talk** HUN-REN Institute for Nuclear Research, Hungary *Correlated Electron Dynamics in Ne^{10+} and He Collisions*
15:10-15:30	**Carolin Frank | O31 Contributed talk** Uppsala University, Sweden and University of Duisburg-Essen, Germany *Rainbow Scattering from Graphene*
15:30-16:00	**Coffee break**
SESSION 12	**chair: Richard Wilhelm**
16:00-16:30	**Pedro Luis Grande | I12 Invited talk** Universidade Federal do Rio Grande do Sul, Brazil *Quantum Trajectories of Energy Loss: Ion Stopping from Bohmian Mechanics to Biological Media*
16:30-16:50	**Claudia Montanari | O32 Contributed talk** CONICET and National University of Salta, Argentina *Antiproton and proton electronic stopping power in transition metals: a non-perturbative model*
16:50-17:10	**Remigio Cabrera-Trujillo | O33 Contributed talk** Institute of Physical Sciences ICF, Mexico and University of Gothenburg, Sweden *Electronic Stopping in Atomic Systems: Effects of Trajectory, Energy Regimes, and Confinement*
17:10-17:30	**Nikola Starčević | O34 Contributed talk** Vinča Institute of Nuclear Sciences, Serbia *Evolution of Crystal and Atomic Rainbows in 2 MeV Proton Scattering Through Ultrathin (001) Si Crystals*
18:30-20:30	**Conference dinner at Bluesun Hotel Elaphusa**
20:30-01:00	**Entertainment: Thursday night fever at Bluesun Hotel Elaphusa Disco**

Friday, 2 October 2026

SESSION 13	**chair: Hermann Rothard**
09:00-09:30	**Arun Persaud | I13 Invited talk** Lawrence Berkeley National Laboratory, USA *Harnessing High-Energy Heavy Ion Irradiation for Engineering Color Center Qubits in Semiconductors*
09:30-09:50	**Satoru Yoshioka | O35 Contributed talk** Osaka Metropolitan University, Japan *XAS investigation of Swift Heavy Ion-Induced Phase Transformations in ZrO_2: From Monoclinic to Orthorhombic and Tetragonal Phases*
09:50-10:10	**Vladimir Skuratov | O36 Contributed talk** Joint Institute for Nuclear Research, Russia *Single ion induced luminescence kinetic in Al_2O_3 in nanosecond range*
10:10-10:40	**Coffee break**
SESSION 14	**chair: Isabelle Monnet**
10:40-11:10	**Shin-ichiro Sato | I14 Invited talk** National Institutes for Quantum Science and Technology, Japan *Rare-Earth Ion Implantation into Nanostructures: Towards Applications in Quantum Light Sources*
11:10-11:30	**Tomás Fernández Bouvier | O37 Contributed talk** University of Helsinki, Finland *Molecular Dynamics insights on single ion implantation for quantum computer manufacturing*
11:30-11:50	**Somar Dibeh | O38 Contributed talk** University of Vienna, Austria *Platinum single atoms and clusters embedded in mono- and few-layer graphene*
11:50-12:10	**Rajdeep Kaur | O39 Contributed talk** Uppsala University, Sweden *Ion-induced tuning of resistive switching properties in amorphous TiO_2 memristors*
12:10-12:30	**Closing ceremony**

The programme is subject to change.

Poster Session 1 (Tuesday, 29 September 2026, 15:30-17:30)

P1. **Djamel Kaoumi**
The use of ion beam coupled with transmission electron microscopy to investigate the irradiation induced phase transformation in polymorphic Ga_2O_3

P2. Yerulan Ungarbayev, Inesh Kenzhina, **Artem Kozlovskiy**
Study of the kinetics of radiation damage accumulation in multicomponent oxide ceramics and determination of the role of phase composition in inhibiting defect formation mechanisms

P3. **Inesh Kenzhina**, Artem Kozlovskiy, A. Zhigalova
Structural changes caused by radiation exposure on the surface layers of oxide ceramics

P4. Yang Jiao, Jinhu Yang, Xinyu Li, Yuzhu Liu, Qiyu Chen, Zongzhen Li, Peixiong Zhao, Pengfei Zhai, Jinglai Duan, **Jie Liu**
Heavy Ion Induced SEUs and Layer Dependence in 3D NAND Flash Memories

P5. **Arno Janse van Vuuren**, Vladimir Skuratov, Anel Ibrayeva, Ruslan Rymzhanov
Exceptional Radiation Hardness of AlN Under Swift Heavy Ion Irradiation: A Comparative Si_3N_4

P6. **Sanjay Kumar Kedia**
Deterministic Control of Interfacial Magnetism via Low and High-Energy Ion Irradiation: Experimental and DFT Study of Spintronic Thin-Film Heterostructures

P7. Sreeja Raghunandanan, Ana Lucia Ferreira de Barros, **Cintia Aparecida Pires da Costa**, Thibault Nguyen Trung, David Dubois, Hermann Rothard, Alicja Domaracka
From Nitrile Ices to Complex N-Bearing Molecules: Simulating Titan's Radiation-Driven Chemistry

P8. Mario Matić, **Andreja Gajović**, Tonči Tadić
Ion beam emulation of neutron radiation damage in reactor materials

P9. **Aaron Herrmann**, Philip Keller, Pascal Schneider, Ina Schubert, Frieder Koch, Pascal Simon, Michael Dürr
Comparison of peptide fragmentation induced by swift heavy ions with low-energy fragmentation processes

P10. Darío Mitnik, Jorge Miraglia, **Claudia Montanari**
Inner-shell ionization by swift heavy ions in matter: CDWEIS calculations, open repository, and neural network model

P11. Platon Karaseov, **Alexander Azarov**, Anton Klevtsov, Andrei Titov
Surface amorphization and fractal analysis of collision cascades in gallium oxide

P12. **Sergey Bragin**, Oleg Bogdanov
Multifrequency laser fields as a tool for generating twisted radiation

P13. **Nandhini Ravindran**, Anna Niggas, Ina Schubert, Somar Dibeh, Filip Vukovic, Vladimir Zobac, Pedro L. Grande, Christina Trautmann, Richard Wilhelm, Toma Susi
Atomic-level characterization of 2D heterostructures modified by swift heavy ions

P14. Nahid Afrin, Shankar Dutt, Maria Eugenia Toimil-Molares, **Patrick Kluth**
Functional ion-track etched nanopores in SiO2 for ultra-sensitive protein detection

P15. Taleb Alwadi, Shankar Dutt, Jessica Wierbik, Nahid Afrin, Raquel Giulian, Christian Notthoff, **Patrick Kluth**
Ion track formation and porosity in InSb and GaSb induced by swift heavy ion irradiation

P16. **Thomas Jarrin**
Average electronic stopping power from ab initio calculations

P17. Roman Voronkov, Danil Zainutdinov, **Nikita Medvedev**, Alexander Volkov
Effect of spatially heterogeneous band gap collapse on formation of swift heavy ion tracks in Al_2O_3

P18. **Danil Zainutdinov**, Alexander Volkov
The shape and composition of swift heavy ion tracks in SiC at high temperatures

P19. Sergey Gorbunov, Alexander Volkov, **Nikita Medvedev**
Spatial inhomogeneities in excitation of matter under high-intensity heavy ion beam

P20. Semion Moskalets, **Ruslan Rymzhanov**, Alexander Volkov
Role of dynamic screening of target atoms in ion track formation in GaN

P21. **BANOTHU SAIDULU**, L.D Varma Sangani, M Ghanashyam Krishna, Anand P Pathak, S V S Nageswara Rao
Fabrication and Radiation Responses of SiC thin-film based device for Sensor Applications

P22. **JINU JOB**, P. JEGADEESAN, VIKAS SINGH GAHLOT, B. SUNDARAVEL, S. AMIRTHAPANDIAN
In-situ FESEM investigations on evolution of fractal morphology of Sb thin films under ion irradiation

P23. Ekaterina Korneeva, Tiep Nguyen Van, **Anel Ibrayeva**, Vladimir Skuratov, Alexander Sohatsky, Alisher Mutali, Nikita Kirilkin, Jacques O'Connell
Size and Matrix Effects on Latent Track Formation in $Y_4Al_2O_9$ Nanoparticles during Swift Heavy Ion Irradiation

P24. **Chloé Nozais**, Aleksi Leino, Flyura Djurabekova
From Damage to Recovery: Atomistic Insights into Swift Heavy Ion Response in Pyrochlores

P25. **Miguel Trigueros Hevia**, Frieder Koch, Pascal Simon, Christina Trautmann, Kersten Hahn, Peter A. van Aken, María Eugenia Toimil Molares, Ina Schubert
Charge-State Effects on Swift Heavy-Ion Damage in Bismuth Nanowires

P26. Danil Zainutdinov, **Nikita Medvedev**, Alexander Volkov
Cross section of nonionizing electron scattering with finite coherence length

P27. **Simon Hoëllard**
Electronic stopping for H, N and Ga projectiles in GaN from first-principles

P28. Narouki Uno, Luca Gerhards, **Vladimir Bacic**, Ilia A. Solov'yov, Hidetsugu Tsuchida
Simulating atomic collisions: theoretical and computational challenges

P29. **Cillian Cockrell**
Simulating radiation in matter: how close can we get?

P30. **Naruki Uno**, Luca Gerhards, Vladimir Bačić, Ilia Solov'yov, Hidetsugu Tsuchida
Orientation effects of MeV C2+ ions on secondary electron emission from graphene: Combined experimental and theoretical study

P31. **Petr Malinský**, Mariapompea Cutroneo, Tereza Dušková, Marek Bouška, Petr Němec, Pereira Jhonatan Rodriguez
Structural and Functional Evolution of GST Thin Films under Carbon Ion Irradiation

P32. **Michael Kendler**, Sophie Wrathall, Lisa Gmainer, Alexander Redl, Anna Niggas, Philippe Roncin, Richard A. Wilhelm
Vacuum compatible printed circuit board anodes for particle detection with electron multiplier devices

P33. **Alexei Zverev**, Aleksi Leino, Joseph Graham, Flyura Djurabekova
First principles parametrization of electron-phonon interaction in swift heavy ion irradiation

P34. **Marko Škrabić**, Marija Majer, Muhammad Alamgeer, Krešimir Salamon, Zdravko Siketić, Maja Mičetić, Željka Knežević, Marko Karlušić
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P35. **Oleg Bogdanov**, Timur Tukhfatullin
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P36. **Gerhard Hobler**
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P42. **K. Tokesi**, R.D. DuBois
Ionization Cross Sections of Hydrogen Molecule by Electron and Positron Impact

P43. **Mandla Msimanga**, Mamogo Masenya, Joseph KO Asante, Abraham Dimtri Kapim-Kenfack
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P44. **Cíntia Aparecida Pires da Costa**, Ana Lucia Ferreira de Barros, Adeline Garcia, Thibault Nguyen Trung, Sreeja Raghunandanan, Ricardo Carrasco-Herrera, David Dubois, Hermann Rothard, Alicja Domaracka, Alexis Bouquet
Ion-Induced Chemistry in H_2O:CO:NH_3 astrophysical ice analogues

P45. **Romana Mikšová**, Matyáš Gary Novák, Petr Malinský, Adéla Jagerová, Martin Kormunda, Anna Macková
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P46. **Vikas Singh Gahlot**, P. Jegadeesan, Md Mofizur Rahman Mollah, Pooja Gupta, Ramnathaswamy Pandian, Soumen Das, Sanjay Rai, S. Amirthapandian
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P47. **Maja Mičetić**, Krešimir Salamon, Kristina Tomić Luketić, Jasminka Popović, Željko Skoko, Tonči Tadić, Andreja Gajović
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P48. **Alexey Dikov**, Sergey Kislitsin, Lyubov Dikova, Anna Shmonina
Effect of Fe Ion Bombardment on the Structure and Elemental Redistribution in the Near-Surface Layers of Ferritic-Martensitic Steel EK-181

P49. Nikita Ashurko, **Oleg Bogdanov**, Yanzhao Wang
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P50. **Krešimir Salamon**, Marko Karlušić, Pavo Dubček, Maja Mičetić, Stjepko Fazinić, Sigrid Bernstorff
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P51. **Muhammad Alamgeer**, Krešimir Salamon, Marko Karlušić, Marko Škrabić, Nataša Vujičić
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P52. **Sergey Kislitsin**, Lyubov Dikova, Alexey Dikov, Alexander Larionov, Sayabek Sakhiyev, Tamara Aldabergenova
The Effect of Low-Energy Irradiation with Light and Heavy Ions on the Structure of Surface Layers and the Physical-Mechanical Properties of Structural Austenitic Steels with Different Nickel Content

P53. **Michael Lee**, Jacques O'Connell, Madeleine Badenhorst, Vladimir Skuratov
In-situ TEM observation of strain annealing in SHI irradiated monoclinic zirconia at intermediate fluences

P54. Ioannis Tzifas, **Christopher Schroeck**, Kay Obbe Voss, Pascal Simon, Jiaxu Liang, Bayarjargal Lkhamsuren, David Merges, Tim H. Reuter, Emanuil Zeqo, Reinhard Boehler, Maik K. Lang, Bjoern Winkler, Christina Trautmann, Maria Eugenia Toimil-Molares
Structural transformations under coupled extreme pressure and swift heavy ion irradiation

P55. **Anirudh Krishna Srinivasa Raghavan**, Miguel Trigueros Hevia, Peter A. van Aken, Kersten Hahn, Maria Eugenia Toimil-Molares, Ina Schubert
Electron microscopy characterization of swift heavy ion impacts in Bi_2Te_3 nanowires

P56. **Leandro Gutierres**, Orlando Deluigi, Ina Schubert, Eduardo Bringa, Maria Eugenia Toimil-Molares
Crystallinity and Track-Parameter Dependence of Swift Heavy Ion Damage in Anatase and Amorphous TiO_2 Ultrathin Films: A ReaxFF Molecular Dynamics Study

P57. Xing-Yu Li, Bin He, Yong Wu, Xiang Gao, Jian-Guo Wang, **Karoly Tokesi**
Interaction of He^{2+} ions with hydrogen isotopes

P58. Z. Li, G. Y. Liang, A Sulyok, J. M. Gong, M. Menyhard, B. Da, R. G. Zeng, **K Tokesi**, Z. J. Ding
Energy loss function of lead determined from the reflection electron energy loss spectroscopy spectra

P59. Lamya El Mesbahi, M. Jakha, S. Mouslih, S. Taj, **K Tokesi**, B. Manaut
Electron-Impact Excitation and Ionization of Hydrogen Atom

P60. **Diana Junisbekova**, **Aigerim Serikbayeva**, Zein Baimukhanov, Alma Dauletbekova, Abdirash Akilbekov
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P61. **Jianrong Sun**, Jian Li
TC-DFT-based Positron Annihilation Spectroscopy Differentiates Irradiation-induced Vacancy Type Defects in 4H-SiC

P62. **Pavo Dubček**, Marko Karlušić
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P63. **István Bányász**, István Rajta, Gyula Nagy, Vladimír Havránek, Stefano Pelli, Gualtiero Nunzi Conti, Simone Berneschi, Miklós Veres, András József Laki, María Cinta Pujol, Ágnes Nagyné Szokol, Robert Magnusson
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P65. **Aldo Artímez Peña**, Nikita Medvedev
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P66. **Raquel Thomaz**, Otávio Berenguel, Khaled Kaja, Hartmut Stadler, Yvette Ngono-Ravache, Maria Eugenia Toimil-Molares
Probing chemical damage induced by individual ion impacts in ultrathin PMMA films by AFM-IR

P67. **Stefan Facsko**, Slawomir Prucnal
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P68. **Reino Piirilä**
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P69. **Pascal Simon**, Frieder Koch, Leon Kirsch, Ina Schubert, Ioannis Tzifas, Kay-Obbe Voss, Michael Wagner, Maria Eugenia Toimil-Molares
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P71. **Masedi Masekane**, Mandla Msimanga, Iva Bogdanović Radović
X-ray production and multiple ionisation in near-symmetric ion-atom collisions

P72. **Stephan Fritzsche**, Aloka Sahoo, Stefan Schippers
Atomic cascade computations for swift ions near surfaces

P73. Eleni Ntemou, Svenja Lohmann, Radek Holeňák, Kevin Vomschee, Gunnar Pálsson, **Daniel Primetzhofer**
Influence of the electronic density of states on the trajectory-dependent energy deposition of keV ions in Silicon

P74. **Kenneth Sanders**, George Adamson, Cale Overstreet, Eric O'Quinn, Tao Liang, Haixuan Xu, Pascal Simon, Maria Eugenia Toimil-Molares, Jesse Smith, Joerg Neuefeind, Joshua Safin, Katharine Page, Xing Wang, Blake Morgan, David Sprouster, Maik Lang
Influence of Compositional Complexity on Transformations in Pyrochlore Oxides under Highly Ionizing Radiation

P75. **Chad Sosolik**, Patrick Johnson, Pooja Dhakal, Grace Orendorff, Julia Brumaghim
Ion transmission through silicon nitride membranes

P76. **Sudip Bhowmick**, Prof. Prasanta Karmakar
Ion-Beam-Induced Ag and C Nanodot Formation on Pre-Patterned Silicon Nano-Templates for Advanced Photonic Applications

P77. **Ankita Ghosh**, Shanu Bandyopadhyay, Tapobrata Som
Fluence-Dependent Nanoscale Resistive Switching Behaviour in Au-Implanted HfO_2 Memristive Devices

P78. **Shanu Bandyopadhyay**, Dipanwita Roy, Anupam Patra, Tanmoy Basu, Tapobrata Som
Defect engineering in 4H-SiC by C and Si ion implantation at room temperature

P79. **Matjaž Panjan**, Domen Korbar
Influence of input parameters on simulated sputtering yields using SRIM and SDTrimSP

P80. **Toreniyaz Shomenov**, Yanwei Wang, Zhandos Utegulov
First-Principles Investigation of Mechanical Stability in Pyrochlore Ceramics

P81. **Zhiwei Ma**, Peng Jin, Tielong Shen, Zhiguang Wang
Effect of He ion irradiation on the early corrosion behaviour of SIMP steel in liquid lead-bismuth eutectic

P82. **Yabin Zhu**, Lijuan Niu, Minghuan Cui, Yanbin Sheng, Zhiguang Wang
Microstructural evolution and irradiation hardening in pressureless sintered SiC irradiated with He ions

P83. **Yanbin Sheng**, Yabin Zhu, Zhiguang Wang
Preliminary Research on High-Performance SOT-MRAM Chips Fabricated by Ion Irradiation Technology

P84. **Sabrina Gouasmia**, Kristina Tomić Luketić, Donny Domagoj Cosic, Fares Boussahoul, Georgios Provatas, Iva Božičević Mihalić
Multipurpose External Ion Microprobe for Irradiation and Analysis at the Ruđer Bošković Institute

P85. **Stjepko Fazinić**, Zdravko Siketić, Milko Jakšić
Status and upgrade of the Ruđer Bošković Institute Tandem Accelerator Centre

Abstracts

(Oral contributions**)**

LL - Experimental and simulation challenges in track formation with swift heavy ions

Christina Trautmann[1]

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This lecture will discuss unresolved questions related to the complex process of swift heavy-ion-track formation. Topics include experimental observations and simulation challenges related to energy dissipation mechanisms, thermal spike evolution, relaxation phenomena such as recrystallization and track annealing, damage morphology, and the influence of stress. Particular attention will be given to surface effects and track formation in nanostructures.

Keywords

swift heavy ions, track formation

Session 1

I1 - Inducing Uniaxial Magnetic Anisotropy in $La_{0.7}Sr_{0.3}MnO_3$ by Means of Surface Nanostructuration with Low and High Energy Ion Irradiation

Mohammad S. Jamal[1], Giuseppe Junior Mosca[2], Iban Llamas[2], Paolo Perna[2], Isabelle Monnet[1], Jimmy Rangama[1], Victor Pierron[3], Bruno Guillet[3], Stéphane Guillous[1], Yann Doublet[1], Stéphane Flament[3], Magali Morales[1], Daniel Chateigner[4], Marko Karlusic[5], Laurence Méchin[3], Mamour Sall[1]

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$La_{0.7}Sr_{0.3}MnO_3$ (LSMO) has been widely used in the form of thin films in the recent years for the development of sensitive magnetic-field sensors based on the anisotropic magnetoresistance effect and operating at room temperature [1]. This requires uniaxial magnetic anisotropy (UMA), which in LSMO thin films is presently obtained using vicinal $SrTiO_3$ (STO) substrates - i.e. substrates where the surface is intentionally misaligned with respect to the crystallographic axis with an angle (in the range 2-10°).

In this study, we present an alternative to the use of vicinal substrates through surface nanostructuring by ion irradiation, either on a flat STO substrate prior to LSMO deposition, or directly on LSMO films deposited on a flat STO substrate:

· Swift Heavy Ion (SHI) irradiation at grazing incidence leads, at the surface of both LSMO and STO, to the formation of highly ordered, anisotropic ripple-like amorphous nanostructures driven predominantly by electronic energy loss [2].

· Low-energy ion irradiation at oblique incidence creates periodic surface amorphous ripples on the surface of bulk STO. This results from a complex interplay between sputtering of matter, surface diffusion, and mass redistribution and is mainly driven by ion potential energy and nuclear energy loss [3].

Using X-ray diffraction and cross-sectional scanning transmission electron microscopy combined with electron energy-loss spectroscopy, we present the structural and chemical modifications accompanying the formation of surface ripple, as well as the thermal stability of the ripples created on irradiated LSMO and STO, and on non-irradiated LSMO layer grown on irradiated STO substrate. In all cases, post-irradiation thermal annealing restored the material crystallinity while preserving the ripple morphology. Furthermore, UMA was demonstrated in both irradiated LSMO and non-irradiated LSMO deposited on irradiated STO.

These results establish ion beam nanostructuring as a robust strategy for designing directionally sensitive magnetic and spintronic devices based on functional oxides.

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[3] M. S. Jamal et al. Small, under revision

Keywords

uniaxial magnetic anisotropy, surface nanostructuration

O1 - Defect-Engineered Charge Transport in ITO/PANI-Graphene/Al Schottky Diodes via Swift Heavy Ion Irradiation

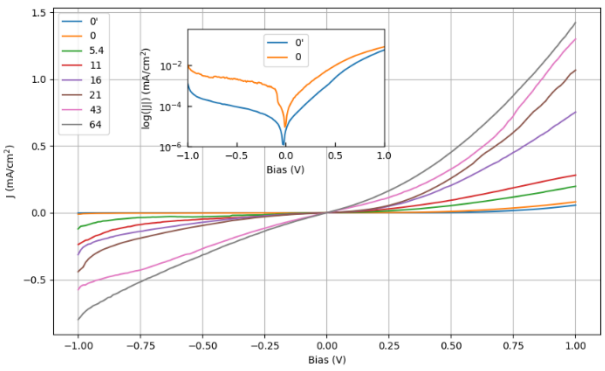
Daniel Chilukusha[1, 2], Jean Jules Mboukam[2], Ncholu Manyala[3], Mandla Msimanga[2]

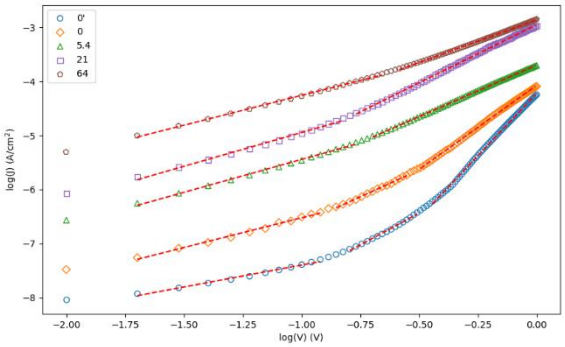
[1]Department of Physics, Mulungushi University, Kabwe, 10101, Zambia, [2]PV NanoComposites R&D Platform, Department of Physics, Tshwane University of Technology, P Bag X680, 0001, Pretoria, South Africa, [3]Department of Physics, University of Pretoria, Pretoria 0002, South Africa

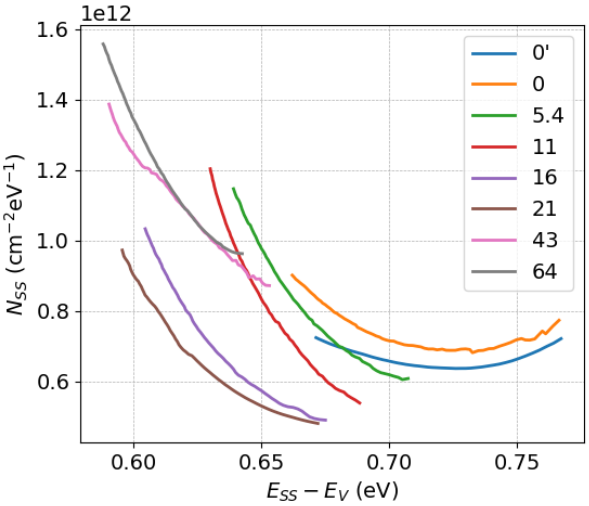
Controlled defect engineering offers a promising pathway for improving the electrical performance of organic Schottky barrier diodes (SBDs), particularly where conventional interface tuning is limited by strong Fermi-level pinning. In this work, we investigate the influence of swift heavy ion (SHI) irradiation on charge transport and interfacial defect states in ITO/PANI-graphene/Al Schottky diodes. Devices were exposed to 36 MeV Cu^{7+} ion irradiation over a wide fluence range under high vacuum at room temperature to induce nanoscale structural and electronic modifications within the active layer and metal-organic junction. Current-voltage analysis revealed a progressive enhancement in carrier injection with increasing irradiation fluence, evidenced by reduced turn-on voltage, increased forward and reverse current, and a systematic decrease in rectification ratio. The Schottky barrier height and ideality factor showed strong fluence dependence, indicating irradiation-induced redistribution of localized states at the interface. Bias-dependent extraction of interface state density confirmed a significant increase in defect-assisted states approaching the valence band edge, suggesting improved hopping-assisted transport pathways. Resistance analysis further showed a pronounced reduction in shunt resistance, supporting the formation of additional conductive channels. At higher electric fields, the dominant transport mechanism shifted from trap-limited conduction to trap-free space-charge-limited conduction, with current-voltage slopes approaching the Child's law regime. These findings demonstrate that SHI irradiation can serve as an effective defect-engineering strategy for tailoring interfacial transport and barrier properties in conducting polymer-based SBDs, offering practical relevance for flexible rectifiers, low-power switching devices, and organic optoelectronic interfaces.

Keywords

Swift heavy ion irradiation, Polyaniline, graphene, Schottky diodes, polymer-metal interfaces







O2 - IBIC characterisation of the charge transport using heavy ions

Milko Jaksic[1], Georgios Provatas[1], Donny Cosic[1], Zdravko Siketić[1], Matija Matijević[1]

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There are several techniques that utilize fast ions of the MeV energy range, focused to a submicrometer spot size, that probe different properties of the material exposed to these ions. Among them, Ion Beam Induced Charge (IBIC), is developed to measure a charge transport of charge carriers induced by a single ion that is being slowed down n the sample. As this transport is influenced by many different parameters and processes, related to the sample itself and to the ions being used, many standard and unique properties of materials and devices exposed to these ions can be studied. The IBIC technique has been primarily used o characterise different properties of radiation detectors made of different materials, but mostly using light ions like protons and He ions, which have long ranges and therefore can often be used to study burred layers which otherwise cannot be reached by laser light or electron beam probes. However, the use of ions like C, O, Si, and heavier, offers new possibilities due to their shorter range and significantly higher density of ionisations along the ion tracks these ions induce. Ideally, the opportunity of creating stronger signals and smaller depth ranges can significantly increase IBIC applicability in the characterisation of micrometer sized volumes of devices, or those devices with poor charge transport properties. However, the high ionisation density of these heavier ions is often accompanied by effects that need to be understood to

interpret the IBIC data properly. Examples of heavy ion IBIC applications that will be presented include studies of micro-dosimeters made of scCVD diamond and GaN, studies of charge multiplication in silicon LGAD and diamond membrane detectors, as well as studies of charge transport properties in diamond as a function of temperature in both the low and high-temperature operation range. Dewvelopment of low-noise IBIC system dedicated o deterministic ion implantation will be presented as well.

Keywords

diamond detector, charge transport, heavy ions, ion microprobe

O3 - Thickness dependence of bond-breaking cross sections in PMMA thin films: new insights from in situ spectroscopic investigations with 9 MeV/u C ions

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Polymer thin and ultrathin films have been applied as a model system to investigate size effects in radiation damage of organic materials [1,2]. Such approach identified strong thickness dependence in cratering induced by single ion impacts [1], but weak size-effects in bond breaking cross sections *s* of carbon bonds, which were largely insensitive to film thickness down to layers of about 5 nm [2]. It was difficult to obtain the thickness dependence of *s* using swift heavy ions (Bi and Au [2]), due to excessive erosion and roughness changes which limit analysis of the thinner films. In this work, we employed ions of intermediate *Z* (9 MeV/u C, electronic stopping power ≈ 200 eV·nm^{-1}) and *in situ* infrared spectroscopy (FTIR) monitoring of bond-breaking to examine chemical damage efficiency in poly(methyl methacrylate) (PMMA) films of various thicknesses (15 and 414 nm). We combine *in situ* spectroscopy with *ex situ* atomic force microscopy (AFM) measurements of film thickness evolution as a function of fluence to disentangle chemical damage from thinning effects. Bond breaking cross sections of the carbonyl (C=O) bond extracted from raw FTIR measurements were similar (around 6.5 × 10^{-15} cm^2) and independent of the tested film thicknesses. Additional XPS analysis of the C1s core level confirms the progressive loss of oxygen-containing functional groups, with an efficiency that is roughly thickness independent. However, correction of FTIR data using post-irradiation thickness values, yields bond-breaking cross sections which decrease in thinner films. We will discuss size-effects on bond breaking efficiency in ultrathin layers on the light of current ion track models.

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Keywords

radiation effects in nanomaterials, polymers, chemical damage,

Session 2

I2 - O_2 plasma-induced modifications in the surface of space-technology polymers

Cíntia Aparecida Pires da Costa[1, 2], Nadhira Laidani[1, 3], Gloria Gottardi[3], Lucrezia Aversa[4], Roberto Verucchi[4], Lorena Maines[5], Matteo Michielan[1], Mirco Rossi[1], Luca Matteo Martini[1], Paolo Tosi[1], Daniela Ascenzi[1]

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Polymeric films are widely employed in aerospace applications because of their low weight, high flexibility, and effective electrical and thermal insulation properties [1]. In the Low Earth Orbit region (LEO) - which reaches altitudes of up to 2000 km above the Earth's surface [2] and includes major space platforms such as the International Space Station (400 - 420 km) and the Hubble Space Telescope (515 km) - these materials experience significant degradation. A key contributor to this deterioration is chemical erosion driven by atomic oxygen (O) and ionized oxygen (O^+), which are the predominant species in the atmosphere at these elevations. The aim of this work is to study the effects of non-thermal oxygen plasmas on spacecraft coating polymers, focusing on the degradation processes at an atomistic level. In particular, to better understand how exposure to atomic oxygen influences the chemical structure of polymers (such as Kapton, Polystyrene, and Graphite), and which components of the macromolecules are more susceptible to oxidation and further erosion. Plasma experiments were conducted at the Fisica Atomica e Molecolare (FAM) laboratory at the Physics Department of the University of Trento. Polymeric samples were exposed to O_2 discharges under controlled conditions to study the effect of the gas pressure, the applied electric power and the exposition time to the O_2 plasma. Atomic oxygen fluxes, Φ_{AO}, were estimated from mass loss measurements, assuming atomic oxygen as the primary erosion agent. Contrarily to Kapton, polystyrene and graphite showed negligible mass losses even after long time expositions (~8 hours). Analysis via Scanning Electron Microscopy (SEM) shows clear erosion effects on Kapton samples characterized by the exfoliation of parts of the material, as well as the formation of round conglomerates after plasma treatment. In each experiment two samples at a time were positioned in the reaction chamber for plasma treatment: i) in direct exposure to the plasma, and ii) in an indirect exposition insured by a quartz shield set 8 mm above it. X-ray Photoelectron Spectroscopy (XPS) reveals chemical and compositional changes. Samples directly exposed present a large amount of metallic contaminants (as Fe, Cr, and Ni), likely sputtered from the sample holder or the chamber walls that were redeposited on top of the samples. This issue is significantly reduced in the case of the samples covered by the quartz window. For the shielded samples, XPS analysis show samples' surfaces enriched with oxygen, and a decrease on the relative quantity of carbon. Figure 1 presents the C1s and O1s XPS spectra for an untreated and a Kapton sample processed by a plasma of 100 W.

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Keywords

Low Earth Orbit; Polymers; Non-thermal plasma; Mass loss; Surface modifications.

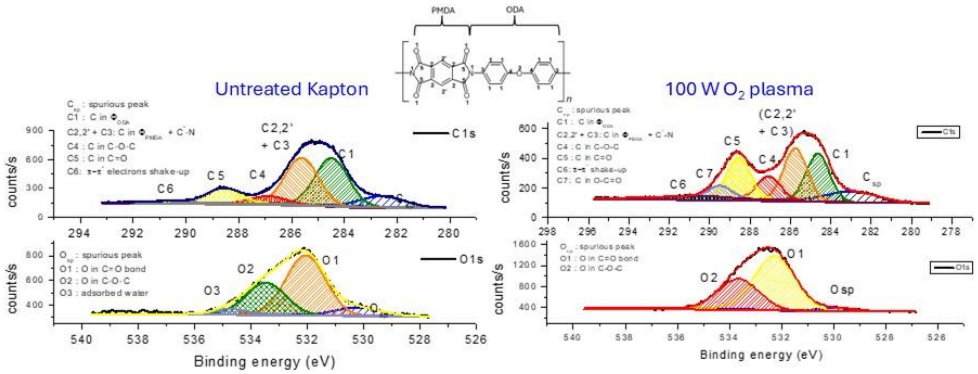


Figure 1: (a) Fitted C1s and O1s spectra from a) an untreated Kapton sample and b) a treated one at 100 W O_2 plasma discharge for 30 minutes, O_2 pressure and flow of 25 sccm and 0.23 mbar. Inserted image depicts the Kapton macromolecule.

O4 - Swift Ion irradiation of ices containing organic molecules at GANIL

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In 2023, France launched the PEPR ("Programmes et équipements prioritaires de recherche") "Origins" (life and universe), program leader CNRS, to address the question of the origin of organics and emergence of life [https://pepr-origins.fr/]. Organic molecules have been observed in space (comets, meteorites, planetary atmospheres, molecular clouds). They can be formed in cold space environments following radiolysis of small molecules (H_2O, CO, CH_4, NH_3 etc.) on cold surfaces of icy bodies in the outer solar system or grains in the dense molecular clouds and by implantation of ions trapped in the magnetospheres of giant planets into the icy surfaces of their satellites (like e.g. S ejected by Io's volcanism impacting Europa and Ganymede). At CIMAP, this was studied in recent years with the "space simulator" device IGLIAS (financed by ANR, operational since 2017) [1]. Infrared absorption spectroscopy FTIR and mass spectrometry QMS allow in situ observation of physico-chemical modifications of thin icy layers. Ex-situ analysis of residues is performed by e.g. high resolution mass

spectrometric methods. At present, MIRRPLA, a unique multibeam irradiation platform (UV photons, keV electrons and keV-GeV ions delivered by the GANIL-Grand Accélérateur National d'Ions Lourds, Caen France) equipped with an infrared spectrometer and a cold head to prepare layers of ices made of mixtures of small molecules is under construction. Complex organic molecules formed during the irradiation of ice layers will be detected using gas phase chromatography and in-situ mass spectrometry [1]. This new versatile MIRRPLA platform [2] will be open to the various scientific communities (astrophysics, radiobiology, environmental and materials sciences) as well as to industry via the CIMAP-GANIL user platform CIRIL [3]. In preparation of the commissioning of MIRRPLA, we performed ion irradiation experiments of ices containing organic molecules (e.g. methanol and aromatic molecules such as benzene) with IGLIAS at GANIL. The results presented here obtained with ionic projectiles will then be compared to electron and UV irradiations performed in MIRRPLA.

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Keywords

organic molecules, ices in space, cosmic rays, radiolysis

O5 - Highly site-selective fragmentation of peptides induced by swift heavy ion impact

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Based on their high energy deposition, swift heavy ions (SHI) can efficiently alter the structure of condensed matter including organic material such as polymers or biological macromolecules. It is generally agreed that the initial excitation proceeds via the electronic subsystem, but the further mechanisms of energy redistribution in organic molecules, finally leading to, e.g., bond cleavage, are to a large extend unclear.

Here we make use of soft cluster-induced desorption/ionization mass spectrometry for a detailed investigation of SHI-induced fragmentation of peptides (Figs. 1(a) and b)). With their different functional groups and bonds, peptides are an ideal model system to investigate selectivity in the interaction of SHI with organic molecules. Furthermore, peptides represent one of the most important classes of biomolecules; therefore, their interaction with SHI is also of interest, e.g., for medical applications as well as in terms of radiation-induced chemical reactions in space.

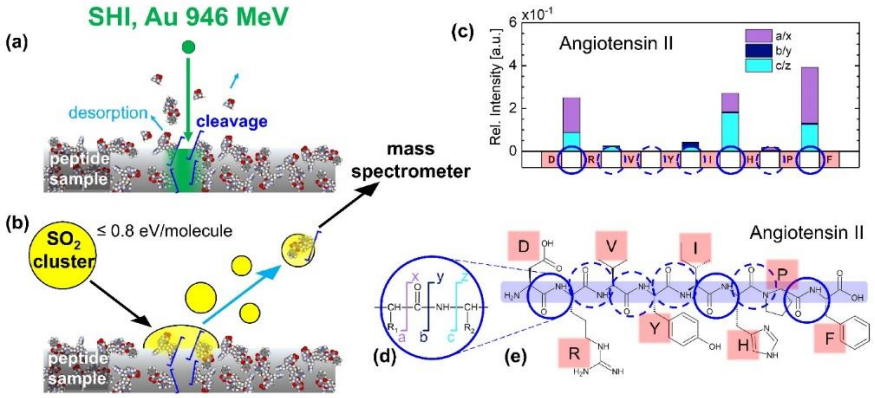
Our experimental results clearly indicate that, despite the high initial energy deposition, SHI-induced peptide fragmentation is highly site-selective with respect to the position of the

cleavage site in the amino acid sequence; only a few of the many chemical bonds in the molecules are cleaved (Figs. 1(c) to (e)). By exchanging single amino acid units in a given molecule, we could further show that the amino acids in the direct neighborhood of the cleavage sites do *not* determine the site selectivity, in contrast to low-energy dissociation processes such as collision-induced or thermal dissociation. The observed selectivity thus rather depends on the whole structure of the peptide; as a result, similar amino acid sub-sequences can behave very differently in different molecules.

Ab initio molecular dynamics calculations suggest multiple electron abstraction as a possible excitation process for SHI-induced peptide fragmentation and the observed site selectivity. Together with the experimental results, they point towards a unique fragmentation channel operative under swift heavy ion impact leading to the surprising site selectivity. The latter might be of particular importance for understanding the contribution of SHI to the formation of biologically relevant molecules in space.

Keywords

mass spectrometry; peptides; radiolysis; selective fragmentation; swift heavy ions



O6 - Velocity-resolved SNMS as a probe of electronically driven sputtering under swift-heavy-ion irradiation

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Sputtering by keV ion bombardment is commonly described in terms of nuclear collision cascades, whereas sputtering under swift-heavy-ion (SHI) irradiation is governed by electronic excitation and the subsequent conversion of deposited energy into atomic motion. This conversion remains difficult to access experimentally, in particular because SHI beams at accelerator facilities are often quasi-continuous and therefore not directly compatible with conventional time-of-flight measuring schemes.

Here, we use velocity-resolved secondary neutral mass spectrometry (SNMS) to compare neutral-particle emission under nuclear and electronic stopping conditions on an identical experimental footing. The measurements combine laser post-ionization with a laser-delay approach, in which the temporal delay between the ionizing laser pulse and pulsed extraction into a time-of-flight mass spectrometer is varied. In contrast to classical extraction-delay

methods, this approach does not require short primary-ion pulses and is therefore applicable to quasi-continuous SHI beams, such as those available at GSI.

Velocity distributions of sputtered neutral species were measured for representative material classes, including indium, bismuth, and sodium chloride. Conventional collision-cascade sputtering was investigated using 5 keV Ar^+ bombardment, while electronically driven sputtering was probed with 4.8 MeV/u $^{48}Ca^{10+/19+}$ and $^{197}Au^{26+/54+}$ projectiles. For all investigated targets, SHI-induced emission exhibits a pronounced shift towards lower velocities compared with the keV reference case. This demonstrates that electronically driven sputtering cannot be described as a simple extension of nuclear collision cascades. At the same time, the measured velocity distributions are not reproduced by a simple Maxwell-Boltzmann distribution, indicating that the emission is not governed by a purely thermal equilibrium process.

These results establish laser-delay-based, velocity-resolved SNMS as a sensitive spectroscopic probe of sputtering mechanisms under electronic stopping conditions. Beyond providing mechanistic insight into SHI-induced emission, the approach offers a route towards quantitative interpretation of SNMS intensities in terms of neutral-particle fluxes and their velocity distributions.

Keywords

SIMS; SNMS; Sputtering

Session 3

I3 - Identifying electronic doorway states in secondary electron emission

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Slow electron emission from ion-surface collisions is important for many applications, yet understanding specific spectral features remains challenging: Ion impacts trigger a cascade of complex, interconnected processes, and the resulting energy spectra of slow electrons are typically broad and mostly featureless, rendering the identification of underlying mechanisms challenging.

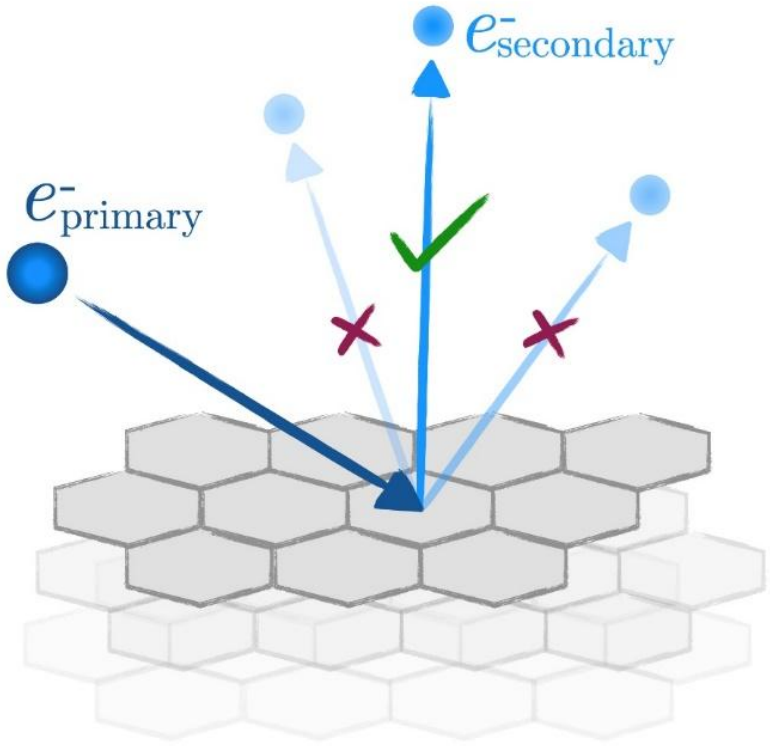
Here we study one specific spectral feature of graphite surfaces — a peak at 3.3 eV often termed X peak in literature [1] — triggered by electron impact instead of ion impact. With electron pair coincidence spectroscopy, we can disentangle the underlying processes leading to this slow electron emission without the complexity of the full ion-induced cascade. In particular, we can associate this feature with excitation of (π+σ) plasmons in the graphite sample [2], followed by emission of secondary electrons based on layer-number-dependent coupling of electronic excitations to the continuum [3]. Interestingly, the angular and energy distribution of this peak remains the same when ions are used as impacting particles, allowing for an assignment of the relevant processes also in ion-surface collisions.

Based on this study, we will discuss how combining electron spectroscopy, coincidence detection, and angle-resolved spectroscopy for both ion and electron impacts enables a comprehensive understanding of electronic excitations at surfaces.

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Keywords

secondary electron emission



O7 - X-ray emissions from slow multiply-charged ions on Si and Nb targets

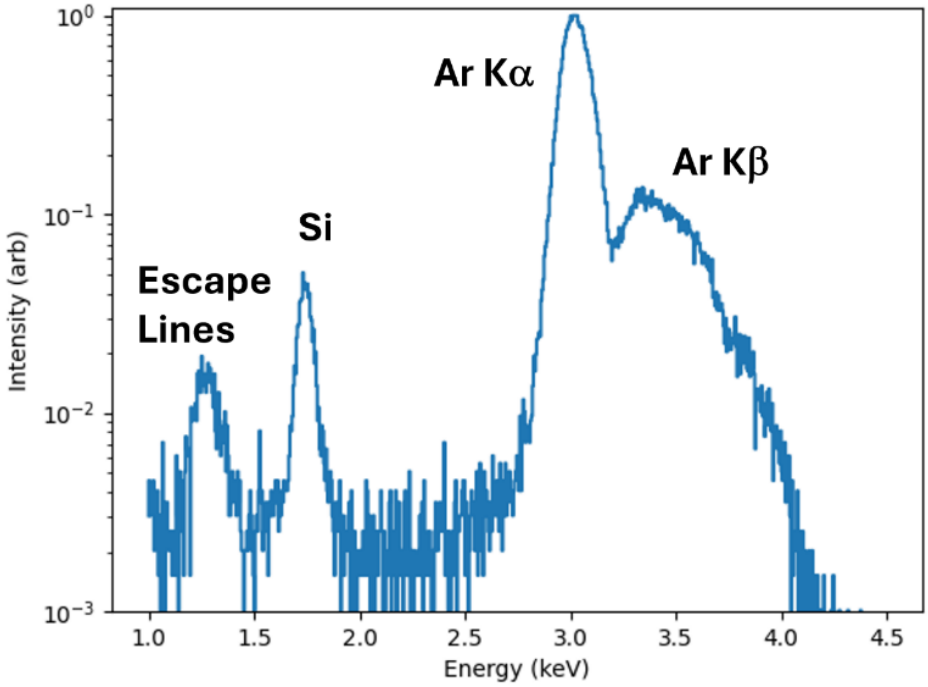
Chad Sosolik[1], Patrick Johnson[1], Sehrish Akhtar[1], Dinesh Gc[1], Pooja Dhakal[1]

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We have investigated the spectrum of x-rays emitted when slow multiply-charged argon ions were used to irradiate well-prepared targets of Si(100) and Nb/Si nanowires. Our goal was to determine the role of hollow atom (HA) formation and x-ray deexcitation on the energy balance in these systems. By varying the impacting ion parameters (energy, angle) we have evaluated the overlapping contributions of collision-promoted and HA-fluorescence x-rays, with an example spectrum for Ar^{17+} incident on Si(100) shown in the figure. Following previous work, a careful examination of the K-shell x-ray emissions in each system was used to evaluate the role of direct vacancy transfers between the projectiles and target atoms across our incident energy range. In particular, we account for the attenuation of HA x-rays onto the target as well as the attenuation of outgoing fluorescence x-rays. Both of our investigated targets serve as candidates for high precision measurements of ion-surface interactions: Si(100) as part of a mechanically resonant system and Nb/Si nanowires for high-fidelity particle detection.

Keywords

x-rays, fluorescence, highly charged ions



O8 - Recent progress in studying the velocity correlated cluster emission (VCCE) effect in surface impact of keV C_{60}-ions

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Over the last few years, we have studied and characterized a new impact interaction mechanism of keV C_{60}^- ions with a variety of targets [1-7]. By measuring kinetic energy distributions (KEDs) of each complete family of secondary clusters sputtered from a given target, we show that they are all moving with nearly the same velocity. Namely, a velocity correlated cluster emission (VCCE) mechanism [1,2,4]. This behavior is very different from that observed using a heavy monoatomic primary ion, and is attributed to the exceptionally high energy density induced in a shallow subsurface region (only a few nm deep) by the impacting polyatomic projectile. KEDs of all the clusters emitted from a given target could be uniquely reproduced by a single shifted Maxwellian, implying a thermal distribution superimposed on a center-of-mass velocity of some superhot moving precursor which is the source of all the outgoing clusters. The large clusters whose KEDs were measured are either purely metallic including Au_n^+ (n=1-15) [1,4], Ag_n^+ (n=1-21) [6] , Cu_n^+ (n=1-9) [4] and Al_n^+ (n=1-14) [3] , emitted from the respective clean metal targets, or carbidic $Ta_nC_m^+$ (n=1-10) [2,4] and $Nb_nC_m^+$ (n=1-9) [4] , as emitted from Ta and Nb targets.

We will briefly analyze the VCCE effect as reported earlier and then focus on three recent aspects which are studied both experimentally and computationally via molecular dynamics (MD) simulations : **(1)** The gradual weakening of the effect for light metallic targets, down to its complete disappearance for beryllium [5]. **(2)** Extending the validity range of the effect to larger clusters and up to Ag_{21}^+ [6]. **(3)** In order to distinguish between decrease of the atomic

mass and other physical properties (structure and bonding) of the target in controlling the VCCE effect, we have very recently extended the KEDs measurements and analysis from the metallic Al to the nearly similar mass but tightly covalently bound, tetrahedrally coordinated Si target [7]. The combined measurements and analysis points at an ultrafast time window for cluster emission, of about 200-500 femtosecond from impact, reflecting the very early stage of the evolution of an extreme thermal spike. Finally, we will discuss astrophysical implications as related to the exceptionally large abundance of C_{60} in the interstellar medium [8].

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[7] V. Bernstein et al, to be submitted

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Keywords

fullerene ion beams, cluster emission, kinetic energy distribution, sputtering mechanism

O9 - Chirality switching in 1T-TaS_2 with Slow Highly Charged Ions

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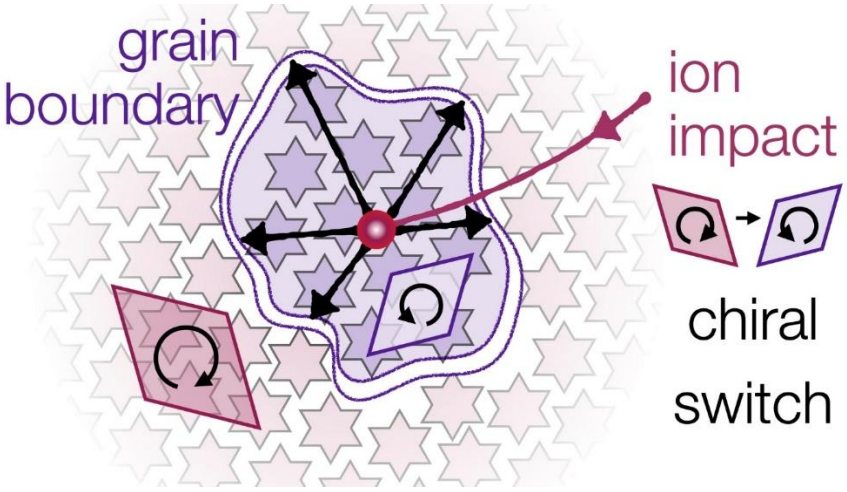
Slow highly charged ions (HCIs) can drive surface modifications in insulating materials with strong electron-phonon coupling. While HCIs carry several keV of potential energy, which is released promptly during the interaction with a surface, the resulting surface modification can be constraint to a single monolayer [1]. Recent charge exchange spectroscopy measurements on freestanding two-dimensional materials explained this by a femtosecond de-excitation channel which becomes active at close interatomic distances when the ion enters the surface [2].

We used a bulk crystal of van-der-Waals layered *1T*-TaS_2 which exhibits a metal-to-insulator transition, where the Mott insulating phase is accompanied by a specific surface reconstruction linked to a commensurate charge density wave. We show that the impact of individual HCIs can induce a specific switch of the surface orientation of the reconstruction from one chirality to another. We probe this chirality switching by *operando* ARPES during the HCI irradiation and deduce the cross section for the chiral switch per ion. Our results compare well with previous findings using laser excitations or electrical pulses to induce this switch and show that HCIs are an efficient tool to electronically modify strongly-correlated quantum materials without significant damage despite the large potential energy stored within them [3].

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Keywords

highly charged ions, surfaces, arpes



Session 4

I4 - Atom and ion irradiation of graphene: disentangling inelastic from elastic scattering and the role of phonons

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Graphene provides the thinnest possible diffraction grating for atom and ion transmission, providing an ideal robust model system for studying the fundamental physics of energy and momentum transfer, and the loss of coherence. Understanding atomic-scale details is only possible with the help of first-principles simulations capable of describing energy loss, which is feasible with the help of time-dependent density functional theory. Our implementation of LCAO Ehrenfest molecular dynamics (ED) method within the projector augmented-wave code GPAW yields satisfactory accuracy at a much-reduced computational cost, which is particularly useful for modeling irradiation processes that require large amounts of vacuum in the simulation cell [1].

After the first demonstration of atom diffraction in transmission through a crystal [2], new measurements have now been performed with an improved graphene sample featuring large monocrystalline domains comparable in size to the beam diameter. In these experiments, the shape of the diffraction pattern is largely determined by the lattice at equilibrium whereas vibrationally-induced distortions are treated perturbatively. By including a model of the target lattice incorporating thermally diffuse scattering via phonon normal modes, we show that the perturbative approach does not hold for helium diffracted at kiloelectronvolt energy through freestanding single-layer graphene. In this case, we enter a new regime of strong coupling, where the projectile strongly interacts with the electron density of several lattice atoms simultaneously, with the weak-coupling regime is retained for atomic hydrogen diffraction [3].

Turning then to ion transmission, the charge of an ion becomes a dynamic quantity when it is in contact with other atoms, molecules, or solids, leading to a complex coupling between stopping processes in matter. We perform experimentally-benchmarked Ehrenfest dynamics simulations of neutral Xe and Xe^{12+} ions transmitted through freestanding single-layer of graphene to reveal the synergy between nuclear and electronic stopping. Importantly, momentum transfer from phonons excludes the high-symmetry bond-center impact parameter from the small acceptance angle of the ion analyzer. Relative to neutral projectiles, ions exert an enhanced nuclear energy transfer, and exhibit non-trivial electronic energy losses. This can result in greater electronic stopping for neutral projectiles compared to ions under certain conditions. Our findings challenge the typical notion that ion stopping force is merely the sum of independent nuclear and electronic stopping components [4].

Funding by the Austrian Science Fund (FWF) via grant P 36264-N is gratefully acknowledged.

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[4] F. Vuković, V. Zobač, A.N. Prohaska, A. Niggas, N. Ravindran, M. Kendler, T. Susi, R.A. Wilhelm, *submitted*

Keywords

Ehrenfest dynamics, atom diffraction, highly charged ion irradiation, phonons

O10 - Two-velocity regimes in nanostructure formation on metal surfaces induced by slow highly charged ions

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Slow highly charged ions (HCIs) are powerful tools for surface modification due to their ability to alter only the topmost atomic layers while leaving the bulk largely unaffected [1]. Depending on the potential energy (charge state), kinetic energy, and collision geometry, the resulting nanoscale modifications may appear as hillocks or craters.

The influence of collision geometry on nanostructure formation is examined within the framework of the two-step cohesive energy model (CEM) [2]. Highly charged ions carry a substantial amount of potential energy, a fraction of which is released upon neutralization at the surface on a femtosecond timescale. This process is modeled using the micro-staircase model (MSCM) in combination with the quantum two-state vector model (TVM).

Beneath the surface, the projectile slows down through interactions with both atomic and electronic subsystems. The associated kinetic energy deposition is described within a charge-dependent energy-loss framework [2]. The combined effects of kinetic energy loss and neutralization energy, dictated by a critical ion velocity, determine the total energy deposited in a small volume around the impact point, thereby increasing the local energy density. The resulting nanostructure is primarily governed by the dominant energy channel: neutralization energy promotes hillock formation, whereas kinetic energy favors crater formation [2,3]. At the critical ion velocity, where the two contributions are comparable, both structures may coexist.

Extending the CEM to arbitrary collision geometries provides a comprehensive description of the underlying energy transfer dynamics. Variation of the incidence angle reveals two distinct velocity regimes [2]. In the low-velocity regime, the process is primarily controlled by the critical ion velocity, whereas at higher velocities, the total deposited energy becomes the decisive parameter. In both regimes, crater formation is favored at small incidence angles, where both energy contributions are enhanced, leading to a higher local energy density, consistent with experimental electron-yield data [4].

A similar distinction arises in the analysis of nanostructure diameter. While the influence of the incidence angle is weak in the low-velocity regime, it becomes dominant at higher velocities, resulting in the largest diameters for both hillocks and craters at the smallest incidence angles.

Finally, for a given ion charge state, specific nanostructures can be deliberately engineered by tuning both the ion velocity and the impact geometry, establishing a framework for ion-induced surface nanostructuring [2].

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Keywords

Highly charged ions, Metal surface, Incidence angle, Surface nanostructure, Velocity effect

O11 - Modeling of Sputtering from Solid Surfaces Under Argon Cluster and Ion Bombardments: Comparison with Experimental and Simulated Data.

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The interaction of energetic ions with solids is a key topic in atomic collision physics, governing energy loss, scattering, and radiation-induced material modification. While atomic ion irradiation is dominated by binary collision cascades and electronic stopping, cluster ion bombardment represents a distinct regime characterized by collective energy deposition within a confined near-surface region. This leads to enhanced sputtering, defect formation (including crater formation), and surface modification compared to single-ion impacts. Argon clusters, composed of weakly bounded atoms, may fragment upon impact and deposit their energy into a small region of the surface, which may result in a shock wave generation in the medium. In this work, a theoretical model for sputtering induced by Argon cluster impacts will be presented. The model was developed on the basis of generated shock wave by argon clusters [1] and validated using experimental data and molecular dynamics simulations[2-5]. The model extends a framework originally proposed for metallic cluster impacts [6] by incorporating the specific properties of Argon clusters (fragmentation dynamics, reduced binding energy…). The analyse of influence of cluster size and cluster-to-target mass ratio revealed a transition from single-ion collision behavior to collective excitation dominated by shock-wave propagation. The results show excellent agreement between theory, experiments, and simulations, and demonstrate significantly higher sputtering yields for Argon clusters compared to atomic ion irradiation at comparable energies. These results improve an understanding of sputtering mechanisms from solid surface impacted by argon clusters and provide a predictive model without adjustable parameters which offers an advantage over existing approaches such as Seah's universal equation [7]. The findings are relevant for applications in thin-film processing, surface modification, and ion-beam-based material engineering.

Keywords

Argon cluster, ion-solid interaction, shock wave, sputtering, energy deposition, molecular dynamics, radiation damage

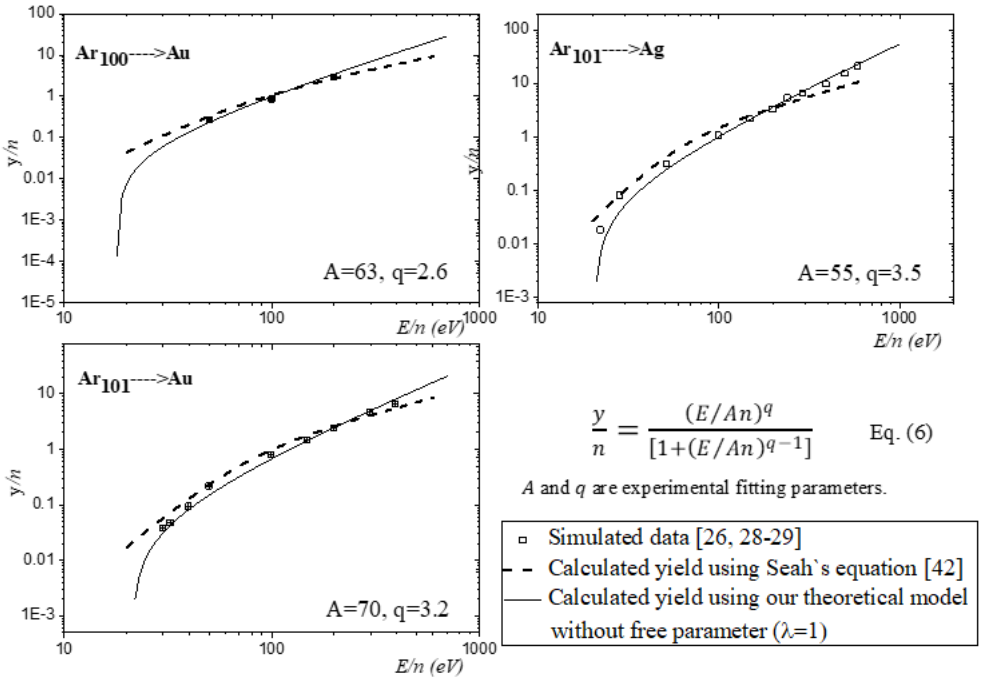


Fig.3: Dependence of sputtering yield (y/n) on scaled impact energy (E/n): (a) Experimental data for Gold bombarded by Ar_{100} clusters at 45° to the normal [29] (b), (c) Simulated data for Gold and Silver bombarded by Ar_{101} clusters at normal incidence [26,28]. The dashed solid line presents the yield calculated from Eq. (6) with two fitting parameters A and q.

O12 - Picosecond Ion Pulses from Laser-Stimulated Desorption at Tungsten Nanotips for Time-Resolved Ion-Solid Interaction Studies

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The understanding of ion-solid interactions on their intrinsic timescales in the picosecond regime requires ion sources capable of delivering well-defined, picosecond pulses in the keV regime. We present the generation and characterization of sub-100 ps ion pulses from adsorbate-covered tungsten nanotips via laser-stimulated desorption (LSD), and outline their usage in a novel time-of-flight-resolved low-energy ion scattering (TOF-LEIS) experiment.

The source is based on an electrochemically etched tungsten nanotip operated under ultrahigh vacuum at bias voltages up to +6.5 kV, resulting in local electric fields in the order of tens of MV/cm at the apex. Selectable gases are introduced and adsorb on the tungsten nanotip surface. Femtosecond ultraviolet laser pulses (<350 fs) trigger desorption and ionization of these adsorbates, producing ions with kinetic energies in the sub-10 keV range. TOF measurements reveal ion pulse durations as short as 84 ps (FWHM) for hydrogen, with intrinsic synchronization to the driving laser [1].

To interpret the temporal structure of the ion pulses, charged-particle trajectory simulations were performed using the SIMION software package [2]. The simulations reproduce the experimentally observed TOF distributions and show that the measured pulse widths are not limited by the desorption process itself, but are dominated by transport-induced dispersion. In particular, the geometric acceptance of the beamline acts as an effective temporal filter, as trajectory-dependent flight times govern the observed pulse duration.

These results demonstrate nanotip-based LSD sources as compact and intrinsically synchronized probes for ion-solid interaction studies with well-defined conditions. Their application in pump-probe schemes, such as laser-pumped TOF-LEIS, enables access to ultrafast processes including transient surface modification, recrystallization, adsorption, and thermal diffusion. The combined experimental and computational approach further provides clear pathways for optimizing the source toward single digit picosecond resolution.

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Keywords

laser-stimulated-desorption, LSD, picosecond, ion-sources, nanotips

Session 5

I5 - Reactivate the rule of "smaller and stronger": breaking the small size limit of mechanical metamaterials by swift heavy ions

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Mechanical metamaterials refer to a class of composite materials with artificially designed structures and exhibit extraordinary mechanical properties that traditional materials do not have. Among them, energy absorption mechanical metamaterials can absorb mechanical energy more efficiently, which requires the material itself to have both high strength and high strain capacity. But in general, high strength and high strain capacity of materials are difficult to obtain at the same time.

Nanolattice is a new class of mechanical metamaterials with characteristic sizes on the order of hundreds of nanometers. Due to extremely special size effects, structural characteristics and material selection, the mechanical properties of this type of porous materials are very different from those of bulk materials, and it can even have better mechanical properties with lighter weight, which is expected to bring revolutionary applications in the field of high-performance functional materials in the future. Beam nanolattice is the main research object of nanolattice materials. However, to date, it is challenging to make breakthrough in the fabrication of metallic beam nanolattice with beam diameter of less than 100 nm, and thus their mechanical properties remain ambiguous.

In our work, a new type of quasi-body centered cubic (quasi-BCC) beam nanolattice mechanical metamaterial is proposed, which is experimentally implemented with ion track technology based on the Heavy Ion Research Facility at Lanzhou (HIRFL). The beam diameter of the quasi-BCC beam nanolattice can be as small as 34 nm, breaking through the size limit of the beam nanolattices mechanical metamaterials. In situ compression experiment results show that the energy absorption capacity of the copper quasi-BCC beam nanolattice exceeds that of the previously reported beam nanolattices. In addition, the yield strength of the gold and copper quasi-BCC beam nanolattices exceeds that of the corresponding bulk materials at less than half the density. Furthermore, experiments and simulations reveal that the supernormal mechanical properties are mainly due to the synergistic effect of size effect, quasi-BCC geometry, and good ductility of metal. This work reactivates the rule of "smaller and stronger", and deepens the understanding of the mechanical properties of beam nanolattices. At the same time, the application of swift heavy ions in the study of nanostructured materials is realized, which provides a new idea for the exploration of beam nanolattice with ultra-high energy absorption capacity. And beyond…

Keywords

Swift heavy ions; Small size limit; Nanolattices; Mchanical metamaterials; Energy absorption

O13 - Osmotic Energy Conversion using Ion Track Etched Conical Nanopores in SiO_2

Xiang Lian[1], Shankar Dutt[1], Aditya Tejas[1], Patrick Kluth[1]

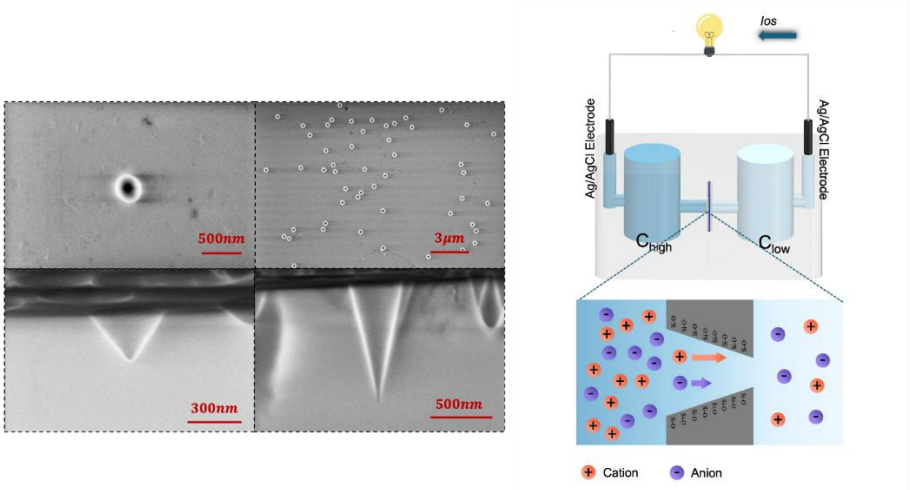
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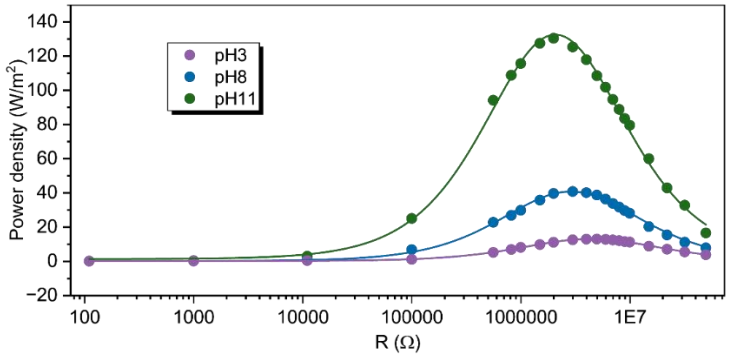
Ion track etching is a versatile method for fabricating nanopores in solid-state membranes. In amorphous SiO2 membranes, this approach enables the fabrication of conical nanopores with systematic control over pore density, pore size, and half-cone angle, including both single-pore and multi-pore configurations. These membranes were investigated for osmotic energy conversion.

We used experiments combined with numerical modelling to investigate the effects of salinity gradient, pH, electrolyte type, pore geometry, and pore density on diffusion potential, osmotic current, resistance, and power output. The results demonstrate that membrane performance is determined by the balance among ion selectivity, ionic conductance, and concentration polarisation, which varies with membrane structure and solution conditions. Representative results further show that changes in half-cone angle and areal pore density affect membrane output. Measurements at different pH values reveal pronounced differences in power density, with the highest performance observed at pH 11. These results highlight the important role of solution-dependent surface charge in osmotic energy conversion.

Keywords

Ion track etching, Conical SiO2 nanopores, Osmotic energy conversion, ion selectivity





O14 - Electrodeposition-Based Fabrication of Hierarchical Nanoporous Au Nanowire Networks with Tunable Electrochemical Functionality

Mohan Li[1, 2], Michelle Schäffer[1, 2], Ina Schubert[1], Harol Moreno Fernández[3], Gideon Henkelmann[4], Christina Trautmann[1], Maria Eugenia Toimil Molares[1, 2]

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Nanostructured materials with hierarchical architectures are of increasing interest due to their tunable surface properties and enhanced functional performance in catalysis, sensing, and energy applications. In this work, we present a versatile approach for the fabrication of three-dimensional (3D) nanoporous Au nanowire networks with controlled composition, morphology, and surface characteristics.

The nanowire networks are synthesized by combining ion-track nanotechnology with electrochemical deposition, using the ion-track etched polycarbonate membranes, to produce self-supported $Au_{1-x}Ag_x$ alloy nanostructures with tailored dimensions and interconnectivity. [1,2] Subsequent selective dealloying of Ag enables the formation of nanoporous nanowires with tunable pore sizes, resulting in a hierarchical structure with dual-scale roughness. This structural evolution leads to a substantial increase in specific surface area and surface roughness, up to ~400 times higher than planar electrodes.

We systematically investigate how alloy composition and structural parameters influence the dealloying process, pore formation, and resulting nanostructure morphology. The correlation between structural hierarchy and electrochemical performance is evaluated using methanol oxidation as a model reaction, demonstrating enhanced catalytic activity of nanoporous networks compared to solid counterparts.

This study highlights the potential of combining template-assisted synthesis and controlled dealloying to engineer functional nanostructures with precisely tunable interfaces and properties, providing a platform for advanced applications in electrocatalysis and energy conversion.

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Keywords

Nanostructure, Ion-track nanotechnology, catalysis

O15 - Ion Track-Etched Silicon Dioxide Nanopores: A Swift Heavy Ion Route to Single-Molecule Biosensing

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Swift heavy ion irradiation of dielectric thin films, followed by selective chemical etching of the ion tracks, offers a uniquely controllable route to fabricating free-standing nanopore membranes with precise control over nanopore geometry, and areal density. In polymeric substrates such as PC and PET, the technique is mature and underpins both commercial track-etched filters and a substantial body of work on pH- and light-responsive ionic transport, biomimetic ion channels, and chemical and biological sensing. By contrast, ion track-etched silicon-based membranes, such as silicon dioxide (SiO_2), remain comparatively unexplored, despite SiO_2 offering mechanical robustness, chemical inertness, well-defined silanol surface chemistry, low electrical noise at high bandwidth, and direct compatibility with standard semiconductor processing.

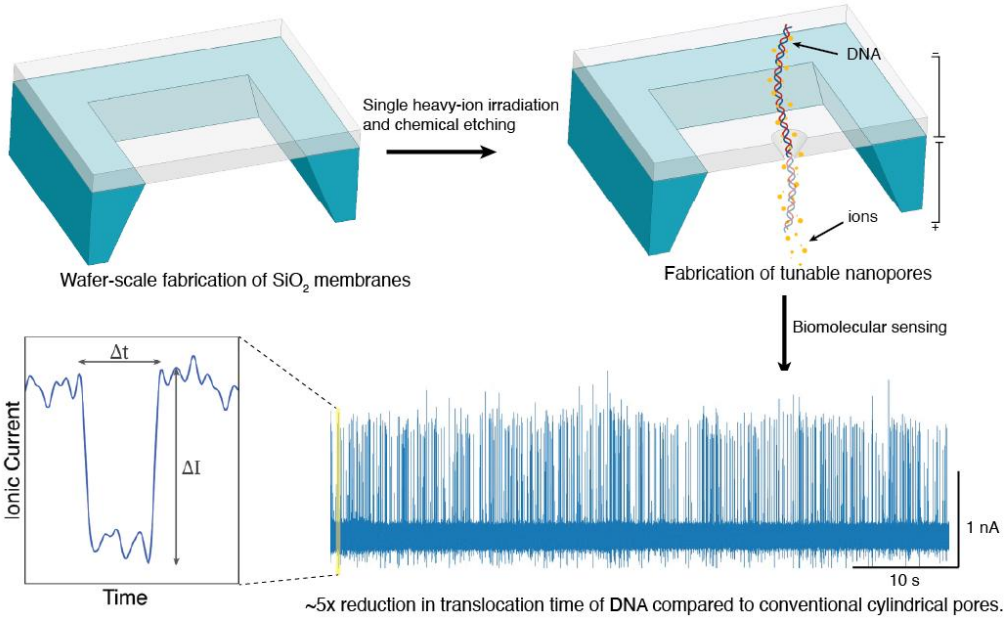
In this work, we report a fabrication framework that combines standard MEMS processing with swift heavy ion irradiation and subsequent selective wet/vapor etching to produce free-standing SiO_2 nanopore membranes with reproducible, geometrically tunable architectures. By systematically varying etching conditions, we can fabricate conical, funnel or hourglass-shaped pores with cone opening angles spanning approximately 5° to 110°. The three dimensional geometry of the nanopores was analysed through synchrotron-based small angle X-ray scattering.

Single-molecule measurements were performed by mounting these membranes with a single nanopore between two electrolyte reservoirs and applying a transmembrane voltage, establishing a steady ionic current through the nanopore (see figure). Individual biomolecules driven electrophoretically into the channel transiently occlude the ion flow and produce characteristic current blockades whose amplitude, duration, and shape encode bio-molecular size, charge, and conformation. Recordings were carried out at bandwidths up to 10 MHz, allowing us to resolve sub-microsecond translocation events. The geometrically tuneable SiO_2 pores slowed biomolecule translocation by approximately fivefold relative to cylindrical pores of comparable constriction diameter, substantially extending the temporal window available for signal extraction while sustaining high event rates per channel. By combining these measurements with a custom machine learning framework that classifies individual translocation events directly from the raw ionic current trace, we have developed a unique nanopore-based sensing platform that enables reliable and highly sensitive detection and identification of different biomolecules in complex solutions. The platform discriminates proteins of similar molecular weight with sensitivity and specificity exceeding 90%.

Together, these results constitute the first demonstration of single-molecule resistive-pulse sensing through ion track-etched SiO_2 nanopore membranes and position the platform as a versatile experimental system for label-free DNA and protein sensing and identification for emerging clinical diagnostics.

Keywords

solid state nanopores, ion-track etching, biosensing, tuneable nanopores



~5x reduction in translocation time of DNA compared to conventional cylindrical pores.

Session 6

I6 - Irradiation-induced phase transformations in Ga_2O_3 polymorphs

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Ga_2O_3 is an ultra-wide bandgap semiconductor, which can be crystalized in several different polymorphs having different physical properties [1]. In general, phase interconversion is a function of temperature and pressure; however, irradiation-induced disorder can trigger polymorph transformation in Ga_2O_3. Thus, in the present talk, recent results on radiation-induced effects in a thermodynamically stable monoclinic (beta) [2] as well as in metastable rhombohedral (alpha) [3] and orthorhombic (kappa) Ga_2O_3 phases will be summarized for a range where nuclear stopping dominates the disorder formation. Specifically, irradiation response of Ga_2O_3 depends on the polymorph and includes such stages as disorder accumulation, phase transformation to defective spinel structure (gamma) and surface amorphization. The competition between these stages is governed by irradiation temperature and density of collision cascades. As a result, controllable formation of polymorphic double or multilayer structures having sharp interfaces was demonstrated. The obtained results pave the way for better understanding of polymorphism in Ga_2O_3 and open possibility to fabricate polymorphic heterostructures which are not achievable through conventional growth techniques.

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Keywords

Ga2O3, polymorphism, phase transformations

O16 - Polymorphism-Driven Thermal Conductivity Degradation in Swift Heavy Ion Irradiated β-Ga_2O_3

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Swift heavy ion (SHI) irradiation provides a unique route to induce non-equilibrium structural transformations in non-metallic materials through intense electronic energy deposition and transient thermal spike processes. In monoclinic β-Ga_2O_3, an ultrawide-bandgap semiconductor widely considered for high-power and radiation-hardened electronics, SHI irradiation leads to a complex interplay between defect accumulation, ion-track formation and

polymorphic transformation [1]. Despite its unique electronic properties, β-Ga_2O_3 suffers from inherently low and anisotropic thermal conductivity, which represents a critical limitation for device performance. In radiation environments, where energetic particles deposit large amounts of energy locally, efficient heat dissipation becomes essential, making the understanding of irradiation-induced thermal transport degradation particularly important.

In this work, we investigate the evolution of thermal conductivity in (010) oriented β-Ga_2O_3 irradiated with 147 MeV Kr^+ ions over a wide fluence range from 1×10^{10} to 1×10^{14} ion/cm^2. X-ray diffraction reveals a multi-stage structural change, including compressive strain accumulation at low fluence, with phase transformation in the overlap regime and partial amorphization at high fluence. High-resolution transmission electron microscopy shows direct evidence of γ-phase tracks formation with typical diameter of 4-6 nm in a β-phase matrix. The structural changes are directly correlated with thermal transport measurements performed using continuum wave laser-based frequency-domain thermoreflectance measurements at kHz modulation rates, which show a monotonic reduction of heat conductivity from 21 W m^{-1} K^{-1} in the pristine crystal to ~1.2 W m^{-1} K^{-1} at the highest ion fluence.

These results demonstrate that irradiation-induced structural evolution critically governs heat transport in β-Ga_2O_3 and highlight the importance of understanding thermal transport degradation for the reliable operation of Ga_2O_3-based devices in extreme radiation environments.

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Keywords

Thermal transport, Ga2O3, swift heavy ions, ion tracks, phase transition

O17 - Amorphization versus defective spinel phase evolution in gallium oxide subjected to different ion beam irradiation conditions

Flyura Djurabekova[1], Tomas Fernandez Bouvier[1], Ru He[1], Junlei Zhao[2]

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High-dose ion irradiation introduces defects that progressively disorder semiconductor materials. While such disorder often drives amorphization, materials whose polymorphs include a defective spinel structure can instead undergo disorder-induced phase transitions that preserve long-range crystallinity. Under the highly non-equilibrium conditions of collision cascades, these transitions are governed largely by kinetic constraints rather than thermodynamic stability.

Although gallium oxide has been shown to exhibit universal radiation tolerance, in this work we examine the mechanisms which may explain why this material undergoes transition to an amorphous state under specific irradiation condition, instead of transition to the defective spinel known as a gamma phase. We identify a clear critical disorder threshold that triggers an irreversible transformation from the beta phase to the gamma defective spinel polymorph. We also show that this transition raises the system's energy to that characteristic of

gamma-Ga_2O_3, the highest-energy crystalline polymorph, which is, however, well below the amorphous state.

We further simulate focused ion beam conditions, where the confined beam spot contrasts with broad-beam irradiation, and demonstrate that ion mass strongly influences whether the material amorphizes or forms the defective spinel. We address whether the resulting structure is truly amorphous and whether any amorphous fraction is stable or will ultimately recrystallize into the defective spinel. These findings open a broader discussion on strategies for engineering this technologically promising material for advanced microelectronic applications. Finally, by extending the analysis to bulk irradiation, we challenge the prevailing assumption that Ga_2O_3 becomes nearly fully amorphous before recrystallizing at irradiation doses reaching hundreds of displacements per atom.

Keywords

gallium oxide; radiation-tolerant materials; molecular dynamics simulations

Session 7

I7 - In-situ investigation of ion beam induced dissolution, displacement and deformation of particles using *i*^{4}-FESEM facility

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In-situ investigation of ion beam induced dissolution, displacement and deformation of particles using *i*^{4}-FESEM facility

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We have recently established a new in-situ ion irradiation and imaging with field emission scanning electron microscope (*i*^{4}-FESEM) facility at our institute[1], This facility is established by integrating a high resolution FESEM (Model: Carl Zeiss CrossBeam 340) with the 10° beamline of 1.7 MV tandetron accelerator. Using the facility investigations were carried out (1) displacement of Au nanoparticles on Si substrate, (2) dissolution of carbide precipitates in P91 steel and (3) deformation of Sb nanocrystals on Al_2O_3 substrate.

In the case of displacement, 2MeV Si^+ ion irradiation on Au nanoparticles decorated FIB patterns reveals that the AuNPs are progressively displaced from the original sites as the ion fluence increases and the displacement of the Au nanoparticles are in the direction of ion beam. The observed displacement of AuNPs is attributed to the inhomogeneous in-plane stress generated by thermal spike temperature in the native SiO_2 layer during ion irradiation and the estimated stress is qualitatively in agreement with Raman measurements[2]. In the case of deformation, antimony (Sb) thin films were grown on sapphire (c-Al_2O_3) by using MBE at room temperature (RT) and at 245 °C (HT), resulting in distinctly different morphologies, well-faceted, discrete square-pyramidal and triangular Sb nanocrystals and nearly continuous film with a worm-like morphology respectively and investigated under *i*^{4}-FESEM facility using 2 MeV Al^+ ion irradiation. For the Sb films deposited at HT, at low ion fluences, irradiation induces disorder within the nanocrystals, effectively lower the melting point of antimony. At high ion fluences, evaporation of Sb occurs, leading to significant shape modifications in the nanocrystals. In contrast, Sb films deposited at RT exhibit a transition from a disordered structure to an ordered crystalline phase. Ion irradiation also drives dewetting of thin film at room temperature itself. This is driven by an in-plane compressive stress of ~0.34 GPa, which is generated during the thermal spike regime. In the case of dissolution of precipitates dissolution of precipitates in P91 steel under 3 MeV Fe+ heavy ion irradiation is investigated using *i*^{4}-FESEM. Nelson, Hudson and Mazey(NHM) model explains the competition between recoil dissolution and temperature dependent diffusion where, the diffusion process enhances the growth of precipitate while recoil mixing increases the dissolution of precipitates. In the

present experiments, the irradiation was carried out at room temperature, the thermal diffusion is significantly low. Hence the dissolution of precipitates and recoil mixed shell structures in the precipitates are observed. These irradiation effects will be discussed in the light of basic ion-solid interaction in materials

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Keywords

i4-FESEM , in-situ, ion irradiation, dissolution

O18 - How boronization alters tungsten erosion: Insights from ion-beam studies of W-B mixed layers

Raphael Gurschl[1], Martina Fellinger[1], Benjamin Burazor Domazet[1], Eduardo Pitthan Filho[2], Daniel Gautam[2], Daniel Primetzhofer[2], Friedrich Aumayr[1]

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Tungsten is the prime candidate for plasma-facing components in ITER and future fusion reactors, yet erosion of tungsten surfaces remains a critical source of high-Z impurities in fusion plasmas. In present-day devices, boronization is widely used as a wall conditioning technique that deposits boron onto plasma-facing surfaces and thereby modifies their erosion behavior.

Here we investigate the sputtering response of tungsten-boron (W-B) mixed layers under fusion-relevant ion bombardment. Thin films with systematically varied W:B composition, from pure tungsten to pure boron, were irradiated with 2 keV Ar^+ and 2 keV D_2^+ ions, representing typical impurity and fuel species in magnetically confined fusion plasmas. Elemental compositions were determined by time-of-flight elastic recoil detection analysis (ToF-ERDA) and high-resolution Rutherford backscattering spectrometry (HR-RBS), while total sputter yields were measured in situ using a highly sensitive quartz crystal microbalance.

A clear and systematic trend emerges: the total eroded mass decreases strongly with increasing boron concentration, particularly for Ar^+ irradiation. Boron enrichment significantly suppresses tungsten sputtering while shifting the composition of the eroded flux toward low-Z species.

These results demonstrate that boronization can substantially mitigate tungsten erosion and thus reduce high-Z impurity sources in fusion plasmas, providing important quantitative input

for plasma-wall interaction modelling and impurity control strategies in ITER-relevant operating regimes.

Keywords

plasma-wall-interaction, nuclear fusion, sputtering, tungsten, boron

O19 - Study of the WTaVCr high entropy alloy for fusion application by irradiation with Cu and He ions in DiFU

Andreja Gajović[1], Kristina Tomić Luketić[1], Toni Dunatov[1], Mario Matić[1], Sandra Drev[2], Vedran Kojić[1], Krunoslav Juraić[1], Jasminka Popović[1], Željko Skoko[3], Miran Čeh[2], Tonči Tadić[1]

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Development of fusion-based power plants (FPPs) is of paramount importance for the European Green Deal initiative of lowering carbon emissions, since FPPs do not generate CO_2 or other substance harmful to the atmosphere. In the context of achieving FPP reliability, one of the important points is the effect of high energy fusion neutrons (MeV range) on the component materials of the fusion reactor. Therefore, the engineering and design of materials for fusion reactors are of key importance [1]. The two processes that are the most relevant when testing a material for fusion environments are its response to (1) displacement damage and (2) transmutation reactions [2]. These processes can be mirrored by ion beam irradiation since effects can be introduced into the material much more simply and quickly than by neutrons generated in fission reactors due to low or no radioactivity and the larger cross-sections of ion beams. Displacement damage can be emulated by heavy ion irradiation, while nuclear transmutation reactions can be mimicked by helium implantation. This is most impactful when these two types of ion irradiation are applied simultaneously, e.g. in the dual-beam irradiation setup, like the Dual-Beam Ion Irradiation Facility for Fusion Materials (DiFU) at Ruđer Bošković Institute [3], which is one of only a dozen worldwide [4].

For fusion applications, the tungsten and tungsten-based alloys, especially refractory high entropy alloys (RHEA), are known as high heat flux (about 10 MW/m^2) materials for plasma facing components e.g. first wall and diverter [5]. Quaternary W-based alloy WTaVCr is expected to be highly resistant upon irradiation [6]. In this study WTaVCr thin films were prepared and its structural properties as well as chemical composition were evaluated before and after irradiation in DiFU.

We deposited 1 mm thick films of WTaVCr on silicon substrate by magnetron sputtering. WTaVCr films were irradiated in DiFU with 8 MeV Cu^{3+} and 200 keV He^+ to Cu^{3+} dose of 1 dpa and 6 dpa. Then they were characterized by XRD, SEM, EDS and (S)TEM before and after irradiation.

As-deposited WTaVCr film dominantly contained body-centered cubic (*bcc*) structure with a unit-cell parameter *a*=3.191(2) Å (Figure 1a). Additionally, a second, minority *bcc* phase with unit-cell parameter *a*=3.126(3) Å was also observed. While the appearance of the second phase indicates a possible phase segregation of lighter element (V or Cr), this assumption has been disproved by EDS measurements in SEM as well as atomic resolution HAADF-STEM imaging in combination with EDS mapping. These results show that all the elements (W, Ta, V and Cr) were homogenously distributed in all the crystal grains as well as at all the atomic positions in *bcc* lattice. These results led to the conclusion that both *bcc* phases are actually the high entropy alloys lattices containing all four metals.

After irradiation in DiFU, high entropy alloy with a unit-cell parameter *a*=3.126 Å becomes dominant crystalline phase, although the presence of HEA structure with *a*=3.191 Å can still be observed. Irradiated sample investigated by atomic resolution STEM imaging in combination with EDS mapping confirmed that all the elements are homogenously distributed in crystal sites (Fig. 2), while the measured atomic ratio of elements observed in crystal lattice of as-deposited sample in comparison to their ratio after irradiation was similar, within statistical deviation. From the atomic ratio of elements, the thermodynamic parameters were calculated by phenomenological approach [7] and the results indicate stable single-phase system, while electronic composition of the valence electrons (VEC) predicts the appearance of a single *bcc* phase.

During Rietveld refinements of XRD patterns, the line broadening analysis has also been conducted. It was found that line profiles of HEA structure with larger unit-cell (present in as-deposited sample) are broader compared to those of HEA structure with smaller unit-cell obtained after the irradiation. Such broadening is caused by the presence of significant distortions within the crystal lattice of as-prepared sample due to the different atomic radii occupying the same crystallographic position yielding the micro-strain value ε that is significantly larger compared to the micro-strain present in the irradiated HEA having smaller unit-cell. Observed decrease in micro-strain indicates that the irradiation causes the significant reduction in number of distortions and the relaxation of deformations originally present within the as-prepared crystal lattice finally also leading to the observed decrease of unit-cell parameters. These results put the studied multicomponent alloy in the forefront as highly resistant to intense irradiation.

Acknowledgment

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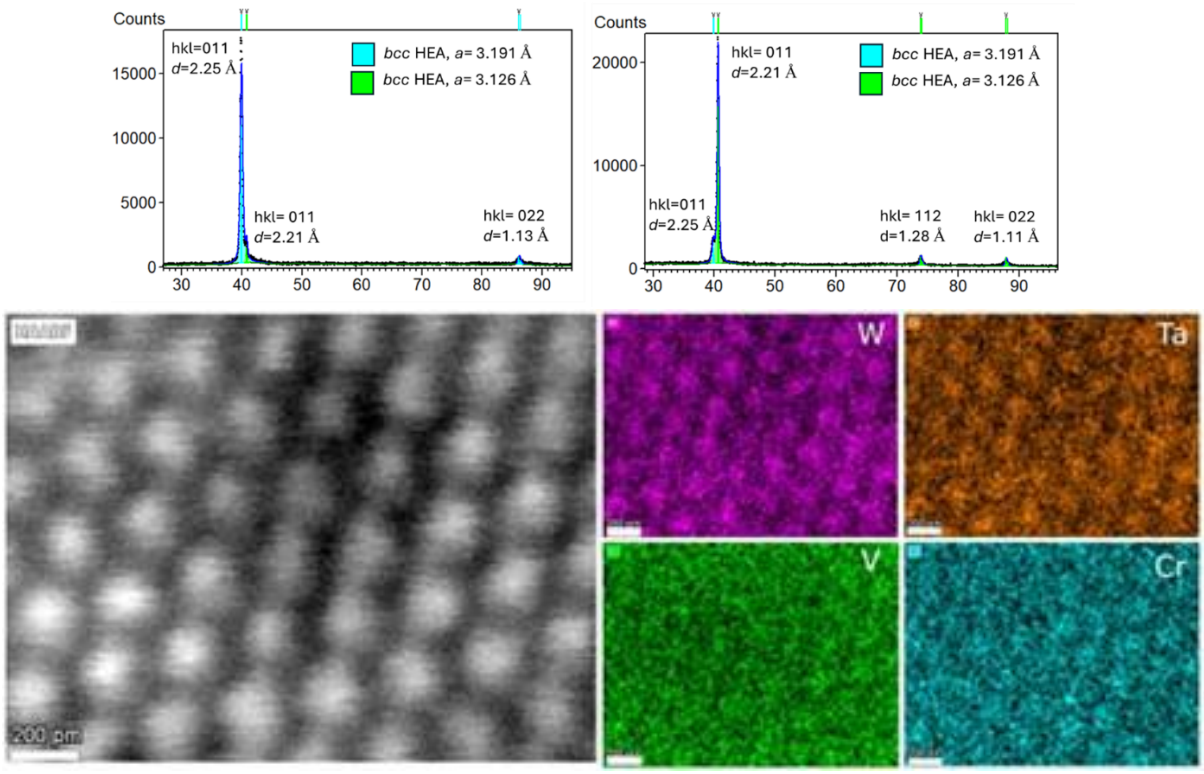
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Keywords

material for fusion application, DiFU, HEA, XRD, STEM



O20 - Production of negative ions at surfaces exposed to a low-pressure deuterium plasma: comparison between boron- and phosphorus-doped diamond, graphite and gadolinium

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Negative ion beams are of significant interest for materials processing and high-energy (>1MeV) neutral beam injection systems for magnetic confinement fusion reactors [1]. Most of negative-ion sources relies on the negative-ion surface generation mechanism in plasmas. Dielectric materials, including doped diamond, are attractive candidates for increasing surface generation as a potential alternative to low work function metals [2] in the context of H^-/D^- production for fusion applications. To this end, it is necessary to better understand the underlying mechanisms of surface charge exchange in a hydrogen (or deuterium) plasma environment. In this study, we have developed an in-situ photoemission yield spectroscopy (PYS) diagnostic coupled with the Fowler model to determine material work-function or material ionization energy. Mass spectrometry is used to measure the negative ion surface production yield. Ionization threshold/work-function (WF) of HOPG, gadolinium, microcrystalline diamond (µc-D), boron-doped microcrystalline diamond (µc-BDD) and phosphorus-doped single-crystal diamond (PDD) are monitored upon plasma exposure at

sample temperature ranging from 30°C to 700° C, and are compared to the evolution of negative-ion yield.

We observe strong correlation between the electronic properties of graphite and gadolinium and their surface electronic properties (WF).

In comparison we observe that exposure of the PDD to deuterium plasma at 400 C reduces its ionization threshold from around 4.0 eV to 2.1 eV. Although the ionization threshold of diamond is sensitive to sample temperature and the dopant used, this appears to have a negligible effect on negative ion production.

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Keywords

plasma-surface interactions, ions-surface interactions, negative ions production at surfaces, electronic properties of surfaces, photoemission yield spectroscopy, work function

Session 8

I8 - Heating mechanisms in SHI tracks: nonthermal effects

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For a few decades, the mechanisms of swift-heavy ion (SHI) track formation in solids were puzzling the scientific community. On the one hand, it was known that the SHI-excited electrons transport away from the ion trajectory within the characteristic time of ~100 fs. Thus, energy transfer from the excited electronic system to the atomic one, leading to the creation of observable nanometric tracks, must take place within this time. On the other hand, the electron-phonon coupling is a slow mechanism, requiring picoseconds to transfer energy from electrons to atoms (phonons) of the target.

In this talk, I will report on our decades long journey to uncover the main mechanisms of energy exchange between the electronic and atomic systems in an SHI track, resolving this apparent contradiction. Systematic studies revealed that the track formation takes place via few main channels: ballistic scattering of fast electrons on atoms (nonequilibrium effect beyond the phononic approximation); coupling of valence-band holes to the atomic system; and - most importantly - nonthermal effects that originate from the ultrafast modification of the interatomic potential energy surface upon intense electronic excitation.

Recognizing that electronic excitation directly alters the potential energy landscape of the solid, causing atoms to accelerate and gain kinetic energy on ultrashort timescales without requiring phonon-mediated energy transfer, allows to transfer significant amount of energy to atoms within ~100 fs. Together, the thermally and nonthermally driven processes govern the structural modifications observed in SHI tracks, with nonthermal effects playing a critical and previously underappreciated role. Knowing these key effects enables us to model the SHI track formation without fitting parameters.

Keywords

Nonthermal melting; Electron-ion coupling; Valence holes coupling; Nonequilibrium processes;

O21 - First-Principles Modeling of Swift Heavy Ion Track Formation

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Energetic ion radiation, including fission fragments produced by spontaneous nuclear decay, leaves narrow damage trails in materials known as fission tracks or swift heavy ion tracks. These tracks have applications in nanotechnology, for example, in the fabrication of nanoscale filters and potentially in the creation of quantum registers from NV centers in diamond [1]. Understanding and modeling track formation is therefore relevant to both technological applications and geochronological methods, such as fission-track dating. The inelastic thermal spike model [2] has been widely used to describe the interaction of swift heavy ions with

materials, but its theoretical foundations and range of validity remain under debate [3]. Recent advances in computational methods now enable the determination of required model parameters using density functional theory in conjunction with semiclassical transport theory. This approach enables us to assess whether the thermal spike model with electron-phonon coupling can explain track formation, or whether additional mechanisms must be invoked. Potential applications of such computations range from improved thermal history reconstruction to the controlled fabrication of nanoscale structures.

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Keywords

swift heavy ions, ion tracks, first-principles modelling

O22 - Simulation of InSb Nanofoams Induced by Ion Irradiation using the Cellular Potts Model

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Semiconductor compounds formed by elements from groups III-IV of the periodic table have been studied over the last few decades. Due to their specific thermoelectric performance, they have enabled a variety of uses in new technologies such as solar cells, vapor and gas detectors, and thermoelectric generators.

Among the various III-IV semiconductors, the binary compounds GaSb and InSb, as well as the ternary (Ga-In)Sb, have shown a remarkable characteristic: they are among the few materials that, when subjected to irradiation with ion beams, undergo a continuous crystalline-porous transformation that ultimately results in a nanometric solid foam. Studies of (Ga-In)Sb thin films using electron microscopy techniques (TEM and SEM), GIXRD, XPS, and ion beam techniques (PIXE, RBS) have yielded significant results, both for formulating models for foam formation and for correlating its dependencies with energy, fluence, and ion beam intensity.

To describe the experimental results, it is necessary to formulate models in terms of fundamental physical quantities such as temperature, electronic structure, band-gap energy, crystalline structure, and energy loss mechanisms in the interaction of ions with matter, especially those occurring in layers very close to the surface of the films (a few nanometers). The use of more common models, especially Molecular Dynamics, has proven impractical due to the very high computational cost. The most recent literature shows some other alternatives, including the CompuCell3D platform.

In this work we present the results of the CompuCell3D simulation for the single crystal InSb thin films deposited by molecular beam epitaxy subsequently irradiated with 17 MeV Au^{+7} at $1x10^{14}$ ions/cm². Our simulation has proved capable of reproducing the formation of the porous structure from the clustering of small pores during irradiation, as well as estimating other parameters for these experimental conditions.

Keywords

antimonide nanofoams, ion irradiation, cellular Potts model simulation

O23 - Non-radial Recovery Kinetics in Swift Heavy Ion Tracks in Monoclinic Zirconia

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Zirconium dioxide (ZrO_2) has emerged as one of the most promising ceramic materials for nuclear applications due to its exceptional radiation resistance, low neutron absorption cross-section, and high solubility for actinides. These properties make it a strong candidate for inert matrix fuel hosts, as well as a potential material for the long-term immobilization and storage of actinide waste generated in nuclear reactors.

In this work, the structural response of natural monoclinic zirconium dioxide (ZrO_2) to swift heavy ion (SHI) irradiation is investigated using a combination of numerical modeling and experimental techniques. The modeling approach includes the Monte Carlo TREKIS model [1] and molecular dynamics simulations [2-3], complemented by transmission electron microscopy (TEM). The mechanisms and kinetics of single-track formation in monoclinic zirconia irradiated with 160 MeV Xe ions are analyzed. Both computational and experimental results demonstrate that SHI irradiation induces a crystalline-to-crystalline phase transformation. Plan-view TEM images reveal the formation of rectangular ion tracks, while cross-sectional observations show segmented regions containing the new phase.

Atomistic simulations further uncover unusual recovery processes following SHI impact, involving significant disordering and subsequent transition to a new crystalline state. The reverse phase transformation is found to occur predominantly in a layer-by-layer manner along the c-axis of the monoclinic structure, resulting in segmented rectangular tracks. This behavior contrasts with the recrystallization of amorphous (molten) regions in other dielectric materials, such as MgO or Al_2O_3, where recovery typically proceeds in a radial direction.

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Keywords

swift heavy ions, zirconia, molecular dynamics

Session 9

I9 - Size-dependent swift heavy ion irradiation effects in nanostructures

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In nanostructures, size effects can modify energy dissipation, thermal transport and recrystallization temperatures, influencing both intrinsic material properties and overall device performances. For reliable operation of nanomaterial-based devices in high-radiation environments, systematic investigations are essential to unravel swift heavy ion-matter interactions in confined geometries.

In this presentation, we will give an overview of our current activities on swift heavy ion irradiation effects in nanomaterials, including Bi nanowires and films as well as TiO_2 nanotubes. Tailored nanostructures are synthesized in ion-track-etched polymer templates: electrodeposition is used to produce nanowires with controlled diameters, while atomic layer deposition enables nanotubes with well-defined wall thicknesses. These nanostructures are exposed to 1-2 GeV heavy ions at the GSI UNILAC linear accelerator, under well-defined beam parameters (initial ion charge state and fluence). High-resolution scanning and transmission electron microscopy reveal, size-dependent morphological changes, demonstrating how nanoscale dimensions affect the response to irradiation. Molecular dynamics simulations based on a thermal spike approach model support our experimental results.

Keywords

nanostructures, size-effects, TEM, molecular dynamics simulation

O24 - Combined S/TEM-MD study on the nanostructure of ion tracks in $MgAl_2O_4$ spinel

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$MgAl_2O_4$ exhibits improved resistance to neutron exposure as compared to Al_2O_3 [1]. However, spinel is sensitive to defect formation through dense electronic excitation with a relatively low threshold energy deposition for ion track formation of about 7.5 keV/nm [2,3]. [4-7] reported on $MgAl_2O_4$ irradiated with 200 MeV Xe and 350 MeV Au. Track morphology was studied in detail using transmission electron microscopy (TEM) and high angular resolution electron channeling X-ray spectroscopy (HARECXS). It was suggested that a phase transformation into a defective rock-salt structure occurs within the track core where Al and Mg ions form

antisite defects and strained regions were detected around the defective structure. No amorphization was reported inside the track core even for electronic stopping powers up to 35 keV/nm deposited by 350 MeV Au ions [4]. Detailed analysis of defect accumulation in $MgAl_2O_4$ irradiated with 152 MeV Xe and 2.24 GeV Au ions using absorption spectroscopy and EPR was published by [8]. Defect concentration was shown to increase with fluence up to 2×10^{12} cm^{-2} with no detectable saturation. The authors interpreted their results based on the creation of complexes of defects, including antisite defects and Al^{3+}, Mg^{2+} vacancies. Such point defects are generally invisible to TEM through direct imaging. On the other hand, molecular dynamics simulation of the relaxation of a system after ion passage offers detailed insight into the production and distribution of single atomic defects provided that a suitable potential is employed. In this work we perform a combined S/TEM-MD study of the nanostructure of SHI induced tracks in $MgAl_2O_4$ by comparing experimental S/TEM images to MD supercells along varying crystallographic directions as well as comparing experimental and simulated diffraction effects. Such a combined approach is further necessitated by the instability of track defect structures under extreme electron doses required to produce high resolution images.

Single crystal stoichiometric $MgAl_2O_4$ with thickness of 500 µm was purchased from Crystal GmbH. The specimens were irradiated with 670 MeV Bi ions to fluences ranging from 1×10^{11} cm^{-2} to 6×10^{12} cm^{-2} at room temperature at the U-400 FLNR JINR cyclotron, Dubna. Plan view TEM lamellae were produced by FIB lift out technique using an FEI Helios NanoLab 650 dual beam. TEM imaging was performed at 200 kV accelerating voltage in a Cs corrected JEOL ARM200F. Simulated STEM images were computed from MD supercells using the abTEM python package [9]

Figure 1 shows a bright field TEM image of the irradiated spinel in plan view. Ion tracks are clearly visible, and a separate track core and halo can be distinguished. Contrast reversal of the track halo in regions with varying local orientation (due to sample bending) shows that the halo is crystalline. Figure 2 shows an experimental HAADF image (b) and simulated (a) image from a 14x14x20 nm MD supercell at the same scale for comparison. The track has a diameter of about 6.5 nm in both cases and shows a different ordering than the surrounding matrix.

Contrast in TEM is a complex function of specimen and beam interactions, even for HAADF STEM, and single point defects are typically not resolvable in bulk specimens. MD offers an opportunity to study such defects in detail provided the employed potential accurately describes the relaxation dynamics after excitation by a fast ion. Combining these two techniques grants the atomic scale defect sensitivity of MD while simultaneously providing verification of the simulation's ability to reproduce experimentally observable features.

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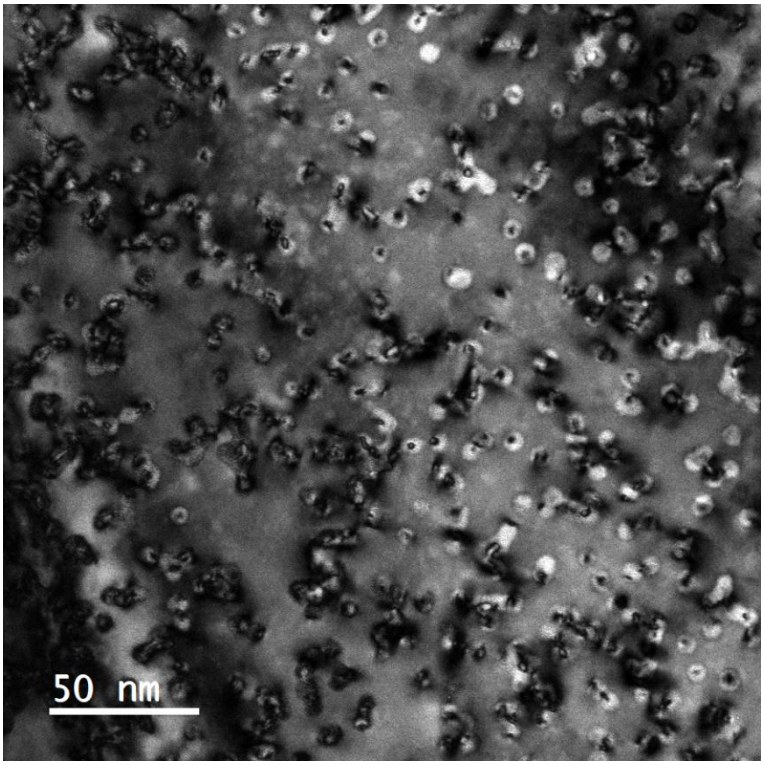
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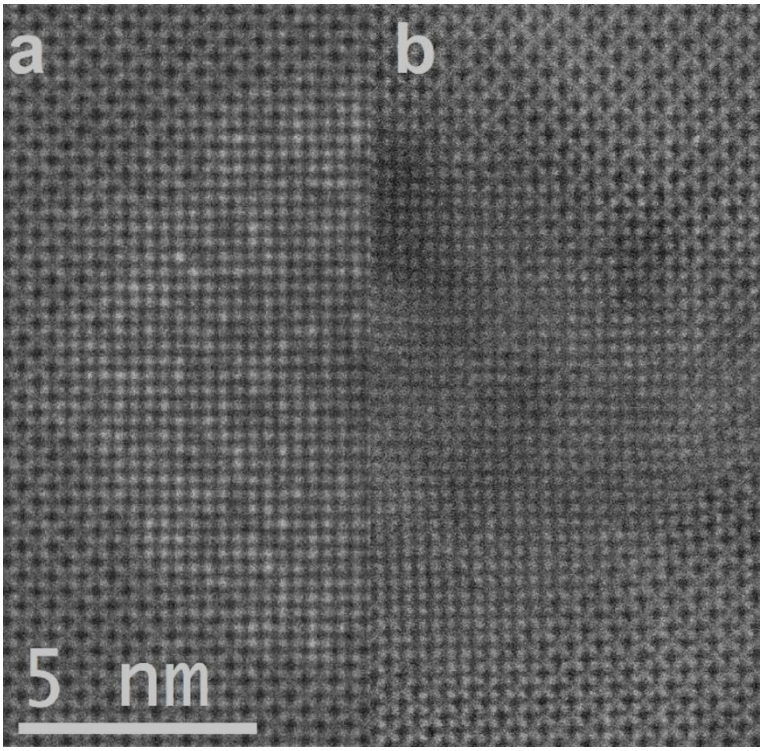
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Keywords

SHI, spinel, TEM, molecular dynamics, image simulation.





O25 - Fluence dependent ion-track formation and transition to self-organized nanodots in Si under 9 MeV C60 ion irradiation

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However high the energies are, any *monatomic* ions have *not* formed ion tracks in crystalline Si (c-Si). Contrary, C_{60} ions of tens MeV formed the tracks in c-Si [1]. Furthermore, recent studies have clarified that the track formation in c-Si is induced at much lower C_{60} energies, below 1 MeV [2], and ultimately to 60 keV [3]. In the case of 60 keV C_{60} irradiation, the track length and diameter are reduced to ~10 nm and ~3 nm, respectively, indicating a quite low aspect ratio of tracks [3].

In the previous studies, we have investigated properties of non-overlapping ion tracks at low fluences. Here we report the interactions between tracks in Si by changing the fluence of C_{60} ions but maintaining the energy to 9 MeV. Regarding the track-overlapping, the Gibbons model [4] is known, in which the ultimate damaged state is assumed within the cylindrical track bodies by a single hit of swift heavy ion. The areal ratio of the track-coverage R at the sample surface is described in the model as,

$$R = 1 - \exp(-sF), \qquad (1)$$

where *s* and *F* denote the track cross-section and the ion fluence, respectively. On the contrary, it is proposed that overlapping of core/shell tracks in amorphous SiO_2 induces partial recovery of the tracks [5]. Therefore, a steady state is attained during the irradiations, in which the material's surface is not fully covered by tracks due to the partial recovery even at infinitely high fluences.

In the case of c-Si irradiated with 9 MeV C_{60} ions, an inter-track interaction was observed at the fluence of 1 x 10^{12} C_{60}/cm^2 where the track diameters became slightly smaller than those of the isolated tracks, indicating the deviation from the eq. (1). With increasing the fluence to 7 x 10^{12} C_{60}/cm^2, a sudden increase of damage due to amorphization was induced, which was confirmed by the electron diffraction. After then, a lot of self-organized nano-dots appeared on the sample surface, which are ascribed to similar phenomena to the nano-ripple formation observed on the surface of compound semiconductors irradiated with high fluence keV ions [6].

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Keywords

ion track; self-organized nano-dot; C60 ion; inter-track interaction; silicon

Session 10

I10 - Advances in Neutron Scattering Characterization of Swift Heavy Ion Irradiated Nuclear Ceramics

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Neutron total scattering with pair distribution function (PDF) analysis provides unique insight into swift heavy ion radiation effects in ceramic materials used in advanced fission and fusion reactors[1]. Unlike conventional diffraction, total scattering reveals both long- and short-range order. This enables detailed investigation of disordered and amorphous materials for which average structural information alone is insufficient. Neutron scattering is particularly useful for probing low-Z materials like oxygen (in contrast with X-rays and electrons[2]), which is often critical to understanding local disorder. Recent results demonstrate that swift heavy ion radiation-induced disorder is more complex than previously recognized. Disordered pyrochlore and spinel retain local structural motifs differing from the long-range average[3]. Similarly, radiation-induced metastable tetragonal zirconia contains nanoscale orthorhombic domains that average to the high-temperature phase[4]. These results highlight why short- and medium-range structural analysis is essential for understanding radiation damage mechanisms. This technique, however, requires large sample masses (~100 mg), which limits studies to swift heavy ions at higher energies with large penetration depths to produce enough homogenously irradiated powder without implantation (>8 MeV/u). Current efforts focus on using the highly collimated neutron beam at the Spallation Neutrons at Pressure (SNAP) instrument to enable similar total scattering analysis on smaller sample quantities, potentially enabling characterization of radiation effects induced by ions with much lower energies.

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Keywords

Neutron Total Scattering Atomic Ordering

O26 - Tailoring Optical Properties of GaP Single Crystals by Irradiation with Energetic Heavy Ions

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Precise control of the optical properties of solids is essential for the development of advanced photonic devices. Here, we focus on Gallium Phosphide (GaP) as a promising wide-bandgap semiconductor. The crystals were irradiated with heavy ions of energies between 1 MeV and 1 GeV applying a wide range of ion fluences [1-3]. By carefully adjusting the beam parameters, we successfully fine-tuned the bandgap of GaP. Correlated structural modifications were studied by means of TEM and Rutherford backscattering spectrometry under channeling conditions. The resulting modifications of both the optical properties and the crystalline structure of GaP are discussed in terms of nuclear and electronic energy loss mechanisms [4].

Acknowledgements:

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Keywords

heavy ions, GaP, optical bandgap

O27 - Investigating Nanomaterials Under High-Pressure and Swift Heavy Ion Irradiation

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The simultaneous exposure of materials to high pressure and swift heavy ion irradiation represents a unique experimental approach, pioneered at the GSI Helmholtz Center Darmstadt [1-3]. When exposed to extreme conditions nanomaterials often display size-dependent stability fields that may significantly deviate from their bulk counterparts [4].

In this contribution, we present how nanowires compressed in diamond anvil cells respond to pressure, both with and without being irradiated with U ions of GeV energy. As samples, $Bi_{1-x}Sb_x$ nanowire networks (NWNWs) with different wire diameters and compositions as well as microcrystals were fabricated by ion-track nanotechnology and electrodeposition. Within pressures up to 25 GPa, the wires display size- and composition-dependent phase transition pressures [5]. In-situ Raman spectroscopy and synchrotron XRD revealed shifts in transition pressures and stabilization of high-pressure phases induced by ion irradiation.

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Keywords

Ion-Track Nanotechnology; High-Pressure; Phase Transitions; Extreme Conditions

O28 - Track morphology in quartz irradiated with swift heavy ions: Thickness and edge effects

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Crystalline SiO_2 quartz samples were irradiated with 1.64 GeV and 200 MeV Au ions and the irradiation induced nanostructures originating from ion track formation were examined using transmission electron microscopy. The analysis revealed not only homogeneous amorphous ion tracks but also tracks with a concentric core-halo structure, characterized by a low-density core along the ion path surrounded by a damaged halo region. The latter type of track was found exclusively in sample regions thinner than 50 nm, suggesting that a thin sample is the prerequisite for the formation of such low-density track cores. Additionally, pitted tracks with a crater-like structure were identified at the sample edges. These findings are discussed in terms of surface phenomena, such as electronic sputtering as well as the role of sample thickness and edge effects, emphasizing the critical influence of sample geometry on the formation of these complex nanostructures. The morphology characteristics of tracks in quartz, Si3N4 and GaN will be compared.

Keywords

Swift heavy ion irradiation, ceramics, ion tracks, nanostructures

Session 11

I11 - Atomic collisions in solids - what can we learn from exit charge states, photon emission and their correlation?

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KeV ions penetrating matter induce a series of different excitations in the material and in the projectile itself. We investigate charge state distributions and the photon emission of He, F and Ne projectiles transmitted through C, Si and SiC. Measurements were conducted utilizing pulsed ion beams at the Time-of-Flight Medium Energy Ion Scattering (ToF-MEIS) setup at Uppsala University [1], which also enables direct, time-resolved studies of processes on a timescale of about 1ns. By separating the charges of projectiles transmitted through Si with a charge state deflector [2] we show that the mean exit charges q_{mean} for Ne and F are strongly trajectory dependent. For ions channeled along the (100) crystal, q_{mean} decreases strongly with respect to the random case. For He, much smaller differences are observed. These observations can be related to the promotion of electrons by formation of molecular orbitals (MO) inside the solid. Our observations for charge state distributions qualitatively match observations in energy loss but contradict a suggested Z_{eff}^2 dependence between energy loss and charge [3]. This contradiction raises questions on the relation between the mean exit charge q_{mean} and the mean charge Z_{eff} in the solid.

This question can be addressed by investigating photon emission induced by He, Ne and F ions interacting with the aforementioned systems. We show that several 10% of transmitted projectiles are excited and that the contribution of the sample to the overall EUV photon emission is negligible if compared to the freely decaying excited projectiles [4]. Charge state resolved photon yields were extracted via photon-charge coincidence measurements [5] and were found to be largely independent of both the target material and trajectory, in contrast to what is observed for energy loss and charge state. We found a strong velocity dependence for He whereas photon yields for F and Ne remain largely constant for the investigated energies. Additionally, the photon yields increase strongly with final charge state and we find close to 100% of the F and Ne particles exiting in an excited state for charges $q \geq 2$. Our observations contradict common models of the charge formation and we propose a new model displayed in fig. 1. Within this model, the velocity and trajectory dependence of charge is mainly based on the time for deexcitation between two subsequent (largely velocity independent) excitations. The model also explains discrepancies for the observed charge state and energy loss: the charge state Z_{eff} inside the solid is smaller than the measured exit charge q_{mean} which is increased by autoionization behind the sample.

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Keywords

Atomic Collisions, Photon Emission, Medium Energy Ion Scattering, Electronic Excitations

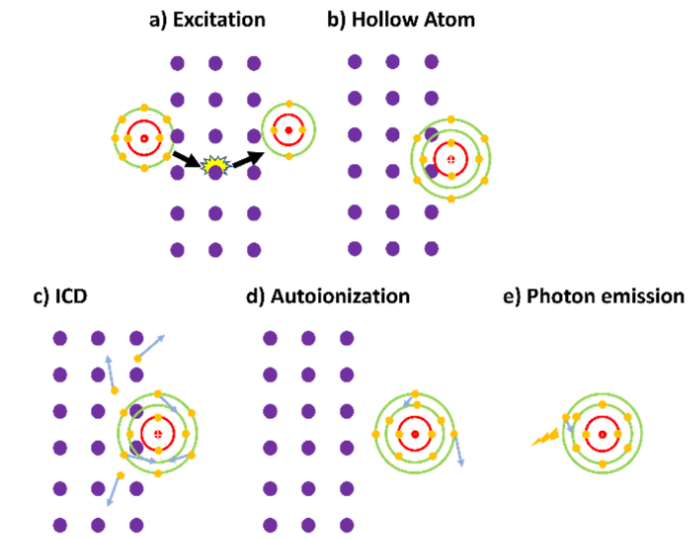


Figure 1 – New model of the charge formation. The projectile repeatedly encounters a) excitation, b) Hollow atom formation and c) Interatomic Coulombic Decay (ICD) inside the solid. Upon leaving the sample, d) autoionization and e) photon emission occur.

O29 - Stopping power measurement of liquid water for heavy ions

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This presentation reports measurements of the stopping power of liquid water using an ion-transmission method with a liquid-film target formed in vacuum. As a major component of the human body, water plays a key role in understanding ion energy loss processes and in dose evaluation for ion radiotherapy.

In this study, carbon ions with energies from 1.5 to 7.5 MeV were used. A stable liquid film with a thickness of several hundred nanometers was formed in a vacuum using a microfluidic chip, enabling direct transmission measurements. The energy loss was measured with a Si detector, while the film thickness was determined by ERDA combined with SIMNRA analysis.

The measured stopping power differs from existing calculations and is discussed in terms of effective charge and related factors.

Keywords

Stopping power, Liquid water, Heavy ions, Bragg peak

O30 - Correlated Electron Dynamics in Ne^{10+} and He Collisions

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The development of the COLTRIMS technique during the 1990s provided insights into the underlying physical mechanisms that mediate collision processes. In particular, the study of processes leading to the two-electron removal from helium (He) highlights the significant role of electron-electron interactions compared to other interactions involved. Notably, this includes advancements in both experimental and theoretical analyses of the photo-double-ionization process [1,2]. More recently, the emission of an electron to the continuum, accompanied by the simultaneous capture of another electron—known as the transfer ionization (TI) mechanism—has offered an alternative approach to examining electron-electron correlation dynamics in He [3,4]. Current analyses involve measuring and theoretically calculating total cross sections, single differential cross sections in terms of the parallel and perpendicular components of the recoil ion momentum, and the electron momentum distribution. For proton impacts, signatures attributed to the Thomas, Two-Step 2, and Shake-Off mechanisms have been identified, and their relative importance has been estimated at various impact energies.

In this work, we utilize three versions of the four-body classical trajectory Monte Carlo method (CTMC) to analyze TI processes for Ne^{10+} collisions with He: i) the nCTMC model, in which electron interactions are completely neglected, with both electrons initialized at an ionization potential of 24.6 eV; ii) the sequential-CTMC model, where electrons are again non-interacting and sorted according to the vertical ionization potentials of 24.6 eV and 54.4 eV [5]; and iii) the EB-CTMC model introduced by Cohen [6], which explicitly considers electron-electron correlation by incorporating energetic constraints into the Hamiltonian, thus preventing atomic collapse due to classical autoionization.

We will present and discuss singly differential cross sections in terms of the parallel component of the recoil momentum p_z and differential distributions for the emitted electron energy as a function of p_z for the three methods. Impact energies ranging from 100 keV/u to 500 keV/u will be considered to assess the sensitivity of the results to the collisional regime. Our current work focuses on identifying timing signatures in two-electron emissions during Ne^{10+}-He collisions. By analyzing correlated electron spectra and angular distributions, we aim to demonstrate how temporal information is encoded in measurable observables and distinguish between competing ionization and charge exchange mechanisms.

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Keywords

Transfer ionization, Monte Carlo simulation, and electron correlation

O31 - Rainbow Scattering from Graphene

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The rainbow effect is a fundamental phenomenon in any scattering theory of waves and particles, describing the accumulation of trajectories at characteristic angles due to extrema of the deflection function. In particular, the atomic rainbow effect - arising in semiclassical particle scattering due to singularities in the classical differential cross section - provides valuable information about the interaction potential between a projectile and target atoms, which is of particular interest for two-dimensional systems. However, experimental observation of the atomic rainbow effect in two-dimensional materials is highly challenging, as both an atomically clean target and a high-resolution detector are required.

Here, we present the experimental observation of rainbow scattering in ion transmission through single-layer graphene using time-of-flight medium energy ion scattering [1]. For 40 keV Xe^+ ions, the scattering pattern shown in Figure 1 exhibits two distinct components: a circular outer rainbow at 5.28°, associated with maximum binary collision deflection from individual carbon atoms, and a hexagonal inner rainbow at 0.43°, originating from projectiles with characteristic trajectories interacting with multiple carbon atoms. Molecular dynamics and binary collision simulations reproduce these regimes and clarify their physical origins, but fail to capture the measured intensity distribution at the smallest deflection angles when using averaged radially symmetric interaction potentials. These results establish graphene rainbow scattering as an experimental benchmark for ion-solid interaction potentials and reveal limitations of commonly used approximations in describing many-body scattering dynamics. The cleanliness of the graphene sample is quantified using a recently developed method based on recoil-projectile coincidence in ion scattering experiments.

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Keywords

rainbow effect, graphene, ion-solid interaction, particle scattering phenomena, interaction potentials

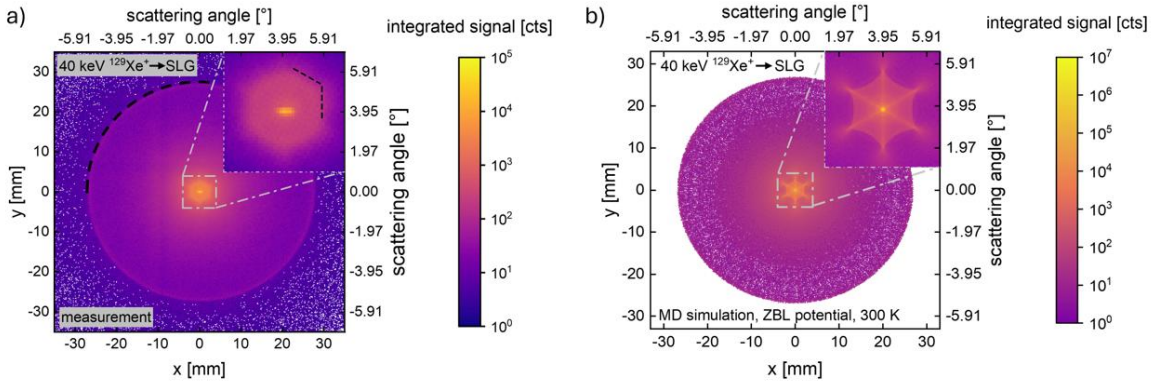


Figure 1: a) Measured 2D distribution of 40 keV Xe^+ ions transmitted through SLG. As a visual guide, the circular shape of the outer rainbow and the hexagonal shape of the inner rainbow, enlarged in the inset, are indicated with dashed lines. b) MD simulated 2D distribution of 40 keV Xe^+ ions transmitted through SLG using the ZBL potential at a thermal displacement of 300 K. The color scale of the inset in a) and b) is adjusted to enhance the visibility of the features.

Session 12

I12 - Quantum Trajectories of Energy Loss: Ion Stopping from Bohmian Mechanics to Biological Media

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The quantification of ion stopping power in matter is central to applications ranging from proton therapy and semiconductor processing to astrophysical studies. Conventional theoretical approaches often involve a compromise between the computational cost of first-principles quantum calculations and the limited applicability of classical or perturbative models, particularly near the stopping maximum.

In this talk, we present two computational frameworks designed to address this challenge. First, we introduce an approach based on Bohmian mechanics in which classical equations of motion are extended to a quantum description through the inclusion of the Bohm quantum potential derived from the electronic density. The method enables the calculation of electronic stopping forces for both fast protons and slow highly charged ions, while naturally incorporating effects such as charge exchange in two-dimensional materials, including graphene [1].

We also discuss the TDDFT-Penn approach for biological media, which combines real-time Time-Dependent Density Functional Theory with the Penn dielectric formalism [2]. This method provides a nonperturbative description of proton energy loss in different phases of water, including vapor, ice, and liquid water. The calculations indicate that the stopping cross sections of liquid water and amorphous ice are equivalent over a broad energy range, supporting the use of amorphous ice as a surrogate target for studies of radiation effects in biologically relevant media.

These developments provide complementary tools for the description of ion energy loss and radiation-induced processes in condensed matter and biological systems.

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Keywords

Electronic stopping power, Bohmian Mechanics, Energy Loss

O32 - Antiproton and proton electronic stopping power in transition metals: a non-perturbative model

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The electronic stopping power of charged particles is a key quantity for understanding energy-loss processes in matter, with applications in ion beam analysis, radiation damage, and nuclear technology [1]. Transition metals present a particular challenge due to their complex electronic structure, characterized by partially filled *d*-orbitals. Particularly, *d*-electrons of elements in groups 8 to 11 of the periodic table, such as Fe, Ni, Cu, Pd, Ag, Pt, and Au, contribute both to conduction and bound states. At low projectile velocities, they play an important role in the stopping process, making non-perturbative approaches necessary for an accurate description. In this regime, differences between proton and antiproton stopping powers (Barkas effect) provide additional insight into the underlying interaction mechanisms.

In this work, we present a non-perturbative model for the electronic stopping power in transition metals [2] based on the momentum distribution of loosely bound *d*-electrons. The model is applied to proton and antiproton impact and compared with available experimental data [3,4]. The results reproduce the expected linear dependence of stopping power at low projectile velocities and provide a consistent description of proton-antiproton differences over a broad energy range, as shown in the figure for Ni. We find that the Barkas effect is more pronounced in contributions from conduction electrons (free-electron gas, FEG) and is strongly reduced in processes involving bound electrons.

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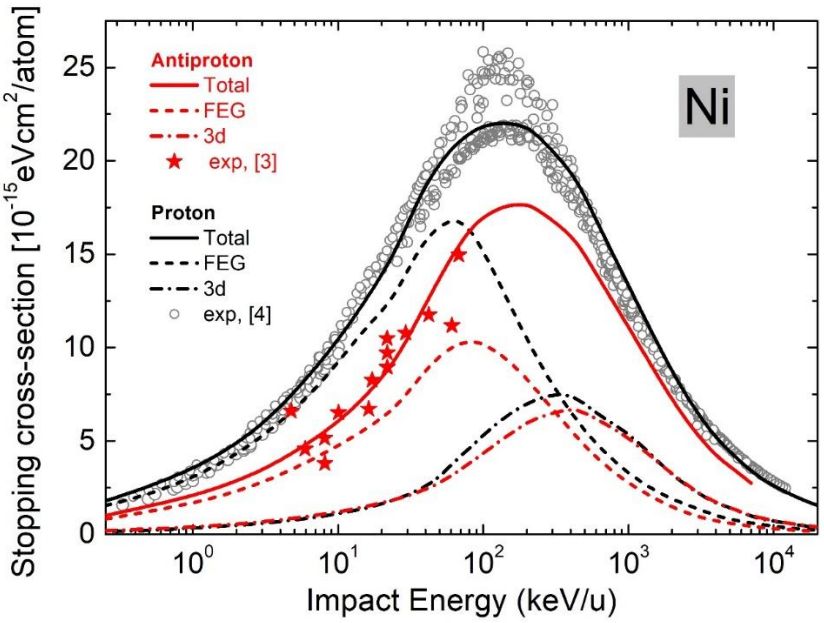
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Keywords

stopping-power, transition-metals, d-subshell, antiprotons, protons



O33 - Electronic Stopping in Atomic Systems: Effects of Trajectory, Energy Regimes, and Confinement

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Understanding energy deposition in atomic and molecular systems is central to applications ranging from radiation therapy to materials science and plasma physics. In this work, we present a unified perspective on electronic stopping processes by integrating recent advances reported in Analytical expression for the electronic stopping cross section of atomic gas targets for hydrogen projectiles, Trajectory effects on the energy loss cross section in ion-atom collisions and Target shape effects on electronic stopping in confined quantum systems. First, an analytical framework for the electronic stopping cross section is established for hydrogen projectiles in atomic gas targets, combining low-energy *ab initio* Electron-Nuclear Dynamics (END) with high-energy perturbative approaches. This formulation captures key processes such as charge exchange, excitation, and polarization effects, yielding accurate energy-loss predictions across a broad energy range and reproducing experimental trends. Second, beyond standard straight-line trajectory approximations, the role of projectile-target dynamics is examined through time-dependent Schrödinger simulations that include coupled END. These results demonstrate that while total charge-exchange cross sections remain largely trajectory-independent, significant deviations arise in energy loss at intermediate and low collision energies, where conventional approximations underestimate stopping power and neglect correlated charge-exchange mechanisms. Finally, the influence of target structure is explored via confined quantum systems modeled using atom-in-a-box approaches. Analytical expressions for dipole and generalized oscillator strengths reveal that geometric confinement and target shape strongly modify excitation spectra and mean excitation energies. Consequently, electronic stopping cross sections exhibit negligible shape dependence at high energies but show pronounced sensitivity at low energies, with confinement enhancing or suppressing energy deposition depending on system size and geometry. Together, these

studies highlight that accurate modeling of stopping power requires a consistent treatment of (i) multi-scale collision dynamics, (ii) charge-transfer and excitation channels, and (iii) target electronic structure, including confinement effects. The combined framework provides a pathway toward predictive, analytically tractable models of energy loss in complex environments, relevant for next-generation radiation technologies and nanoscale material design.

Keywords

Electronic stopping power, Ion-atom collisions, Charge exchange, Quantum confinement, Energy loss cross sections

O34 - Evolution of Crystal and Atomic Rainbows in 2 MeV Proton Scattering Through Ultrathin (001) Si Crystals

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[1]Vinča Institute of Nuclear Sciences

This study presents a theoretical investigation of rainbow scattering of 2 MeV protons through ultrathin (001) silicon crystals. The crystal thickness was varied within the range of 20 to 50 nm to observe the transition in scattering dynamics. Calculations were performed using the Rainbow Molière (RM) proton-silicon interaction potential under the continuum approximation. To determine the angular distributions of transmitted protons, we utilized the FLUX computer program, which employs a hybrid methodology: a binary collision model for small impact parameters and the continuum approximation for large impact parameters.

Our results identify two distinct categories of rainbows: Crystal Rainbows, arising from large impact parameters and the collective influence of atoms forming the crystal channel and Atomic Rainbows, corresponding to small impact parameters and individual atomic interactions.

The evolution of both rainbow types was analyzed in detail as a function of crystal thickness. These findings provide a deeper understanding of the interplay between individual and collective atomic forces in the ultrathin regime.

Keywords

Ion Channeling, Rainbow Scattering, Interaction Potential

Session 13

I13 - Harnessing High-Energy Heavy Ion Irradiation for Engineering Color Center Qubits in Semiconductors.

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High energy (~1 GeV), heavy ion (e. g. gold) irradiation of single crystal diamonds leads to the conversion of native nitrogen atoms to nitrogen-vacancy centers (NV) along the ion trajectories. The resulting self-aligned quasi-1D chains of coupled NV centers with lengths in the tens of micron range can be building blocks for quantum information processing and they provide insights into harsh radiation-matter interactions [1].

Here, we report on the study of individual quasi-1D chains of NV centers created by using 1 GeV Au ions with a low fluence of 10^8 ions/cm^2. By using 3D-resolved confocal photoluminescence (PL), we visualized individual 1D NV chains appearing as isolated bright luminescence strings, which indicates the presence of densely coupled NV centers created along a single ion trajectories. The up to 30 µm length of 1D chains of NV centers is consistent with Monte Carlo simulations of the range of high energy, heavy ions. Molecular dynamics simulations further indicate that both isolated vacancies and defect clusters form along ion trajectory through electronic stopping processes. We further quantify the electron spin properties of 1D NV chains through optical detection of magnetic resonance (ODMR). Importantly, individual 1D NV chains show enhanced electron spin resonance contrast and coherence time compared to a background of NV centers that are present in the nitrogen doped diamonds. Our findings suggest the possibility that NV centers in 1D chains with dipolar interaction between NV centers can improve sensitivity in NV-based magnetometry applications and provide guidance on the engineering of 1D chains of NV centers with minimal disorder for applications in quantum information processing.

Acknowledgments:
Work at Berkeley Lab was supported by the Office of Science, Office of Fusion Energy Sciences, and by the Molecular Foundry, a DOE Office of Science User Facility supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

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Keywords

SHI, MD, color center, diamond,

O35 - XAS investigation of Swift Heavy Ion-Induced Phase Transformations in ZrO_2: From Monoclinic to Orthorhombic and Tetragonal Phases

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[1]Osaka Metropolitan University, [2]Kyushu University, [3]Japan Atomic Energy Agency, [4]Linköping University

Zirconium dioxide (ZrO_2) is well known for its polymorphism, with the monoclinic phase being thermodynamically stable under ambient conditions. Since the high-pressure cubic and tetragonal phases exhibit various functional properties, such as high ionic conductivity and biocompatibility, their stabilization at room temperature is typically achieved through doping. Swift heavy ion (SHI) irradiation has emerged as a powerful tool for inducing phase transformations in ZrO_2. Recently, a specific orthorhombic phase (oIII-ZrO_2, space group $Pbc2_1$) has attracted significant interest due to its potential ferroelectric properties. In this study, we explored metastable phase transformations in ZrO_2 polymorphs induced by SHI irradiation.

Polycrystalline sintered monoclinic ZrO_2 was irradiated with 200 MeV Xe ions up to a fluence of 1×10^{13} cm^{-2}. At a lower fluence of 1×10^{12} cm^{-2}, we observed a local structural transformation to an orthorhombic phase. This was confirmed by Zr L_3-edge X-ray absorption spectroscopy (XAS) combined with theoretical spectra obtained from first-principles calculations. Subsequent irradiation to higher fluences resulted in a second transformation to the tetragonal phase. These fluence-dependent transitions suggest that the tetragonal phase originates from ion impacts within regions already transformed to the orthorhombic phase. Consequently, precise control of irradiation fluence is identified as a critical factor for phase engineering in ZrO2.

Keywords

Zirconium dioxide, Polymorph, X-ray absorption spectroscopy, First principles calculation

O36 - Single ion induced luminescence kinetic in Al_2O_3 in nanosecond range

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Being recorded in-situ over a wide time domain, from picoseconds to hours, the luminescence generated by swift heavy ions is a potential source of important information related both the irradiation-induced defects and relaxation of dense electronic excitations in particle tracks. The main objective of this work is to compare the luminescence kinetic in nanosecond range during irradiation of Al_2O_3 crystals with 3 MeV helium and high energy Xe (230 MeV, 395 MeV)

and Bi (670 MeV) ions having significantly different electron stopping powers. First, we describe new method of the start pulse production in measurements of time-resolved luminescence generated by single projectiles. In order to minimize any effects connected with dispersion in ion energy, we have used a design in which electron emission generated by the incident ion directly from the target surface is taken to produce the start pulses. As was found, no significant contribution of the ultrafast component, dominating in decay curves gathered during Xe and Bi ion irradiation and associated with enhanced decay rate ion the ion track region, is registered for He ions. When analyzing the experimental data, the results of modeling the processes of energy dissipation in the electronic and atomic subsystems of sapphire based on the Monte-Carlo code TREKIS and molecular dynamics simulations with LAMMPS software are considered

Keywords

swift heavy ions; ionoluminescence; luminescence decay; ion tracks; radiation damage

Session 14

I14 - Rare-Earth Ion Implantation into Nanostructures: Towards Applications in Quantum Light Sources

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Reliable single-photon sources (SPSs) that provide on-demand single photons are indispensable for rapidly growing quantum technologies, including quantum computing, quantum sensing, and quantum communication. To be maximally useful, such sources must operate at room temperature, be compatible with mature fabrication processes, and integrate seamlessly with other photonic systems. These requirements have driven intensive research into gallium nitride (GaN)-based photon emitters and devices. Rare-earth (RE)-doped GaN exhibits temperature-insensitive, spectrally sharp, and stable visible to near-infrared emission. This behavior originates from the localized 4f-shell energy levels responsible for the optical transitions, which are shielded by filled 5s and 5p orbitals and thus weakly coupled to free carriers in the host material. In addition, RE-doped GaN benefits from the well-established GaN platform, enabling integration into more complex devices. However, the spontaneous emission rate of RE ions based on 4f-4f transitions is generally lower than that of other SPS candidates, such as quantum dots. Therefore, enhancing photon emission through coupling between RE ions and nanostructures is crucial for the realization of RE-doped GaN SPSs. In this study, we present two types of nanostructures—nanopillar structures and photonic crystal nanocavities—that enhance photon emission from implanted RE ions in GaN, and discuss the underlying enhancement mechanisms. We also discuss the importance of advancing ion-beam technologies and of deepening the understanding of ion-matter interactions, since ion implantation is an essential technology for the development of solid-state SPSs. This work was financially supported by the JST FOREST Program (JPMJFR203G, Japan), JSPS KAKENHI (JPKK0137, JP18H01483, JP22H03880, Japan), and the Foundation for Promotion of Material Science and Technology of Japan.

Keywords

Rare-Earth Ions, Ion Implantation, Photoluminescence, Single Photon Source, Quantum Technology

O37 - Molecular Dynamics insights on single ion implantation for quantum computer manufacturing

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Single-atom dopants in silicon are considered among the most promising candidates for scalable quantum computing architectures[1]. However, two key manufacturing challenges remain unresolved[2]. First, achieving placement precision below 15 nm is essential for enabling qubit entanglement. Second, acceptable activation rates have so far been limited to the lightest impurity species[3]. This limitation is believed to stem from radiation damage caused by solid ion interactions during single-ion implantation[3].

To develop more effective damage recovery protocols, molecular dynamics simulations offer valuable insights into underlying mechanisms and provide a practical framework for testing and benchmarking potential solutions. Although radiation damage in silicon caused by dopant implantation has been extensively studied, a key limitation remains: the absence of an interatomic potential capable of accurately capturing the interactions between implanted dopants and the resulting damage. This gap hinders the reliability of simulation-based approaches.

In this work, we introduce a molecular dynamics framework specifically designed to model dopant-silicon interactions, enabling accurate simulations at scales far beyond the reach of ab initio methods. The model's transferability is demonstrated across group V dopants, allowing us to investigate key phenomena such as vacancy-mediated diffusion, dopant-interface interaction during recrystallization, and binding to complex defects. Based on these insights, we propose strategies to improve both implantation precision and dopant activation rates. Our findings offer computational guidance that could inform and enhance current manufacturing approaches.

Keywords

Molecular Dyanamics, Radiation Damage, Quantum Computer, Spin Donor

O38 - Platinum single atoms and clusters embedded in mono- and few-layer graphene

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Graphene, a single atomic layer of carbon atoms arranged in a honeycomb structure, exhibits exceptional properties, including excellent thermal and electrical conductivity. Combining graphene with noble metal catalysts, such as platinum (Pt), has the potential to develop efficient single-atom catalysts (SACs).

Here, we use a two-step implantation approach for the controlled incorporation of Pt single atoms into mono- and few layer- of graphene [1]. Specifically, we first use Ar^+ ion irradiation, generated using a microwave plasma source, to create vacancies in the graphene lattice. Next, we introduce Pt atoms via electron beam evaporation. The density of defects, and consequently the number of incorporated dopants in the lattice, can be controlled by adjusting the plasma irradiation time. Similarly, the size of the introduced structures—from single atoms to nanoclusters—is regulated by controlling the duration of evaporation [2]. The resulting Pt-graphene system is characterized using electron energy-loss spectroscopy (EELS) in the context of scanning transmission electron microscopy (STEM) to confirm single-atom incorporation, while 4D-STEM provides insights into the exact atomic structure. Our results show the successful incorporation into both mono- and multilayers of graphene. We also demonstrate that our method works similarly for any thickness of the substrate, as the density of the created defects on the top layer is the main factor controlling the density of the resulting Pt single atoms and nanoclusters. Additionally, we investigate the thermal stability of Pt single atoms in graphene by annealing the sample at different temperatures and highlight the difference between rampant annealing of the surface using a diode laser and steady gradually increasing temperature using an ultra-high vacuum heating chamber.

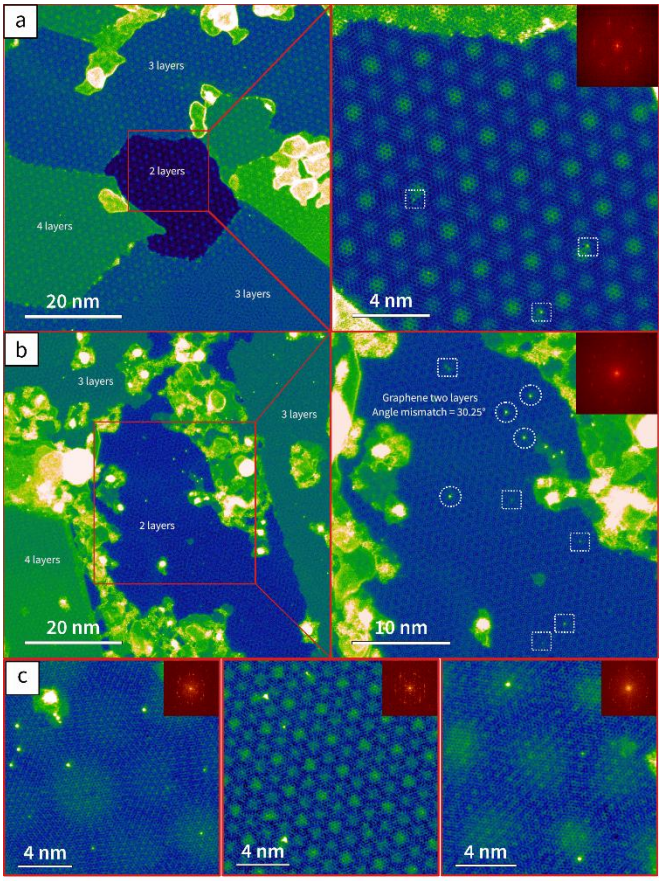
We acknowledge funding from the Austrian Science Fund (FWF) [10.55776/COE5] (Cluster of Excellence Materials for Energy Conversion and Storage).

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Keywords

Heteroatom Doping, Graphene, Ion Irradiation, Defect Engineering, Scanning Transmission Electron Microscopy



(a) A MAADF image of clean area of multilayer graphene showing two, three and four layers of graphene with a zoomed image marked in the red square showing a closer view of the two layers with some impurities of light elements (probably silicon). (b) A MAADF image of a region of multilayer graphene sample after Pt incorporation. Here, we can clearly distinguish the Pt atoms from the other elements due to the contrast difference. Pt atoms are marked in white dashed circles and lighter impurities with white dashed squares. (c) MAADF smaller field of view images of two, three and four layers of graphene. The number of layers is determined from the fast fourier transform (FFT) presented in the inset of the images, where the number of the spots in each direction in the FFT outer spots corresponds to the number of randomly oriented layers. All images in the figure were subjected to gamma correction ($\gamma = 0.5$) and contrast enhancement. A mild Gaussian smoothing ($\sigma = 1$) was applied, and the images are displayed using the Kindlmann color scale.

O39 - Ion-induced tuning of resistive switching properties in amorphous TiO_2 memristors

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Memristors, or resistive switching (RS) memory devices, are widely investigated for next-generation data storage and neuromorphic computing [1]. The intrinsic properties of the memristive material strongly govern the RS properties and underlying mechanisms. Ions offer a versatile approach for defect engineering, enabling controlled modification of material properties and tuning of switching properties in memristors. In this contribution, we study ion-induced defect formation and localised structural and stochiometric modifications in amorphous TiO_2 (a-TiO_2) thin films, which modify the RS properties.

Sputter-deposited Pd/TiO_2/Pd memristors exhibit bipolar RS after an initialisation step known as electroforming. Implantation with 8 keV ^{20}Ne ions creates a reservoir of oxygen vacancies in the near-surface half of the TiO_2 film, enabling electroforming-free RS and tuning properties such as electroforming voltage. In contrast, implantation with 8 keV ^{16}O ions primarily introduces local structural modifications, leading to distinctly different switching properties. In parallel, irradiation with MeV energy ions induces changes in the TiO_2 film, such as mass density and atomic structure, which potentially influence the switching mechanism and properties.

To investigate the switching mechanisms in O-implanted samples by selectively tracking oxygen migration in ion-implanted memristors, ^{18}O isotope tracking was performed using nuclear reaction analysis (NRA). Further investigation focuses on operando NRA and X-ray Photoelectron Spectroscopy (XPS) measurements to study the real-time evolution of ^{18}O and oxygen vacancy concentrations, respectively, in Pd/TiO_2/Pd memristors. Such operando studies can provide insights into the fundamental switching mechanisms.

These results demonstrate ions as both a defect-engineering tool and a direct probe of atomic migration processes, providing insights into ion-induced defect dynamics in memristors based on amorphous metal oxides.

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Keywords

Resistive switching, ion implantation, oxygen vacancies

Abstracts

(Poster contributions)

P1 - The use of ion beam coupled with transmission electron microscopy to investigate the irradiation induced phase transformation in polymorphic Ga_2O_3

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Ga_2O_3 has the potential to be used as a semiconductor in harsh environments involving irradiation. Hence, it is important to probe the effects of radiation damage and temperature on the stability gallium oxide crystal structure. This is all the more important than Ga_2O_3 is known to be polymorphic that can be present in six different phases: *α, β, γ, δ, ε* and *κ.* Monitoring radiation effects in terms of possible phase changes and radiation damage is critical to understanding the possible changes in physical properties. In the literature, a phase transformation from *β to κ* was reported in bulk Ga_2O_3 irradiated with ions at room temperature for a given dose. Later, it was reported that the actual phase forming was *γ and not* κ. In order to bring more light onto this irradiation induced phase transformation, a systematic study was done not only to further investigate the mechanisms of the phase transformation in Ga_2O_3 but also the effect of temperature (which has not been reported in the literature). For that matter, irradiations of Ga_2O_3 (grown either by Czochralski (CZ) or Edge-defined Film-Fed Growth (FFG) techniques) were done using 1 MeV Kr ions *in situ* in a TEM. Detailed Diffraction Pattern analysis was performed as a function of irradiation dose, which brought more insight onto the phase transformation and temperature dependence. The experiments showed that, unlike what was suggested in the literature, the phase transformation does not require implantation of ions. The possible mechanisms are discussed in this presentation which showcases how the combination of ion beam with TEM results in a powerful in-situ characterization tool for radiation effects in materials.

Keywords

ion beam; gallium oxide; in situ TEM; radiation damage; phase transformation

P2 - Study of the kinetics of radiation damage accumulation in multicomponent oxide ceramics and determination of the role of phase composition in inhibiting defect formation mechanisms

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Studying the kinetics of radiation damage accumulation in multicomponent oxide ceramics is an important area of modern materials science aimed at understanding the degradation mechanisms and improving the radiation hardness of materials used in nuclear power. Of particular interest is the analysis of defect structure evolution as a function of irradiation dose, temperature, and chemical composition of the material. In multicomponent oxide ceramics (such as solid solutions, high-entropy oxides, and composite systems), phase composition plays a key role in defect formation and subsequent evolution. The presence of multiple cationic sublattices and differences in ionic radii and valence states leads to the formation of

a complex energy landscape that influences the mobility of point defects, their recombination, and agglomeration. Furthermore, phase composition significantly influences resistance to amorphization. For example, the presence of secondary phases, nanoscale inclusions, or grain boundaries can act as effective traps for defects, facilitating their recombination and reducing the likelihood of the formation of extended damaged areas. In some cases, a "self-organized repair" effect is observed, in which defects are redistributed and annihilated without significant disruption of the crystal structure. Thus, a detailed study of the kinetics of radiation damage accumulation and the role of phase composition in multicomponent oxide ceramics allows us to identify mechanisms that inhibit defect formation, optimize the composition and structure of materials, and develop new radiation-resistant ceramics with improved performance characteristics for use under intense irradiation.

Keywords

radiation defects, ceramics, distortion, degradation

P3 - Structural changes caused by radiation exposure on the surface layers of oxide ceramics

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Structural changes caused by radiation exposure to the near-surface layers of oxide ceramics are a complex, multi-stage process involving defect accumulation, phase transformations, and changes in the morphology of the material. The near-surface region is the most vulnerable, as it concentrates the bulk of the energy of incident ions or neutrons, leading to intense damage to the crystalline structure. One of the key consequences of radiation exposure is partial or complete amorphization of the near-surface layer. The loss of long-range order in the crystalline structure is accompanied by changes in the physical properties of the material—a decrease in thermal conductivity, deterioration in mechanical strength, and changes in optical characteristics. In some cases, the formation of metastable phases or radiation-induced phase transformations is possible. This paper presents the results of an assessment of the mechanisms of defect formation in beryllium oxide-based ceramics caused by ion irradiation, as well as gas swelling processes occurring during high-dose irradiation. Particular attention is paid to the analysis of the formation and evolution of the defect structure, including the generation of point defects, their agglomeration into clusters, and the subsequent formation of extended defective regions. The studies revealed that changes in irradiation conditions associated with variations in irradiation temperature lead to increased destabilization of the ceramic surface layer, as well as an increase in the concentration of gas-filled inclusions associated with helium agglomeration in the damaged layer. It was established that the growth of gas bubbles is accompanied by an increase in internal pressure, causing local mechanical stresses in the crystal lattice. This promotes the initiation of microcracks, structural disorder, and accelerated amorphization processes. As a result, a pronounced damage gradient is formed along the depth axis, including an amorphized surface layer, a transition zone with a high defect density, and a relatively unchanged crystalline region.

Keywords

Radiation damage, oxide ceramics, amorphization, ion irradiation, defect structure

P4 - Heavy Ion Induced SEUs and Layer Dependence in 3D NAND Flash Memories

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The single event upsets (SEUs) in 128-layer dual-deck 3D NAND Flash memories have been investigated under heavy ion irradiation with LET from 11.4 to 82.5 MeV·cm²/mg and ion range up to 988 um in silicon. By mapping error addresses into 3D spatial distributions, we found that multiple cell upsets (MCUs) align along the ion track, with both number and size increasing with LET. The string cross section, the probability of upsetting an entire vertical string, scales linearly with LET, due to radial energy deposition following an inverse square law. Threshold voltage measurements reveal an exponential tail in programmed cells after irradiation, indicating charge loss from the proximity effect, the number of degraded cells also increases linearly with LET.

Layer-dependent analysis showed a slight but systematic increase in upset counts with device depth, particularly in the upper deck, with a noticeable dip at the deck interface. This trend is not caused by LET variation but by tapered channel hole etching, top cells have larger diameter, lower initial threshold voltage, and thus higher radiation vulnerability. Multiple-bit upsets (MBUs) account for less than 1% of total errors, supporting the suitability of 3D NAND for space applications.

Keywords

Single event effects, 3D NAND Flash, Heavy ions, Multicell upsets

P5 - Exceptional Radiation Hardness of AlN Under Swift Heavy Ion Irradiation: A Comparative Si_3N_4

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The integration of advanced ceramics in extreme radiation environments, such as nuclear fusion reactors and high-energy physics facilities, necessitates materials capable of maintaining structural integrity under intense electronic excitation. This study investigates the microstructural response of Aluminum Nitride (AlN) to swift heavy ion (SHI) irradiation, demonstrating its superior radiation tolerance compared to Silicon Nitride.

In this research, we subjected polycrystalline samples of AlN to heavy ion bombardment at various energy regimes to simulate the displacement damage and electronic stopping power (S_e) encountered in severe radiation fields. Despite undergoing electronic energy deposition exceeding the threshold typically required for track formation in many dielectric materials, AlN exhibits remarkable resistance to amorphization and significant defect accumulation. X-ray diffraction and high-resolution transmission electron microscopy analyses reveal that AlN maintains its long-range crystalline order, with minimal dislocation loop formation or void swelling even at high fluences.

In stark contrast, Si_3N_4 - a structural nitride frequently utilized for its mechanical robustness - shows rapid structural degradation under comparable SHI irradiation parameters. Experimental data confirms that Si_3N_4 undergoes significant lattice dilation and eventual phase transition to an amorphous state at lower electronic stopping power thresholds than those required to induce detectable lattice damage in AlN.

These findings suggest that the specific nature of the Al-N bond and the local electronic structure of AlN facilitate efficient dissipation of energy through non-radiative channels, effectively suppressing the formation of permanent radiation-induced defects. This work highlights AlN as an exemplary candidate for next-generation radiation-hardened components. The results provide critical insights into the design of non-metallic ceramics for structural applications, emphasizing the significance of electronic stopping power thresholds in governing the long-term stability of nitride-based materials in extreme environments.

Keywords

Aluminium Nitride; Silicon Nitride; Transmission Electron Microscopy; Radiation Hardness; Nitride Ceramics

P6 - Deterministic Control of Interfacial Magnetism via Low and High-Energy Ion Irradiation: Experimental and DFT Study of Spintronic Thin-Film Heterostructures

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Engineering the interfacial spin structure and magnetic anisotropy in ferromagnet/antiferromagnet (FM/AF) heterostructures is central to spintronic device performance. We present a combined experimental and theoretical study of exchange bias and coercivity modulation in top and bottom pinned FM/AF multilayers subjected to low and high energy ion beam irradiation. Multilayer stacks based on $Si/SiO_2/Cu/Ir_8Mn_{92}/Co_2FeAl/Ta$, $Si/SiO_2/Cu/Ni_{80}Fe_{20}/ Ir_8Mn_{92}/Ta$, and related systems were deposited at room temperature by ion-beam sputtering under an *in situ* in-plane magnetic field of ~1 kOe to induce deterministic magnetic anisotropy. Low-energy He^+ irradiation (25 keV) under an in-plane magnetic field leads to a pronounced enhancement of both positive and negative exchange bias up to a critical ion dose. This enhancement originates from controlled defect generation within the antiferromagnetic layer, which increases pinning centers and stabilizes uncompensated spins, thereby strengthening interfacial exchange anisotropy. At higher doses, irradiation-induced atomic displacements and interfacial mixing dominate, resulting in interfacial disorder and suppression of exchange bias. In contrast, high-energy ion irradiation induces stronger interfacial mixing even at lower fluences, leading to an earlier crossover from enhancement to degradation. These trends are consistent with hyperthermal effects described by the thermal spike model. Structural characterization using X-ray reflectivity and Rutherford backscattering spectroscopy confirms irradiation-induced interface modification as the governing mechanism. Density functional theory calculations further reveal defect-mediated redistribution of spin polarization near the Fermi level, supporting the experimentally observed evolution of exchange bias and coercivity. Overall, this study establishes ion irradiation energy and dose as effective tuning parameters for interfacial magnetism in FM/AF heterostructures.

Keywords

Interfacial Magnetism, Spin resolved density of states, spin polarization, ion beam irradiation, magnetic anisotropy

P7 - From Nitrile Ices to Complex N-Bearing Molecules: Simulating Titan's Radiation-Driven Chemistry

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Propionitrile (C_3H_5N, PCN) is a nitrogen-bearing molecule of astrochemical relevance, particularly for Titan, where nitriles play a key role in low-temperature organic chemistry and can be identified through their infrared signatures [1]. Laboratory studies have shown that irradiation of nitrile ices drives molecular transformation and increases chemical complexity [2]. In this work, we present new results on the irradiation of propionitrile ices with 40 MeV ^{40}Ar heavy ions at the GANIL facility, simulating cosmic-ray processing in astrophysical and planetary environments. Experiments were performed at 80 K and 110 K, and the chemical evolution was monitored by infrared spectroscopy. We observe significant modifications in the C≡N stretching region (2300-2200 cm^{-1}) [3], together with the appearance of new absorption features associated with irradiation products, as shown in Fig. 1.

Among the newly formed species, we identify smaller nitriles and related molecules such as hydrogen cyanide (HCN), methane (CH_4), cyanoacetylene (HC_3N), and methyl isocyanide (CH_3NC), indicating efficient fragmentation and subsequent recombination pathways. Similar irradiation experiments on nitrile-bearing ices have shown that such products arise from bond cleavage and molecular rearrangement processes [4]. These findings demonstrate that energetic processing of propionitrile ices is an efficient pathway for the production of chemically diverse N-bearing molecules, some of which are potential precursors of complex organic species. This provides important experimental constraints for the interpretation of infrared observations of Titan and similar environments and reinforces the role of heavy-ion irradiation in driving molecular complexity and prebiotic chemistry in cold astrochemical ices [3,4].

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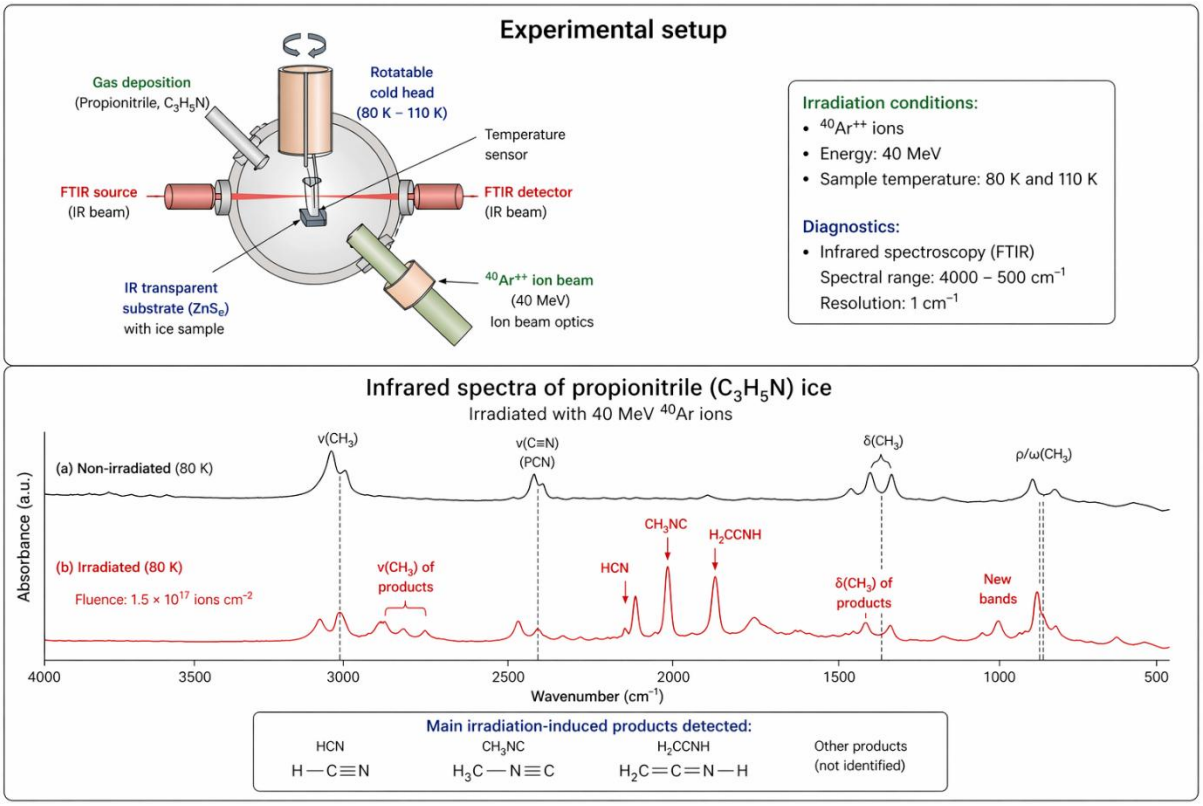
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Keywords

Titan; Nitrile ices; Heavy-ion irradiation; Infrared spectroscopy; Astrochemical evolution



P8 - Ion beam emulation of neutron radiation damage in reactor materials

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Understanding material response to intense neutron irradiation is essential for the development of advanced nuclear systems, particularly fusion reactors. Fast 14 MeV neutrons produce displacement damage and transmutation reactions, leading to defect formation and accumulation of gases such as hydrogen and helium, which degrade mechanical properties.

Reduced activation ferritic-martensitic (RAFM) steels are leading candidates for structural components in fusion devices due to favorable radiation resistance and low activation. Long-term performance under simultaneous irradiation and gas production at fusion-relevant neutron energies requires further investigation.

Ion beam irradiation provides an efficient alternative to neutron testing by enabling rapid damage accumulation and controlled simulation of transmutation products without sample activation. At the Ruđer Bošković Institute, the Dual Beam Ion Irradiation Facility for Fusion (DiFU) enables simulation of neutron-induced effects through simultaneous implantation of hydrogen or helium combined with displacement damage by heavy ions. Precise control over

irradiation parameters, including dose, dose rate, and temperature, supports systematic investigation of coupled radiation and thermal effects.

Keywords

ion irradiation, fusion, neutron damage, reactor materials

P9 - Comparison of peptide fragmentation induced by swift heavy ions with low-energy fragmentation processes

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The interaction of swift heavy ions (SHI) with organic matter is of relevance for applications such as ion-beam cancer therapy and the controllable modification of biomaterials using SHI. It is also of fundamental interest with respect to the mechanisms of energy deposition by SHI and redistribution in complex molecular systems. In this context, SHI-induced fragmentation of peptides represents a very well-suited model system due to the structural diversity of peptide molecules; it has been studied for many other, low-energy fragmentation processes.

The study of molecular fragmentation by external stimuli, however, requires an analytical tool that does not introduce fragments itself. Therefore, we make use of Desorption/Ionization induced by Neutral SO_2 Clusters (DINeC), an extremely soft desorption method [1] which is sensitive to structural changes but does not introduce further fragmentation, in combination with mass spectrometry (MS). DINeC-MS has proven to be an ideal tool for analyzing fragmentation processes [2].

Using DINeC-MS, we find that SHI-induced peptide fragmentation is characterized by a dominance of specific bond cleavages in the peptide backbone over non-specific cleavages in the amino acid side chains [2]. Moreover, the specific fragmentation exhibits a high site selectivity with respect to the amino acid sequence.

Here, we give a detailed comparison of SHI-induced peptide fragmentation with results from a variety of other fragmentation processes, including collision-induced dissociation (CID), surface-induced dissociation (SID) [3] which is closely related to CID, thermal dissociation, electron transfer dissociation (ETD) [4], and CID of radical peptide ions [5]. In particular, the exchange of amino acid units and its influence on the distribution of fragments is compared for SHI-induced fragmentation and CID. Whereas the latter shows a pronounced dependence of the observed site selectivity on the amino acids present in the direct neighborhood of selectively cleaved peptide bonds, site selectivity in SHI-induced fragmentation is found to be largely independent on the single amino acid units in the direct neighborhood of the cleavage site.

Considering the site selectivity as well as the distribution of the three types of peptide bond cleavages (a/x, b/y, and c/z), we thus find that the fragmentation process operative under SHI irradiation is specific for the interaction of SHI and organic molecules.

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Keywords

collosion-induced dissociation, mass spectrometry, peptides, radiolysis, selective fragmentation

P10 - Inner-shell ionization by swift heavy ions in matter: CDWEIS calculations, open repository, and neural network model

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Particle-induced X-ray emission (PIXE) is a widely used analytical technique whose accuracy relies on reliable inner-shell ionization cross sections. In this work, we present *ab initio* calculations based on the continuous distorted-wave eikonal initial-state (CDWEIS) model [1,2]. We emphasize the study on Z = 11-30 (Na-Zn) targets, impacted by ions with different charges as well as by antiprotons. This group of elements includes key components in pigments, steels, and reactor materials [3,4], highlighting the relevance of the present results for PIXE applications.

A systematic analysis of the CDWEIS results is performed to identify scaling laws and their dependence on projectile charge and velocity. As an example, we display in Fig 1, the present K-shell ionization cross sections of targets with Z=21-30 by swift protons. Due to the high computational cost of CDWEIS calculations, we will introduce an open-access database providing tabulated cross sections for a wide range of projectiles, targets, and initial states. In addition, we will present the CDWEIS-NN, a neural network model [5] trained to extend the calculated cross sections to other systems and impact energies. The model shows good agreement with both CDWEIS results and available experimental data for K- and L-shell ionization, as shown in Fig. 2. As a next step, we are developing a physics-informed neural network framework to incorporate fundamental physical constraints into the learning process.

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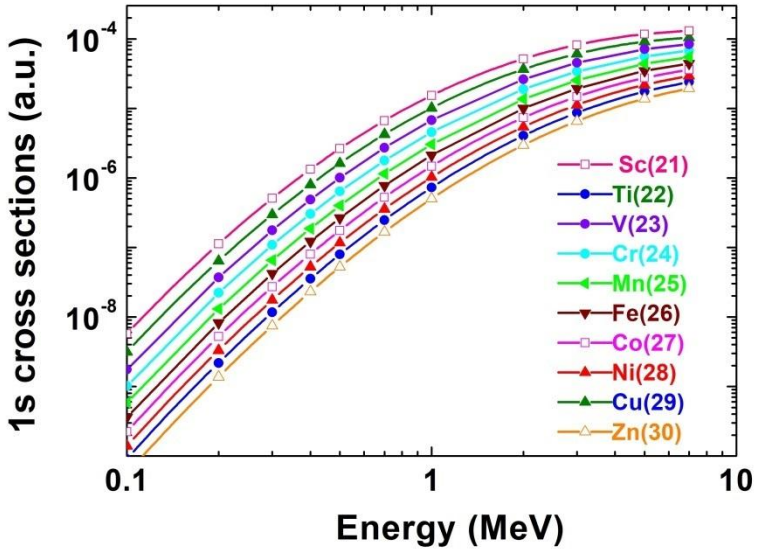
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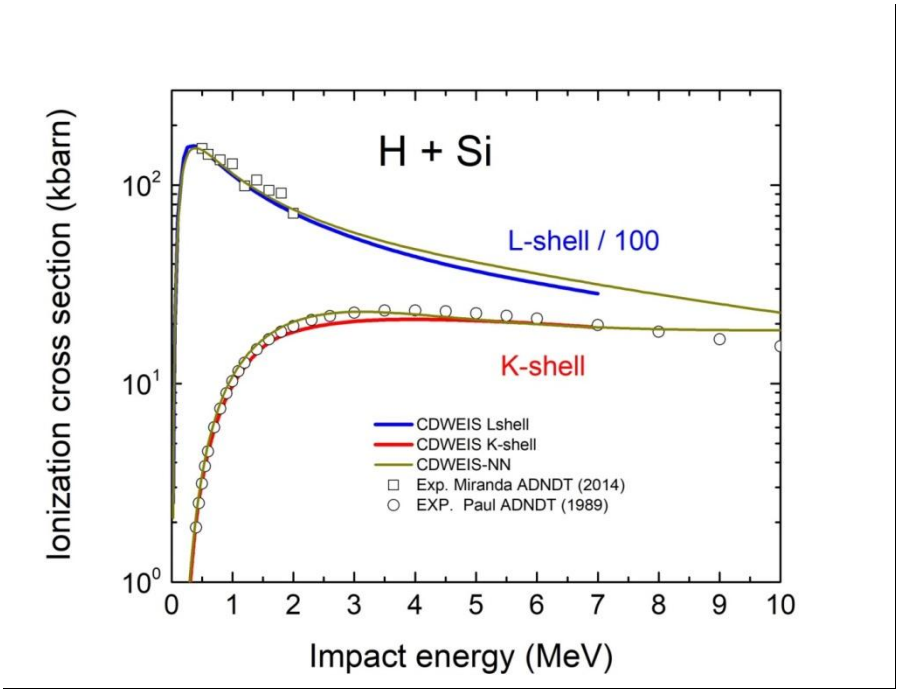
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Keywords

ionization, heavy-ions, CDWEIS, neural-network,PIXE





P11 - Surface amorphization and fractal analysis of collision cascades in gallium oxide

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It is well established that generation of structure damage in a crystalline solid by accelerated ion proceeds in two major stages, namely, (i) atoms are shifted from their lattice sites in a cascade of ballistic collisions initiated by impinging ion, and (ii) primary defects diffusing in the target interact each other, various sinks or centers forming stable damage. Amount of such stable damage appeared after irradiation is determined by ion energy and mass, ion flux and dose, target temperature, etc. Indeed, collision cascade play key role in damage formation.

Therefore, the quantitative description of collision cascades is vital for understanding of radiation phenomena in new materials. Collision cascade produced by an energetic ion has a complex 3D structure involving a number of sub-cascades. Similarities between ion-induced collision cascades and fractals let treating complex 3D cascade shapes in the framework of the fractal geometry [1].

We study damage accumulation in a- and β-Ga_2O_3 under keV monoatomic and small cluster ion irradiation. Further, density and fractal dimension of collision cascades formed by different ions were calculated using different algorithms based on the binary collision approximation. The rate of surface amorphization in both Ga_2O_3 polymorphs as experimentally measured, increases with increasing collision cascade density which is a function of ion mass as well as cluster size. Fractal dimension of collision cascades in Ga_2O_3 could be correlated with the cascade density [2]. The fractal analysis is more generic and this approach can be applied to practically any type of collision cascades, irrespective of its morphology. These results enhance the understanding of radiation defects in Ga_2O_3 polymorphs, applicable in the development of the ion beam technology in these interesting materials. Particularly, the prediction made by, Winterbon, Sigmund et al.[1] quite a long time ago “that at some time the knowledge of fractals will become useful in further understanding some aspects of collision cascades,” has been proven in the case of Ga_2O_3.

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Keywords

Gallium oxide; radiation damage; collision cascade; fractal analysis

P12 - Multifrequency laser fields as a tool for generating twisted radiation

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The problem of generating photons possessing orbital angular momentum (twisted photons) ranks among the actively developing areas of modern high-energy physics and quantum optics [1]. Traditional approaches, in particular the method of phase plates, demonstrate high efficiency in the optical range but prove inapplicable in the domain of X-ray and gamma radiation. As a promising alternative for obtaining hard twisted photons, schemes based on inverse Compton scattering are considered [2], in which the configuration of the laser field interacting with relativistic electrons plays a decisive role. Variation of the parameters of this field enables targeted control over the angular momentum of the generated photons. In works [3,4], the radiation of relativistic particles in intense laser fields with circular and linear polarizations was investigated, taking into account quantum recoil effects. Additionally, the generation of twisted photons in multifrequency undulators was studied [5], where the influence of the complex spectral structure of the field on the intensity, asymmetry, and selection rules of the radiation was analyzed.

In the present work, the process of twisted photon generation in multifrequency laser fields is considered. By analogy with how multi-frequency undulators enable the production of

photons in states that are superpositions of states with different projections of total angular momentum [6], the application of multifrequency lasers in the inverse Compton scattering scheme opens the possibility for controlled generation of twisted radiation with specified quantum numbers. The aforementioned approach provides a mechanism for controlling the spectral and angular characteristics of the radiation, which, in turn, creates the prerequisites for the development of compact sources of hard radiation with desired properties.

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Keywords

twisted photons, multifrequency laser fields, total angular momentum, inverse Compton scattering

P13 - Atomic-level characterization of 2D heterostructures modified by swift heavy ions

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When ions with mega-electron-volt (MeV) kinetic energies impact materials, several physical processes can occur depending on the irradiation energy and dose. When bulk materials are irradiated with swift heavy ions (SHI), ion tracks are formed [1], but freestanding 2D materials present a distinct case. Very recently, Liebsch and colleagues demonstrated controlled nanopore formation in monolayer MoS_2 by SHI irradiation [2].

Previous studies of highly-charged ion irradiation of molybdenum disulfide (MoS_2) and its heterostructures with graphene showed that material order plays a significant role. Apparently, in the case of graphene facing the ion beam, it absorbed all the potential energy while shielding

the underlying MoS_2 layer. By contrast, a single layer of MoS_2 facing the ions gets perforated, but when there are two or more layers, the second or third layers show reduced or no damage [3].

These studies prompted us to explore the effect of SHI irradiation on heterostructures. MoS_2 flakes grown on silicon wafers by chemical vapour deposition (CVD) were transferred onto a single-layer graphene-coated transmission electron microscopy (TEM) grids. For this study, we made sure that the MoS_2 side is on top of graphene, facing the ion beam.

Three freestanding MoS_2-on-graphene heterostructures were irradiated by SHI of gold at 4.8 MeV/u with charge states of Au^{25+}, Au^{54+}, Au^{58+} and a fluence of 5×10^{10} ions/cm^2 per sample. To characterize the samples both before and after ambient transfer to the ion irradiation facility at GSI, we imaged them in Vienna at atomic resolution at 60 keV on an aberration-corrected scanning transmission electron microscope Nion UltraSTEM100 [4]. We used standard medium-angle annular dark-field imaging, where the graphene contrast is weak compared to MoS_2.

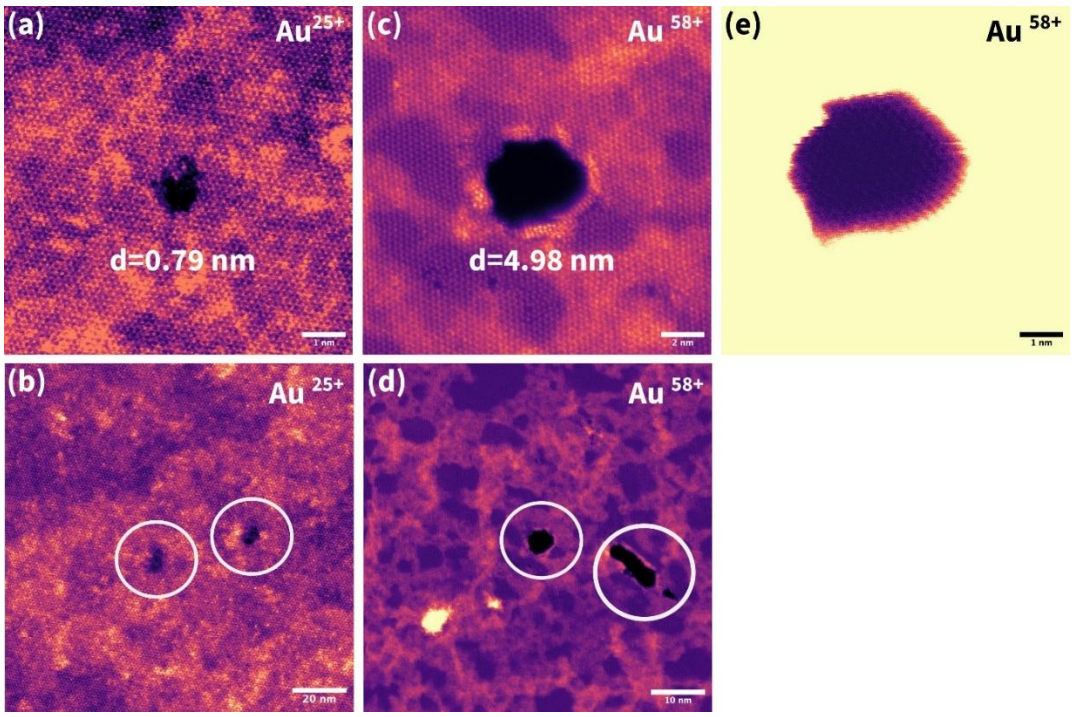
The mean pore diameters in the irradiated samples were 1.5 ± 0.4 nm for Au^{25+}, 4.7 ± 0.5 nm for Au^{54+} and 4.4 ± 0.4 nm for Au^{58+}. We thus reach the following findings. i) Remarkably, graphene remains intact even after such extreme swift heavy ion impact (see figure), consistent with prior findings for highly charged ions. ii) Increased charge of the ion increases pore size in MoS_2 for swift heavy ions of the same element and kinetic energy. iii) The pore density closely matches the applied ion fluence, indicating a pore creation efficiency of approximately unity.

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Keywords

van der Waals heterostructures, swift heavy ions, scanning transmission electron microscopy



P14 - Functional ion-track etched nanopores in SiO_2 for ultra-sensitive protein detection

Nahid Afrin[1], Shankar Dutt[1], Maria Eugenia Toimil-Molares[2], Patrick Kluth[1]

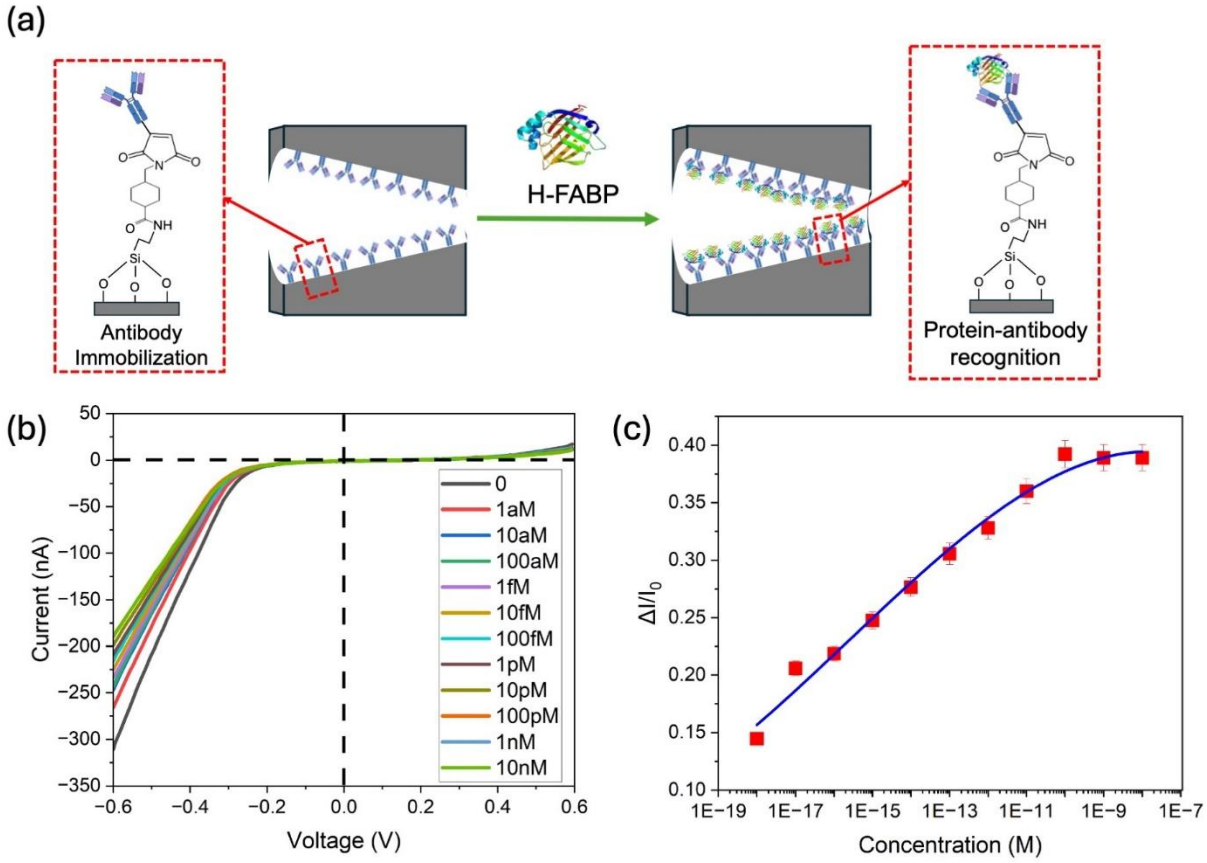
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When highly energetic heavy ions traverse through a target material, the high electronic excitations can generate long cylindrical damaged regions so called 'ion tracks'. Ion track damage often exhibits preferential chemical etching over the undamaged material. This etch-anisotropy can be used to create pores of up to tens of micrometers in length, with pore diameters as small as several nanometers. The resulting nanopore membranes are well suited to a range of advanced applications including ultrafiltration, biomedical sensing, nano-fluidics, and nano-electronic devices. A key feature of the technique is the ability to generate single pores as well as large highly parallel pore arrays with extremely narrow size distributions and tunable pore areal density.

We have demonstrated that ion track etching can be used to fabricate conical nanopores in SiO_2 membranes. The nanopore size and cone angle can be readily tuned by adjusting the etching conditions. In this presentation we demonstrate the use of our nanopore system for ultra-low concentration sensing of proteins, which remains a central challenge for early disease diagnosis and monitoring. The anisotropic pore geometry, together with the intrinsic charge of the SiO_2 surface display high ion current rectification in an appropriate electrolyte solution. To functionalize the membrane, antibodies were covalently immobilized on the nanopore surface through siloxane chemistry. The functionalized nanopores generate a characteristic rectifying current-voltage response, which shows a distinct shift upon binding to the target protein due to partial neutralization of the negatively charged pore surface. We have utilized the sensor for the rapid detection of heart-type fatty acid binding protein (H-FABP), a well-established biomarker of cardiac injury that enables early differentiation between unstable angina and acute myocardial infarction. Elevated H-FABP levels have also been reported in cerebrospinal fluid from patients with neurodegenerative disorders, including Alzheimer's disease and synucleinopathies. Our sensor exhibits excellent sensitivity in the attomolar to nanomolar concentration range with a detection limit (LOD) of this biomarker of 0.4 attomoles. The sensitivity is demonstrated in the figure which shows (a) the pore functionalization, (b) the I-V curves and (c) the current rectification ratio as a function of H-FABP concentration. The platform also exhibits high selectivity, distinguishing H-FABP from non-target proteins (HSA and Hb) at concentrations six orders of magnitude higher. Each measurement requires only seconds and does not require sophisticated analytical equipment. Nanopores can be regenerated using standard chemistry, enabling repeated functionalization and reuse. The technique can be readily adapted to other molecular receptors and thus provides a versatile platform for future low-cost biomarker screening and diagnostics.

Keywords

ion track etching, nanopores, biosensing, silicon dioxide



P15 - Ion track formation and porosity in InSb and GaSb induced by swift heavy ion irradiation

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Swift heavy ion irradiation of InSb and GaSb can induce ion-track formation, amorphization, strain, swelling and porosity, yet the interplay among these processes remains incompletely understood. Here, we investigate the damage evolution in InSb and GaSb under 125 MeV and 150 MeV ^{107}Ag and 185 MeV ^{197}Au irradiation as a function of fluence, irradiation angle and film thickness using scanning electron microscopy (SEM), Raman spectroscopy, grazing-incidence X-ray diffraction (GIXRD), Rutherford backscattering spectrometry in random and channelling geometries (RBS/C), and particle-induced X-ray emission (PIXE). In bulk InSb irradiated with ^{107}Ag ions, RBS/C yields track radii of of track radii of ~ 5 nm and ~ 8 nm for 125 MeV and 150 MeV, respectively, while the damage fraction saturates near 90%, indicating that partial recrystallization limits complete amorphization. In bulk InSb irradiated with ^{107}Ag ions, porosity emerges at fluences of 8.8x10^{12} ions/cm^2 and above, with pore size and density depending on energy loss and the irradiation angle. Higher-energy irradiation enhances pore

growth and angle sensitivity, while lower-energy irradiation produces finer and more uniformly distributed pores. Cross-sectional SEM of polycrystalline InSb and GaSb thin films irradiated with 185 MeV ^{197}Au ions at normal incidence reveals progressive, thickness-dependent porosity accompanied by pronounced swelling, reaching ~ (50 − 60)% in InSb, and ~ (75 − 100)% in GaSb at high fluences. Raman spectroscopy indicates irradiation induced tensile strain in both materials. In addition, GIXRD reveals pronounced increased disorder accompanied by a reduction in crystallite size decreasing from ~ 40 (pristine) to ~ 13 nm at a fluence of 2.0×10^{12} ions/cm^2 in 314 nm InSb films and from ~ 26 (pristine) to ~ 11 nm at a fluence of 5.6×10^{12} ions/cm^2 in 278 nm GaSb films. RBS and PIXE confirm that elemental composition remains stable within experimental uncertainty. These results provide insight into track overlap, porosity onset and strain evolution in InSb and GaSb, highlight how energy deposition governs the structural evolution of antimonides under swift heavy ion irradiation.

Keywords

SHI, InSb, GaSb, Porosity, Ion track formation

P16 - Average electronic stopping power from ab initio calculations

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The electronic stopping power S_e is one of the most fundamental quantity to assess the effects of heavy ions in matter. It is therefore a quantity at the heart of many applications, from cancer treatments to microelectronic devices hardening. SRIM is the most common and general purpose tool used to calculate S_e. It is based on theoretical models adjusted to reproduce experimental data. However, for many (projectile, target) combinations there exists no or very few experimental data. There is thus no comparison points to judge SRIM's accuracy for those cases. However, Real-Time Time Dependent Density Functional Theory (rt-TDDFT) now allows to calculate S_e, and thus to compare to SRIM, at an *ab initio* level for any (projectile, target) combination. rt-TDDFT is a heavy atomic scale method giving access to a lot more information on the stopping process than SRIM, among which the anisotropy of S_e in crystals. Indeed, in rt-TDDFT, each S_e calculation is carried out in a specific crystal direction, and thus each calculation yields a S_e value valid for this direction only. The other side of the coin of this atomic scale description of S_e is that it can be very difficult with rt-TDDFT to obtain reliable average S_e values that can be compared to SRIM as many rt-TDDFT simulations in various crystal directions have to be performed.

In this contribution, we introduce a method that proposes to calculate average S_e with rt-TDDFT by carefully choosing a single crystal direction. We use the electronic density as a descriptor of S_e: we search for a crystal direction along which the electronic density distribution experienced by the projectile is the closest possible to a probability density function of the electronic density representative of the whole material. Our hypothesis is that a projectile following such a path will experience an electronic stopping power close to the average one obtained in experiments and given by SRIM. The method is validated on Si, with 80 Å long projectile trajectories, for protons and Si ions projectiles. We choose Si as this a material for which there are many experimental data available to compare to and for which SRIM performs

well. Our calculated data agrees very well with SRIM and experiments. The objective in the future is to apply this method to materials for which there are very few S_e experimental results.

Keywords

Electronic stopping power; ab initio; radiation effects; semiconductors

P17 - Effect of spatially heterogeneous band gap collapse on formation of swift heavy ion tracks in Al_2O_3

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Irradiation of insulators with swift heavy ions (SHI) initially leads to extreme excitation of the target's electronic system, initiating sharp changes in the interatomic potential energy surface. Atomic displacements caused by nonthermal acceleration of atoms due to these changes result in a quick, shorter than 100 fs, collapse of the material band gap [1]. The potential energy of the electronic system, released during the collapse, transfers to the atomic system. Together with the electrons and holes scattering, it heats up the lattice, inducing damage detectable in the experiments [2].

The Monte-Carlo code TREKIS takes into account this energy transfer mechanism by the conversion of the potential energy of valence holes generated around the ion trajectory to atoms by the end of calculation (100 fs) when the electronic system cools down [2,3].

However, the electronic excitation in a track quickly decreases from the center outwards resulting in radial heterogeneity in the changes of the band structure in the proximity of the ion trajectory.

In this work, we employed the density functional theory, in combination with the TREKIS code, to estimate the effects of such heterogeneity on the excitation and material damage in SHI tracks in Al_2O_3. We simulate the initial SHI passage and subsequent electronic cascades as well as electrons and holes scattering on the lattice with the TREKIS code and determine the electronic and atomic temperatures in the cylindrical layers around the SHI trajectory. Then, using these temperatures as initial conditions, we perform DFT molecular dynamics calculations for each layer with the Quantum Espresso code tracing changes in alumina's band structure.

We demonstrate that an impact of 700 MeV Bi ion causes, after approximately 50 fs, a transient metal-semiconductor heterojunction in alumina: the metallization associated with the band gap collapse occurs within ~2 nm radius from the ion trajectory. The band gap shrinks at distances of about 3-5 nm, while it remains almost unaffected at radii >5nm.

The transfer of valence holes' potential energy to the lattice according to the degree of band gap shrinkage improves the damage simulations along the ion path manifesting itself in more distinct discontinuous nature of the track for all crystallographic directions compared to the case when the entire holes ensemble' energy is transferred, although both approaches correctly predict the track radius.

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Keywords

swift heavy ion track, monte-carlo simulation, density functional theory, band gap collapse, nonthermal transition

P18 - The shape and composition of swift heavy ion tracks in SiC at high temperatures

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Silicon carbide (SiC) is highly resistant to swift heavy ion (SHI) irradiation. However, our modeling [1] has revealed that SiC loses this tolerance at elevated temperatures, and SHIs create structurally modified tracks in it.

We report here on the patterns of structural modifications caused by SHIs in silicon carbide under high-temperature irradiation:

First, we reveal the formation of two types of nanostructures [2], nanohillocks and nanocraters, on the surface of SiC films of various thicknesses irradiated with 710 MeV Bi ions over a wide temperature range. The transition from hillocks to craters occurs with increasing irradiation temperature. The temperature of this transition increases with film thickness, approaching ≈1534 K for film surfaces with thicknesses exceeding 100 nm.

Second, we observed the formation of nanocavities in the near-surface layer of the irradiated SiC films. At room temperature, carbonization of the surfaces of both the film itself and the voids within was detected. Moreover, we have determined that this carbonization occurs due to the redistribution of defects inside the film and is not associated with excessive silicon ejection from it. We have also found that an increase in irradiation temperature suppresses the carbonization process, resulting in a surface composition that is nearly homogeneous.

Third, we found that in bulk SiC targets, the irradiation in the temperature range $T_{irr} \geq 1800$ K induce structural modifications not only near the surface but also in the bulk of the material. Depending on the energy of an incident Bi ion, at $T_{irr} = 2200$ K the cross-section of the pores in the track core can be circular, triangular, or elliptical (see Fig. 1).

Fig. 1. The shape and size of nanopores in SiC after irradiation with Bi ions of various energies at 2200 K.

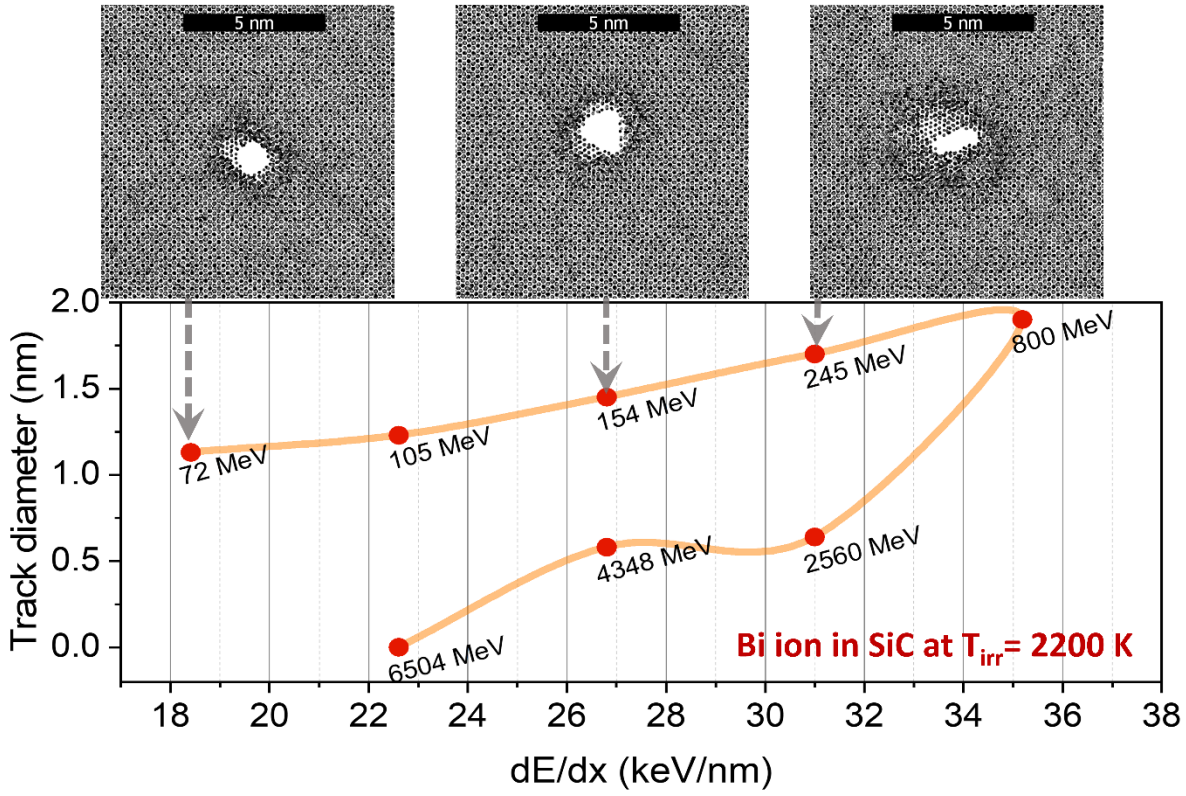
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Keywords

ion-solid interactions; modeling; multiscale; ceramic



P19 - Spatial inhomogeneities in excitation of matter under high-intensity heavy ion beam

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Heavy-ion accelerator facilities under construction, such as HIAF and FAIR, will provide unique experimental conditions for investigating unusual extreme states of matter produced by irradiation with intense beams - up to 10^{12} ions/mm^2 in 100 ns bunch [1, 2]. Describing the evolution of these states requires accurate source terms of energy deposition by the excited electrons accounting for changes in the electronic state of a target during the bunch.

To study these changes, we develop a hybrid model that simulates the temporal and spatial kinetics of target excitation under such ion bunch with nanometric resolution. The Monte-Carlo code TREKIS [3] provides radial distributions of the electron concentration and their energy density after each ion impact, accounting for nonequilibrium electron kinetics, core hole decays, and particle transport. The dynamic structure factor formalism describes the cross sections of electron-lattice coupling at various evolving atomic temperatures [4]. The thermal diffusion approach traces the further spatial spreading of the cooling electrons and the lattice excitation.

We demonstrate at fluxes below ~10^{19} ions cm^{-2} s^{-1}, new ions in the bunch of Xe 156 MeV ions pass through Al_2O_3 target areas with already relaxed electron system. The overlap of hot tracks of ions in the sample starts from the flux intensity of ~10^{20} ions cm^{-2} s^{-1}. At the flux of

$4 \cdot 10^{21}$ ions cm^{-2} s^{-1}, the concentration of excited electrons and the lattice temperature affect the relaxation of tracks of new ions, creating a spatially inhomogeneous state. Significant overlap of tracks with the hot electronic system occurs at the extreme flux of $4 \cdot 10^{22}$ ions cm^{-2} s^{-1}

The results suggest that not only transient heating and ionization of a target should be taken into account during a bunch simulation, but also the variations of these values over the target area with nanometric resolution.

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Keywords

Swift heavy ions, intense beams, track overlap, FAIR, HIAF

P20 - Role of dynamic screening of target atoms in ion track formation in GaN

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We conducted atomic-level modeling to analyze the structural changes in nanometric proximities of trajectories of swift heavy ions (SHI) decelerated in GaN in the electronic stopping regime [1]. The multiscale model we used integrates the Monte Carlo code TREKIS-3 [2], which describes the excitation of the electronic and atomic systems around the ion trajectory, with molecular dynamics simulation (LAMMPS [3]) of GaN atomic system's response to the excitation.

We show for Au 185 MeV, Pb 132 MeV, Pb 930 MeV, and U 900 MeV ions that the simulated track structure agrees with the experimental data only when dynamic screening of target atoms [4] in the scattering cross-sections and the Tersoff-Brenner interatomic potential are used in the TREKIS-3 and MD respectively.

For all mentioned ions, the formation of cylindrical amorphous tracks was observed, with nitrogen cavities located in the cores of these tracks (Fig. 1a,b).

Fig. 1. (a) Size and (b) structure of Au 185 MeV tracks in GaN. (c) Lattice defects surrounding Au 185 MeV track core. Edge dislocations are indicated as green lines.

The analysis of the crystalline lattice structure showed the presence of edge dislocations and stacking faults in the crystalline halo surrounding track cores (Fig. 1c). It is believed that the presence of edge dislocations elongated along the track impedes the recrystallization process of the damaged GaN structure.

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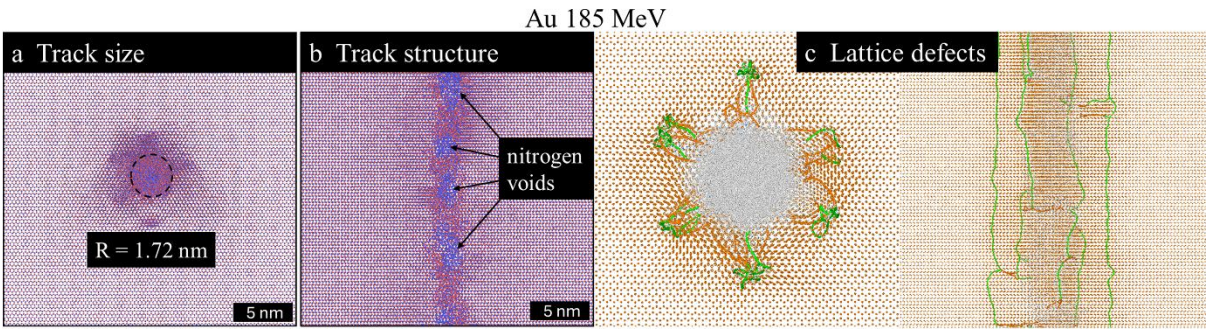
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Keywords

GaN; swift heavy ions; track; dynamic screening; dislocations



P21 - Fabrication and Radiation Responses of SiC thin-film based device for Sensor Applications

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A detailed study on the fabrication and radiation response of SiC thin-film based high-temperature and high-power electronic devices will be presented. Their applicability to various sensing applications has been examined. SiC thin-films were deposited on different substrates by RF magnetron sputtering technique. Metal contacts were deposited by employing thermal / e-beam evaporation. The influence of various growth parameters on the formation of thin-films is interpreted by invoking the underlying physical mechanisms. The optimized devices will be employed for sensing applications such as temperature, gas and radiation sensors. The influence of gamma and/or ion irradiation on the structural properties of SiC thin-films and consequents effects on the performance of corresponding devices will be discussed in this conference. The research aims to explain the electrical characteristics of SiC thin-film devices subjected to various thermal, gamma and ion irradiation treatments, with a particular focus on parameters such as leakage current, barrier heights, and breakdown voltage. The findings of this research are expected to provide useful information for applications in aerospace, nuclear, and defence sectors, where reliability of devices in harsh environments is critical.

Keywords

Silicon carbide, RF sputtering, sensor, ion, gamma, irradiation

P22 - In-situ FESEM investigations on evolution of fractal morphology of Sb thin films under ion irradiation

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The two-dimensional (2D) antimony, which is widely known as antimonene, has high potential for technological applications. In bulk (3D) form, antimony is a semimetal; as thickness decreases, it transitions to a topological insulator and a trivial semiconductor due to quantum confinement and surface coupling effects. Our earlier *in-situ* investigations [Jinu Job, *et al, Scientific Reports* 16 (2026**)** 13475] on 2 MeV Al^+ ion irradiation effect on Sb films deposited on *c*-Al_2O_3 demonstrates that in the Sb film deposited at 245 °C, the ion irradiation causes disorder within the nanocrystals, effectively lowering the melting point of antimony. In contrast, Sb films deposited at room temperature (RT), exhibit a transition from a disordered structure to an ordered crystalline phase. These observed transitions (disordered to crystalline and crystalline to disordered) under ion irradiation demonstrate the potential of antimony for future phase-change material applications.

In the present work, Sb(5 nm)/Si(100) films deposited at RT possess snowflake-like dendritic Sb islands exhibiting pronounced self-similarity with radially branched structures, which are characteristic signatures of fractal growth. The average fractal dimension obtained for the Sb islands was D_f ~ 1.65, which is in good agreement with the fractal dimension (D_f ~ 1.7) predicted for diffusion-limited aggregation (DLA) systems. The morphological evolution of the film is investigated under high-energy ion (2 MeV Al^+) irradiation for various ion fluences with the help of i^4- FESEM facility [P. Jegadeesan, *et al*. *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms 566* (2025) 165759], where FESEM is coupled with the beamline of 1.7 MV tandetron accelerator.

It is observed that with the increase in the ion fluence of 2 MeV Al^+ ion irradiation, the dense fractals of Sb narrow and the dendrite becomes thinner (shown in Fig.1). The average fractal dimension has decreased significantly from 1.73 to 1.61 (shown in Fig. 2), leading to a larger effective contact area with the water droplet and thereby enhancing the interaction between the liquid and the Si surface. The contact angle measurements show a reduction in contact angle from 83°(un-irradiated sample) to 74°(irradiated sample) (shown in Fig. 3) upon ion irradiation. The observed change in fractal dimension is attributed to the evaporation of Sb during the thermal spike regime of ion irradiation. These observations will be discussed in the light of MBE thin-film growth and ion-solid interactions.

Keywords

Molecular beam epitaxy (MBE), Fractal, In-situ ion irradiation and imaging with FESEM (i4-FESEM), Ion irradiation, Thermal spike

Fractal evolution in Sb(5 nm)/Si(100) deposited at RT under 2 MeV Al^+ ion irradiation

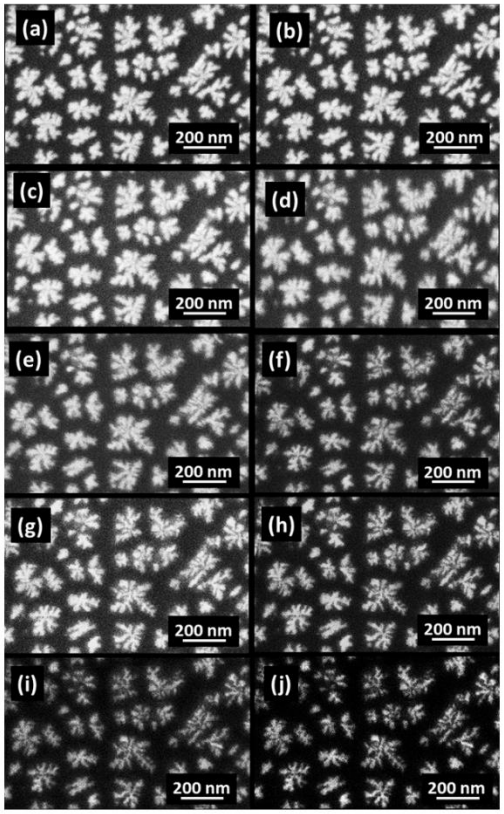


Fig. 1. Sequence of SEM images showing the evolution of Sb islands on Si(100) under 2 MeV Al^+ ion irradiation. The images were recorded (a) before irradiation, and after irradiation at the following ion fluences (b) 0.025, (c) 0.334, (d) 1.23, (e) 2.48, (f) 4.12 (g) 5.18, (h) 6.78, (i) 8.97, and (j) 12.20 $\times 10^{16}$ ions/cm^2

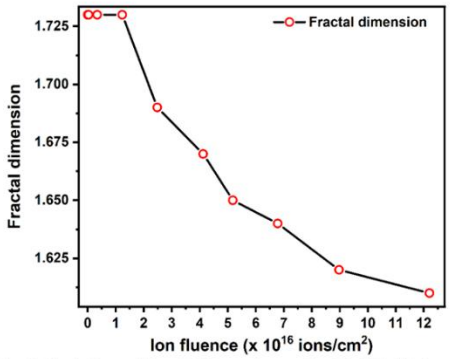


Fig. 2. Evolution of fractal dimension under 2 MeV Al^+ ion irradiation in Sb film

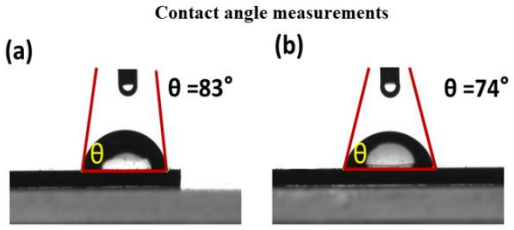


Fig. 3. Contact angle measurements in Sb(5nm)/Si(100) (a) unirradiated (b) After 2 MeV Al^+ ion irradiation (Ion fluence: 1.22 $\times 10^{17}$ ions/cm^2)

Observations

- **The average fractal dimension reduces from 1.73 to 1.61 upon ion irradiation**
- **After ion irradiation, the contact angle decreases from 83° to 74°.**
- **The observed reduction in contact angle upon ion irradiation is due to an increase in surface roughness.**

P23 - Size and Matrix Effects on Latent Track Formation in $Y_4Al_2O_9$ Nanoparticles during Swift Heavy Ion Irradiation

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Oxide dispersion strengthened (ODS) alloys are promising structural materials for next-generation nuclear reactors due to their high-temperature strength and radiation resistance [1,2]. Their performance is largely determined by nanoscale oxide particles, typically yttrium-based compounds, embedded in a metallic matrix. Irradiation-induced morphological and structural changes in these nanoparticles can significantly influence the macroscopic behavior of the material under swift heavy ion irradiation.

Previous studies have shown that isolated Y-Al-O nanoparticles exposed to ions with electronic energy losses $S_e \geq 8$ keV/nm develop well-defined cylindrical latent tracks, indicating efficient energy deposition with limited heat dissipation [3]. In contrast, nanoparticles embedded in ODS steels behave differently under irradiation. In particular, in the KP4 alloy no

visible tracks are detected even at very high stopping powers (S_e>30 keV/nm, corresponding to 700 MeV Bi irradiation), demonstrating a pronounced matrix effect [4]. At high irradiation fluences (up to 1.5×10^{15} cm^{-2} at 167 MeV Xe ion irradiation), a size-dependent response is observed: irradiation-induced amorphization occurs only in larger particles (~20 nm), whereas smaller nanoparticles (~5 nm) remain crystalline [4].

In this work, we present a transmission electron microscopy study of structural changes in $Y_4Al_2O_9$ nanoparticles irradiated with swift Xe ions. Both isolated nanoparticles and particles embedded in ODS matrices (PM2000, MA956, KP4) are investigated. We analyze the influence of electronic stopping power, nanoparticle size, and the surrounding metallic matrix on the formation of latent tracks.

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Keywords

ODS alloys, Y-Al-O nanoparticles, transmission electron microscopy (TEM), swift heavy ions (SHI), latent tracks.

P24 - From Damage to Recovery: Atomistic Insights into Swift Heavy Ion Response in Pyrochlores

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Pyrochlores are a class of crystalline oxides that have attracted significant interest for applications in the long-term immobilization of radioactive waste. Their suitability arises from their ability to incorporate a wide range of elements into their structure, combined with their inherently high chemical durability. However, long-term performance critically depends on their resistance to radiation damage arising from self-irradiation, which can progressively alter structure and properties over time. Given the large compositional space of pyrochlores, which encompasses hundreds of compounds, not all exhibit sufficient radiation tolerance, making it essential to understand the underlying mechanisms that govern their response to irradiation.

In this work, the effect of swift heavy ions (SHIs) on pyrochlores is investigated using a coupled two-temperature model and molecular dynamics framework. This approach provides a physically realistic description of the phenomena by accounting for the role of the electrons during irradiation, while simultaneously considering the structural evolution of the lattice. Two representative systems are considered: the ordered cubic pyrochlore $Ho_2Ti_2O_7$ and the defect-fluorite $Ho_2Zr_2O_7$, allowing direct comparison between structurally distinct but compositionally related materials. By analyzing their response to SHI irradiation at the atomic level, we identify key properites that enable recovery and prevent permanent damage. Rather than relying on compositional predictors, this study highlights how crystal structure and atomistic interactions

collectively determine whether a material recovers or accumulates permanent damage. These findings provide deeper insight into radiation effects in pyrochlores and pave the way for the rational design of oxide materials with improved radiation tolerance.

Keywords

SHI, pyrochlore, molecular dynamics, two-temperature model

P25 - Charge-State Effects on Swift Heavy-Ion Damage in Bismuth Nanowires

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Irradiation experiments were performed by exposing nanowires to swift heavy ions with different initial charge states. When ions enter a material with non-equilibrium charge state, their charge, and consequently the electronic energy loss, evolves rapidly within the near-surface region, typically over the first tens to hundred nanometres [1,2]. In nanostructures with dimensions comparable to or smaller than this equilibration depth, these effects become particularly pronounced [3]. In this work, we investigate how the initial charge state affects heavy-ion-induced damage in bismuth nanowires as a function of their diameter and determine the charge equilibration depths for these nanostructures.

Bismuth nanowires of systematically varied diameters of 20, 30, and 50 nm were fabricated by electrodeposition into ion-track etched polycarbonate templates. After template removal and transfer onto TEM grids, nanowires were irradiated at the M-Branch of the UNILAC (GSI Helmholtz Center) with 4.8 MeV/u Au ions at three selected charge states: 25^+, 54^+, and 60^+. Ion-induced structural modifications were analysed by scanning transmission electron microscopy (STEM in SEM), high-resolution TEM and electron energy-loss spectroscopy (EELS), complemented by SEM imaging of surface morphology. Experimental observations are compared with charge-state evolution calculations performed using the ETACHA4 code [4].

Our results demonstrate that damage formation in bismuth nanowires is governed by the interplay between charge-state evolution and nanowire diameter. Distinct and opposite trends are observed for ions below and above equilibrium charge state converging toward that of equilibrium conditions as the nanowire diameter increases. These findings underline the importance of accounting for non-equilibrium charge-state effects when assessing radiation damage and resilience in nanoscale systems.

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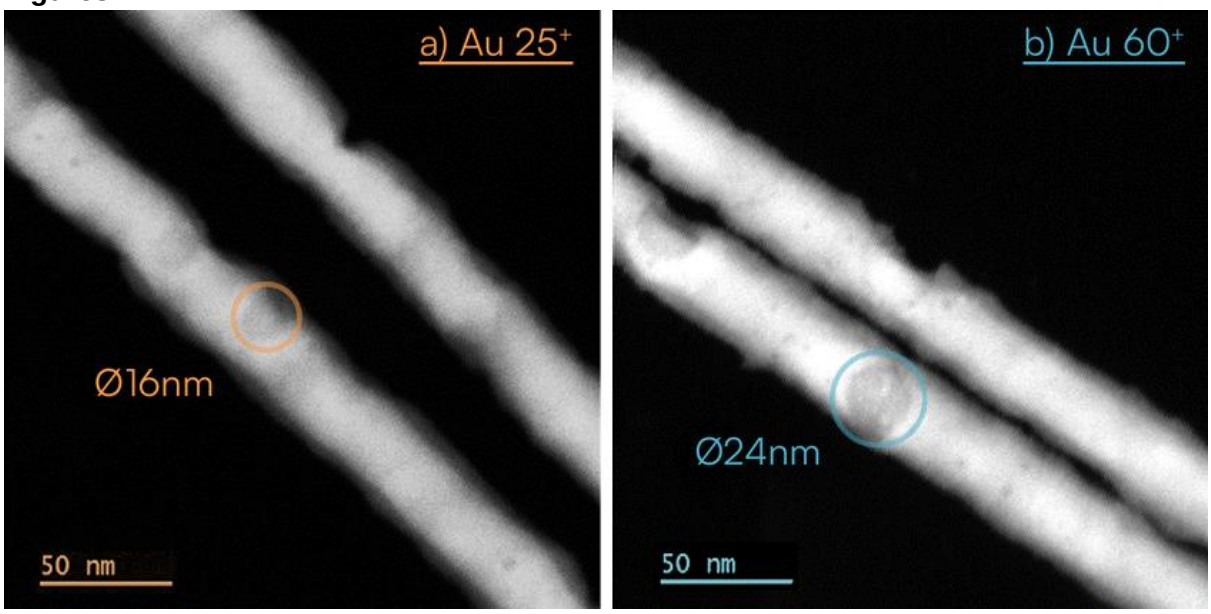
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Keywords

Ion Charge State, Swift Heavy Ion Irradiation, Bismuth, Nanowires

Figures



P26 - Cross section of nonionizing electron scattering with finite coherence length

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Transport of excited electrons and their energy exchange with an atomic lattice in swift heavy ion tracks are commonly modelled with Monte Carlo transport codes [1]. They rely on differential cross sections describing the interaction between electrons and atoms.

The Rutherford cross section works well for nonionizing scattering of fast electrons with wavelengths smaller than the lattice constant. In contrast, the Van Hove cross section [2] is suitable for slow electrons with a wavelength exceeding the lattice constant, which describes both phonon scattering and scattering on the static lattice.

We have bridged the gap between these two limiting cases, unifying the description of the scattering for arbitrary (nonrelativistic) electron energies.

A common approach to this problem, in which the electron is represented as a wave packet, encounters the issue of the packet spreading. To circumvent it, we considered that an electron

moving through a medium experiences decoherence, since its wave functions become entangled with the medium [3]. In this case, the scattering can be described in terms of the density matrix, which we take in the form: , where is the electron coherence length, which in our model is proportional to its de Broglie wavelength. Accounting for the finite coherence length (FCL) enabled us to incorporate a finite scattering time in the model.

The FCL cross section used naturally describes the three modes of scattering with increasing energy of the incident electron (decreasing wavelength): (i) scattering on phonons, (ii) scattering on the static lattice, and (iii) scattering on isolated atoms accounting for the dynamical screening (DS) by their core electrons. We observe these modes not only in the total scattering cross section but also in the angular dependence of the differential cross section.

The energy dependence of the electron mean free path in SiC obtained using the FCL cross section is shown in Fig. 1, which reproduces the limiting cases of the Rutherford and Van Hove mean free paths, while showing complex behavior in between.

Fig. 1. The nonionizing mean free path of electrons in SiC with FCL, Rutherford, and Van Hove cross sections.

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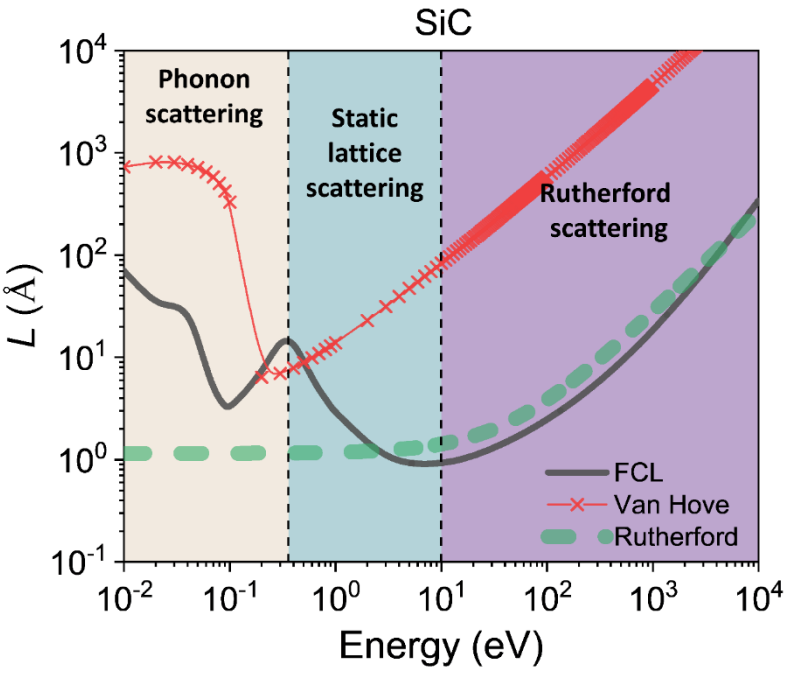
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Keywords

scattering cross section; decoherence; dynamic screening



P27 - Electronic stopping for H, N and Ga projectiles in GaN from first-principles

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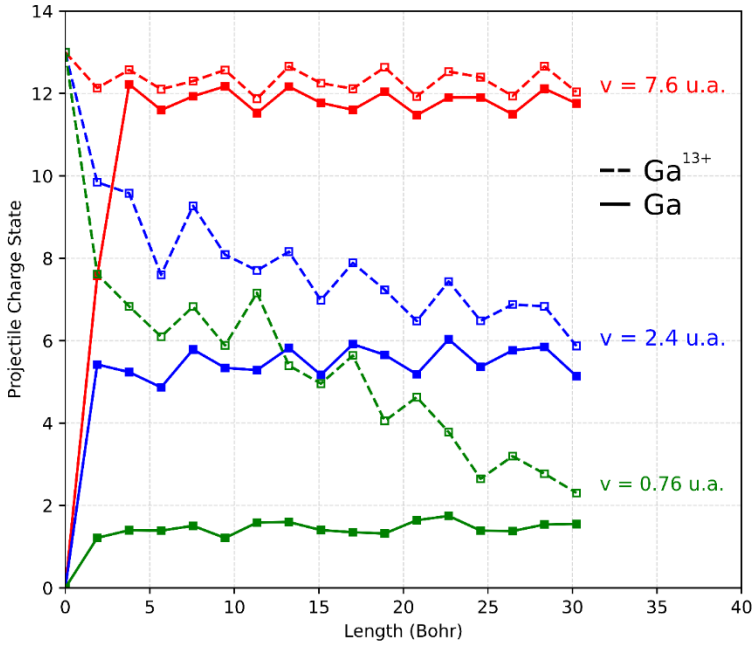
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Gallium nitride (GaN) is a material of interest for high-power and high-frequency microelectronic components operating in extreme environments such as space or other high-radiation settings, where devices are continuously exposed to energetic particles. However, despite its technological relevance, available experimental data on the electronic stopping (ES) power behaviour in GaN are sparse, leading to potential large uncertainties in modelling tools based on experimental data such as SRIM. First-principles calculations used to calculate ES could thus bring insights for GaN.

In this contribution, we use real-time Time Dependent Density Functional Theory (rt-TDDFT) to compute ES in GaN. We examine channeling directions, evaluating the effect of different impact parameters, as well as selected off-channeling directions to obtain average ES from first principles. This approach enables direct comparison with existing experimental data and with SRIM predictions. We calculate the ES of protons in GaN over a broad energy range and compare our results with the empirical SRIM model, highlighting regimes where first-principles calculations refine or correct existing estimates. We identify a kink velocity around v = 0.3 a.u. which we believe comes from the excitation of d-electrons. Finally, we extend the study to heavier projectiles and investigate the evolution of their charge states (Fig. 1) to assess the influence of the projectile's initial charge state on the ES. We observe that the projectile equilibrium charge state is a lot longer to reach when the projectile is initially charged than when it is initially neutral.

Keywords

Electronic stopping power, RT-TDDFT, GaN, channeling, Charge-state



P28 - Simulating atomic collisions: theoretical and computational challenges

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In recent years, *ab-initio* computational methods, such as time-dependent density functional theory (TDDFT), have become an important tool in supplementing experimental data on colliding ions and electrons with molecules and solids. Although seemingly straightforward, practical application of these methods is met with a variety of challenges regarding the setup of collision simulations, as well as processing simulation results. For example, when using a real-space type TDDFT code, such as Octopus[1], care must be taken when choosing reasonable values for parameters like time step, grid spacing, box size etc. to ensure both accuracy and numerical stability while retaining the feasibility of the simulation in terms of memory requirements and execution speed. By simulating the collision of C_2^+ ions on the graphene flakes, we investigate the impact the aforementioned and other parameters on the simulation outcome in detail. We show how small deviations from optimal parameter values can sometimes lead to qualitatively different results. Our simulations are carried out using Octopus code and are benchmarked against experimental results. At last, we introduce VIKING[2]: a free, user-friendly web interface (available at www.viking-suite.com) which provides an intuitive and easy way to set up and run collision and other types of nanoscale simulations. VIKING not only executes various state-of-the-art programs on a user's behalf on a computational facility, but it also manages all technical details of a typical simulation pipeline, including parameter validation as well as collection and analysis of the results. This way, VIKING greatly facilitates computational exploration on the nanoscale level, especially for novices and non-experts.

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Keywords

simulation, TDDFT, collision, VIKING

P29 - Simulating radiation in matter: how close can we get?

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The radiation resistance of nuclear materials is notoriously difficult to characterise, with licencing, shielding, transportation, and training all presenting formidable obstacles to an institution setting up experimental studies of fundamental and applied nuclear materials research. For this reason, the community has leaned heavily on theory and simulations in order to infer material degradation and inform nuclear materials design. Meanwhile, ion beam irradiation offers an accessible and efficient method to introduce a given fluence, or energy, to a material, however the method of energy deposition and subsequent non-equilibrium effects at the atomic scale are completely different between swift ions and recoil nuclei. The ability of ion beam irradiation to act as a surrogate for experimentally inaccessible environments is therefore predicated on a comprehensive understanding of energy deposition and relaxation in condensed matter.

Here, we give a perspective the state of molecular dynamics simulations in the context of this “incomplete bridge” between experiments and theory. As materials simulations techniques become more sophisticated and computational power ever grows, simulations become more accessible and best practice becomes increasingly important. Using work on two nuclear ceramics: iron phosphate and lithium metatitanate, we explore how analytical model framework, interatomic potential choice, integration algorithms, and the handling of electronic stopping affect molecular dynamics trajectories, and to what extent the observed phenomena constitute faithful physical mechanisms. We will conclude with an outlook on how further methods development can help bridge the gap between theory and experiments, and on how the simulations community can better align with experimental data.

Keywords

molecular dynamics; radiation cascades; electronic stopping; threshold displacement energy; ceramics;

P30 - Orientation effects of MeV C_{2+} ions on secondary electron emission from graphene: Combined experimental and theoretical study

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The transfer of energy in ion-solid interactions is significantly influenced by electronic excitation during the initial collision phase. Studying these dynamics, particularly with cluster ions in conventional solid targets, poses two main challenges. First, as the cluster’s individual atoms move through the solid, their increased internuclear distances complicate the determination of molecular orientation at the moment of collision. Second, the secondary electrons (SEs) produced undergo transport processes, such as multiple scattering and energy loss, which obscure information about the initial excitation. To address these challenges, we used self-supporting single-layer graphene, which allows us to study collision dynamics under conditions suitable for single collisions. In this study, we focused on how the

molecular axis orientation of 3.6 MeV C_2^+ ions influences the energy distributions of secondary electrons generated.

To explore the relationship between SE emission and projectile orientation, we conducted event-by-event coincidence measurements. We collected SE energy spectra using a tandem-type electron spectrometer, while the corresponding orientation angles were determined using the foil-induced Coulomb explosion method. Our results indicate that the yield of secondary electrons is higher when emitted in the forward direction compared to the backward direction. Notably, in forward emission, there is a clear orientation dependence: when the molecular axis is aligned parallel to the beam, the SE yield near the peak of the distribution (around 5 eV) increases. Conversely, the energy distributions of SEs emitted backward showed no significant orientation dependence across the entire energy range.

To evaluate these experimental findings, we performed real-time time-dependent density functional theory (RT-TDDFT) simulations. The theoretical results align well with our experimental observations in three key aspects: (1) the asymmetry between forward and backward yields, (2) the orientation dependence near the peak of the forward SE distribution, and (3) the lack of orientation effects in the backward emission. Based on the consistency between the experiments and simulations, we will discuss the electronic excitation processes that occur within a few femtoseconds following the collision. Specifically, by calculating the SE energy distributions for individual impact positions on the graphene lattice, we provide a microscopic analysis that enhances the spatially averaged experimental results.

Keywords

secondary electron emission, swift clutser ion, graphene, TDDFT

P31 - Structural and Functional Evolution of GST Thin Films under Carbon Ion Irradiation

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Phase-change materials (PCMs), particularly ternary Ge-Sb-Te (GST)-based alloys, represent promising systems for modern technologies, including memory devices, neuromorphic computing, and advanced sensor technology. However, their broader application is limited by two factors: the thermal instability of the amorphous phase restricts reliable switching at elevated temperatures and the drift in electrical resistance caused by structural relaxation hinders their overall performance.

Our research focuses on the targeted modification of GST thin films deposited on glass substrates using carbon (C) ion implantation. Previous studies indicate that the irradiation of GST with light elements, such as carbon, introduces stabilizing defects into the structure. This process has been shown to significantly increase the crystallization temperature and mitigate resistance drift. To investigate this phenomenon, GST layers were exposed to C ions at an energy of 800 keV, at fluences ranging from 1×10^{12} to 1×10^{16} cm^{-2}. A combination of analytical

techniques was utilised to comprehensively evaluate the effects of implantation on the material. Elemental depth profiles, dopant distribution, and layer stoichiometry were analysed using Rutherford Backscattering Spectrometry (RBS) and Elastic Recoil Detection Analysis (ERDA). Changes in chemical states and vibrational modes across the layer profile were investigated via X-ray Photoelectron Spectroscopy (XPS) and Raman Spectroscopy. The effect of the ion beam on surface homogeneity and topography was monitored using Atomic Force Microscopy (AFM) and Scanning Electron Microscopy (SEM).

The primary objective of this study is to correlate the structural and compositional modifications with the macroscopic functional properties of the material. We evaluate the effect of ion fluence on the modulation of electrical conductivity, the shift in the structural phase transition temperature, and the potential of these modified layers for applications in electronics and sensor technology. The results demonstrate that controlled defect engineering via ion implantation is an effective tool for optimising the optoelectronic and sensing properties of p-block tellurides.

Keywords

GST, chalcogenides, carbon ion implantation, phase transitions, defect engineering

P32 - Vacuum compatible printed circuit board anodes for particle detection with electron multiplier devices

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Electron signal amplification devices, including microchannel plates (MCPs) and channeltron electron multipliers (CEMs), are widely used in particle detection and beam diagnostics for both industrial applications and R&D. To capture and analyze the amplified electron output, different anode configurations are employed, enabling the extraction of spatial and/or temporal characteristics from the charge distributions produced by particle impacts [1].

In this work, we introduce a novel anode concept utilizing ultra-high-vacuum-compatible polyimide laminates as a substrate for printed circuit board (PCB) layouts [2]. This design provides outstanding timing performance by incorporating polyimide-core decoupling capacitors and impedance-matched transmission lines directly on top of the substrate [3]. Unlike conventional approaches that depend on external decoupling electronics, our design integrates an *in vacuo* high-pass filtering stage, allowing fast timing signals to be extracted with increased bandwidth and enhanced signal-to-noise ratio. This results in a higher detection efficiency for MPCs as well as in increased energy resolution for time-of-flight, coincidence and pump-and-probe experiments. Furthermore, the concept supports customizable arrangements of parallel, segmented anode regions, enabling spatial discrimination of particle impact positions, for instance in combination with an MCP.

Thanks to the flexibility of the laminate material, flat waveguide strips can be implemented, and sections of the PCB can be bent in various directions without compromising mechanical integrity or electrical performance. Compared to rigid coaxial cables commonly used for high-frequency signal transmission, these printed waveguide-like structures offer clear advantages, particularly in compact vacuum environments. Overall, this technology opens up new possibilities for compact, application-specific, and more sophisticated in-vacuum electronic circuits.

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Keywords

MCP, vacuum electronics, printed circuits boards, impedance matching, high-speed anodes

P33 - First principles parametrization of electron-phonon interaction in swift heavy ion irradiation

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Recent experiments showed that swift (high-energy) heavy ions (SHI), when passing through a solid such as a diamond, leave a trail of nitrogen-vacancy (NV) centers along the track [1]. An NV center is a vacancy defect that forms a two-state system that can function as a qubit. This observation indicates the possibility of creating thousands of qubits over several micrometers, which is beneficial for quantum computing.

To guide the experiments on controlled defect formation, computational models are needed. However, most of the existing models rely on experimental data and can be applied only to metals. The two-temperature model (TTM) is a widely used approach to simulate SHI-induced effects in materials. It is based on two heat diffusion equations coupled through the electron-phonon coupling constant *G*. In this work, we implement the first-principles parameterization of the TTM, making it applicable to semiconductors and insulators.

We verify our approach by conducting simulations on various well-studied metallic structures (aluminum, nickel, gold, and titanium). The obtained *G*-constant values are compared against the existing data [2], showing a good agreement. Additionally, we apply our model to semiconductors and insulators. The consistency in the results highlights the potential of this method for further applications in experiments.

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Keywords

Swift heavy ion irradiation, electron-phonon coupling, two-temperature model, nitrogen-vacancy centers, first-principles calculations

P34 - FTIR Study of Ion Irradiation and Thermal Effects on Magnetron-Sputtered Amorphous Oxides

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Thin films based on SiO_2, Al_2O_3, and MgO were fabricated via magnetron sputtering. Their elemental composition was verified using elastic recoil detection analysis. The prepared layers were then subjected to irradiation using several ion beams (23 MeV I, 18 MeV Cu, and 2.5 MeV Cu, in addition to gamma-ray exposure. Furthermore, all samples underwent annealing at a range of temperatures to examine the effect of thermal treatment. Post-irradiation and post-annealing characterisation was carried out using infrared spectroscopy. The findings demonstrate a notably high resistance of all oxide films to radiation damage under both ion and gamma irradiation conditions, while the observed changes in the infrared spectra after annealing were attributed to early-stage c within a predominantly amorphous matrix.

Keywords

sputtering, amorphous oxide, FTIR, irradiation, annealing

P35 - RADIATION FROM POSITRONS CHANNELED IN THE SYSTEM OF FAN-ORIENTED HALF-WAVELENGTH SILICON CRYSTALS

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Over the past decade, numerous experiments have been conducted on the channeling [1] of relativistic particles in crystals. These studies include investigations of electron dechanneling at GeV energies under planar channeling conditions [2], as well as the deflection of proton and ion beams in bent crystals [3]. Special attention has been given to channeling radiation of relativistic electrons in periodically bent crystals [4]. The phenomenon of rainbow scattering of electrons in ultrathin crystals was also predicted theoretically and confirmed experimentally [5].

Further progress has been achieved in beam steering using half-wavelength crystals (HWC) [6, 7]. These studies demonstrated that HWC channeling is a novel efficient method for controlling proton [8] and electron [9] beams, with deflection efficiencies reaching 58% and 29%, respectively. To increase the deflection angle, systems of fan-oriented HWCs have been proposed [10], allowing ion beams to be deflected by several critical channeling angles according to numerical simulations.

Of particular interest is the radiation spectrum formed during electron channeling in such systems. The radiation includes contributions from both under-barrier and over-barrier electrons, with their relative contributions depending on the incidence angle. Numerical simulations for 255 MeV electrons in silicon HWCs aligned along the (111) planes show a rapid decrease in radiation intensity with increasing incidence angle [11].

In the present work, we report, for the first time, numerical simulations of 255 MeV positron trajectories in a system of three fan-oriented silicon HWCs. Angular beam distributions in each crystal are calculated, and the radiation spectra in the forward direction are analyzed.

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Keywords

positron, channeling, channeling radiation, half-wavelength crystal

P36 - Controlling the maximum impact parameter in BCA simulations

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One of the merits of the TRIM computer program [1,2] was the introduction of an energy dependent free flight path (FFP), which leads to a drastic reduction in simulation times at high energies while still including all relevant collisions at low energies. This was achieved by using relationships between the average scattering angle and the path length, and between the minimum energy transfer to recoils and the maximum impact parameter (pmax) used in the simulation. To avoid numerical integration during simulation, analytic approximations to these relationships are used in TRIM [1,2]. They are specific to the ZBL interatomic potential.

Recently, new interatomic potentials have been proposed for all pairs of atomic numbers [3]. In addition, finite-range versions of these potentials have been developed for use in BCA simulations. Significant differences at high energies and huge differences at low energies compared to the ZBL potential have been found [4]. Apparently, the TRIM formulae for the FFP length would be inaccurate when used with the new interatomic potentials.

In this contribution, I present a unified framework for determining pmax for arbitrary, purely repulsive interatomic potentials including finite-range ones. It will be shown that the impulse approximation provides a close upper limit to the smallest pmax which guarantees that only scattering angles and energy transfers below chosen limits are neglected. The calculation of pmax involves the numerical evaluation of an integral. This can be done during the initialization phase to generate tables of energy-pmax pairs for use during trajectory simulation. From pmax, the mean FFP length in amorphous targets is calculated as to guarantee the correct atomic density of the target.

The algorithm has been implemented in our BCA codes [5,6]. Beyond its application in the bulk of amorphous targets, like in TRIM, it may also be used with a smaller angle limit to include gentle collisions during the reflection of glancingly incident ions at surfaces and during channeling in crystalline targets.

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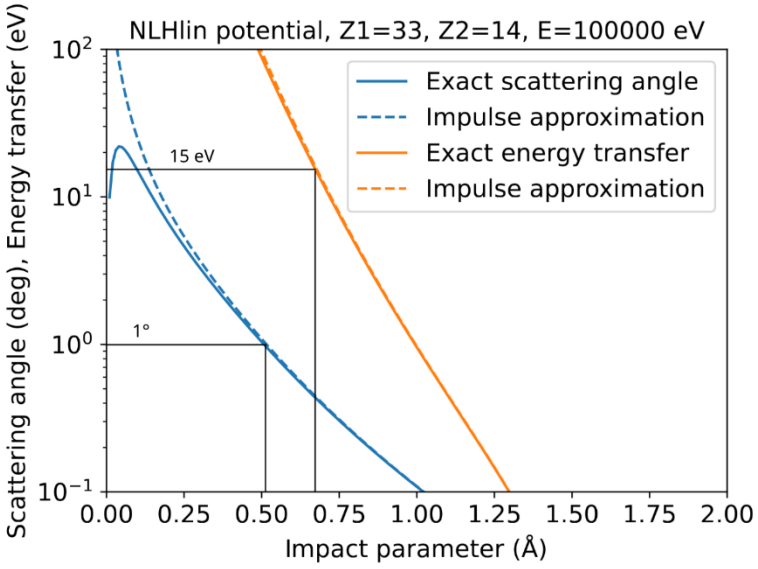
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Keywords

Binary collision approximation; impulse approximation; free flight path



P37 - The role of irradiation temperature on optical and structural properties of swift heavy ion irradiated alumina

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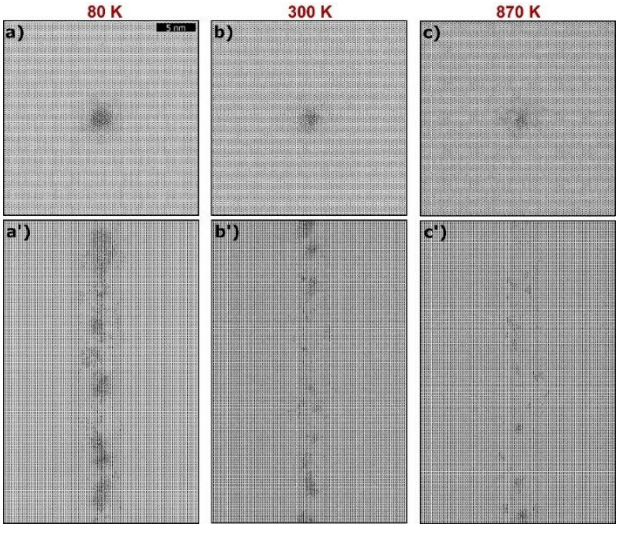
Aluminum oxide α-Al_2O_3 exhibits excellent mechanical, optical, and electrical properties, which account for its wide application in various fields of science and technology. In addition, the high radiation resistance of corundum makes it one of the promising materials for use in nuclear and thermonuclear energy, which is why it has remained an object of systematic research for a long time.

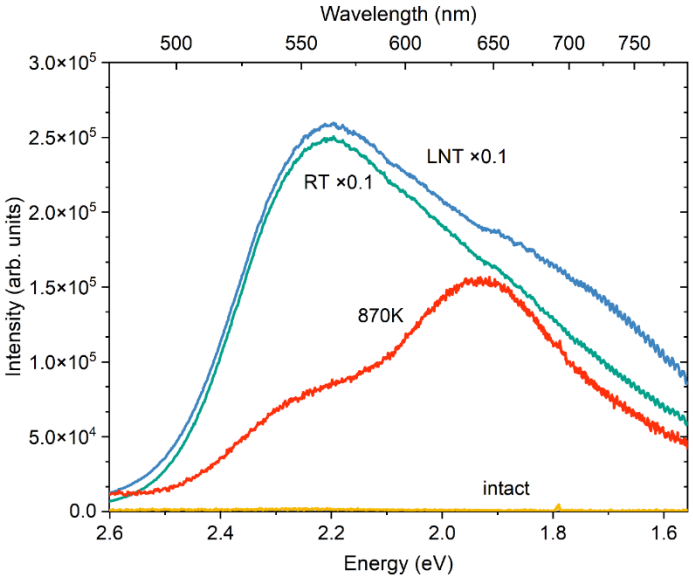
In this work, the effect of irradiation temperature by high-energy Xe ions on the defect morphology and optical characteristics of single-crystal aluminum oxide was studied. Electron microscopy analysis and molecular dynamics modeling showed that the impact of swift heavy ions leads to the formation of specific radiation damage in the near-surface region — latent tracks, which are nanometer-scale cylindrical zones containing clusters of vacancy-type defects located along the ion trajectory. The morphology of the tracks strongly depends on the irradiation temperature: at low temperatures (77 K), an increased accumulation of defects is observed, whereas at 300 K and especially at 870 K, the higher mobility of point defects leads to partial relaxation of radiation damage.

Photoluminescence measurements, including time-resolved spectroscopy, showed that excitation at a wavelength of 445 nm stimulates emission whose spectral composition changes with irradiation temperature. It is assumed that the observed broad, overlapping bands with maxima at 560 nm, 630 nm, and 775 nm, and characteristic lifetimes in the range of 1-10 ns, are associated with three different states of F_2^{2+} color centers.

Keywords

Aluminum oxide, swift heavy ions, photoluminescence, ion tracks, radiation damage





P38 - Swift heavy ion irradiation of astrochemical model systems with in situ analysis for cosmic radiation simulation

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Complex organic molecules have been detected in the interstellar medium (ISM) and in protoplanetary discs, both in the gas phase and increasingly also in the solid phase through observations with the James Webb space telescope (e.g.[1-3]. These molecules are thought to form in the solid phase within the ISM, where particles and molecules are exposed to various types of electromagnetic and particle radiation.

Among these, heavy ions are of particular interest because they deposit large energy densities in highly localized regions. This leads to very specific effects on sputtering and radiolysis of molecules, as well as on the morphology and structure of cosmic dust analogs. Although heavy ions represent only a minor fraction of cosmic radiation, their specific interaction mechanisms must be considered separately to obtain a complete picture of chemical processes in the ISM.

Here, we provide an overview on the in situ experimental techniques available at the M-Branch of the GSI heavy ion accelerator facility, including ice deposition, FTIR and Raman spectroscopy, X-ray diffraction and time-of-flight mass spectrometry for the detection of secondary ions and neutrals. We highlight selected results from various experimental user campaigns on the radiolysis and desorption of complex organic molecules. Additionally, we discuss the role of dust grain surfaces in promoting the formation of new molecular species in irradiated ices, an aspect that is often neglected in studies on the effects of cosmic radiation

(cf. section 37 in [4]), and present new results on evolution of ices on cosmic dust analogs and the analogs' surface properties, obtained both at M-Branch and IRRSUD at the GANIL facility in Caen, France.

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Keywords

swift heavy ions, cosmic rays, astrochemistry, cosmic dust, ice

P39 - Ion Beam Shaping of Catalytic Nanoparticles

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Metallic nanoparticles can be used to catalyze chemical reactions, such as the water gas shift reaction, an important step in the production of hydrogen through steam methane reforming [1]. The catalytic performance depends heavily on the size and shape, as well as the composition of the nanoparticle [2]. An interesting path to optimize catalytic particles is shaping them such that more surface atoms at low-coordinated sites are exposed to the reactant.

We investigated ion beam irradiation as a method of shaping spherical 10nm AuCu alloy particles. Nanoparticles deposited on glassy carbon substrates were irradiated with 2 keV Ar^+ beams. The samples were measured using atomic force microscopy (AFM) before irradiation and after fluences of 0.5 ions/Å^2 and 1.0 ions/Å^2. AFM shows a decrease in the average height of the particles after irradiation.

This process was also simulated using the binary collision approximation code SDTrimSP-3D. Simulation results show that the spherical particles are eroded into a conical shape at fluences between 0.5 ions/Å^2 and 1.0 ions/Å^2. Beyond 2.0 ions/Å^2, the nanoparticles are almost fully removed. The simulated heights of the irradiated nanoparticles coincide with the AFM results. The simulations also predict an enrichment of Au on the surface of the nanoparticles.

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Keywords

nanoparticles, catalysis, sputtering, ion beam

P40 - CasP Express: A Web-Based Platform for Swift Ion-Solid Interaction Calculations

Henrique Fonteles[1], Flávio Mathias[2], Douglas Newton Bilhalva[1], Felipe Ferreira Selau[1], Raul Fadanelli[1], Gustavo Azevedo[1], Henrique Trombini[3], Johnny Dias[1], Pedro Luis Grande[1]

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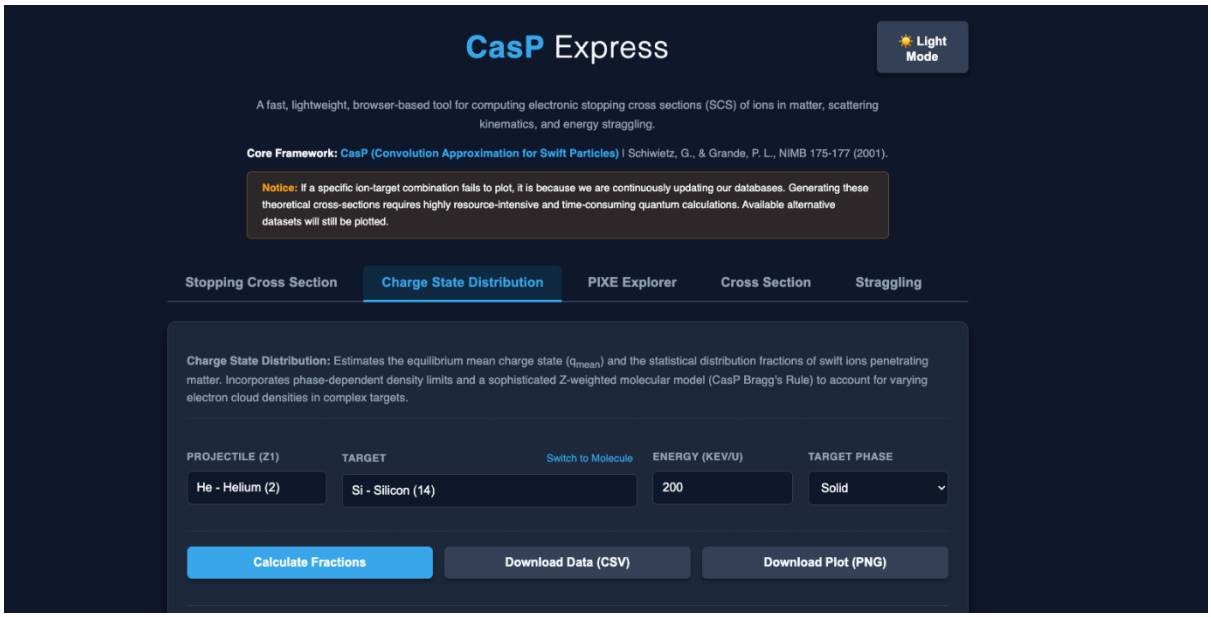
Accurate modeling of ion-solid interactions is fundamental to the advancement of ICACS/SHIM community. However, accessing state-of-the-art theoretical calculations often requires researchers to navigate complex, computationally heavy codes or compile legacy software. To bridge the gap between rigorous theoretical physics and modern accessibility, we introduce ***CasP Express***, a fast, lightweight, and fully browser-based application designed to compute and visualize swift ion interactions with matter on the fly.

Built around the Convolution Approximation for Swift Particles (CasP) parametrization framework, the platform utilizes a modular, client-side JavaScript architecture that eliminates the need for server-side processing. CasP Express centralizes millions of pre-calculated data points into an intuitive interface, allowing users to instantly evaluate and compare multiple physical phenomena. The application features five core modules: **(1) Stopping Cross Sections (SCS)**, which overlays CasP 6.0 data, analytical Double Konac fittings, SRIM tables, and the IAEA experimental database; (**2) Charge State Distributions**, for gases and solids. Besides the CasP data, the plataform offers **(3) PIXE Cross Sections**, interrogating ISICS-generated databases (PWBA and ECPSSR) alongside Helmut Paul's empirical database for protons; **(4) Differential Scattering Cross-Sections**, computing exact laboratory-frame cross-sections using analytical screened potentials; and (**5) Energy Straggling**, which implements updated straggling formulas and intra-atomic electron bunching effects.

We present this tool as both a powerful analytical resource for experimentalists in the laboratory and an interactive pedagogical platform for the broader IBA community.

Keywords

CasP; Ion Beam Analysis; Stopping Cross Section; Energy Straggling; Charge State



P41 - Characterization of SpaCal-Pb Modules and a Novel Deep-Drilling Technique for the PicoCal Calorimeter of Large Hadron Collider beauty (LHCb) experiment

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After the second major upgrade (Upgrade II), the Large Hadron Collider beauty (LHCb) experiment will operate at a peak luminosity of about $1 \cdot 10^{34}$ $cm^{-2} \cdot s^{-1}$ and accumulate 300 fb^{-1} of pp collision data. At this luminosity, the electromagnetic calorimeter will face a substantial increase in accumulated radiation dose (up to 10^{16} $n \cdot cm^{-2}$) and channel occupancy, motivating the development of the new PicoCal calorimeter with radiation resistant spaghetti-type modules (SpaCal). The electromagnetic calorimeter of the LHCb experiment is scheduled for a two-phase upgrade. The first phase, during CERN Long Shutdown 3 (2026-2029), will introduce two new spaghetti-type module technologies (SpaCal-Pb and SpaCal-W). The second phase, the PicoCal upgrade (2034-2035), will further increase granularity in the inner region and introduce timing capabilities.

The SpaCal-Pb modules consist of a lead absorber with containing a 56×56 array of channels (1.6 mm diameter) filled with scintillating fibres. The inter-channel wall thickness is below 0.5 mm. Located in the central region of the calorimeter, these modules are subjected to a static load from the overlying structure of approximately 1 ton per module. This imposes stringent requirements on compressive strength and long-term dimensional stability, as the channel geometry must remain stable over the detector's 15-year lifetime.

For the LS3 upgrade, SpaCal-Pb modules are produced using a low-pressure casting technique. For the subsequent PicoCal phase, the significantly increased number of modules motivates further technological optimization. A novel deep-drilling technique for lead absorbers, initially developed at the CERN Main Workshop, has been transferred to industry, with multiple prototypes manufactured in Karaganda, Kazakhstan.

This work presents the characterization of prototype absorbers made during the R&D process. Neutron tomography at the WWR-K pool-type reactor (Institute of Nuclear Physics, Almaty, Kazakhstan) was used. The technique demonstrated the effectiveness of non-destructive testing for assessing module structural integrity and will be applied at the mass production stage for quality verification. Short-term uniaxial compression tests and creep measurements conducted over 1100 hours showed higher strength values for casting prototypes though both modules satisfy the applicable technical requirements. Due to the limited data on radiation effects in lead alloys, neutron irradiation experiments at the WWR-K reactor are currently being prepared to assess modules performance up to the maximum expected fluence of $1 \cdot 10^{16}$ n/cm^2 in the PicoCal calorimeter.

Keywords

LHCb, Lead, Neutron tomography, strength, neutron irradiation

P42 - Ionization Cross Sections of Hydrogen Molecule by Electron and Positron Impact

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We present ionization cross sections of hydrogen molecule by electron and positron impact for impact energies between 20 and 1000 eV. The calculations were performed classically using a three body CTMC approximation where the H_2 target is described using a central core and a single active electron approximation [1]. We found that using this model the total cross sections for positron impact agree reasonably well with experimental data. For electron impact our calculated cross sections are in good agreement with the experimental data in impact energies between 80 eV and 400 eV but are smaller at higher impact energies and larger at lower impact energies.

In the intermediate energy region where good agreement with experimental total ionization cross sections was found, the singly differential cross sections were also analysed. For the case of energy distributions an excellent agreement with experimental data was found with no differences associated with the sign of the projectile charge. However, the angular distributions for electron ejection by positrons and electrons have shown noticeably differences. We present also impact parameter information for total and differential ionization. For total ionization the most notable feature is a shift toward smaller impact parameters with increasing impact energy. For differential ionization, the average impact parameters for positron and electron impact were quite similar for the scattered projectile and for lower energy electron emission but quite different for higher energy emission and for all ejection angles.

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Keywords

classical trajectory MonteCarlomodel; ionization; chargeexchangecrosssections; electron impact processes; positron impact processes

P43 - Irradiation effects of 25 MeV Cu^{7+} ions on the electrical characteristics of $CsSnBr_3$ thin films

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Perovskite thin films have garnered a lot of interest in photovoltaics in recent years as Generation III semiconductors due to their relatively low production cost and favourable optoelectrical properties. Device instability due to environmentally induced structural and electronic defects unfortunately still hinders widespread production of perovskite based solar cells. Swift Heavy Ion (SHI) irradiation, at appropriate doses, has been used in traditional generation I & II semiconductors for suppression of intrinsic defects. Not much has been reported in the literature on SHI effects on generation III semiconductors like perovskites. This study presents results of an experimental investigation carried out to determine the effect of

SHI irradiation on the electrical properties of CsSnBr3 thin films. The films were grown on flexible polyethylene terephthalate substrates, coated with aluminium, using thermal deposition. Schottky contacts were then formed on the perovskite layer through Au-deposition via RF magnetron sputtering. The irradiation runs were performed using 25 MeV Cu7+ ions (ion energy chosen to completely traverse the layer stack) for different doses ranging from 1011 - 1013 ions/cm2. Current-voltage (I-V) measurements were then carried out over several weeks post-irradiation to monitor temporal variation of the electrical characteristics (barrier height, ideality factor and reverse saturation current) of the irradiated devices. The observed trends are discussed in terms of the evolution of the charge transport properties of the irradiated devices over the monitoring period.

Keywords

perovskite, ion irradiation, defects, Schottky

P44 - Ion-Induced Chemistry in H_2O:CO:NH_3 astrophysical ice analogues

Cíntia Aparecida Pires da Costa[1], Ana Lucia Ferreira de Barros[2, 3], Adeline Garcia[1], Thibault Nguyen Trung[2], Sreeja Raghunandanan[2], Ricardo Carrasco-Herrera[1], David Dubois[2], Hermann Rothard[2], Alicja Domaracka[2], Alexis Bouquet[1]

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Due to low temperatures, molecules tend to condense into the solid phase in astrophysical regions (such as in comets or in ice mantles on dust grains). Energetic particles from the solar wind, planetary magnetospheres [1], or galactic and extragalactic cosmic rays [2] continuously impact the surfaces of bodies such as asteroids, moons and comets, interacting with molecules present in astrophysical ices, usually embedded in water and carbon oxide ices. Since the interaction with incoming radiation depends on the surrounding ice matrix, it is important to investigate the dependence of destruction cross sections on concentration, when the target molecules are embedded in analogues of interstellar ices to determine their radioresistance. Interstellar ice mantles are mainly made of H_2O, but they also contain a variety of other small molecules such as CO_2, CO, CH_3OH, and NH_3 [3]. From these small compounds, cosmic ionizing radiation may drive the formation and destruction of more complex molecules. Samples of H_2O:CO:NH_3 ice mixtures at 10 K and at concentrations of 10:0:1, 5:0.7:1, 3:0.8:1, and 1:1:2, have been irradiated using 40 MeV Ar^{9+}, as a projectile to mimic heavy ions present in the interstellar medium, at the IRRSUD beamline at the Grand Accélérateur National d'Ions Lourds (GANIL). The evolution of the samples with the beam fluence was followed by in situ Fourier Transform Infrared (FTIR) spectroscopy. Figure 1 shows the decrease of the precursor molecules (H_2O:CO:NH_3) with increasing fluence, as well as the formation of the main product detected, CO_2. For all the samples at different concentrations, water exhibits a slow, nearly linear decrease due to its high radioresistance. Destruction cross sections of CO and NH_3 are close and in the order of 2×10^{-13} cm^2. The formation of CO_2 is slightly more efficient at samples with mixtures with lower water content, with formation cross sections in the order of 5×10^{-15} cm^2. A multilayer deposition procedure was also employed to produce a solid residue to be analyzed by ex situ GC-MS (Gas

chromatography Mass Spectrometry). Figure 1 shows the results of the irradiation of the first layer, which is ~0.8 µm thick. From layer 2 to layer 8, each layer was ~2.5 µm thick. New irradiation products to be identified were detected in the infrared spectra only after layer 2 (as small features at 2276, 2092, and 657 cm^{-1}).

Figure 1: Column density evolution of H_2O (Band 760 cm^{-1}), CO (Band 2139 cm^{-1}), NH_3 (1300-950 cm^{-1}), and CO_2 (Band 2342 cm^{-1}) as a function of projectile fluence (40 MeV Ar^{9+} beam).

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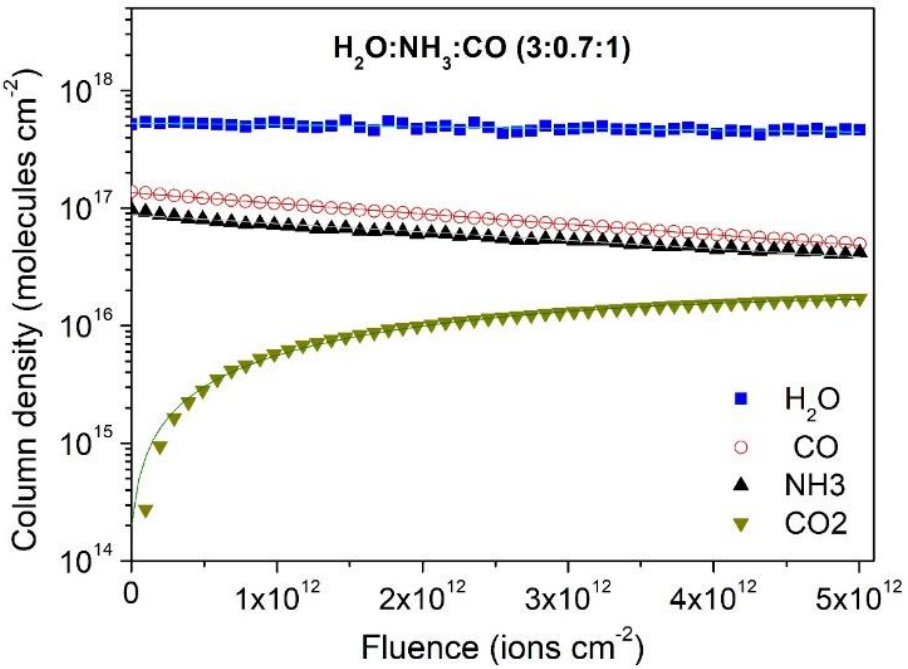
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Keywords

Ion irradiation; astrophysical ices; infrared; astrochemistry.



P45 - Improved photocatalytic degradation of rhodamine B over MoS_2/PET heterostructures modified by MeV ion irradiation

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Two-dimensional (2D) nanomaterials, particularly transition metal dichalcogenides (TMDCs) like molybdenum disulfide (MoS_2), represent a highly promising field for electronics and photocatalysis due to their exceptional optical and catalytic properties. This work investigates the modification of MoS_2/PET heterostructures, comprising a 20 nm MoS_2 thin layer deposited on a flexible polyethylene terephthalate (PET) substrate, using energetic ion beams. The primary goal was to evaluate how ion irradiation influences the structural and functional properties of these layers to optimize them for flexible devices and water treatment applications. The experimental phase involved irradiation with light ions (C, O) and heavy ions (Ag, Au) at MeV energy levels, with fluences ranging from 1×10^{12} to 5×10^{14} cm^{-2}. Quantitative elemental analysis using RBS and ERDA revealed that ion irradiation leads to progressive carbonization of the PET substrate, characterized by significant hydrogen and oxygen loss. In the MoS_2 layer, the process induced structural defects, specifically sulphur vacancies, which shift the stoichiometry toward a Mo-rich state. XPS analysis further confirmed these changes, showing a partial phase transition from the semiconducting 2H phase to the metallic 1T phase and surface oxidation at defect sites. Surface morphology characterization via AFM and SEM showed that while light ions gradually increase surface roughness, heavy ions (specifically Au) cause dramatic topographical changes and layer delamination due to high mechanical stress. Functional testing demonstrated a significant enhancement in photocatalytic activity for the degradation of rhodamine B. The highest degradation constant was observed in the case of Au ions. ion modification.

Keywords

MoS_2, ion irradiation, nanostructuring, photocatalysis, PET, flexible electronics

P46 - Irradiation growth in U-6 wt.% Zr alloy under ion irradiation; in-situ FESEM investigations

Vikas Singh Gahlot[1, 2], P. Jegadeesan[1], Md Mofizur Rahman Mollah[3], Pooja Gupta[2, 4], Ramnathaswamy Pandian[1, 2], Soumen Das[2, 3], Sanjay Rai[2, 4], S. Amirthapandian[1, 2]

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Uranium-zirconium (U-Zr) alloys are widely used as promising metallic fuels in sodium cooled fast reactors, offering superior fuel economy, high thermal conductivity, high burnup capability, rapid thermal response rendering inherent safety, high fissile and fertile atom density, and favorable fuel cycle characteristics [G. Hofman, *et al*., *Prog. Nucl. Energy* 31(1997) 83-110]. The addition of zirconium increases the solidus temperature, reduces fuel-cladding chemical interaction, and enhances dimensional stability during thermal cycling, ensuring reliable reactor performance. In the present work, the use of *in-situ* FESEM technique led to better understanding of the evolution of morphology under ion irradiation.

The alloy U-6 wt.% Zr was prepared by using arc melting technique under a UHP Ar atmosphere by taking appropriate amount of uranium and zirconium metals. The ingots were then air cooled to room temperature, sectioned, ground and polished. The morphological evolution of the as-cast U-6 wt.% Zr was examined under 3.6 MeV Zr^{+} ion irradiation over a range of ion fluences using our in situ *i*^{4}-FESEM setup [P. Jegadeesan, *et al*., *NIMB* ,566 (2025) 165759]. The grazing incidence X-ray diffraction (GI-XRD) measurements were carried out on the ion irradiated and unirradiated region of the sample by using BL-02 beamline at INDUS-2 synchrotron facility.

Figure 1 presents a series of SEM images of the unirradiated U-6 wt.% Zr alloy alongside irradiated one at different ion fluences. In the marked regions (Figure 1), cracks are clearly visible at certain ion fluences; however, these features disappear at higher ion fluences. This behavior indicates a dynamic deformation process, primarily associated with the formation and evolution of dislocation loops during ion irradiation. For anisotropic materials such as α-U (orthorhombic structure), irradiation growth is expected even at room temperature. Energy-dispersive X-ray (EDX) analysis further confirms the presence of Zr-rich regions embedded within the α-U matrix. In α-U, the [001] plane shows minimal change in interplanar spacing under ion irradiation, whereas the [100] and [010] planes exhibit lattice expansion and contraction, respectively [Arunkumar Seshadri,*et al., Materials,* 2022, 15(12), 4106].

GIXRD results (Figure 2) align with these observations, showing that most crystallographic planes undergo significant lattice constant changes compared to the relatively stable [002] plane. The irradiation growth behavior of the U-6 wt.% Zr alloy is therefore interpreted based on fundamental ion-solid interactions under the present experimental conditions.

Keywords

In-situ ion irradiation and imaging with FESEM (i4- FESEM), Ion irradiation, Irradiation growth, U-6 wt.% Zr

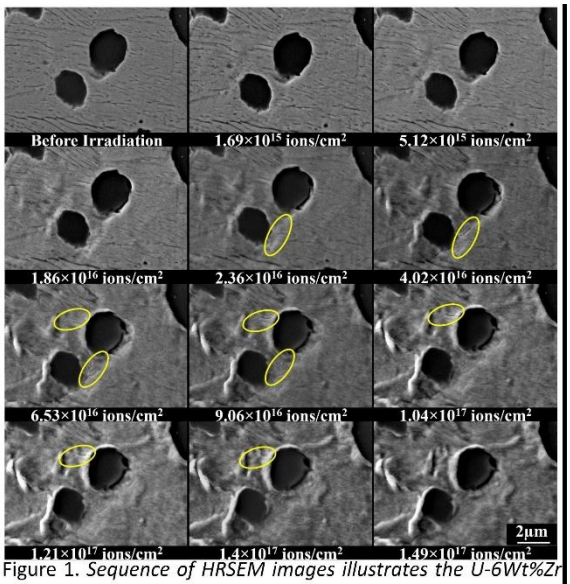


Figure 1. *Sequence of HRSEM images illustrates the U-6Wt%Zr alloy irradiated with 3.6 MeV Zr^+ ions for ion fluences ranging from 1.69 × 10^{15} to 1.49 × 10^{17} ions/cm² are presented. The marked regions show cracks appearance. All the images are in same magnification.*

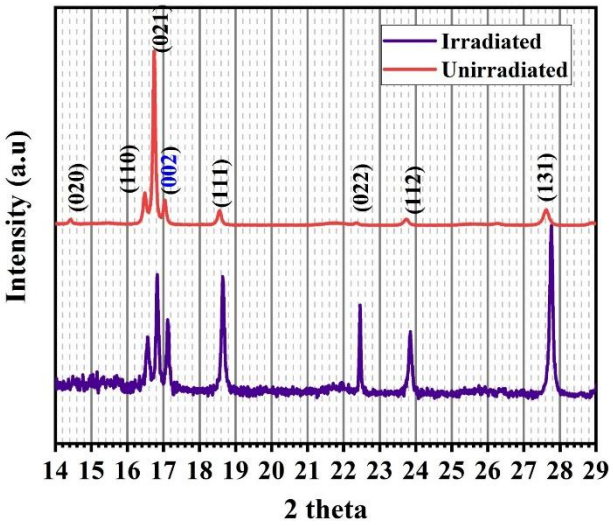


Figure 2. Synchrotron *X-ray diffraction (XRD) patterns of unirradiated and 3.6 MeV Zr^+ ion irradiated(ion fluence: 1.49 × 10^{17} ions/cm²) U-6Wt%Zr alloy. The measurements were carried out in grazing incidence with an angle of 1.5°.*

P47 - Structural Evolution of W-Ta-V-Cr-Ti High-Entropy Alloy Thin Films Prepared by Magnetron Sputtering

Maja Mičetić[1], Krešimir Salamon[1], Kristina Tomić Luketić[1], Jasminka Popović[1], Željko Skoko[2], Tonči Tadić[1], Andreja Gajović[1]

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High-entropy alloy (HEA)-based materials have attracted significant interest due to their resistance to high-energy neutron irradiation, making them promising candidates for fusion reactor wall applications. This study focuses on the preparation of a series of HEA thin films by magnetron sputtering and on the characterization of their structure, morphology, and elemental composition.

A series of 3-5 thin-film samples composed of five refractory metals (W, Ta, V, Cr, and Ti) was prepared. The deposition conditions, including substrate temperature and the volumetric fraction of individual elements, were systematically varied, while post-deposition annealing was applied to obtain a single-phase crystalline material. The relationship between the preparation conditions and the resulting thin-film structure was investigated with the aim of developing HEA materials expected to exhibit high resistance to high-energy neutron irradiation under fusion reactor operating conditions. The irradiation resistance was evaluated by irradiation experiments performed in the DiFU chamber.

Keywords

HEA materials, magnetron sputtering

P48 - Effect of Fe Ion Bombardment on the Structure and Elemental Redistribution in the Near-Surface Layers of Ferritic-Martensitic Steel EK-181

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Simulation experiments using particle accelerators play a critical role in modern materials science. As part of the development of accelerated simulation testing methods for characterizing the performance properties of ferritic-martensitic materials, EK-181 steel was irradiated with 0.5 MeV $^{56}Fe^{+}$ ions to a fluence of 5×10^{17} cm^{-2} at 350 °C. Surface morphology and composition were examined by SEM-EDS, while depth-dependent mechanical properties were evaluated using instrumented nanoindentation (Oliver-Pharr method). The irradiation produced a distinct two-zone structure. In the near-surface layer (~250 nm), Fe depletion with Cr, C, and Al enrichment was observed, consistent with selective sputtering, resulting in modest hardening and a reduced Young's modulus. At greater depths (~250-500 nm), where the composition approaches the pre-irradiation state, pronounced hardening and an increased modulus occurred. These deeper changes may be associated with the accumulation and migration of irradiation-induced defects beyond the primary damage zone predicted by SRIM. The results demonstrate how selective sputtering and radiation-induced segregation together produce a two-zone mechanical response in EK-181, providing insights for optimizing ferritic-martensitic steels in nuclear applications.

Keywords

EK-181; ferritic-martensitic steel; Fe ion irradiation; selective sputtering; radiation-induced segregation; instrumented indentation

P49 - Excitation of GDR in Yttrium Nuclei by Channeling Radiation of Relativistic Electrons in Crystals

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The study of collective nuclear excitations, such as the giant dipole resonance (GDR) [1], remains highly relevant. Of particular interest is the application of channeling radiation (CR) from electrons in crystals as a novel method for investigating photonuclear reactions. Numerical calculations [2] have shown that GDR excitation by CR gamma photons is a more efficient and cost-effective approach compared to the conventional method based on bremsstrahlung (BS).

Radioactive isotopes of yttrium are important in nuclear medicine due to their theranostic pair: diagnostic and therapeutic isotopes with identical chemical properties enable personalized treatment with preliminary dosimetry assessment, making them indispensable in oncology.

In this work, we present the results of a study on GDR excitation in yttrium nuclei using radiation produced during the channeling of relativistic electrons in crystals. Numerical calculations of the total GDR yield in the (γ, n) and (γ, 2n) photonuclear reactions are presented. It is shown that this method can offer advantages over the conventional BS-based approach and can serve as a pulsed neutron source with controllable parameters.

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Keywords

giant dipole resonance, channeling radiation, relativistic electrons, crystals

P50 - Nanoripples on thin amorphous oxide surfaces produced by grazing incidence high-energy heavy ion irradiation

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High-energy heavy ion irradiation can produce permanent nanoscale damage in materials, also known as ion tracks. These nanostructures can be easily observed on surfaces by means of atomic force microscopy, especially if the ion irradiation is conducted under grazing incidence geometry. For prolonged irradiation exposures, when ion tracks start to overlap, nanoripples can arise. Grazing incidence small angle X-ray scattering is a very useful technique for nanoripples characterisation, as it yields detailed statistical information about the whole irradiated surface. In the present work, response of thin oxide films to high-energy iodine and copper ion irradiation was studied, and suitable irradiation conditions for nanoripple formation were found.

Keywords

amorphous oxides, nanoripples, ion irradiation, AFM, GISAXS

P51 - SWIFT HEAVY ION IRRADIATION OF LAYERED AMORPHOUS SEMICONDUCTING AND METAL-OXIDE THIN FILMS

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Swift heavy ion (SHI) irradiation provides a potent method for customising material characteristics through strong electronic energy deposition and subsequent non-equilibrium relaxation processes. This study examines how SHI affects the morphology and structure of oxide based thin films. Magnetron sputtering was used to prepare (Ge+MgO)/MgO and

(Cu+MgO)/MgO multilayer thin films. As grown films are amorphous, with pure MgO layers well separating mixed (Ge+MgO) layers having homogeneously dispersed Ge or Cu atoms. To promote the precipitation and crystallisation of Ge and Cu nanoparticles, thin films were subsequently vacuum-annealed at various temperatures (600-800 °C). Concurently, as-grown films were irradiated with SHI (23 MeV I ions were utilised) in order to compare electronically generated energy deposition with the thermally driven structural and morphological changes during annealing. Infrared spectroscopy, Raman spectroscopy, X-ray diffraction (XRD), `and grazing-incidence small-angle X-ray scattering (GISAXS) were among the methods used to characterise the annealed and irradiated thin films. The purpose of this work is to provide light on how embedded metal and semiconducting nanoparticles regulate energy transfer and structural evolution in MgO amorphous multilayer systems under either annealing or irradiation condititions.

Keywords

Swift heavy ion irradiation, amorphous multilayer thin films, magnetron sputtering, nanoparticle crystallization, structural evolution

P52 - The Effect of Low-Energy Irradiation with Light and Heavy Ions on the Structure of Surface Layers and the Physical-Mechanical Properties of Structural Austenitic Steels with Different Nickel Content

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The study results of the effects of low-energy proton and iron ion irradiation on the structure and physical-mechanical properties of austenitic steels AISI 304, C0.12Cr18Ni10Ti, and 316NL are presented. One of the features of these steels is their different nickel content. According to the specifications, AISI 304 steel contains 8 wt.% nickel, C0.12Cr18Ni10Ti steel contains 10 wt.%, and 316 NL steel contains 12 wt.%. The nickel content in steel is known to largely determine how its properties and structure change under irradiation. So, in steels with low nickel content, irradiation leads to the formation of a martensite phase, which affects the structure and mechanical properties. This work is devoted to studying the effect of low-energy ion irradiation on the structure and properties of the mentioned above steels. This work is devoted to studying the effect of low-energy ion irradiation on the structure and properties of the mentioned above steels. A distinctive feature of this work is that it focuses on the effect of ion irradiation on the surface layers of these steels, as this issue is given significantly less attention compared to studying the effects of irradiation in the bulk of the material.

Ion irradiation was performed at the Institute of Nuclear Physics (Almaty, Kazakhstan) using the UKP-2-1 tandem accelerator, which accelerates both light and heavy charged particles in the energy range from 300 keV to 2 MeV. To correct compare the effects of proton and iron ion irradiation, the regions of ion stopping and the radiation defects which they generate must be located at the same depth from the irradiated surface. Therefore, irradiation with 300 keV iron ions and 850 keV protons through a 5-μm-thick nickel foil were chosen. With this irradiation, the braking regions of both proton and iron ion, as well as defect generations regions, are located within 100-150 nm from the surface. A series of proton and iron ion irradiations was performed. The final proton irradiation fluence was 10^{17} cm^{-2}, and the iron ion

fluence was $2 \cdot 10^{15}$ cm^{-2}. Irradiations were performed at room temperature (~25°C). The calculated radiation dose at these proton and iron ion fluences is comparable and amounts to ~0.1 dpa.

Post-irradiation studies of the surface structure and elemental composition were performed using electron microscopy (SEM), energy-dispersive spectroscopy (EDS), and conversion electron Mössbauer spectroscopy (CEMS). Hardness and Young's modulus were measured using nano - and microhardness testers.

The results of the studies can be shortly summarized as follows:

- proton irradiation at room temperature up to fluence does not lead to significant changes in the surface morphology and elemental composition of the steels;

- iron ion irradiation leads to noticeable changes in surface morphology and elemental composition;

- irradiation with low-energy protons and iron ions leads to noticeable changes in hardness and Young's modulus in a region exceeding the ion ranges by 4-5 times;

- radiation damage in the near-surface region of austenitic steels depends on both the energy of the bombarding ions and the nickel content.

This work was implemented under financial support of the Program of targeted financing of the Agency of Republic of Kazakhstan on Atomic Energy No BR23891779.

Keywords

austenitic steel, proton, iron ion, irradiation, mechanical properties

P53 - In-situ TEM observation of strain annealing in SHI irradiated monoclinic zirconia at intermediate fluences

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SHI irradiation studies for monoclinic zirconia have shown that the transformation to the high temperature tetragonal phase was stabilized at room temperature (RT) after exposure to suitable irradiation fluences [1-3]. The tetragonal transformation has been quantitatively demonstrated using techniques such as Raman spectroscopy and X-ray diffraction (XRD) for SHI irradiation fluences down to 2×10^{12} for heavy ions and 5×10^{13} cm^{-2} for light ions [4]. This "apparent" fluence threshold for the monoclinic to tetragonal transformation is most due to the detection limit (~ 1-2 vol%) for the Raman and XRD techniques. O'Connell *et al* [5] reported on the direct observation of individual ion tracks, containing interlocking tetragonal segments, which formed in monoclinic zirconia (m-ZrO_2) as a result of 167 MeV Xe irradiation (fluence 2×10^{10} cm^{-2}) at room temperature. However, information on the direct TEM observation and analysis of microstructural evolution of m-zirconia at intermediate SHI fluences has not been previously reported.

The formation of the tetragonal SHI track formation and the effect, specifically induced strain, on the surrounding monoclinic lattice could possibly provide evidence for the formation and stabilization of the tetragonal phase at higher fluences. In this work we report on the direct observation, by transmission electron microscopy (TEM), of the response by monoclinic zirconia to SHI irradiation at intermediate fluences, covering both the single track and track

overlapping regimes, followed by the in-situ TEM observation of the annealing behaviour of these irradiated samples.

Experimentally, sections of single crystalline m-zirconia were irradiated with 150 MeV Xe ions at a fluence in the range 5 × 10^{11} - 1 x 10^{13} cm^{-2} at room temperature. Electron transparent lamellae were prepared by FIB lift out technique using an FEI Helios NanoLab 650 and analysed using a double Cs corrected JEOL ARM200F operated at 200 kV. TEM in-situ thermal annealing was implemented using a DENSsolutions Wildfire micro-electro-mechanical system (MEMS) based heating system allowing for closed loop temperature control up to 1 300^0C.

The TEM analysis of the irradiated specimens will be shown to exhibit extensive strain in the monoclinic lattice surrounding the tetragonal tracks, which increases with increasing fluence. Subsequently, at a fluence of 1 x 10^{13} cm^{-2}, it was observed that the tracks are no longer visible due to the excessive strain contrast. However, it will be shown that nano-size areas of different or mixed crystalline character indicating the possibility of structural evolution due to the excessive strain in the material between the SHI tracks. The possibility of the presence of additional phases such as cubic or orthorhombic cannot be excluded, in agreement with recent work [6].

In-situ annealing of the SHI irradiated specimens at 400^0C were observed to reduce the strain in the monoclinic material whereas the tetragonal segments transformed to monoclinic phase and a line of defect loops in the original SHI tracks as shown in the TEM bright field image in figure 1. The insert is a magnified (x2) image of the line of defect loops within the tracks. The SHI direction is indicated by the arrows. These results and the possible mechanisms during the formation and annealing process will be discussed in detail.

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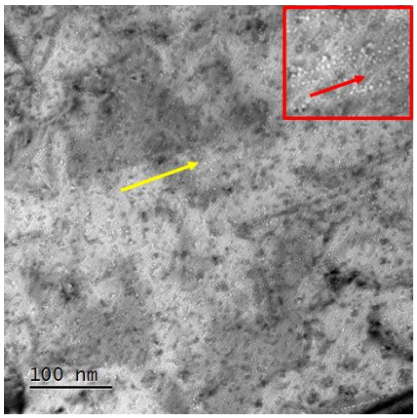
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Keywords

zirconia, monoclinic, annealin, in-situ, TEM



P54 - Structural transformations under coupled extreme pressure and swift heavy ion irradiation

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The response of materials to the simultaneous application of high pressure and intense ionizing radiation remains largely unexplored, despite its relevance for functionality in extreme environments and for non-equilibrium materials synthesis [1]. This unique combination of extremes is accessible using the high-pressure irradiation platform installed in Cave A at the heavy-ion synchrotron SIS18 (GSI, Darmstadt, Germany) [2]. Micrometer-sized samples are compressed in diamond anvil cells (DACs) and irradiated with 200-480 MeV/u uranium ions. In-situ Raman spectroscopy and optical microscopy enable real-time tracking of structural and optical modifications as a function of accumulated fluence. In this contribution, we present recent results on ion-induced transformations in various materials under high pressure, including molecular compounds such as carbon monoxide (CO) and sulfur (S), the inorganic compound sodium azide (NaN_3), and selected nanomaterials [3]. Effects identified by Raman spectroscopy and synchrotron X-ray diffraction include polymerization, decomposition, bond rearrangement, and phase transformations, highlighting the rich landscape of radiation-pressure-coupled processes.

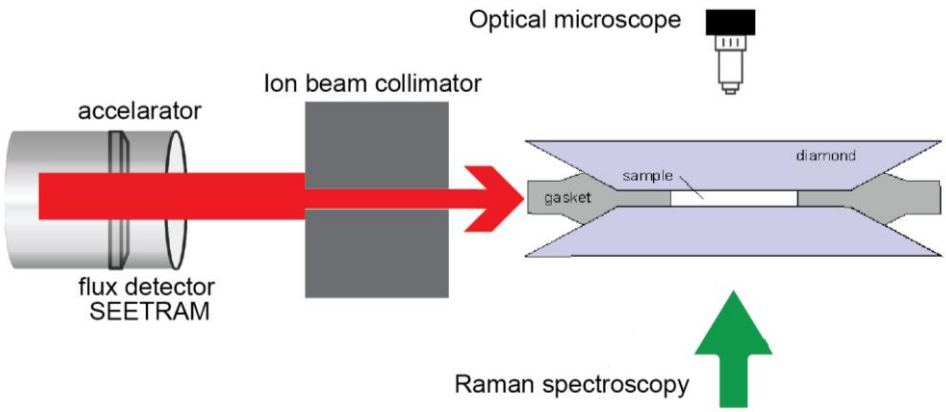
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Keywords

high pressure, swift heavy ion irradiation, irradiation effects



P55 - Electron microscopy characterization of swift heavy ion impacts in Bi_2Te_3 nanowires

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Bismuth telluride (Bi_2Te_3) is a well-established room-temperature thermoelectric material with intrinsically low thermal conductivity [1]. When confined to nanowire geometries, reduced dimensions and high surface-to-volume ratios further modify thermal transport and energy dissipation pathways. These characteristics make Bi_2Te_3 nanowires excellent model systems for investigating size-dependent energy deposition and structural modifications by swift heavy ions, with implications for the stability and performance of nanowire-based thermoelectric devices in a radiation environment.

In this work, we analyze the effects of swift heavy-ion irradiation on Bi_2Te_3 nanowires synthesized by electrodeposition into ion-track-etched polymer templates [2]. Nanowires with diameters of 20, 30, and 50 nm were irradiated with ^{108}Ag and ^{197}Au ions at specific energies of 4.8 and 8.3 MeV/u, fluence of $1x10^{11}$ and $5x10^{10}$ ions/cm^2, respectively, at the UNILAC linear accelerator of GSI Helmholtz Center for Heavy Ion Research.

Post-irradiation characterization was performed using scanning electron microscopy (SEM) and transmission electron microscopy (TEM). Advanced imaging techniques, including STEM-in-SEM and high-resolution HR-TEM, provide direct evidence of pronounced ion-induced modifications that depend on both nanowire diameter and the ion's electronic stopping power. Observed effects include surface crater formation, cavities, and segmentation of the nanowires. These results demonstrate the strong and clear impact of swift heavy ions on the morphology and structure of bismuth telluride nanowires, providing insights into nanoscale energy deposition and damage mechanisms.

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Keywords

Swift heavy ions , Nanomaterials , Bismuth telluride , Electron microscopy , Ion matter interaction

P56 - Crystallinity and Track-Parameter Dependence of Swift Heavy Ion Damage in Anatase and Amorphous TiO_2 Ultrathin Films: A ReaxFF Molecular Dynamics Study

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Titanium dioxide (TiO_2) is a semiconductor with numerous technological applications, including dye-sensitized solar cells, photocatalysis, sensors, or medical implants. Exploring methods to modify the physical properties of TiO_2 at the nanoscale in a controlled manner, such as through swift heavy ion (SHI) irradiation, is therefore of great interest[1]. Here we investigate, by means of MD simulations, the transient processes of energy transfer, damage production, and the resulting structural changes induced in freestanding anatase and amorphous TiO_2 ultrathin films bombarded by individual swift heavy ions.

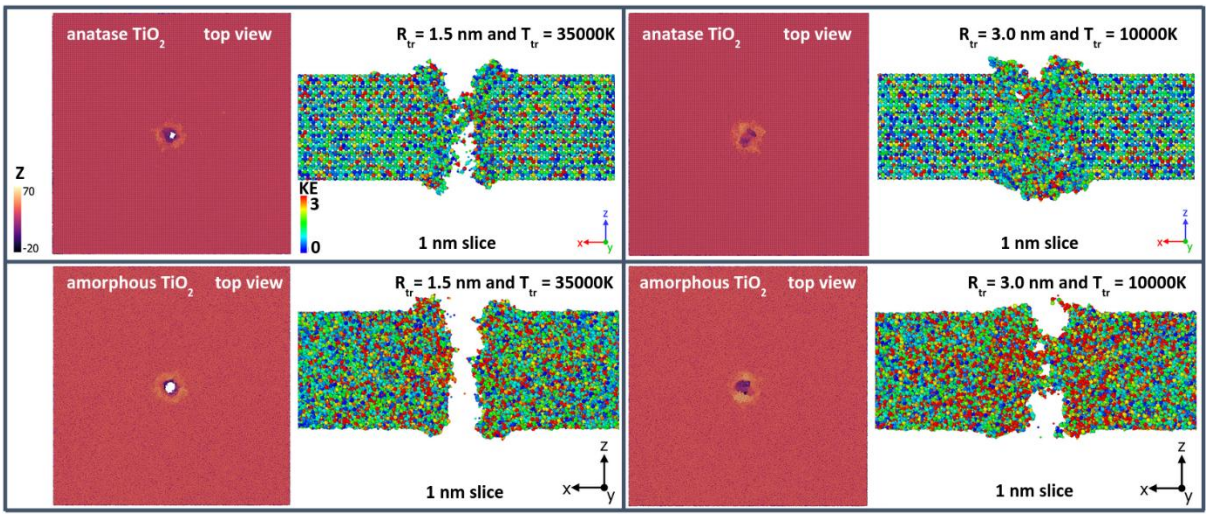
MD simulations were performed using the ReaxFF interatomic potential[2] for anatase and amorphous TiO_2 samples, with 7-15 nm thickness. A cylindrical hot track with a radius of 1.5-3.0 nm and an initial nominal temperature of 10000-35000 K (corresponding to electronic energy losses of 15-30 keV/nm) was evolved for up to 100 ps. The simulations were compared with experimental data obtained for TiO_2 nanotubes of similar thickness irradiated with swift heavy ions under comparable energy loss conditions. The results will be discussed and provide atomistic insight into the mechanisms of SHI-induced damage in TiO_2 nanostructures and establish a framework for tailoring radiation-induced structural modifications through controlled irradiation conditions.

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Keywords

Swift Heavy Ion Tracks, Molecular Dynamics Simulations, ReaxFF, TiO_2 Ultrathin Films, Crystallinity



P57 - Interaction of He^{2+} ions with hydrogen isotopes

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The current methods of energy production will not be able to meet humanity's energy needs in the long run. One of the most promising solutions for the future is the implementation of fusion power plants. In this context, accurate knowledge of the cross sections in collisions between He^{2+} ions and hydrogen isotopes is critical for controlled nuclear fusion research.

The standard three-body classical trajectory Monte Carlo (CTMC) model is a well-known classical approach for modeling atomic collisions [1]. However, due to the absence of quantum features in this standard model, the CTMC is unable to accurately describe cross sections, particularly at lower impact energies where quantum mechanical effects are dominant. To address this limitation, we developed a three-body quasi-classical trajectory Monte Carlo (QCTMC) model that incorporates the quantum characteristics of the collision system. In this model, a Heisenberg correction term is added to the standard classical Hamiltonian to simulate the Heisenberg uncertainty principle [2-7].

We present ionization, total, and state-selective charge exchange cross sections for collisions between He^{2+} ions and hydrogen isotops at impact energies ranging from of 2.5 keV/u to 885.0 keV/amu, utilizing both the CTMC and QCTMC models. Our findings indicate that the QCTMC model significantly enhances the accuracy of the cross sections, particularly at lower projectile energies. The results obtained are in close agreement with previously reported quantum-mechanical findings. Our model efficiently provides accurate results with greater simplicity, where quantum mechanical approaches may become complicated. Thus, our QCTMC model serves as a viable alternative for calculating accurate cross sections, yielding results comparable to those derived from quantum-mechanical methods [2-7].

Keywords

Classical trajectory Monte Carlo simulations, ionization,charge exchange cross section

P58 - Energy loss function of lead determined from the reflection electron energy loss spectroscopy spectra

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An accurate quantitative description of surface excitation is essential for resolving the contributions of bulk and surface excitations, especially when electrons crossing the surface are necessary for quantifying electron-beam-related techniques. This is particularly true for

surface-sensitive electron spectroscopies, including X-ray photoelectron spectroscopy, Auger electron spectroscopy, and reflection electron energy loss spectroscopy (REELS). REELS spectra provide valuable information on surface excitation, as they result from the dielectric response of a solid surface to an external electric field carried by electrons. Moreover, REELS measurements are easier to perform experimentally, as they do not require special sample preparation.

In this work present a detailed semi-classical theoretical model of surface excitation to describe the electron differential inverse inelastic mean free path (DIIMFP) in the surface region. By formulating the model in a cylindrical coordinate system of momentum transfer, we can explicitly incorporate a surface plasmon dispersion that relates to the parallel component of momentum transfer, enhancing our description of surface plasmon excitation. The bulk dielectric function is represented using the Drude-Lindhard oscillator parameters, from which we derive the associated surface dielectric function and its depth-dependent form.

We demonstrate example calculations for lead (Pb). By integrating our improved surface excitation model into the RMC method, we successfully simulate the REELS spectrum shape of Pb, achieving closer alignment with the measured REELS spectra at incident electron energies of 1 keV, 1.5 keV, and 2 keV compared to simulations using Li's earlier semi-classical model [1]. The corresponding averaged energy loss function (ELF) reveals a prominent bulk plasmon peak around 13 eV. Furthermore, we conduct first-principles calculations of the ELF for Pb, showing excellent agreement in both position and intensity for this bulk plasmon peak. Through our enhanced theory that accounts for surface excitation and a unique surface dispersion relation, we have established a framework for the quantitative analysis of surface excitations in REELS spectra, highlighting its potential to explain unusual surface plasmon peak intensities observed in certain metals.

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Keywords

optical properties, Monte Carlo technique, surface and bulk excitation

P59 - Electron-Impact Excitation and Ionization of Hydrogen Atom

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Electron-hydrogen collisions represent one of the most fundamental benchmark problems in atomic collision physics [1]. Due to the simplicity of the hydrogen atom, this system serves as an ideal testing ground for theoretical approaches applied to inelastic scattering, playing a crucial role in evaluating both classical and quantum collision models. In our present work, we investigate total and differential cross sections for electron-impact ionization and excitation of ground-state hydrogen as a function of the incident electron energy in the eV range. For excitation, we separately study the 1s→2s and 1s→2p transitions and also determine the total excitation cross section to the n = 2 manifold. These channels provide a useful basis for

analyzing the energy dependence of excitation and for comparing the relative importance of different final states.

Two complementary approaches are employed. In the first, the collision dynamics is described within the classical trajectory Monte Carlo (CTMC) framework, where a large ensemble of trajectories is generated with statistically selected initial conditions [2]. In the second, non-relativistic analytical quantum calculations are performed, allowing for a direct comparison between classical and quantum descriptions of the same elementary processes [3]. The calculated cross sections reproduce the expected overall behavior for both ionization and excitation. In particular, the excitation and ionization probabilities exhibit the characteristic dependence on projectile energy, with marked variations near threshold and smoother trends at intermediate and higher energies.

A satisfactory agreement between the CTMC and quantum results is obtained mainly in the intermediate-energy region, whereas more pronounced differences arise near threshold and at higher energies, where the role of quantum effects becomes more significant and the limitations of the classical approximation become more apparent. The comparison presented here provides valuable information on the applicability of classical and quantum approaches to electron-atom collisions. It also contributes to a better understanding of the mechanisms governing ionization and low-lying excitation in simple atomic systems and offers a clear benchmark for future extensions toward more complex targets and collision processes.

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Keywords

ionization, excitation, electron impact,classical trajectory Monte Carlo method, non-relativistic analytical quantum calculations.

P60 - Synthesis and characterization of doped SnO_2 nanowires in SiO_2/Si track templates for sensor applications

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Currently, the development and study of sensitive elements for gas sensors is a pressing task for many researchers [1-3]. To improve the sensitivity of such elements, we propose the production of nanoscale crystals (NCs) and nanowires (NWs) of tin and its oxides using template synthesis methods. We also propose heat treatment in an oxidizing environment of the obtained arrays of nanoscale structures, as well as a study of the effect of metal impurities (Me (Pd, Sb, Ni, and Au)) on their electrophysical and optical properties. In our research, we use SiO_2/Si track templates as an effective technological route for the synthesis of Me/SnO_2-NWs(NCs)/SiO_2/Si composites. Nanostructured metal oxide films doped with various impurities are promising for increasing the sensitivity of sensors.

The Me/SnO_2-NWs(NCs)/SiO_2/Si composites considered in this work were prepared by template synthesis, namely, chemical deposition (CD) of tin oxide with activating impurities in SiO_2/Si track templates. Track structures in the nanostructured SiO_2/Si systems were created by irradiation with 200 MeV swift heavy xenon ions at a fluence of 10^7-10^8 cm^{-2} using a DC-60 cyclotron (Astana, Kazakhstan). Nanopores in the track templates were formed using a 4% aqueous solution of hydrofluoric acid (HF). The analysis of filled pores after the chemical deposition process, as well as the surface morphology of the SiO_2/Si track templates, were examined using a Zeiss Crossbeam 540 dual-beam scanning electron microscope. The phase composition and crystallographic structure of the Me/SnO_2-NWs(NCs)/SiO_2/Si composites were studied using X-ray diffraction (XRD) on a D8 ADVANCE ECO X-ray diffractometer. Bruker AXSDIFFRAC.EVAv.4.2 software and the international ICDD PDF-2 database were used to identify the phase composition and determine the crystal cell parameters.

The research results obtained in this area will enable the future development of highly sensitive gas sensors based on tin oxide nanowires, thanks to their unique physical properties, which depend on their size and shape. These gas sensors are designed to detect explosive, flammable, and toxic volatile substances.

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Keywords

SiO2/Si track template; activating metal impurities; tin oxide-based nanowires; template synthesis; highly sensitive gas sensors

P61 - TC-DFT-based Positron Annihilation Spectroscopy Differentiates Irradiation-induced Vacancy Type Defects in 4H-SiC

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[1]Institute of Modern Physics, Chinese Academy of Sciences

Irradiation introduces defects into materials, of which vacancy-type defects play an important role. Especially for ceramic materials such as silicon carbide (SiC), which rely on covalent bonding to form their crystal structure, vacancy-type defects are difficult to move freely once

they are formed and may remain for a long time, adversely affecting various micro and macro properties of the material. To effectively utilize materials working in irradiation environments and prevent structural damage and collapse, it is necessary to carry out in-depth studies on vacancy-type defects. Positron Annihilation Spectroscopy (PAS) is a well-established method for sensitive and efficient nondestructive detection of vacancies, and there are two commonly used methods, namely, Positron Annihilation Lifetime Spectroscopy (PALS) and Slow Positron-beam Doppler Broadening Spectroscopy (SPDBS). However, both methods have problems and challenges when applied to SiC. Among them, PALS has long been considered incapable of distinguishing between defect-free crystals and carbon monovacancy (V_C) in SiC, leading researchers to attribute the wide range (170~210 ps) of lifetime signals to the contribution of silicon monovacancy (V_{Si}) only. SPDBS usually yields a total spectrum that mixes all the signals of different types of vacancies, from which it is difficult to extract the contribution of a particular type of vacancy and cannot be used to distinguish between different types of vacancies.

For the problems faced by PALS, this study accurately calculates the structural changes occurring in different types of vacancies in 4H-SiC in the presence of positrons via Two-Component Density-Functional Theory (TC-DFT), obtains more accurate theoretical lifetimes as references, and successfully distinguishes defect-free crystals, V_C and V_{Si} from the experimental data for the first time. For the problems faced by SPDBS, this study calculated the theoretical spectrum of positron annihilation occurring independently in various types of vacancies in irradiated 4H-SiC using a customized high-completeness Projector Augmented-Wave (PAW) basis, and a set of relative statistical parameters “P” is constructed and be used to identify different types of vacancies. For the first time, two basic types of monovacancies in irradiated 4H-SiC are distinguished and the variation of these two types of vacancies as a function of irradiation doses is quantified, which further proves the effectiveness and accuracy of the above novel method.

In conclusion, this study not only provides a solution for the challenge of identifying coexisting multiple vacancy types using PAS technology but also extends the applicative scope and depth of PAS in fields such as nuclear energy, aerospace, semiconductors, etc.

Keywords

Irradiation; Vacancy-type defects; Positron Annihilation Spectroscopy (PAS); Density Functional Theory (DFT); SiC

P62 - Grazing Incidence Swift Heavy Ion Tracks Evolution with Grazing Angle

Pavo Dubček[1], Marko Karlušić[1]

[1]Ruđer Bošković Institute

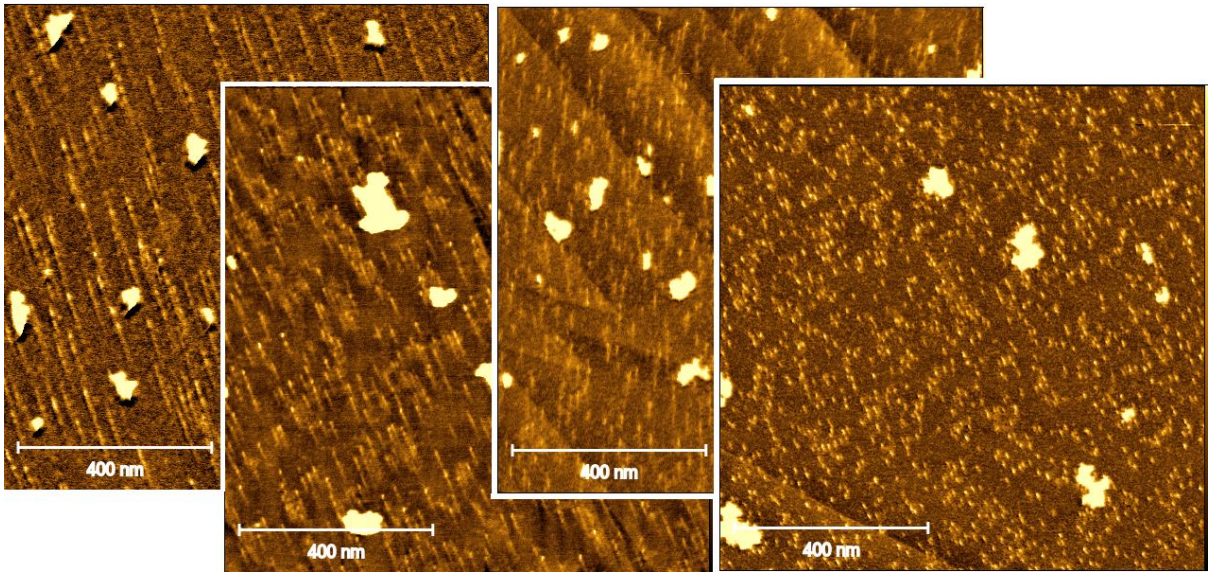
Swift heavy ions passage through insulators leaves permanent structural damage, provided the ion energies are above the threshold level for the given material. When the irradiation is done at grazing angles, long tracks of uneven height are formed on the surface. Usually, these have continuously increasing profile upon which several hillocks are superimposed.

We applied 12MeV Si ion grazing incidence irradiation on CaF_2 in order to follow the track properties as a function of incidence angle, and surface tracks images were obtained using atomic force microscopy (AFM). In order to have isolated tracks, the dose was adjusted aiming to form about 100 tracks on 1μm by 1μm AFM image. As the formation of tracks is a statistical

process, we applied software which autonomously locates tracks and analyses the details of their features, determining statistical distributions for these. Finally, these properties (track length and number of hillocks, as well as hillocks height and location along the tracks) are studied as a function of grazing incidence angle.

Keywords

swift heavy ion, grazing incidence irradiation, atomic force microscopy



P63 - Direct writing of optical microstructures in glasses and crystals by swift heavy ion microbeams: What we have learnt so far

István Bányász[1], István Rajta[2], Gyula Nagy[3], Vladimír Havránek[4], Stefano Pelli[5], Gualtiero Nunzi Conti[5], Simone Berneschi[5], Miklós Veres[6], András József Laki[7], María Cinta Pujol[8], Ágnes Nagyné Szokol[6], Robert Magnusson[9]

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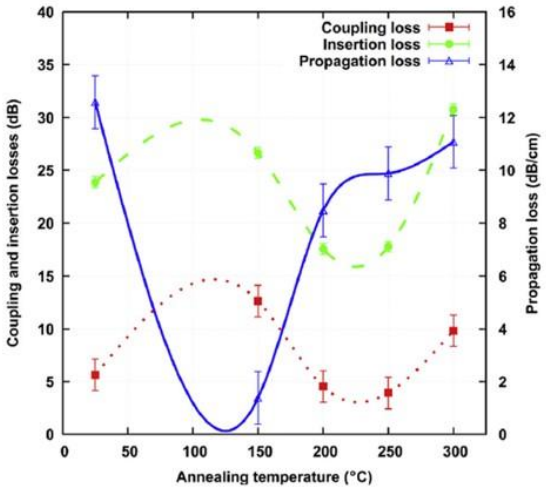
Microbeams of carbon, nitrogen and oxygen ions were used for direct writing of channel waveguides and transmission optical gratings in rare-earth ion doped and undoped optical glasses and $LiNbO_3$, $Bi_{12}GeO_{20}$. Energies of the ion beams were in the 5 MeV - 11 MeV range. Based on simulations with the SRIM code, creation of channel waveguides either directly under the sample surface or slightly buried in the sample was expected. It was found that stepwise thermal annealing resulted in a significant decrease of the propagation losses of the

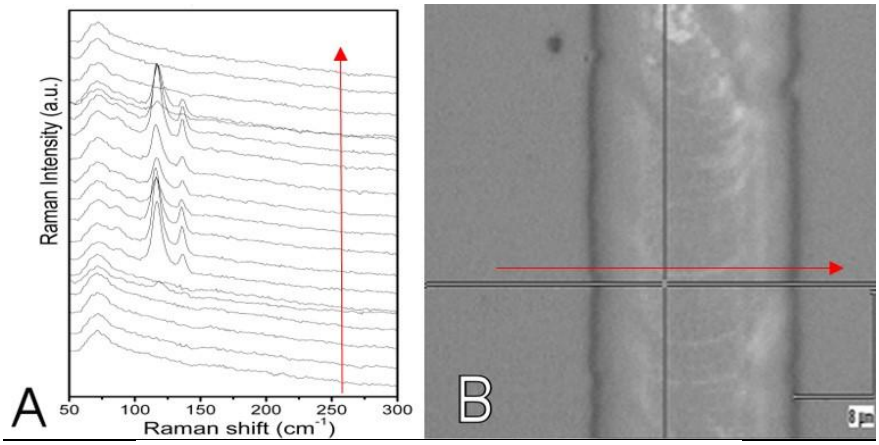
as-implanted channel waveguides. In the case of an Er-doped tungsten-tellurite target direct writing of channel wavguides with a 11 MeV C^{4+} ion beam at fluences in the range of $1 \cdot 10^{14}$ - $5 \cdot 10^{16}$ ion/cm^2 resulted in channel waveguides with very high propagatio losses, around 14 dB/cm at a wavelength of 1400 nm. Stepwise annealing of the implanted sample up to 150 °C in air reduced propagation losses to 1.5 dB/cm. Similar results were obtained when implanting channel waveguides in optical crystals with microbeams of swift heavy ions. Micro Raman spectroscopic measurements of the ion microbeam implanted channel waveguides proved to be very useful, since they revealed the fluence-dependent ion beam induced structural changes in the target material. Expansion or compaction of the target under the ion microbeam was an unwanted effect when channel waveguides were inscribed in the samples. However, it was found that local volume changes induced by the ion microbeam could be controlled very well by the spatial modulation of the implanted fluence. Surface relief transmission optical gratings with quasi-sinusoidal and sawtooth profiles were written successfully with C, N and O microbeams. The samples were IOG glass, Pyrex glass, and $Bi_{12}GeO_{20}$, Er: $LiNbO_3$ and Er: Fe: $LiNbO_3$ crystals. Lateral dimensions of the microbeams were around 2 micron x 2 micron. Ion beam energies were between 5 and 11 MeV. Implanted fluences were between 1 x 10^{14} and 1 x 10^{16} ion/cm^2. The highest diffraction efficiencies measured in gratings implanted in all the samples were between 24 and 26%, close to the theoretical maximum of 33 %, derived from the Raman-Nath theory. Besides of single integrated optical elements, fabrication of complicated integrated optical devices based on modification of both the refractive index and the surface profile of the samples can also be envisaged. Using nanobeams could reduce the feature size of those optical devices to about 200 nm.

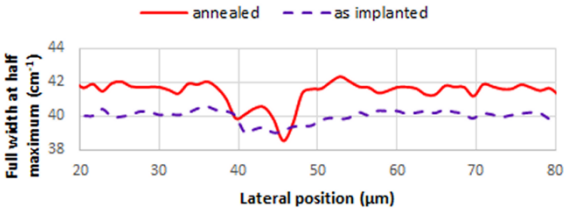
Keywords

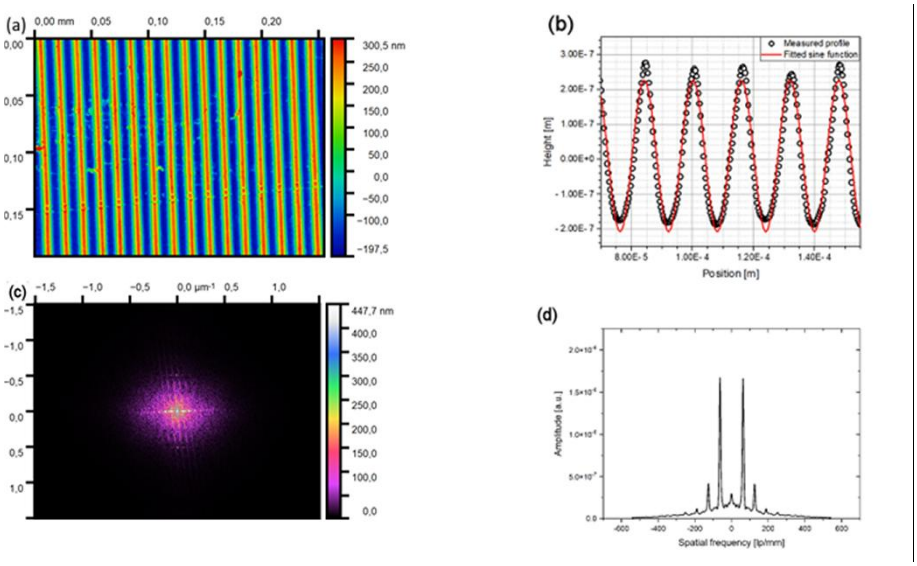
swift heavy ion, ion microbeam, ion beam implantation, channel waveguide, surface relief transmission optical grating

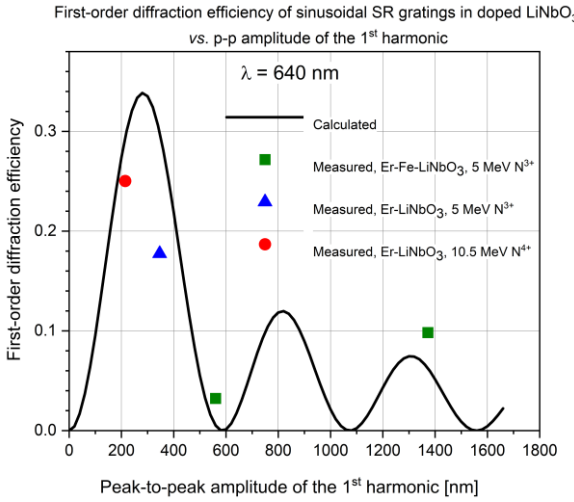





A
Raman Intensity (a.u.)
50
100
150
200
250
300
Raman shift (cm^{-1})
B
3 µm


annealed
as implanted
Full width at half maximum (cm^{-1})
44
42
40
38
20
30
40
50
60
70
80
Lateral position (µm)


(a)
0,00 mm
0,05
0,10
0,15
0,20
300,5 nm
250,0
200,0
150,0
100,0
50,0
0,0
-50,0
-100,0
-197,5
(b)
Measured profile
Fitted sine function
Height [m]
3.00E-7
2.00E-7
1.00E-7
0.00E+0
-1.00E-7
-2.00E-7
8.00E-5
1.00E-4
1.20E-4
1.40E-4
Position [m]
(c)
−1,5
−1,0
−0,5
0,0 µm-1
0,5
1,0
447,7 nm
400,0
350,0
300,0
250,0
200,0
150,0
100,0
0,0
(d)
Amplitude [a.u.]
Spatial frequency [lp/mm]


First-order diffraction efficiency of sinusoidal SR gratings in doped LiNbO$_3$
vs. p-p amplitude of the 1st harmonic
λ = 640 nm
Calculated
Measured, Er-Fe-LiNbO$_3$, 5 MeV N^{3+}
Measured, Er-LiNbO$_3$, 5 MeV N^{3+}
Measured, Er-LiNbO$_3$, 10.5 MeV N^{4+}
First-order diffraction efficiency
0.0
0.1
0.2
0.3
0
200
400
600
800
1000
1200
1400
1600
1800
Peak-to-peak amplitude of the 1st harmonic [nm]

P64 - Experimental diffraction of helium through graphene

Carina Kanitz[1], Jakob Bühler[1], Francois Aguillon[2], Vladimir Zobac[3], Toma Susi[3], Philippe Roncin[2], Maxime Debiossac[1], Christian Brand[1]

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Diffracting an atomic matter wave through a two-dimensional material such as graphene provides unprecedented insights into the interaction of atoms with the material [1, 2], as well as opening new perspectives for material research. The understanding of material properties to which the matter wave is susceptible is increased by probing a monocrystalline graphene sample and comparing experimental data to simulations.

In this contribution, we qualitatively describe the influence of lattice distortions and the interaction strength on the diffraction pattern [3]. Due to the comparatively strong projectile-grating interaction leading to phase shifts up to multiple π radians this method explores a previously inaccessible diffraction regime. Commonly used models lose validity in that regime, so a simulation model incorporating explicit treatment of large phase variations due to thermal displacement of lattice atoms was established. Based on this, we gained insights into the potential limits of atomic diffraction through 2D materials due to thermal decoherence.

[1] Kanitz et al. *Science*, **389**, 724-726 (2025)

[2] Guichard et al., *Phys. Rev. Lett*. **135**, 263403 (2025)

[3] Kanitz et al., *in preparation*

Keywords

grapene; atoms; 2D material; matter wave

P65 - Multiscale Modelling of Swift Heavy Ion Irradiation in CdTe

Aldo Artímez Peña[1, 2], Nikita Medvedev[1, 3]

[1]Institute of Physics, Czech Academy of Science, [2]Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, [3]Institute of Plasma Physics, Czech Academy of Sciences

Cadmium telluride (CdTe) is a II-VI semiconductor of broad technological relevance, finding applications in photovoltaic devices, radiation detectors, and optoelectronic systems[1]. Understanding its structural response to swift heavy ion (SHI) irradiation is essential for predicting performance degradation and exploiting ion-beam-induced modifications in device engineering. In this work, we model the response of bulk and surface CdTe to irradiation with Au ions over a wide range of energies (10-600 MeV) using a multiscale approach that couples Monte Carlo and molecular dynamics simulations.

The electronic energy deposition is modelled with the TREKIS-3 Monte Carlo code[2] using the complex dielectric function formalism within the single-pole approximation. Taking into account that generated electron-hole pairs contribute directly to the total energy transferred to

the lattice via nonthermal effects, the resulting radial energy distributions serve as initial conditions for classical molecular dynamics simulations performed with LAMMPS[3]. We compare the Stillinger-Weber and the bond-order interatomic potentials against experimental melting points and cohesive energies.

Nonthermal effects constitute the dominant channel of energy transfer to the lattice, dominating over the electron-ion and valence-band hole-phonon coupling. The atomic temperature and density evolve radially on a picosecond timescale, giving rise to amorphous ion tracks. Track growth proceeds up to approximately 5 ps post-irradiation through progressive melting of the surrounding crystalline matrix, followed by recrystallisation to the zinc-blende structure without evidence of a wurtzite phase transformation or dislocation formation. Track radii and damage thresholds are quantified as a function of ion energy, and structural modifications at the surface are compared to those in the bulk.

These results provide a microscopic basis for interpreting experimental track morphologies in CdTe and for guiding the design of ion-beam processing conditions in CdTe-based device applications.

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Keywords

swift heavy ions, cadmium telluride, molecular dynamics, track formation, multiscale modelling

P66 - Probing chemical damage induced by individual ion impacts in ultrathin PMMA films by AFM-IR

Raquel Thomaz[1], Otávio Berenguel[2], Khaled Kaja[3], Hartmut Stadler[3], Yvette Ngono-Ravache[4], Maria Eugenia Toimil-Molares[1]

[1]Materials Research Department, GSI Helmholtz Centre for Heavy Ion Research, Darmstadt, Germany, [2]National Laboratory of Nanotechnology, Brazilian Center for Research in Energy and Materials (CNPEM), Campinas, Brazil, [3]Bruker Nano Surfaces and Metrology, Karlsruhe, Germany, [4]CIMAP, UMR CEA-CNRS-ENSICAEN-UCBN, Caen, France

Radiation-induced chemical modifications in polymers are driven by complex processes initiated by ionizing radiation, leading to bond scission, mass loss, and structural rearrangements at the nanoscale. These effects are commonly assessed using macroscopic techniques and expressed in terms of damage cross sections, which rely on averaged responses and provide limited access to the local modifications produced by individual ions. In this context, techniques capable of probing chemical damage with nanometric spatial resolution are essential.

In this work, atomic force microscopy-based infrared spectroscopy (AFM-IR) is used to investigate chemical modifications induced by individual ion impacts in poly(methyl methacrylate) (PMMA) thin films. Films with thicknesses ranging from a few nanometers to

several tens of nanometers, deposited on Si, Cr, and Au substrates, were irradiated with both swift heavy ions (MeV-GeV range) and slow highly charged ions (keV range). Swift heavy ion irradiations were performed at the 3 MV Tandetron accelerator (Porto Alegre, Brazil) and at the UNILAC accelerator at GSI Helmholtz Centre for Heavy Ion Research, while highly charged ion irradiations were carried out using the HICS setup at University of Duisburg-Essen.

The results show that AFM-IR enables the detection of characteristic vibrational bands of the polymer, even in ultrathin films. Clear chemical contrast associated with individual swift heavy ion impacts is observed, with spatial features comparable to the corresponding ion-induced surface modifications. In contrast, impacts from highly charged ions could not be resolved, most likely due to limitations in spatial resolution imposed by the AFM tip.

The AFM-IR response also depends strongly on film thickness and substrate material, highlighting the combined influence of confinement and local field enhancement effects in nanoscale infrared measurements. Although AFM-IR provides direct access to nanoscale chemical information, several technical challenges remain for a full, quantitative interpretation of the data. These include control of the probing depth, AFM-tip changes and tip-convolution effects during analysis, damage induced by the IR laser beam, and crosstalk between chemical contrast and topography. These aspects are discussed in comparison with conventional approaches based on averaged spectroscopic measurements.

Keywords

Thin films; AFM-IR; polymer; ion irradiation

P67 - Defect Formation in Monolayer WS_2 Induced by Argon Gas Cluster Ion Irradiation

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[1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf

Monolayers of transition metal dichalcogenides (TMDCs) such as WS_2 are promising materials for future electronic and optoelectronic applications due to their direct bandgap, strong excitonic response, and high carrier mobility. Controlled defect engineering is an important route for tailoring their physical properties. In this work, we investigate defect formation in CVD-grown monolayer WS_2 induced by argon gas cluster ion beam (GCIB) irradiation.

WS_2 monolayers were irradiated using Ar cluster ions with varying cluster energies (30-100 keV), fluences (10^{12}-10^{14} cm^{-2}), and cluster sizes (Ar_{500}-Ar_{2000}). The resulting structural, optical, and morphological modifications were analyzed using atomic force microscopy (AFM), Raman spectroscopy, photoluminescence (PL), optical microscopy, scanning electron microscopy (SEM), and Auger electron spectroscopy (AES).

The measurements reveal a strong dependence of defect formation on irradiation conditions. At low energy per atom (60 eV/atom), substantial sputtering and loss of optical contrast were observed, while intermediate conditions (120 eV/atom) led to localized defect formation and edge erosion without complete destruction of the monolayer. AFM and SEM measurements revealed the formation of nanoscale triangular defects within the WS_2 flakes. Raman spectroscopy showed only minor shifts of the E_2g^1 and A_1g phonon modes, indicating preservation of the monolayer structure despite irradiation-induced disorder. PL

measurements exhibited reduced intensity and the emergence of broadened excitonic features, particularly near flake edges.

These results demonstrate that ion irradiation provides a controllable method for defect engineering in monolayer WS_2 while mostly preserving the overall two-dimensional structure.

Keywords

2D materials, WS2, defects, cluster ion irradiation

P68 - Potential energy environment of SiO_2 ion tracks

Reino Piirilä[1]

[1]University of Helsinki

Gaining a more fundamental understanding of the mechanisms responsible for the annealing of ion tracks in minerals can be of practical use in thermochronological applications where thermal histories of rocks are estimated based on the densities and length distributions of ion tracks present in the samples [1]. Ion tracks form in rocks when heavy unstable impurities like uranium defects decay into fission fragments whose mass-to-kinetic-energy ratios lie in the Swift-Heavy-Ion regime. To improve the existing phenomenological methods' accuracy, as well as to place them on a firmer theoretical bedrock, we characterize the potential energy environment of an ion track in a model atomic system of SiO2 in various different pressure conditions using a recent Atomic-Cluster-Expansion interatomic potential [2]. We invoke the Activation-Relaxation Technique [3] to investigate the distribution of energies associated with the available transitions to metastable states. The properties of this distribution should provide an initial step towards understanding track annealing, making them relevant for the development of track length profile models.

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Keywords

Computational materials science, swift-heavy ions, fission tracks, potential energy surface

P69 - Materials Research Target Stations at GSI

Pascal Simon[1], Frieder Koch[1], Leon Kirsch[1], Ina Schubert[1], Ioannis Tzifas[1], Kay-Obbe Voss[1], Michael Wagner[1], Maria Eugenia Toimil-Molares[1, 2]

[1]Material Research, GSI Helmholtz Center for Heavy Ion Research. Darmstadt, Germany, [2]Department of Materials- and Geoscience, Technical University Darmstadt, Germany

The Materials Research department at GSI operates several target stations dedicated to swift heavy ion irradiation, providing unique in-situ analysis capabilities for fundamental radiation-matter interaction studies, applied radiation hardness testing, and ion-track nanotechnology for a broad international user community.

At the M-Branch, GSI's UNILAC accelerator provides beams from carbon to uranium at energies between 3.6 and 11.4 MeV/u, typically 4.8 MeV/u, to three target stations: M1 with time-of-flight secondary ion/neutral mass spectrometry and in-situ SEM; M2 with on-line X-ray diffraction; and M3, a versatile multi-purpose target station equipped for ionoluminescence, FTIR and Raman spectroscopy, laser Doppler vibrometry, IR thermography, and cryogenic-to-high-temperature irradiations. M-Branch serves as the primary platform for radiation hardness assessments of functional materials such as high-entropy alloys, amorphous metals, ceramics and accelerator components [1-3] as well as fundamental ion-matter interaction studies [4].

At X0, an automated irradiation system processes up to 500 samples per hour for ion-track nanotechnology and high-energy irradiations up to 11.4 MeV/u. The heavy ion microprobe, providing sub-micrometer single-ion irradiation with ions as heavy as gold and uranium, allows in-operando testing of detectors and electronics. At Cave A (SIS18), a recently commissioned high-pressure platform combines diamond anvil cells at pressures up to tens of GPa with focused, fast-extracted heavy ion beams and in-situ Raman spectroscopy to study novel phenomena such as ion-induced phase transitions under extreme conditions or the stabilization of high-pressure phases [5, 6].

We present the current status of our infrastructure and give an outlook on the beams and capabilities that will be available when our user program resumes in 2028, including planned upgrades to experimental setups and the availability of new beam parameters.

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Keywords

In-situ analysis, radiation hardness, ion-track nanotechnology, high-pressure irradiation, user facility

P70 - Compositional Dependence of Strain and Radiation Resistance in AlGaN Alloys Analyzed with Channeling Rutherford Backscattering Spectrometry

Steven Frankowski[1], Joseph Graham[2, 3, 4], Miguel L. Crespillo[1], Pascal Simon[5], Maria Eugenia Toimil-Molares[5, 6], José Olivares[2, 4], Sunil Kumar[2], Thaddeus J. Asel[7], Shin Mou[7], Adam T. Neal[7], Alexander Chaney[7], Maik Lang[1]

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$Al_xGa_{(1-x)}N$ is a wide bandgap semiconductor with a direct bandgap tunable from the near-UV to deep-UV by varying Al composition. This material's large breakdown electric field allows for higher power density and switching speeds in power electronics. Such properties are attractive for use in aerospace environments with demanding size, mass, and power constraints. Space is a high radiation environment; therefore, understanding the resistance of AlGaN to radiation damage is critical. Here we present a study of AlGaN films across several compositions grown by metal modulated epitaxy and disordered with 946 MeV swift heavy Au ions. Rutherford backscattering spectrometry in channeling configuration was used to disentangle strain arising from ion-induced damage, lattice mismatch at the film-substrate interface, and alloying. Compositions with greater Al content exhibit enhanced resistance to structural modification following radiation, demonstrating that bandgap tuning through alloying also governs radiation tolerance, which may impact device performance and longevity.

Keywords

Swift Heavy Ion, Semiconductors, Rutherford Backscattering Spectroscopy (RBS), Channeling, Strain

P71 - X-ray production and multiple ionisation in near-symmetric ion-atom collisions

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The calculation of ionisation atomic parameters based on single-hole vacancy production post ion-atom collisions is not valid for heavy ion-atom interactions. This is due to significant electronic screening associated with the prolonged dwell times of heavy ions at energies relevant to Ion Beam Analysis (IBA) techniques such as MeV SIMS and ToF-ERDA. Under these conditions, multiple ionisation (MI) states in both the projectile and the target atom are formed, where the presence of spectator subshell vacancies results in proportionally modified X-ray emission probabilities. The extent to which MI effects manifest increases at lower impact energies and with projectile mass, thereby promoting the formation of transient molecular orbitals (TMO). Understanding these MI states is important for both potential quantitative application of PIXE using heavy ions at various ion energies and collision symmetries; and for fundamental studies of ion-atom interactions.

Previous evaluations of MI effects across different ion-atom systems have been carried out using X-ray Doppler shifts, changes in intensity ratios for specific transition series, and vacancy distributions. Shifting vacancy distributions were extracted from analyses of satellite progressions in the L-shell for Sn-induced carbon ions before.

In the present study, MI effects are evaluated through experimental X-ray production cross sections measured for C, Ag, and I projectiles in the energy range 0.1-0.5 MeV/u, incident on Si, Zr, and Sn targets. The dependence of MI effects on projectile mass and collision symmetry is discussed. TMO formation is discussed in the context of Resonant Transfer and Excitation processes in near-symmetric collisions.

Keywords

Multiple ionisation, X-ray production, Ion-atom collisions, Ion Beam Analysis

P72 - Atomic cascade computations for swift ions near surfaces

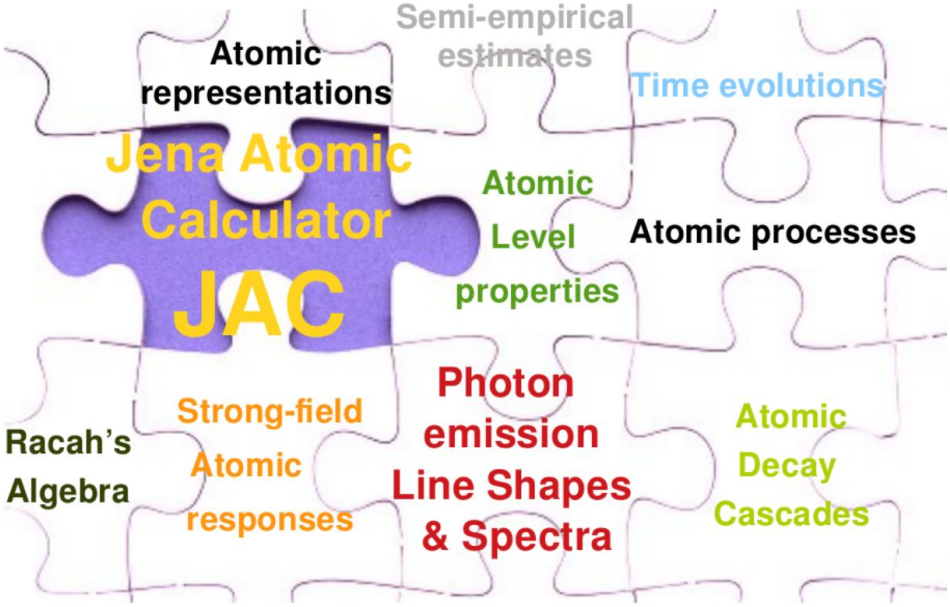
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Atomic cascades occur frequently in Nature and have therefore been studied in different fields of physics and elsewhere, from precision measurements to the modeling of astrophysical spectra, and up to ion near surfaces. We here discuss a classification of atomic cascades and shall demonstrate how such cascade processes can be readily modeled within the framework of JAC, the Jena Atomic Calculator.

Keywords

atomic cascade; atoms and ions; Jena Atomic Calculator; hollow atoms



P73 - Influence of the electronic density of states on the trajectory-dependent energy deposition of keV ions in Silicon

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We investigate how the electronic density of states (DOS) in condensed matter influences the electronic excitations induced by penetrating keV ions. Using single crystalline, self supporting Si membranes, a prototypical band gap material, we measure the specific electronic energy deposition of ions transmitted along well defined crystallographic trajectories. For Ne ions channeled along the ⟨100⟩, ⟨211⟩, and ⟨111⟩ orientations, the measured energy transfers agree well with density functional theory (DFT) predictions based on the unperturbed electron densities of an electron gas. This agreement indicates that atomic collision processes are strongly suppressed under channeling conditions and that the dominant interactions involve valence and conduction electrons. In contrast, for H and He ions, the measured specific energy deposition is found to be systematically lower than predicted, suggesting additional excitation channels or non-linear interaction mechanisms not captured by simple electron gas models. Across all studied low index orientations, Ne ions exhibit non-linear velocity dependence of the specific energy deposition. For random orientations, an inverted trend is observed relative to channeling conditions. We discuss how experimental challenges, particularly the difficulty of constraining ion trajectories at the lowest velocities, can obscure signatures of electronic excitation thresholds in the target DOS.

Keywords

Electronic stopping, channeling

P74 - Influence of Compositional Complexity on Transformations in Pyrochlore Oxides under Highly Ionizing Radiation

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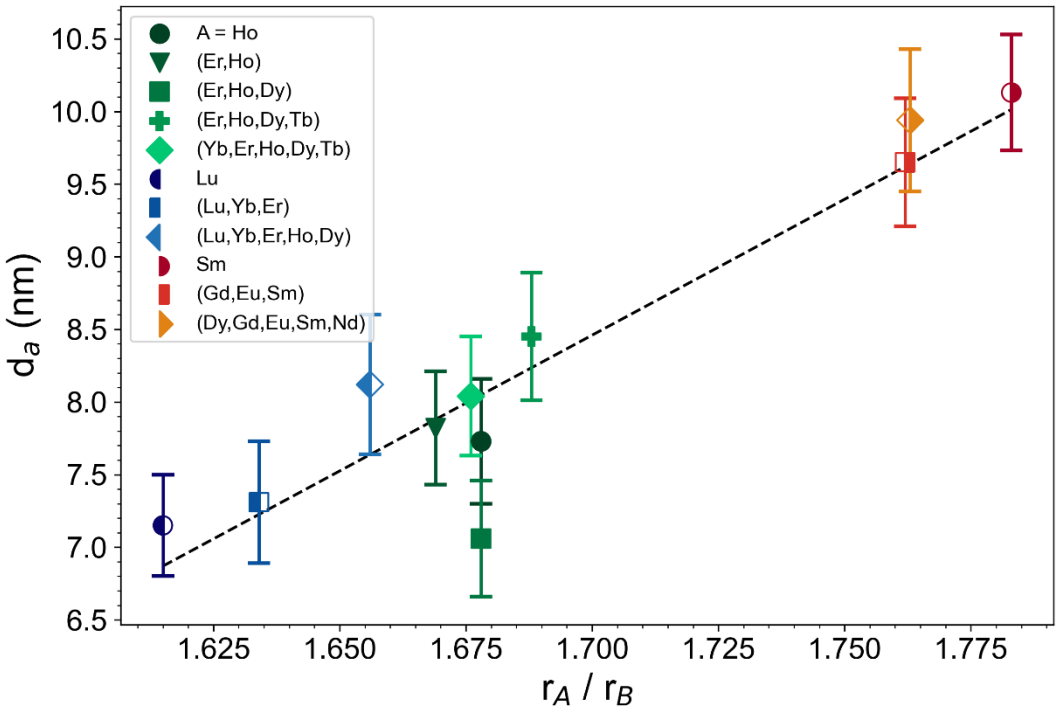
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Compositionally complex ceramics with several principal components offer the opportunity to study how material behavior in harsh environments is influenced by the simultaneous incorporation of many cations, as well as potentially improved properties for harsh environments expected in advanced technologies like nuclear waste immobilization matrices. To examine these effects, series of titanate and zirconate pyrochlores were irradiated with 946 MeV Au ions at the GSI Helmholtz Centre, with subsequent characterization performed using synchrotron-based X-ray scattering, neutron total scattering, high resolution TEM, and Raman spectroscopy. Ion track diameters calculated from diffraction measurements showed that

amorphization rates in compositionally complex titanate pyrochlores are comparable to that of conventional endmembers, exhibiting a mostly linear relationship between amorphous track core diameter and relative cation size. However, a secondary non-linear effect was observed that suggests 'medium entropy' compounds may outperform more complex compositions (Fig. 1), which is supported by calculations of calculations cation antisite defect energy using density functional theory. An amorphous core / defective shell morphology is indicated by HRTEM images of track cross-sections and X-ray diffraction measurements, suggesting epitaxial recrystallization occurs in a similar fashion to traditional pyrochlores. Sensitivity to irradiation was observed in complex zirconate pyrochlores from synchrotron X-ray diffraction measurements, which does not occur in the analogous single-component oxide ($Ho_2Zr_2O_7$).

Keywords

Amorphization, advanced characterization, high-entropy materials



P75 - Ion transmission through silicon nitride membranes

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In an effort to develop high-throughput screening of radiation damage assays for aqueous biological targets, we have investigated ion transmission through silicon nitride membranes. Our measurements utilize two-by-two arrays of 30 nm thick silicon nitride (Si_3N_4) grown on a 200 micron thick Si frame. Each windowed membrane target was mounted on a custom-built stainless steel holder (see Figure) mounted in front of an electron multiplier detection system. Normal incidence beams of alpha particles (^{210}Po) and multiply charged Argon ions obtained from an electron beam in source were used to determine the membrane transmission

characteristics. These data are compared to SRIM simulations, and x-ray emissions measured during select irradiation runs are also presented. To validate the use of these samples as a platform for biological irradiations, we have performed pressure tests with the windowed membranes serving as a vacuum barrier under configurations suitable for aqueous targets.

Keywords

membranes, HZE ions, alpha particles, multiply charged ions



Figure: Si_3N_4 window in a stainless-steel holder.

P76 - Ion-Beam-Induced Ag and C Nanodot Formation on Pre-Patterned Silicon Nano-Templates for Advanced Photonic Applications

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The controlled fabrication of optically active nanostructures on semiconductor platforms is highly promising for advanced photonic, plasmonic, sensing, and optoelectronic applications [1,2]. In this work, we demonstrate a scalable ion-beam-driven strategy for engineering isolated Ag- and C- nanodots on self-organized silicon nano-templates. The templates were synthesized via grazing-incidence 14 keV N_2^+ ion irradiation at 70° on crystalline Si, producing pyramidal silicon nitride nanostructures that promote selective ion incorporation and nanodot formation. Subsequent broad-beam implantation of Ag and C ions enabled the formation of embedded nanodots with enhanced optical properties [3,4].

Cross-sectional TEM revealed shallow embedded nanodots of 5-15 nm localized on pyramidal faceted structures. XPS confirmed the formation of elemental Ag nanodots in Ag-implanted templates [4] and the presence of graphitic carbon, SiC, and graphitic nitrogen (NC) phases in C-implanted templates [5]. Raman studies confirmed the dominance of D-band carbon (amorphous carbon) over G-band carbon (crystalline carbon), while subsequent annealing at 800 °C for 3 hours resulted in significant enhancement of the G-band intensity, indicating improved carbon's crystallinity. Ag nanodots exhibited strong localized surface plasmon resonance effects, significantly enhancing local electromagnetic fields. Optical

measurements demonstrated a significant change of reflectivity and bandgap tuning from ~1.88 eV to ~0.8 eV due to defect-state evolution and interface reconstruction. Surface-enhanced Raman spectroscopy of 10 µM Rhodamine 6G showed more than 20 times Raman enhancement in the presence of Ag-dots contained templates with excellent reusability. Simultaneously, C nanodots displayed excitation-dependent photoluminescence extending from green to deep-red emission highlighting its potential for white LEDs and photosensors. Therefore, those nanodots contained template offer a versatile platform for reusable SERS substrates and next-generation integrated photonic devices.

Figure 1: Schematic of Ag/C nanodots formation on pre-patterned Si nano template

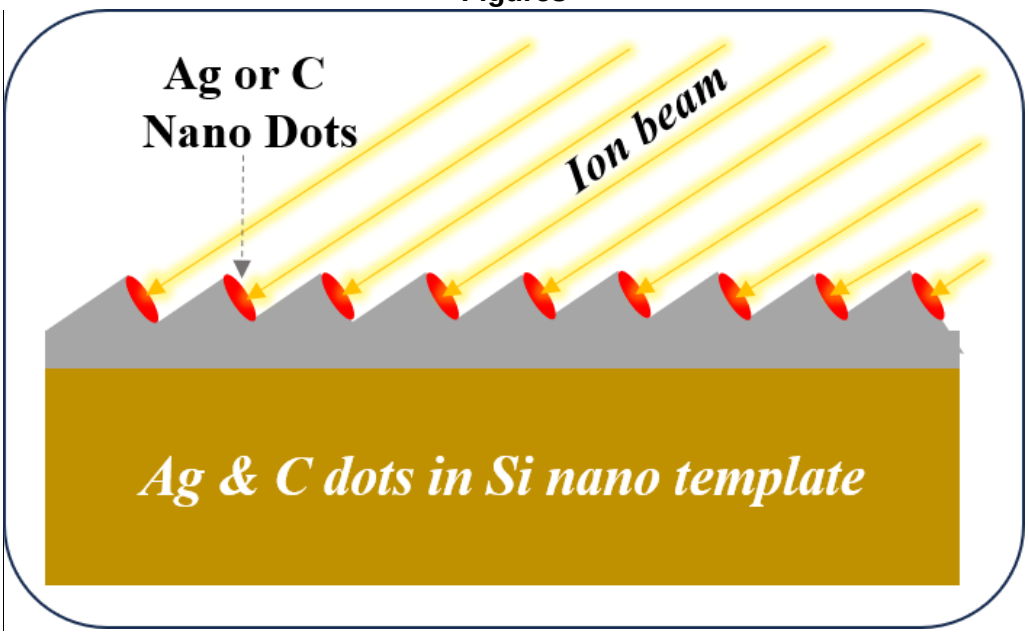
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[5] S. Bhowmick et.al., Nanotechnology, 35 (12) (2024).

Keywords

Nanodots, Ion beam modification, Nano template, Irradiation, SERS

Figures



P77 - Fluence-Dependent Nanoscale Resistive Switching Behaviour in Au-Implanted HfO_2 Memristive Devices

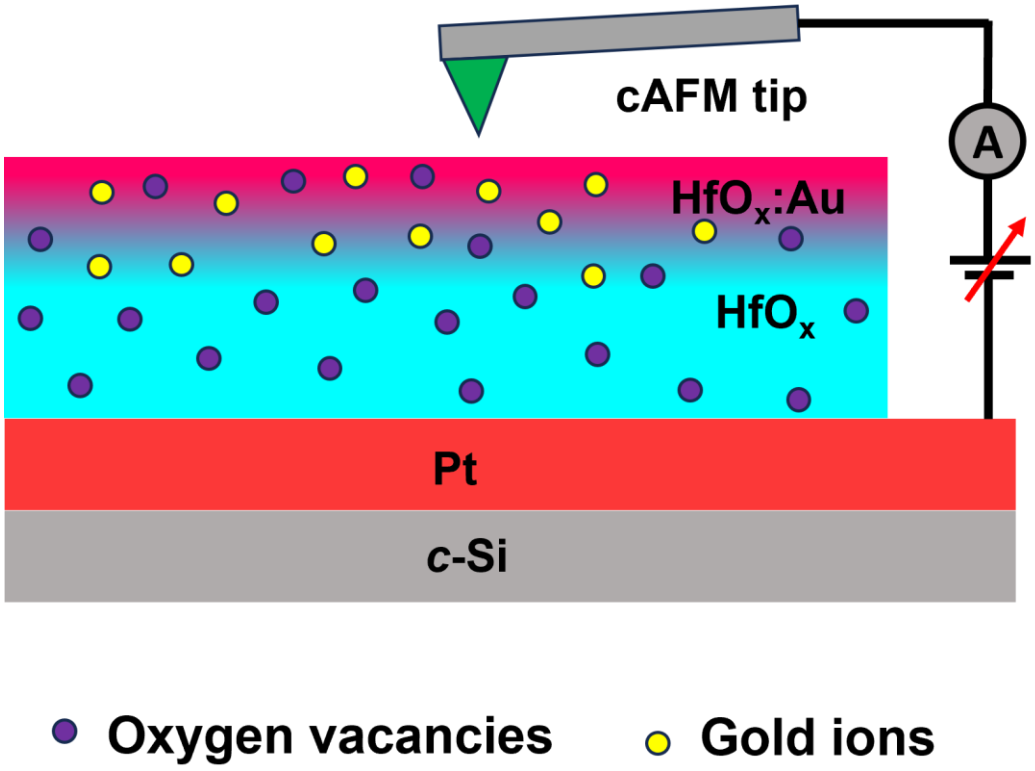
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With the increasing demand for high-density, low-power, and energy-efficient data storage technologies, nanoscale resistive random-access memory (RRAM) devices have emerged as highly promising candidates for next-generation non-volatile memory and neuromorphic computing applications. In this work, the effect of Au-ion implantation on nanoscale resistive switching behaviour of HfO_2 thin films is systematically investigated. Au-ions are implanted into HfO_2 films using various fluences to tailor the defect distribution, oxygen vacancy concentration, and local conductive pathways within the oxide layer. The device implanted at low fluence (viz. 1×10^{16} ions/cm^2) shows a noticeable cycle-to-cycle variation over 50 switching cycles, indicating non-uniform conductive filament formation and unstable defect distribution. In contrast, the device implanted to a higher fluence (viz. 1×10^{17} ions/cm^2) exhibits highly stable (~500 cycles) and repeatable switching behaviour with a reduced operating voltage and improved switching uniformity. This observation suggests easier ion migration and lower filament formation energy, highlighting its potential to exhibit neuromorphic behaviour. The results confirm that the fluence of Au-ion fluence plays a crucial role in defect engineering and nanoscale resistive switching performance in HfO_2-based RRAM devices.

Keywords

resistive switching, memristors, ion implantation, HfO2 film, conductive atomic force microscopy



P78 - Defect engineering in 4H-SiC by C and Si ion implantation at room temperature

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In the quest for the development of advanced quantum technology, designed to overcome the limitation of the conventional classical architecture, Single Photon Sources (SPSs) in wide band-gap materials have emerged as key alternate due to its ultrafast computation, precise sensing, and secure communication. Among the various SPS platforms (i.e. defects in diamond, *h*-BN etc.), Silicon vacancies (V_{Si}), Carbon-antisite vacancies pair (V_CC_{Si}), and divacancies ($V_{Si}V_C$) in single crystal Silicon Carbide (4H-SiC) have gained significant attention. These defect centers exhibit several advantageous properties including room-temperature operation, a broad emission spectrum, long spin coherence times, and a low second-order correlation function, making them promising candidates for quantum applications. In this work, we have produced defects by C and Si ion implantation having energy of 30 keV and using fluences in the range of 10^{12} - 10^{14} ions/cm^2 and systematically studied their influence on life time and the photoluminescence (PL) of the defect centres. Using the dynamic Monte Carlo based TRIDYN simulation to evaluate the defect densities, ion implantation profiles and the depth profile for the above implantation conditions. These simulations are expected to guide the optimization of experimental parameters to localize defect formation within the desired depth range, while minimizing unwanted damage and the creation of non-radiative recombination centers.

Keywords

Single Photon Source (SPS), Ion implantation.

P79 - Influence of input parameters on simulated sputtering yields using SRIM and SDTrimSP

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Accurate sputtering yields are essential in the thin-film deposition, fusion research, space science, semiconductor fabrication, and several other scientific and technological fields [1]. In this work, we focus on sputtering conditions relevant to thin-film deposition techniques. For this purpose, we employ two widely used binary-collision-approximation-based simulation codes, SRIM and SDTrimSP [2].

We present a comparative analysis of sputtering yields obtained for Ar ion bombardment in the energy range of 100-1000 eV for period-4 and period-6 transition-metal targets. Particular attention is given to the influence of several input parameters available in SDTrimSP, including the interaction potential (KrC, ZBL, Moliere, and Nakagawa-Yamamura), electronic energy-loss model (Lindhard-Scharff, Oen-Robinson, and Ziegler tables), integration method (numerical and geometrical), and surface binding energy. The simulations reveal significant differences in the predicted sputtering yields depending on the selected interaction potential. These differences are most pronounced for lighter transition metals such as Ti, Cr, and Cu, for which the KrC and ZBL potentials give similar values, whereas the Moliere screening function yields considerably higher sputtering yields.

The choice of electronic energy-loss model also has a noticeable effect on the calculated sputtering yields, despite the relatively small contribution of electronic stopping compared with nuclear stopping at ion energies below 1000 eV. In contrast, the numerical and geometrical integration methods generally produce similar yield values, except in calculations using the KrC potential. When default surface binding energies are used (approximated by the heat of sublimation in both programs), SDTrimSP shows better agreement with experimental data, whereas SRIM generally overestimates the sputtering yields, particularly for heavier elements. These results highlight the importance of careful parameter selection for obtaining reliable sputtering yields in the thin-film growth processes.

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Keywords

sputtering, binary collision approximation, SDTrimSP, SRIM

P80 - First-Principles Investigation of Mechanical Stability in Pyrochlore Ceramics

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The development of advanced nuclear energy technologies requires structural materials capable of maintaining their integrity under intense irradiation. Pyrochlore ceramics ($A_2B_2O_7$-type) such as $La_2Zr_2O_7$, $Nd_2Zr_2O_7$, $Sm_2Zr_2O_7$, $Yb_2Ti_2O_7$, $Eu_2Ti_2O_7$, $Y_2Ti_2O_7$, and $La_2Hf_2O_7$, have emerged as promising candidates owing to their exceptional resistance to radiation-induced amorphization, high chemical stability, and favorable thermo-mechanical properties. Understanding the atomistic response of these materials to irradiation-induced defects is therefore essential for the rational design of next-generation nuclear waste forms and radiation-tolerant ceramics. In this work, first-principles density functional theory (DFT) calculations are employed to investigate the influence of intrinsic point defects, including oxygen vacancies, cation vacancies, and antisite defects, on the structural and mechanical properties of representative pyrochlore ceramics. Defect formation energies, local structural distortions, elastic constants, bulk modulus, shear modulus, and Young's modulus are systematically evaluated to quantify the effects of defect formation on mechanical performance and structural stability. The calculations reveal that vacancy defects generally reduce elastic stiffness and mechanical robustness, whereas selected antisite disorder configurations exhibit improved resistance to structural degradation. These results establish clear correlations between defect chemistry and the thermo-mechanical response of pyrochlore ceramics, providing atomistic insights into the mechanisms governing their radiation tolerance. This study extends our previous combined computational and experimental investigations of irradiated ceramic materials (V. Bessonov, J. O'Connell, T. Shomenov, *et al*., *Applied Surface Science*, **725**, 165730, 2025) and provides a computational framework for the future design and multiscale modeling of radiation-resistant pyrochlore ceramics for advanced nuclear applications.

Keywords

Density Functional Theory (DFT), Molecular Dynamics (MD), Elastic constants, Thermal conductivity, Ion irradiation, Nuclear materials, Ceramics.

P81 - Effect of He ion irradiation on the early corrosion behaviour of SIMP steel in liquid lead-bismuth eutectic

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He-ion irradiated and pristine SIMP steel samples were corroded in oxygen-saturated liquid LBE at 550°C for 24 h. The results show that the oxide layer on the irradiated sample is significantly thicker than that on the pristine sample. In the irradiated sample, the inner oxide layer is notably enriched with Si and Cr at the martensitic lath boundaries, causing severe depletion of these elements within the laths. This significantly accelerates the oxidation of the irradiated sample in liquid LBE in combination with the increased surface roughness of the irradiated sample, the radiation enhanced elemental diffusion and the voids in the inner oxide layer.

Keywords

Ferritic/martensitic steels; TEM; Irradiation; Lead-bismuth eutectic; Corrosion

P82 - Microstructural evolution and irradiation hardening in pressureless sintered SiC irradiated with He ions

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Pressureless sintered silicon carbide (PLS-SiC) ceramics, combining outstanding material performance with superior cost-effectiveness, represent a highly promising candidate for structural components featuring complex geometries or large dimensions in advanced nuclear systems. In this study, the microstructural evolution and mechanical response of PLS-SiC under helium ion irradiation were systematically investigated. Irradiation was performed using 500 keV He ions at 500 °C over a fluence range of 2.0×10^{16} to 1.0×10^{17} ions/cm^2. Grazing-incidence X-ray diffraction (GIXRD) and Raman spectra results confirm irradiation-induced lattice expansion caused by the accumulation of interstitial-type defects, and the formation of homonuclear Si-Si and C-C bonds. Transmission electron microscopy observations reveal that helium bubbles nucleate at a fluence of 5.0×10^{16} ions/cm^2, with preferential segregation and coarsening observed at grain boundaries. The average bubble size increased from 0.93 nm to 1.66 nm with rising fluence, accompanied by an increase in the density of black-spot defects and dislocation loops. Nanoindentation results reveal an increase in hardness across all irradiated regions relative to the unirradiated counterpart, with the irradiation-induced hardening degree (ΔH/H) following a fluence-dependent power-law relationship: $\Delta H/H = 3.05 \times \Phi^{0.69}$. The hardening behavior is primarily ascribed to the impediment of dislocation motion by helium bubbles and defect clusters, showing good consistency with the Friedel-Kroupa-

Hirsch model. Overall, our findings are essential for evaluating the service reliability of PLS-SiC ceramics in irradiation environments, and promoting its nuclear applications.

Keywords

SiC; He-ion irradiation; defects; helium bubbles; irradiation hardening

P83 - Preliminary Research on High-Performance SOT-MRAM Chips Fabricated by Ion Irradiation Technology

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In the post-Moore era, emerging technologies such as artificial intelligence (AI) have driven a surging demand for high-performance in-memory computing chips. Spin-orbit-torque magnetic random-access memory (SOT-MRAM) offers compelling advantages, including high-speed operation (nanosecond-scale), low power consumption, and non-volatility, making it a promising candidate for next-generation memory and in-memory computing architectures. However, current SOT-MRAM devices still suffer from insufficient spin-orbit torque (SOT) efficiency, relatively high write current, and inadequate magnetization switching stability, which severely hinder their development for low-power in-memory computing applications.

Ion irradiation technology, characterized by high energy density and precise controllability of processing parameters, provides a powerful means for developing high-performance SOT-MRAM chips for in-memory computing. It enables the modulation of spin transport and magnetization switching properties in SOT heterostructures through the engineering of irradiation-induced defects, interfacial reconstruction, and local strain. In this work, we conduct a systematic investigation into the underlying mechanisms of ion-irradiation-modulated free layers and heavy-metal/ferromagnetic interfaces, the design of SOT heterostructures with high charge-to-spin current conversion efficiency, and the device-level performance verification. This study aims to provide theoretical foundations and technical support for the development of key materials, device design, and subsequent industrial-scale chip applications of high-performance SOT-MRAM.

Keywords

SOT-MRAM Chips; Ion irradiation; Heterostructures

P84 - Multipurpose External Ion Microprobe for Irradiation and Analysis at the Ruđer Bošković Institute

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A new experimental end station is currently under development at the Ruđer Bošković Institute, designed for advanced irradiation and Ion Beam Analysis (IBA). Equipped with a quadrupole focusing system, an exit nozzle for in-air beam delivery, a precise motorized sample stage, and specialized IBA detectors, this end station will be capable of delivering

micrometer-sized beams in ambient air. Additionally, a specialized vacuum chamber positioned before the exit window will house large solid-angle Particle Induced X-ray Emission (PIXE) and other IBA detectors, allowing for submicron-sized beam delivery, irradiation and analysis within a vacuum environment.

The end station will be coupled to a new 5.0 MV tandem accelerator, enabling the delivery of higher-energy protons (up to 10 MeV) and a diverse range of heavy ions. Precise dose control for irradiation studies will be maintained via integrated ion beam fluence monitoring systems in the vacuum chamber. Following installation and commissioning in 2027, this beamline will extend ongoing dosimetric research-specifically the proton and heavy-ion irradiation of radiophotoluminescent (RPL) glass detectors used in hadron therapy [1]. Furthermore, ongoing studies on the radiobiological effects of ion beams on cancer cells will expand using these higher-energy protons and heavy ions for irradiation [2]. This work will present the current status of the new end station and the 5.0 MV tandem accelerator, highlighting its capability for vacuum submicron and in-air (micron-sized and broad) beam delivery with precise beam dose monitoring, together with its potential for future heavy-ion irradiation research.

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Keywords

External Ion Microprobe, IBA, proton irradiation, heavy-ion irradiation

P85 - Status and upgrade of the Ruđer Bošković Institute Tandem Accelerator Centre

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Through the Laboratory for Ion Beam Interactions, the Division of Experimental Physics of the Ruđer Bošković Institute (RBI) operates and maintains the Tandem Accelerators Centre (RBI-AC). RBI-AC was established in 1987 on the basis of a 6 MV EN Tandem VDG accelerator. In 2005 complementary 1 MV Tandetron accelerator was acquired. Recently low energy ion implanter has been developed and installed as well. The accelerators can deliver various ions with energies from 0.1 to tens MeVs to numerous beam-lines and end-stations. They are used for ion beam analysis (IBA) and ion beam materials' modification (IBMM) studies, including measurements of related fundamental parameters, such as relevant nuclear reactions and inner shell ionization cross sections, ion stopping powers, etc. Occasionally measurements in experimental nuclear physics are performed as well. Regular users of the Center are researchers from Croatia, the EU and beyond, as well as users from industry and the wider community.

Recognizing the strategic importance of the Center and the need to maintain it at a high level, the RBI included its improvement in its strategic ESIF project O-ZIP, considering that: (i) the existing hall of the Center is inadequate for maintenance and development after 60 years; (ii)

6 MV Tandem is over 60 years old, obsolete and unreliable. Thus, a new hall for the Center has been recently built and a new 5MV tandetron accelerator has been ordered and delivered. Installation of new 5 MV Tandetron is in progress. Over the coming period, this new accelerator will be installed, while the 1 MV Tandetron and all the existing experimental beamlines and end-stations will be relocated to the new hall.

In addition to O-ZIP, the upgrade of the RBI-AC is also supported by the ERDF project CEMS through significant modernization of the equipment and the expansion of the expertise of new generations of scientists; then by the UNIMAC project, co-financed by EU funds from the Recovery and Resilience Facility (RRF) financial instrument, as well as by the project OTARI co-financed by the Ministry of Science, Education and Youth through the IBDR loan as the Digital, Innovation, and Green Technology Project (DIGIT Project) financial instrument.

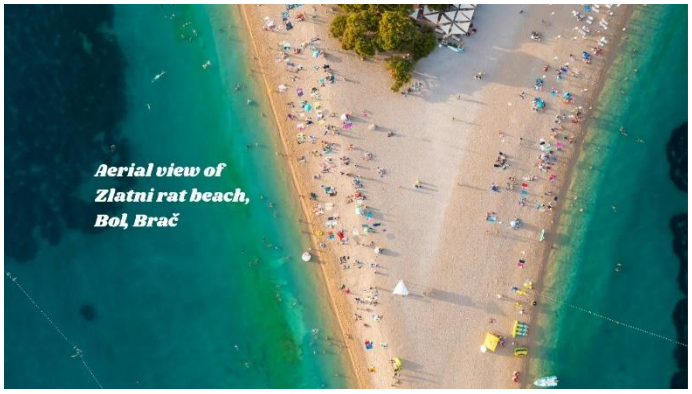
UNIMAC support is focused on the provision of the equipment necessary for the new experimental line for ion irradiation of larger surfaces, including the electrostatic ion beam deflection system, the end-station support, and the entrance ion optics for the new 5 MV accelerator.

The objectives of the OTARI project are to enhance professionalization of organizational and operational model to run the RBI-AC; to optimize transparent access to RBI-AC and services; to enhance capacity of the staff involved in RBI-AC activities; to strengthen collaboration with industry and other research infrastructures; and to increase visibility and user base of the RBI-AC.

The status of the RBI-AC upgrade is presented.

Keywords

RBI-AC, IBA, IBMM


Aerial view of
Zlatni rat beach,
Bol, Brač



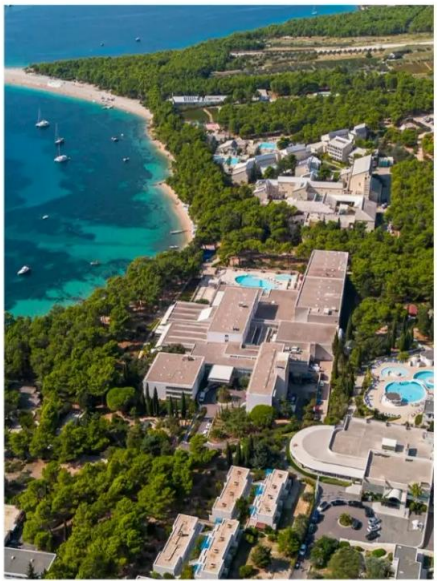

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Croatian Science
Foundation


Chapel within
Dominican monastery,
Brač


Aerilal photo of Bol,
Brač


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scan
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