



IBMM2024

International Conference on Ion Beam Modification of Materials (IBMM)

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ABSTRACT BOOK

	IBMM 2024 Draft Programme				
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INVITED ABSTRACTS

Radiation damage of high temperature superconductors for fusion magnets

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High temperature superconductors (HTS) in the form of coated conductors are an enabling technology for the next generation of compact nuclear fusion reactors that require higher magnetic fields than Nb₃Sn can provide. However, in operation, the superconducting magnet windings will be exposed to a flux of fast neutrons which will introduce structural damage at cryogenic temperatures. Many previous studies using both fission spectrum neutrons and ions at room temperature (or slightly elevated temperatures) have shown that an initial increase in the superconducting current carrying performance upon irradiation is followed at higher fluences by a severe degradation of the properties and eventually complete loss of superconductivity. The superconducting transition temperature is found to decrease monotonically with fluence, strongly suggesting that radiation-induced defects occur throughout the entire crystal lattice, even at relatively low fluence. Here we will report on two facets of the work being carried out by the Oxford group to improve understanding of radiation damage of HTS materials. The first involves innovative in situ ion irradiation experiments carried out at Surrey Ion Beam Centre to assess radiation damage of HTS at cryogenic temperatures relevant for operation in a fusion magnet. These are crucial experiments because early work has shown that excursions to room temperature lead to an evolution of the defect landscape and a partial recovery of the superconducting performance which could be exploited to extend magnet lifetime.

Secondly, we will report results of our recent studies aimed at understanding the nature of the lattice defects that cause the degradation in transition temperature using polarisation dependent high energy resolution x-ray absorption spectroscopy (HERFD-XAS) to probe small changes in the bonding environment of the copper ions that cannot be easily imaged using atomic resolution electron microscopy. We have successfully modelled the experimental spectra using DFT core hole calculations, allowing the origin of the various spectral features to be identified. The nature of the defects responsible have been investigated by calculating spectra from a range of defect structures and comparing with the experimental results. We have found that samples irradiated neutrons exhibit similar spectral differences to those irradiated with light ions (He⁺), suggesting that light ions may be a useful safe proxy for understanding the degradation of the fundamental properties of high temperature superconductors.

Using Ion Irradiation for Fast Simulation of Reactor Neutron Damage: Credibility, Issues, and Mitigation

Lin Shao¹

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Accelerator-based ion irradiation has been widely used as an emulation of neutron irradiation, due to its capability to achieve a damage level up to 1000 displacements per atom, at a speed several orders of magnitude higher than that of a testing reactor. Accelerator testing significantly accelerates materials screening in both fission and fusion reactor development. However, the acceptance of accelerator testing data in materials qualification and certification has been challenging due to size effects and artifacts. The former primarily arises from length scale challenges in post-irradiation mechanical property testing, while the latter are mainly caused by (1) surface effects, (2) injected interstitial effects from extra atoms introduced, and (3) dpa rate effects. In this talk, the current status of linking or equating accelerator and reactor irradiation data is summarized. The artifacts and the best practices for mitigating these artifacts are discussed. Both the surface effect and the injected interstitial effect can be mitigated through the appropriate selection of a safe data analysis zone based on data self-consistency, but the dpa rate effect has not yet been fully resolved. Fundamentally, addressing this issue requires revisiting both void nucleation theory and non-conservative Ostwald ripening theory. The currently available model, known as the temperature shifting model, is valid only for the void growth stage. After modifying the early void nucleation theory developed by Katz and Wiedersich, we have shown that the new model can reasonably predict void swelling data. Furthermore, it provides guidance on experimental parameter selection to (1) maximize the safe analysis zone and (2) select irradiation temperatures to compensate for the dpa rate difference. In summary, although accelerator-based irradiation involves complex data interpretation, it remains a trustworthy method and the only realistic option for rapid nuclear materials testing.

Synaptic transistor based on charge trapping in ion-implanted gate dielectrics

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Neuromorphic computing aims to emulate the human brain using parallel networks of solid state synapses and neurons[1]. Novel devices, including: memristors, ferroelectric transistors, synaptic transistors and memtransistors are currently being investigated for such applications [2, 3]. Here, we report the fabrication of a synaptic field effect transistor (FET) based on charge trapping and de-trapping in the gate dielectric.

Back-gated field-effect transistors (FETs) with ultra-thin indium-oxide channel layers were fabricated by squeezing a droplet of In between 300nm SiO₂/p++ Si substrates heated to 250°C in air. After separation and cleaning, this produced a uniform area of InOx with a thickness ~5 nm that serves as the semiconducting channel of the transistor. Electron beam lithography was subsequently used to define Cr/Au Source/Drain electrodes. The synaptic response of the transistors was achieved by ion-implanting the gate-dielectric prior to InOx deposition, with the memory effect arising from the capture and emission of charge carriers. Details of these devices and the mechanisms underlying their synaptic response will be discussed.

References

- 1) M.K. Kim, Y. Park, I.J. Kim, J.S. Lee, 'Emerging Materials for Neuromorphic Devices and Systems', *iScience* 23(12) 101846 (2020).
- 2) S. Dai, Y. Zhao, Y. Wang, J. Zhang, L. Fang, S. Jin, Y. Shao, J. Huang, 'Recent Advances in Transistor-Based Artificial Synapses', *Adv Funct Mater* 29(42) (2019).
- 3) Z. Li, W. Tang, B. Zhang, R. Yang and X. Miao, 'Emerging memristive neurons for neuromorphic computing and sensing', *Sci Technol Adv Mater.* 24, 2188878 (2023)

Ion beam controlled polymorph transitions in gallium oxide

Andrej Kuznetsov¹

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On many occasions, structural defects bare a negative connotation, provoking efforts to reduce their contents. On the other hand, many unique material properties may become possible only with defects in materials. In this talk, I review our recent observation of the disorder-induced ordering in gallium oxide controlled by the accumulation of intrinsic defects (Physical Review Letters 128, 15704 (2022) resulting in remarkably high radiation tolerance of the gamma-polymorph obtained by this modification (Nature Communications 14, 4855 (2023)) and outline a possible explanation of the mechanisms (Physical Review Letters, in-review (2024) and arXiv:2401.07675v3). Altogether, it comprises an interesting story of the ion beam controlled modification in materials not reported in literature before this work.

Ion beam synthesis of earth-abundant electrocatalysts for Hydrogen evolution and Ammonia production

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Electrocatalysts are at the heart of green hydrogen and ammonia production. Cost-competitive hydrogen requires GW-scale electrolyser production coupled with a significant drop in current manufacturing costs. Earth-abundant alternatives to platinum compatible with large-scale manufacturing is therefore highly desirable. On the other hand, realising electrochemical ammonia production demands highly selective catalysts for dinitrogen activation. In this work, we present a novel electrocatalyst fabrication approach based on ion implantation that can be customised for both hydrogen evolution reaction (HER) and nitrogen reduction reaction (NRR).

Transition metal carbides (TMC) and nitrides (TMN) have attracted significant interest as cathode electrocatalysts for HER and NRR, respectively. The inability to manufacture TMCs as ultra-fine nanoparticles (to achieve high surface area) has prevented realisation of their catalytic potential for HER. Conventional routes require high synthesis temperatures leading to uncontrollable agglomeration, drastically reducing their active surface area. Using ion implantation, we demonstrate ion beam synthesis of tungsten and molybdenum carbides with high activity towards HER [1-3]. With high-resolution TEM and X-ray photoelectron spectroscopy, we demonstrate synthesis of rare metastable phases of TMCs (e.g., γ' -MoC known for HER activity comparable to Pt) at dimensions as low as 2-3 nm. We show that by careful selection of synthesis parameters, the phase and size of the TMC particles can be controlled consequently affecting their HER activity.

Using a similar approach, we demonstrate fabrication of TMN catalysts such as VN and ZrN, known for their unique ability to selectively reduce nitrogen via., Mars-van Krevelen mechanism. We apply stringent protocols to evaluate their electrochemical performance and quantify the ammonia produced (ion chromatography). The ion beam synthesised TMNs drive nitrogen reduction to ammonia with a Faradaic efficiency of ~20% and ~160 nmol cm⁻² h⁻¹ production rate. In summary, we present a novel manufacturing technique to fabricate promising cathode catalysts for HER and NRR.

References

- 1) Fiedler, H. et.al 2023. Small, Online: 9 p.; doi: 10.1002/smll.202304118
- 2) Malone, N. et.al 2023. ASC applied engineering materials, :24 p.; doi: 10.1021/acsaenm.3c00298
- 3) Malone, N. et.al 2024. ASC applied nano materials, 7(5): 4843-4852; doi:10.1021/acsanm.3c05497

Competitive effects of electronic and nuclear energy loss in pre-damaged KTaO₃: A possible ion velocity dependence

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In the scientific excitement stirred by the awareness that optical and electronic properties of potassium tantalate (KTaO₃) can be tailored through irradiation-induced defects[1], interest in ion beam modification of KTaO₃ properties has recently been renewed [2,3]. Its optical and electronic properties tunability makes KTaO₃ a promising candidate for future optoelectronic and spintronic applications [1,4]. All these applications require effective control of the structural modification, but this is an extremely difficult task, since it demands in-depth knowledge of the interactions of ions with the local defect states in the corresponding material and the resulting evolution of radiation damage[5]. In this regard, effects of ionizing energy deposition on damage evolution in defective KTaO₃ have been investigated by irradiating pre-damaged single crystal KTaO₃ with intermediate energy O ions (6 MeV, 8 MeV and 12 MeV) at 300 K. By exploring these processes in pre-damaged KTaO₃ containing a fractional disorder level of 0.35, the ion channelling results reveal the occurrence of a precursory stage of damage production before the onset of competitive recovery process in defective KTaO₃ that decreases with O ion energy. In addition, the reduction of disorder level is accompanied by the broadening of the disorder profiles into greater depth with increasing ion fluence, and enhanced migration is observed with decreasing O ion energy. Since Se ($\sim 3.0 \text{ keV nm}^{-1}$) is nearly constant at all 3 ion energies, the difference in behaviour is a natural consequence of the “velocity effect”. As consequence of the so-called “velocity effect”, the Se is confined to a smaller volume in case of the low velocity ions leading to a higher energy density. Therefore, for nearly equal values of Se, much more pronounced ionization-induced annealing process is expected for the smaller ion velocity/energy (i.e., 6 MeV O). The inelastic thermal spike calculation has further confirmed the existence of a velocity effect, not previously reported in KTaO₃ or very scarcely reported in other materials for which this competitive recovery process has also been reported.

References

- 1) A. Gupta, H. Silotia, A. Kumari, M. Dumen, S. Goyal, R. Tomar, N. Wadehra, P. Ayyub, S. Chakraverty, KTaO₃—The New Kid on the Spintronics Block, *Advanced Materials* (2022) 2106481. <https://doi.org/10.1002/ADMA.202106481>.
- 2) G. Velişa, E. Zarkadoula, D. Iancu, M.D. Mihai, C. Grygiel, I. Monnet, B. Kombaiah, Y. Zhang, W.J. Weber, Near-surface modification of defective KTaO₃ by ionizing ion irradiation, *J Phys D Appl Phys* 54 (2021) 375302. <https://doi.org/10.1088/1361-6463/AC0B11>.
- 3) D. Iancu, E. Zarkadoula, M.D. Mihai, C. Burducea, I. Burducea, M. Straticiuc, Y. Zhang, W.J. Weber, G. Velişa, Revealing two-stage phase transition process in defective KTaO₃ under inelastic interactions, *Scr Mater* 222 (2023) 115032. <https://doi.org/10.1016/J.SCRIPTAMAT.2022.115032>.
- 4) X. Han, E. Zarkadoula, Q. Huang, M.L. Crespillo, C. Liu, M. Zhang, X. Wang, P. Liu, Nanostructures evolution assessment and spectroscopic properties modification induced by electronic energy loss in KTaO₃ crystal, *Mater Des* 223 (2022) 111248. <https://doi.org/10.1016/J.MATDES.2022.111248>.
- 5) Y. Zhang, W.J. Weber, Ion irradiation and modification: The role of coupled electronic and nuclear energy dissipation and subsequent nonequilibrium processes in materials, *Appl Phys Rev* 7 (2020) 041307. <https://doi.org/10.1063/5.0027462>.

Exploring the Versatility of MeV Focused Heavy Ion Beams for Diamond Modification

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Diamond, renowned for its exceptional properties, is increasingly utilised in various scientific and technological applications. Traditionally, keV ion implantation has been the standard method for doping and modifying the optical and electrical properties of diamond. However, this technique presents several challenges that need addressing.

In recent years, MeV ion implantation has emerged as a promising alternative, offering novel possibilities that merit thorough investigation. The greater depth penetration of MeV ions results in a higher graphitisation threshold, thereby enabling new avenues for diamond modification. To maximise the benefits of this approach, it is essential to gain a comprehensive understanding of the effects induced by MeV heavy ions on diamond.

In addition to altering electrical and optical properties, focused heavy ions with MeV energies are particularly effective for creating micrometric structures on diamond samples. This is due to the expansion of material to the surface, which occurs because of the density decrease at the end of the ion range, leading to superficial tomography. This capability is of significant interest for applications requiring precise material modification at microscale levels.

This presentation will review recent research conducted at the Centro de Micro-Análisis de Materiales (CMAM) using MeV focused ion beams. Insights gained from studies of MeV carbon and boron ion beams will be presented. Additionally, the presentation will cover the fabrication process of microstructures using focused ion beams of carbon, oxygen, and silicon, as addressed at CMAM internal microbeam line.

Tellurium-implanted Silicon: correlation between impurity lattice location and electrical/optical properties

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Hyperdoping of silicon (Si) with deep-level impurities, which involves doping well above the solid solubility limit, has attracted renewed interest due to the resulting unique physical properties. These properties include broad sub-bandgap absorption in the infrared wavelength range at room temperature. Here, tellurium (Te) hyperdoped Si has been prepared by ion implantation and pulsed laser melting. The resulting Te-hyperdoped Si layers are epitaxially grown on substrates. With increasing the Te concentration, the samples undergo an insulator-to-metal transition [1,2]. Surprisingly, the electron concentration is approaching 10^{21} cm^{-3} and does not show saturation [3]. It is even higher than that of shallow donor (P, As, Sb) doped Si and potentially meets the criteria of source/drain applications in future nanoelectronics. The infrared optical absorptance is found to increase with dopant concentration [1]. Based on Te-hyperdoped Si, we demonstrate the room-temperature operation of a mid-infrared photodetector [4,5] and the occurrence of mid- and far-infrared localized surface plasmon resonances [6].

To understand the microscopic picture, we have performed Rutherford backscattering/channeling angular scans and first-principles calculations [3,7]. The Te-dimer complex sitting on adjacent Si lattice sites has the lowest formation energy and is thus the preferred configuration at high doping concentrations. Those substitutional Te-dimers are effective donors, leading to the insulator-to-metal transition, the non-saturating carrier concentration as well as the sub-band photoresponse. Moreover, the Te-hyperdoped Si layers exhibit thermal stability up to 400 °C with a duration of at least 10 minutes [8,9]. Therefore, Te-hyperdoped Si presents a test-bed for electrical and optical applications utilizing deep-level impurities. It is unlocking the route toward the direct integration of infrared photonics within a single-chip complementary metal-oxide-semiconductor (CMOS) platform.

References

- 1) M. Wang et. al., Physical Review Applied 10, 024054 (2018).
- 2) M. Wang et. al., Physical Review B 102, 085204 (2020).
- 3) M. Wang et. al., Physical Review Applied, 11, 054039 (2019).
- 4) M. Wang et. al., Advanced Optical Materials, 9, 4, 2001546 (2020).
- 5) M. S. Shaikh, S. Wen, M. T. Catuneanu, Mao Wang, et. al. Optical Express 31, 26451 (2023).
- 6) M. Wang et. al., Nanoscale, 14, 2826 (2022).
- 7) M. Hoesch, O. Fedchenko, Mao Wang et. al. Applied Physics Letters, 122, 252108 (2023).
- 8) M. Wang et. al., Physical Review Materials 3, 044606 (2019).
- 9) M. S. Shaikh, M. Wang et. al., Applied Surface Science, 567, 150775 (2021)

Electron, Exciton, and Defect Kinetics of the Ion-Matter Interaction in Amorphous Silica

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Electronic modifications brought about by ion irradiation in insulators take place over several time and length scales, from the initial deposition of ion energy into the electronic and atomic structures, to the thermalization and transfer of energy from the hot electron-hole plasma to atoms, and the thermal diffusion and recombination of cool charged and neutral carriers. Recent experimental and computational efforts to better understand each of these stages in amorphous silica are presented. In-situ cryo-ionoluminescence studies using light and heavy ions and complementary ex-situ absorbance measurements reveal the kinetics of self-trapped excitons (STEs), oxygen deficient centers, non-bridged oxygen hole centre (NBOHC) defects, and E' centers following and ion impact. The STE kinetics, in particular, provide several insights into STE formation, migration, recombination, and competitive removal by Auger recombination and the thermal spike. The role that the dielectric screening plays on both STE formation competitive non-radiative Auger recombination is discussed and generalized to other oxide dielectrics. Two contributions to the NBOHC emission are observed. The intensity of the first contribution is independent of fluence but proportional to electronic energy loss. It has been attributed to scission of silanol groups (OH impurities). The second contribution increases with ion fluence in a manner correlated with the STE population, suggesting that the decay of STEs contributes to the accumulation of optically active point defects in pristine silica. Recent efforts to develop methods to calculate the electron-phonon coupling in insulators from first principles are also discussed in the context of the ion matter interaction.

Swift heavy ion irradiation of graphene and graphite

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In this contribution, we present results of systematic investigations of swift heavy ion irradiation effects in graphite [1] and graphene [2-5]. Such a dedicated approach enabled us to study the role of electronic and nuclear stopping, i.e., to identify the energy dissipation channels responsible for damage formation in these two studied materials. In the case of graphene samples, we have additionally investigated the role of the number of layers [3], and the influence of the substrate [2]. With the obtained experimental results (by means of atomic force microscopy and Raman spectrometry), complemented by molecular dynamics simulations, we were able to identify the thresholds for ion track formation in both materials.

References

- [1] D. Iveković, P. Dubček, A. Gajović, T. Čižmar, B. Radatović, A.L. Brkić, M. Kralj, M. Karlušić, High-energy heavy ion irradiation of HOPG, *J. Nucl. Mater.* 578 (2023) 154370.
- [2] K. Tomić Luketić, J. Hanžek, C.G. Mihalcea, P. Dubček, A. Gajović, Z. Siketić, M. Jakšić, C. Ghica, M. Karlušić, Charge State Effects in Swift-Heavy-Ion-Irradiated Nanomaterials, *Crystals* 12 (2022) 865.
- [3] D. Iveković, S. Kumar, A. Gajović, T. Čižmar, M. Karlušić, Response of Bilayer and Trilayer Graphene to High-Energy Heavy Ion Irradiation, *Materials* 16 (2023) 1332.
- [4] D. Iveković, K. Tomić Luketić, H. Vázquez, A. Leino, F. Djurabekova, K. Nordlund, L. Madau, Y. Liebsch, M. Schleberger, M. Karlušić, Suspended nanoporous graphene produced by swift heavy ion bombardment, *Mat. Chem. Phys.* 313 (2024) 128729.
- [5] M. Karlušić et al., unpublished

Ion Beam Synthesis of Layer-Tunable and Transfer Free Graphene for Device Applications

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Direct synthesis of layer-tunable and transfer-free graphene on technologically important substrates is highly valued for various electronics and device applications. State of the art in the field is currently a two-step process: a high-quality graphene layer synthesis on metal substrate through chemical vapor deposition (CVD) followed by delicate layer-transfer onto device-relevant substrates. Here, we report a novel synthesis approach combining ion implantation for a precise graphene layer control and dual-metal smart Janus substrate for a diffusion-limiting graphene formation, to directly synthesize large area, high quality, and layer-tunable graphene films on arbitrary substrates without the post-synthesis layer transfer process.

Carbon (C) ion implantation was performed on Cu-Ni film deposited on a variety of device-relevant substrates. A well-controlled number of layers of graphene, primarily monolayer and bilayer, is precisely controlled by the equivalent fluence of the implanted C-atoms (1 monolayer $\sim 4 \times 10^{15}$ C-atoms/cm²). Upon thermal annealing to promote Cu-Ni alloying, the pre-implanted C-atoms in the Ni layer are pushed towards the Ni/substrate interface by the top Cu layer due to the poor C-solubility in Cu. As a result, the expelled C-atoms precipitate into graphene structure at the interface facilitated by the Cu-like alloy catalysis. After removing the alloyed Cu-like surface layer, the layer-tunable graphene on the desired substrate is directly realized.

This presentation will focus on graphene layer formation mechanism, detailed characterizations, and performance characteristics of select devices fabricated through this ion beam approach.

Ion Beam Modification of High-Entropy Pyrochlore and Perovskite Oxides

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High-entropy oxides (HEOs) have recently gained recognition for their low thermal conductivity, improved mechanical properties and tunable functionalities [1,2], but little is known about their response to high energy heavy ion beams. In this work, the heavy-ion irradiation response of HEOs with the pyrochlore ($\text{HE}_2\text{Ti}_2\text{O}_7$) and perovskite (SrHEO_3) structures has been investigated, where HE represents 5 equal-molar elements. The damage accumulation behavior at 300 K due to 4 MeV Au ion irradiation of a $\langle 100 \rangle$ -oriented HEO titanate pyrochlore single crystal has been investigated by Rutherford backscattering spectrometry in channeling geometry and transmission electron microscopy (TEM) [3]. In addition, in situ TEM irradiation of the same HEO titanate pyrochlore with 600 keV Xe ions has been employed to reveal the dose and temperature dependence of amorphization. In another single-crystal HEO titanate pyrochlore composition, amorphization due to 23 MeV Ni ions has been characterized by Raman spectroscopy, which indicates a much higher dose for amorphization, suggesting significant athermal recovery during irradiation due to the high electronic energy loss of the Ni ions. Ion tracks formed in a Sr-HEO perovskite structure irradiated with 774 MeV Xe ions have been characterized by HRTEM, and the stability of these ion tracks under electron beam irradiation has been evaluated. The irradiation response of these HEO structures, as well as other HEO compositions, are compared to those of their single-component counterparts.

References:

1. A. Sarkar, Q. Wang, A. Schiele M. R. Chellali, S. S. Bhattacharya, D. Wang, T. Brezesinski. H. Hahn, L. Valasco, B. Breitung, *Advanced Materials* 31 (2019) 1806236.
2. T. Z. Ward, R. Wilkerson, B. L. Musicó, A. Foley, M. Brahlek, W. J. Weber, K. E. Sickafus, A. Mazza, *Journal of Physics: Materials* 7 (2024) 021001.
3. Kinsler-Fedon, L. Nuckols, C.T. Nelson, Z. Qi, Q. Huang, D. Mandrus, Y. Zhang, W.J. Weber, V. Keppens, *Scripta Materialia* 220 (2022) 114916.

Radiation Damage in Nuclear Reactor Materials

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When considering the development of new materials for use in advanced nuclear reactor designs – both fission and fusion – conducting neutron irradiation studies can be costly and time inefficient, particularly exacerbated during the phase of down-selection of potential compositions to be considered. Ion irradiation of materials offers an alternative method of efficient pre-screening of materials to aid in rapid development of potentially radiation tolerant materials. In this talk, some examples of how ion beam irradiations have been conducted on novel materials to evaluate their radiation tolerance will be discussed – MAX phases and high entropy alloys. Additionally, the differences between ion and neutron irradiation induced microstructural changes will be discussed, and how this can be used as an advantage in the rapid development of new alloys for nuclear power systems use.

ORAL ABSTRACTS

Helium Ion Beam Irradiation of Plutonium Surrogates

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At 140te, the UK currently possesses over half of the world's stockpile of civil plutonium, which is stored as calcined powder in sealed stainless steel canisters at Sellafield. This work aims to investigate radiogenic helium release from this plutonium powder. Due to the issues involved in working with plutonium, cerium oxide and yttria-stabilised zirconia have been used as surrogates. Since helium is not radiogenically produced within these surrogates, helium ion beam implantation has been used. This process uses an ion beam to bombard a sample with helium ions of sufficient energy to implant the ions into the samples.

The samples produced by ion beam implantation have then been characterised using a range of analytical techniques. The results of these characterisation experiments have then been compared against a control unirradiated sample, allowing conclusions to be drawn regarding the impacts of the irradiation.

A notable observation during the helium ion beam irradiation of cerium dioxide samples was the discolouration of the cerium dioxide samples post-irradiation, theorised to be oxygen vacancies being formed, which is supported by the Raman Spectra of the irradiated samples. In contrast, XPS studies show no presence of Ce(III) sites that might be expected with oxygen vacancies. However, this is likely due to XPS only having a penetration depth of 2-3 nm whilst Raman interrogates 1-10 microns into the bulk. The observations by Raman of oxygen vacancies in the material bulk is significant as DFT and molecular dynamics-based simulation data suggest that oxygen vacancies in a plutonium dioxide lattice are an energetically favourable location for helium ions to occupy.

Further experiments in progress include:

- The characterisation of helium ion beam irradiated yttria-stabilised zirconia samples;
- TGA analysis of the temperature at which the implanted He is discharged from the samples.

The results of these studies will also be reported at the conference.

Retention and desorption of deuterium implanted and co-deposited in mixed boron-tungsten layers for fusion applications

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In magnetic confinement fusion reactors, modification of Plasma Facing Materials (PFM) by Plasma-Wall Interaction (PWI) such as implantation, erosion, heating, re-deposition, and co-deposition of fuel atoms with species eroded from the wall are key processes that will limit performance, durability, safety, and maintenance of these devices [1]. Aiming to improve the understanding and predictability of PWI in PFM and its potential effects in future devices, laboratory-scale studies to investigate the formation and modification of PFM under reactor-relevant conditions were performed. Special focus was given to the formation of boron-containing layers since boronization, being a critical step for the upstart of a fusion device operating with a tungsten wall, might result in mixed layers of boron with PFM. Fuel retention, atomic migration, and changes in the microstructure of these layers caused by thermal annealing and ion exposure were assessed in-situ and in real-time by ion beam techniques supported by ex-situ analysis.

Specifically, we sputter-deposited thin films from tungsten (main PFM candidate) simultaneously with boron under argon and deuterium atmospheres to obtain mixed layers of these materials [2]. Deuterium implantation under low energies (< 1 keV) and fluences up to 1×10^{22} atoms/m² in selected structures was followed by in-situ analysis to investigate the influence of incorporation route in the retention and desorption of fuel-atoms. An experimental set-up at Tandem Laboratory, that allows growth, thermal annealing, and ion irradiation without breaking the vacuum was used for the in-situ experiments [3]. The detailed composition and depth profiling by ion beams before, during, and after annealing up to around 600°C will be presented and discussed.

References

- [1] S. Brezinsek et al., Nucl. Fusion. 57, 116041 (2017).
- [2] E. Pitthan et al., Nucl. Mater. Energy 35, 1449 (2023).
- [3] K. Kantre et al. Nucl. Instrum. Meth. B 463, 96 (2020).

Enhanced analysis of ferritic-martensitic steel through ion-beam modification

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High chromium ferritic-martensitic steels are being explored as potential construction materials for the core structures of next-generation lead-cooled fast reactors. This study aims to investigate the Pb ion implantation profile and diffusion behavior of Pb in 9wt% chromium ferritic-martensitic steel T91 using ion beam analysis techniques. Additionally, the synergistic impact of Pb ion irradiation and exposure to a liquid lead environment on the corrosion behavior of T91 steel was assessed.

Specimens, obtained from 15mm thick hot rolled plates, underwent ion irradiation at room temperature with Pb ions under two conditions: at ion energies of 250 keV to a total fluence of 6.5×10^{14} ions/cm², and at 500 keV to a total fluence of 1×10^{15} ions/cm². The depth profile of injected Pb atom concentrations was measured using RBS and TOF-ERDA techniques and compared to theoretical calculations with SRIM/TRIDYN. Following heat treatment of the irradiated specimens at 450°C for 100 hours, the diffusion of Pb atoms within the ferritic-martensitic matrix was characterized. The microstructure of the irradiated specimens was examined using transmission electron microscopy.

Local mechanical properties were evaluated through nanoindentation using a Berkovich indenter. Cyclic unloading measurements were conducted to determine the depth-dependent hardness in both irradiated specimens and unirradiated references.

Subsequently, both irradiated and unirradiated materials were subjected to exposure to liquid lead at 400°C. The dissolved oxygen content in the lead was continuously monitored during the tests and maintained at approximately 10^{-6} wt.%. We examined the potential synergistic effects resulting from both ion implantation and exposure to liquid lead on T91 steel.

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Ion irradiation induced changes in Al-Cu-Co multilayer stacks

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This study investigates the impact of ion-beam assisted annealing and mixing on the compositional and structural changes in Al-Cu-Co multilayers. The multilayers, 800 nm thick and composed of successive single-metal Al, Cu, and Co nanolayers, were prepared by magnetron sputtering deposition. Thermal annealing at temperatures of 300°C, 400°C, and 500°C, as well as ion irradiation using 30 MeV Cu⁵⁺ ions at fluences ranging from 1×10^{13} to 5×10^{14} at/cm² were employed. Characterization was conducted using SEM, EDX, XRD, SIMS and TEM, including HAADF. Irradiation caused a transformation in the treated samples, with two distinct types of alternating nanolayers observed. One type consists of wider coarse-grained structurally and chemically homogeneous single-phase nanolayers composed of Al₂Cu, while the other type comprises narrower fine-grained two-phase nanolayers. These two-phase nanolayers exhibit a heterogeneous composite structure, with a central Co sublayer (remnant of the original single-metal Co nanolayer) surrounded by Al-Co sublayers, primarily comprising Al₉Co₂. The Co sublayer was found to act as a diffusion blocker for Al and Cu and impedes the migration of borders between individual nanolayers. Notably, no evidence of ternary phase formation was observed in any of the samples.

Ion channeling and defect modeling in ion-implanted Ga compounds

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Ion beams are widely used in materials science, e.g., to tune material properties through ion implantation. However, the process creates structural defects due to its ballistic nature, which may weaken the intended effects or even prevent them entirely. Therefore, additional processing, such as thermal annealing, may be necessary. Moreover, different defect types can transform into extended forms upon increasing fluences. Thus, it is crucial to understand the mechanisms of ion beam-induced defect formation and transformation under various conditions to ensure optimal material properties.

One well-established technique used to analyze structural defects in single crystals is Rutherford backscattering of light ions in the channeling mode (RBS/C). However, interpreting RBS/C energy spectra can be challenging due to convoluted signals from various defect types. Analyzing these spectra without computational methods like Monte Carlo simulations can be misleading. One such code used for this purpose is McChasy, which simulates the trajectories of light ions in virtual structures. McChasy-1 is designed for relatively small crystal cells ($\sim 10^2$ atoms) [1], while McChasy-2 can handle larger structures (up to $\sim 10^8$ atoms), generated using, e.g., Molecular Dynamics [2].

In this talk, we will demonstrate how to model ion beam-induced defects for use in the McChasy-1 and McChasy-2 codes, focusing on randomly displaced atoms, edge dislocations, and dislocation loops. We will show how to parametrize these defects using Transmission Electron Microscopy and Molecular Dynamics. We will describe how to determine preferable dislocation loop orientations based on RBS/C results of the anisotropy research of radiation-induced defects in β -Ga₂O₃ implanted with rare earth. We will also present the influence of polarity and the manufacturing method of the material on different kinetics of damage buildup observed in ion-implanted N-polar and Ga-polar c-GaN.

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References

- [1] P. Jóźwik, A. Caçador, K. Lorenz, R. Ratajczak, C. Mieszczczyński, Nucl. Instrum. Methods Phys. Res., Sect. B 538 (2023) 198.
- [2] C. Mieszczczyński, P. Jóźwik, K. Skrobas, K. Stefańska-Skrobas, R. Ratajczak, J. Jagielski, F. Garrido, E. Wyszkowska, A. Azarov, K. Lorenz, E. Alves, Nucl. Instrum. Methods Phys. Res., Sect. B 540 (2023) 38.

Local measurement of surface energy via blistering of light-ions implanted materials

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In the Smart Cut™ technology, light ions implantation is used to create a buried damaged layer composed of nano-sized defects. Upon annealing, after bonding to a host substrate, these defects form pressurized micro cracks, by capturing surrounding implanted atoms [1]. Their evolution is controlled via a balance between i) their mechanical energy (i.e. their internal pressure) and ii) the surface energy (i.e. energy cost to open new surfaces) of the surrounding material. Our last studies on the Smart Cut™ technologies have focused on the first point [2], however, the impact of ion implantation and fracture annealing on the material properties, and more particularly its surface energy, has not been yet well characterized, leading to difficulties to establish quantitative models for micro cracks growth.

This work proposes a methodology to evaluate the local interface energy of implanted semiconductors using the shape analysis of hydrogen and/or helium blisters. The blistering is modelled using mechanical theories coupled with Finite Element Modelling [3]. Experimental data are obtained using atomic force microscopy on implanted and annealed samples. The method enables the extraction of a local interface energy of implanted materials. It gives a new tool to investigate the dependencies of surface energy versus implantation conditions (ions, doses) and thermal budget. In silicon, we found surface energies close to the bulk value (2.5 J/m^2) with helium implantation, whereas in H-implanted silicon surface energies are smaller. The chemical affinity between hydrogen and silicon weakens the implanted interface, thus decreasing the cost of opening new surfaces. The study in silicon will be discussed regarding implantation and annealing parameters and extended to other semiconductors.

References

- [1] J.D. Penot et al., J. Appl. Phys., 114, 123513 (2013).
- [2] L. Colonel et al., Phys. Status Solidi A, 2100219 (2021).
- [3] N. Cherkashin et al., J. Appl. Phys. 118, 245301 (2015).

Radiation Effects in Uranium Nitride and Zirconium Nitride

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UN is a promising accident tolerant fuel (ATF) concept with numerous benefits over conventional UO_2 fuel, such as increased uranium density and thermal conductivity with a similar melting point [1]. Thus, understanding its stability under extreme conditions in a high temperature steam and radiation environment becomes critically important. The current work will discuss the radiation response of coarse-grained ZrN fabricated using spark plasma sintering and magnetron sputtered monocrystalline UN thin films. 600 keV Ar ion irradiations were carried out to understand material modifications by primary knock-on atoms (PKAs) from neutrons and gas accumulation as a function of damage dose from 1 dpa – 100 dpa. As ZrN is isostructural to UN, it is used as its model material [2], while the thin film configuration of UN presents a unique opportunity to study its radiation response due to its negligible activity and therefore ease of handling during characterisation. The irradiated samples were characterised by x-ray diffraction, transmission electron microscopy and Raman spectroscopy. Nanoindentation is used to understand corresponding changes in hardness and modulus. Throughout its operational lifetime, UN and ZrN will experience harsh reactor environments. Accordingly, observed microstructural modifications are correlated with physical property changes with relevance to nuclear fuels.

Results have shown that the chemical composition and lattice parameter of ZrN is minimally perturbed at all fluences, while crystallinity displays a significant increase of ~50% in the irradiated region. Pronounced hardness and modulus increases are observed post-irradiation. Cross-sectional TEM and SAED observations revealed the radiation-induced formation of an epitaxially matched surface layer of cubic ZrO_2 to the underlying bulk ZrN. Furthermore, evidence of a correlated disorder and commensurate ordering is displayed through selected area electron diffraction analysis of irradiated ZrN regions. These results will assist in our understanding of fuel degradation over its lifetime and shed light on the effects of PKAs in nuclear fuel, as well as the accumulation and diffusion of gas bubbles due to fission processes.

Alongside this project, we are investigating the effects of 600 keV Ar and higher energy ion irradiations of 1.5 MeV Si, 9 MeV Si and 7 MeV Au in nanocrystalline IBAD ZrN films. Nanocrystalline materials hold promise for possessing increased radiation tolerance owing to its high density of large angle grain boundaries [3,4]. This work primarily explores the distinct effects of ionising and displacive interactions and target material grain size.

References

- [1] Yun, D. et al. Materials Reports: Energy 1 (2021) pp. 100007.
- [2] Wheeler, K. et al. Journal of Nuclear Materials 366(3) (2007) pp. 306–316.
- [3] Zhang, Y. et al. (2014) Physical Chemistry Chemical Physics, 16(17), pp. 8051–8059.
- [4] Lu, F. et al. (2012) Applied Physics Letters, 101(4).

Modelling for Novel Applications of Industrial Implantation of Semiconductor Devices

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The flexibility and precision of ion implantation when doping semiconductors with different species, angle, energy and fluence has historically enabled transistor manufacturing to follow Moore's Law. Now, new implanter architectures deliver directional ion, neutral and radical beams to control both physical and chemical mechanisms of deposition and etch processes that are increasingly being applied to process steps outside of transistor formation. For example, the Applied Centura® Sculpta® patterning system [1] can reduce the complexity of critical patterning schemes by precisely modifying simple starting patterns generated by EUV lithography.

Modelling can enhance the performance and time to market of advanced equipment and manufacturing steps through improved understanding of the interplay of multiple mechanisms within an overall process and efficiency in the design and interpretation of physical experiments. Up to now, TRI3DYN [2] has been applied to model implant processes such as plasma doping of 3D structures that are dominated by physical deposition, sputtering and knock-in [3]. However, novel processes must now consider chemistry. Whilst 3D chemistry modelling codes exist, they often follow chemical reactions through multiple intermediate steps, each requiring knowledge of their rate and threshold energy, and only approximate angular scattering for low energy particles [4]. This paper will show that process outcomes can be reproduced using a modelling approach in which physical processes such as scattering and sputtering for the more energetic beams of an implanter are calculated by TRI3DYN and chemistry is considered using simplified single step reactions.

References

- [1] <https://www.youtube.com/watch?v=GSuTyOMq1Bg>
- [2] Moller, Nucl Instrum Meth B 322 (2014) 23
- [3] England et al, Nucl. Instrum. Meth. B 409 (2017) 60
- [4] Guo et al J. Vac. Sci. Technol. A 27 (2009) 388

Avalanche annealing mechanism of disordered damage pockets in silicon

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It is well established that most kinds of ion implantation in silicon produce damage in disordered (amorphous) damage pockets. However, even though there is also evidence that these pockets may partly anneal even below room temperature, the annealing mechanisms are not well understood. This issue is highlighted by recent efforts to develop dark matter detectors that can detect individual radiation events down to about 20 eV. Tests of these detectors, operating at sub-Kelvin temperatures, show an unexpected excess of low (below 50 eV) energy recombination effects that is not consistent with dark matter or known radioactive background sources.

To understand the damage annealing mechanisms in silicon and in particular the origin of this excess signal, we have carried out systematic studies of annealing of damage pockets created by 5 keV recoils in silicon. The annealing of these was studied over time scales up to 30 ns in the temperature range 0.05 - 500 K. For the lower temperatures, a quantum thermal bath was employed to describe the effect of quantum mechanical zero-point vibrations on atom dynamics.

The results show that annealing of disordered pockets in silicon can proceed by an avalanche-like events, where a metastable defect configuration first crosses an energy barrier of about 0.1 eV. Crossing this kind of small barrier can then trigger a rapid additional bond recombinations that lead to partial recrystallisation and energy releases exceeding 10 eV. These events occur randomly on time scales of at least tens of nanoseconds after the initial picosecond time scale radiation event. This mechanism explains why large energy release events can occur even down to cryogenic temperatures. The recombination events are shown to have a very similar exponential dependence of energy as that observed in experiments.

Ion-irradiation induced magnetic phase transition in 2D semiconductor CrSBr

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CrSBr is rapidly gaining attention as a prominent candidate within the family of van der Waals magnetic semiconductors [1-3]. Below the Néel temperature of 132 K, the material is supposed to exhibit prototypical A-type antiferromagnetic order, as predicted by mean-field theory years ago. Recently, however, several groups reported the observation of unusual magnetic signatures indicating a second magnetic phase transition at temperatures around 40 K. In this contribution, we are going to discuss: (1) whether these signatures reflect an intrinsic property of the material or are caused by extrinsic influences; (2) if not the former, whether one can tailor the magnetic properties after growth.

We start with CrSBr single crystals synthesized by chemical vapor transport. Surprisingly, by extensive magnetization measurement utilizing SQUID magnetometry, we cannot detect the second, 40 K magnetic phase transition [4]. Our magnetometry measurements confirm the theoretically predicted magnetic phase diagram and thus demonstrate that the 40 K phase observed by other groups is not an intrinsic element of the magnetic phase diagram of CrSBr. The pure antiferromagnetic CrSBr crystals and flakes were then subjected to non-magnetic ion irradiation, which produces structural defects in the crystals in a controllable way. We observe a transition from antiferromagnetic to ferromagnetic behavior in CrSBr [5]. Already at moderate fluences, ion irradiation induces a remanent magnetization with hysteresis adapting to the easy-axis anisotropy of the pristine magnetic order up to a critical temperature of 110 K. Structure analysis of the irradiated crystals in conjunction with density functional theory calculations suggest that the displacement of constituent atoms due to collisions with ions and the formation of interstitials favor ferromagnetic order between the layers. Increasing irradiation fluences gradually lowers the Curie temperature, reflecting the impact of crystalline degradation. This suggests that by finely tuning the irradiation parameters and employing precise lithography techniques, it is possible to selectively modulate induced ferromagnetism in CrSBr in terms of magnetization strength, critical temperature, and spatial distribution. However, in our opinion, the origin and nature of the second phase with a transition temperature around 40 K reported in pristine CrSBr samples by various studies still remains elusive.

References

- [1] N. P. Wilson, K. Lee, J. Cenker et al., *Nat. Mater.* 20, 1657 (2021).
- [2] F. Dirnberger, J.M. Quan, R. Bushati et al., *Nature* 620, 533 (2023).
- [3] K. Lin, X. Sun, F. Dirnberger et al., *ACS Nano* 18, 2898–2905 (2024).
- [4] F. Long, K. Mosina, et al., *Appl. Phys. Lett.* 123, 222401 (2023).
- [5] F. Long, M.Ghorbani-Asl, K. Mosina, et al., *Nano Lett.* 23, 8468–8473 (2023).

Novel Energy-Filtered Implantation Technique for Field Stop Formation in Silicon Power Devices

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Insulated Gate Bipolar Transistors (IGBTs) power devices require high blocking capability as well as adaptable switching behaviour [1]. The technique presented in this work aims to realise continuous deep ($> 40 \mu\text{m}$) n-type profiles as field stop structures in high voltage silicon-IGBTs ($> 1200 \text{ V}$) to adjust the soft switching capability. Hydrogen-related donor (HD) defect complexes perform as n-type dopants in single crystalline silicon [2] and they are formed by a combination of H or He implantation inducing lattice defects and a subsequent annealing step in a H atmosphere.

Up to now, these IGBT field stop profiles are generated using multiple high energy (up to 2 MeV) implantation steps. In contrast, we achieve continuous deep HD profiles in a single implantation step by inserting a micro-patterned silicon membrane (energy-filter) of max. $50 \mu\text{m}$ thickness into the primary ion beam to provide a beam with broad customisable energy distribution.

In this work we investigate, how filter structure, implanted dose ($1\text{e}13$ to $5\text{e}15 \text{ cm}^{-2}$) and annealing conditions affect the depth distribution of HD defect complexes.

The energy-filters were manufactured by KOH etching of single crystalline (100)-oriented silicon.

Using these energy-filters, H was implanted into silicon substrates at 2.0 to 2.5 MeV, resulting in fully buried profiles. After annealing under H atmosphere, the samples were analysed by Spreading Resistance Profiling.

We found that the annealing efficiency, i.e., the electrically active dose divided by the implanted dose, depends on the pattern type of the energy-filter (long grooves or squares), the implanted dose and the annealing temperature (270°C to 470°C). Annealing efficiency ranges from 0.3 % to 1.1 %, with highest values reached for groove-structured filters, lowest ion doses and an annealing temperature of 295°C .

References

1 - T. Laska et al., doi: 10.1109/ISPSD.2000.856842

2 – Y. Ohmura et al., 1973, physica status solidi (a), Vol. 15, No. 1, p. 93

Oxygen sublattice as a backbone of exceptional stability of gallium oxide

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Remarkable radiation tolerance of Ga₂O₃, as demonstrated in Ref [1], brings this ultrawide bandgap semiconductor to the frontiers of power electronics applications that are able to operate in challenging environments. Understanding the mechanism of radiation

tolerance is crucial for further material modification and tailoring of the desired properties. In this study, by using machine-learning interatomic potential [2] we performed atomistic simulations of high fluence ion irradiation of β -Ga₂O₃ to follow the gradual transition from β to γ phase. The observed stages of phase transformation are remarkably close to those seen in experiment. We also assess separately the stability of both the gallium (Ga) and oxygen (O) sublattices under various levels of damage. Our study [3] uncovers the high resilience and exceptional stability of the O-sublattice, attributing this property to the strong tendency of recovery of the O defects, especially within the stronger disordered regions. On the other hand, we observe the opposite behavior of the Ga-related defects. These appear more stable in the same regions where disorder is increased. We also observe that highly defective β -Ga₂O₃ is able to transform into γ -Ga₂O₃ during annealing runs due to strongly preserved lattice organization of the O-sublattice.

This result clearly indicates ultrahigh stability of the O-sublattice, which provides the backbone for the exceptional radiation tolerance of the γ/β double-polymorphic structure. Moreover, we observe that our computational insights compare closely with experiments, opening avenues for further exploration of polymorphism in Ga₂O₃ and potentially in analogous polymorphic families spanning a broad range of diverse materials of complex polymorphic nature.

References:

- [1] A. Azarov, J. G. Fernández, J. Zhao, F. Djurabekova, H. He, R. He, Ø. Prytz, et al. "Universal Radiation Tolerant Semiconductor." *Nature Communications* 14, no. 1 (2023) 4855
- [2] J. Zhao, J. Byggmästar, H. He, K. Nordlund, F. Djurabekova, and M. Hua, Complex Ga₂O₃ Polymorphs Explored by Accurate and General-Purpose Machine-Learning Interatomic Potentials, *npj Computational Materials* 9, (2023), open access
- [3] R. He, J. Zhao, J. Byggmästar, H. He, and F. Djurabekova "Ultrahigh stability of O sublattice in β -Ga₂O₃", submitted to PRM, <https://arxiv.org/html/2404.10451v1>

Ion implantation for β -Ga₂O₃ microtubes and nanomembranes fabrication: experiment & simulation

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Due to its wide bandgap (~ 4.8 eV at room temperature) and high breakdown electric field (~ 8 MV/cm), monoclinic β -Ga₂O₃ has been gaining increased interest as one of the most promising semiconductors for future applications, including high power or transparent electronics. Moreover, thanks to the (100) easy-cleavage plane, this material lends itself to the production of thin flakes produced by conventional mechanical exfoliation techniques, such as the scotch tape method, which have been applied in different devices [1].

In this work, we report a novel process for β -Ga₂O₃ microtubes and nanomembranes by ion implantation into (100)-oriented single-crystals [2]. Under specific implantation conditions, the induced strain profile promotes the rolling-up of the surface layer, forming a microtube. These strains can then be relaxed upon annealing, triggering the unrolling of the microtubes, forming nanomembranes with bulk-like crystalline quality. Hence, such a nanomembrane fabrication method may be advantageous over other conventional methods, offering improved reproducibility and control of parameters such as the membrane thickness or its optical, magnetic or electrical properties, which can be customised to the desired application.

Aiming at understanding the physical processes underlying this newly-reported implantation-induced exfoliation phenomenon, we will present a detailed study of β -Ga₂O₃ samples implanted with Cr under different conditions, combining X-Ray Diffraction, Rutherford Backscattering Spectrometry in the Channelling Mode and Molecular Dynamics simulations. In particular, experiment and simulation show excellent agreement on the defect profiles and subsequent strain and stress fields created by the implantation. Such fields can be correlated with the anisotropic monoclinic lattice in order to explain the physical processes leading to exfoliation. Furthermore, implantation damage is seen to recover at moderate temperatures, revealing the excellent quality of the nanomembranes and showing the high potential of ion implantation in this emerging semiconductor.

References

[1] M. Peres, K. Lorenz, et al., ECS J. Solid State Sci. Technol. 8, Q3235 (2019)

[2] Patent “Process of Production of Roll and Submicrometric Membrane of Ga₂O₃ by Ion Implantation”: PT 117063; EU PCT/PT/2022/050006; USA R6157.0189/189US

Thermal stability of double-layer gamma/beta Ga₂O₃ structures fabricated by ion beams

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Polymorphism can be a limiting factor in technology due to uncontrollable polymorphic transformations; however, it can also provide additional opportunities for the functionalization of the surfaces and interfaces. This holds, in particular, for Ga₂O₃ which is an ultra-wide bandgap semiconductor having 5 different polymorphs. Recently, it was demonstrated that monoclinic (β -) to cubic spinel (γ -) phase transitions in Ga₂O₃ can be stimulated by disorder-induced ordering under ion bombardment [1]. The resulting double γ/β layer structure demonstrates unprecedentedly high radiation tolerance and the aim of the present study is to investigate the role of temperature variations on optical and structural properties of such structures. For these purposes ~ 300 nm thick γ layer was prepared on the top of the (010) oriented β -Ga₂O₃ single wafer by ion irradiation. Temperature dependent photoluminescence in combination with diffuse reflectance spectroscopy was used for the investigation of optical properties of such double γ/β layer structure. In its turn, RBS/C combined with high resolution TEM and XRD were used for the structural analysis and phase identification. The results show two distinct annealing stages, where the low temperature stage ($<700^\circ\text{C}$) is characterized by the shrinkage of the γ layer due to its epitaxial recrystallization. In contrast, the high temperature stage ($>700^\circ\text{C}$) leads to the degradation of the structure complicated by the non-epitaxial β -phase formation in the near surface region.

References

[1] A. Azarov, J. García Fernández, J. Zhao, F. Djurabekova, H. He, R. He, Ø. Prytz, L. Vines, U. Bektas, P. Chekhonin, N. Klingner, G. Hlawacek, and A. Kuznetsov, "Universal radiation tolerant semiconductor", Nat. Commun. 14, 4855 (2023).

Spatially resolved polymorph conversion in Galliumoxide

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Monoclinic gallium oxide (β -Ga₂O₃) is a promising wideband gap semiconductor with a bandgap of 4.7 eV and a high breakdown voltage. However, the existence of several metastable polymorphs and the immature fabrication technology limits its applications. The research is based on the recent observation that β -Ga₂O₃ can reliably be converted into γ -Ga₂O₃ using high energy ion beams [1,2]. It could also be shown that the resulting γ -Ga₂O₃ layer exhibits an exceptional tolerance towards high fluence ion beam irradiation [3].

Here, we use focused ion beam (FIB) induced processing to convert β -Ga₂O₃ into γ -Ga₂O₃ in a spatially controlled way. We employ focused Ne ions from a helium ion microscope (HIM) and liquid metal alloy ion sources (LMAIS) based FIB with Co, Si, and In to induce the polymorph conversion. Electron backscatter diffraction (EBSD), transmission electron microscopy (TEM) and atomic force microscopy (AFM) are used to confirm, in a spatially resolved way, the successful polymorph conversion. From the obtained EBSD data the orientation relationship between the irradiated and unirradiated material is resolved. Broadbeam irradiated reference samples have been used to corroborate these results with channeling Rutherford backscattering spectrometry (c-RBS), X-ray diffraction (XRD) and Doppler broadening variable energy positron annihilation spectroscopy (DB-VEPAS) results. The obtained crystal structure and defect distribution data supports the model suggested for the conversion mechanism [3].

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References

- [1] A. Azarov, C. Bazioti, Disorder-Induced Ordering in Gallium Oxide Polymorphs, Phys. Rev. Lett. 128 (2022), 015704.
- [2] J. Garcia-Fernandez, S.B. Kjeldby, Formation of γ -Ga₂O₃ by ion implantation: Polymorphic phase transformation of β -Ga₂O₃, Appl. Phys. Lett. 121 (2022), 191601.
- [3] A. Azarov, J. G. Fernández, J. Zhao, F. Djurabekova, H. He, R. He, Ø. Prytz, L. Vines, U. Bektas, P. Chekhonin, N. Klingner, G. Hlawacek, A. Kuznetsov, Universal radiation tolerant semiconductor (2023), doi:10.48550/ARXIV.2303.13114.

Tuning 2D transition metal carbides (MXenes) architecture and properties by ion irradiation

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2D transition metal (TM) carbides or nitrides (so-called MXenes) with chemical formula $M_{n+1}X_nT_z$ ($n = 1-3$), where M is a TM, X is carbon and/or nitrogen and T are surface functionalization groups like O(H) or F have emerged as a peculiar family exhibiting an original combination of tunable hydrophilicity, and very good electronic and mechanical properties [1]. These 2D materials can be easily and cost-effectively processed as thin films and are studied for a constantly growing number of applications including optoelectronic devices and energy storage. One of the main interests for MXenes is their rich chemistry. Being commonly obtained from the chemical exfoliation of the A atomic planes from $M_{n+1}AX_n$ phases (A being essentially Al), the M or X elements in the MXene sheets can be modified by using different MAX phases precursors. In addition, the T surface groups can be modified by adjusting the chemical etching process or using post-synthesis annealing or reaction in various atmospheres. All these modifications have a deep impact on MXenes properties, but most of them suffer from a major lack of control, flexibility and reproducibility on the final MXene. In this context, ion implantation/irradiation appears to be a very promising approach to modify, in a controlled way and with possible access to out-of-equilibrium states, the structure and physical properties of MXene. For instance, we recently demonstrated that ion implantation can be used to incorporate foreign species (Mn) into MXene sheets up to several percent [2].

In this work, we show further that ion irradiation offers high flexibility for the design of MXenes, allowing to shape their properties on demand which is a unique asset for applications. In particular, we demonstrate the efficiency of He⁺ irradiation in tuning the optical properties of $Ti_3C_2T_x$ (T=F, Cl, or O(H) and $x \approx 2$) spin-coated thin films. The introduction of a controlled amount of structural modifications both on the surface and into the MXene layers, by fine tuning the irradiation fluence, allows for the increase of the thin films transparency from IR to UV, while preserving the electrical conductivity. The modification of the properties is rationalized using a combination of structural, electronic and optical characterization methods including (S)TEM-EELS, thereby giving insights on the correlation between structural defects, and the induced modifications of the Ti-d bands which are responsible for the optical/electrical properties in this system [3]. This innovative method can be generalized to other chemistries as well as upscaled and can be expected to become a standard approach to tailor MXenes properties

Interaction of low-energy ions with plasma-facing materials from the perspective of time-of-flight low-energy ion scattering

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Candidate materials for the first wall in controlled thermonuclear fusion devices such as EUROFER97 and W are modified in different ways due to interactions with energetic plasma species. Time-of-flight low-energy ion scattering (ToF-LEIS) is a non-destructive method to study the near-surface composition of such materials with high depth resolution and the capability of in-situ analysis [1]. Herein, ToF-LEIS together with Auger electron spectroscopy have been used to study the influence of elevated temperatures on the near-surface composition of EUROFER97 [2].

Moreover, ToF-LEIS allows us to investigate the electronic stopping cross-sections (ϵ_e) of plasma species in these materials and address the lack of relevant accurate experimental ϵ_e [3], a prerequisite for modelling particle range or sputter yields. Employing ToF-LEIS, we experimentally deduce unprecedented data of ϵ_e of W [4] and EUROFER97 for H, D and He ions below 10 keV. For both W and EUROFER97, ϵ_e is extracted from relative measurements, and from absolute measurements on sputter-deposited thin films of W, and thin film stacks of sputter-deposited EUROFER97 and W after characterisation using IBA and microscopy techniques [5]. In all the studies, Monte Carlo simulations using TRBS code [6] are employed to evaluate the data and account for plural and multiple scattering. The deduced ϵ_e are compared to existing semiempirical and theoretical models for W, and SRIM [7] predictions based on Bragg's rule of stopping power additivity for EUROFER97.

References

- [1] D. Primetzhofer et al., Appl Phys Lett. 92 (2008).
- [2] J. Shams-Latifi et al., Nucl Mater Energy. 30 (2022).
- [3] C. C. Montanari et al., Nucl Instrum Methods Phys Res B. 408, 50–55 (2017).
- [4] J. Shams-Latifi et al., Nucl Mater Energy. 36 (2023).
- [5] J. Shams-Latifi et al., Mater Res Express. 11, 016518 (2024).
- [6] J. P. Biersack et al., Nucl Instrum Methods Phys Res. 861, 77–82 (1991).
- [7] J. F. Ziegler et al., Nucl Instrum Methods Phys Res B. 268, 1818–1823 (2010).

Elastic backscattering during boron implantation in Si(1-x)Ge(x)

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Ion implantation is a well-controlled process that is used extensively in the semiconductor industry, e.g., to modify the electrical properties of materials. Much research has focused on the range of the implanted ions in the material, on the generation of crystallographic defects and damage, and on the surface sputtering in the case of large doses. Remarkably, the dose loss which results from the elastic backscattering of the implanted species has received little experimental attention and is often assumed to be negligible. We show that this assumption is not always justified, and that the retained dose can be as much as 15% lower than the implantation fluence in the case of the implantation of 10 keV boron in germanium [1].

To demonstrate the effect, a series of 11 Si(1-x)Ge(x) ($0 \leq x \leq 1$) samples were implanted with boron ions under identical conditions to a dose of 5×10^{14} atoms/cm². Following implantation, nuclear reaction analysis (NRA) using the $^{11}\text{B}(p, \alpha_1)2\alpha_{12}$ reaction was carried out to quantify the retained boron dose in each sample. The experimental results showed a linear decrease in retained boron dose with increasing germanium concentration, with a retention factor ranging from 97% (for pure silicon) to 85% (for pure germanium). Our experimental findings perfectly agree with Monte Carlo simulation results using SRIM-2013 software.

Hence, our results demonstrate that the backscattering effect must be considered – and corrected for – when targeting a specific concentration in ion implantation. In particular, the dose-loss is important when interpreting the electrical properties in terms of the doping level after ion implantation, or when ion-implanted samples are used as reference materials in other techniques, for example, in secondary ion mass spectrometry.

References

[1] Quan Bai et al., Elastic backscattering during boron implantation in Si(1-x)Ge(x), *Vacuum* 219 (2024) 112740. <https://doi.org/10.1016/j.vacuum.2023.112740>

Secondary-electron emission from first principles and electronic stopping power predictions from machine learning

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Multi-length and time-scale relaxation processes connect the initial non-equilibrium excited electron distribution in a target material after ion irradiation with characteristic properties of these electrons when they are emitted as secondary electrons. This talk will explore the use of such secondary electrons as high-resolution thermalization probes, by studying secondary electron emission dynamics using first-principles real-time electron dynamics simulations. The simulation work presented here focuses on graphene as a prototypical two-dimensional material and accounts for high electron and lattice temperatures. The data shows signatures of kinetic and potential emission and generally good agreement for electron yields between experiment and theory. The duration of the emission pulse is about 1.5 femtoseconds, indicating high time resolution when used as a probe. These simulations show that lattice temperature significantly increases secondary electron emission, whereas electron temperature has a negligible effect.

While such quantum-mechanical electronic-structure simulations can yield very accurate predictions, their computational cost is a limiting factor that impedes applications to length and time scales that are required to model ion beam modification of materials. This talk will also describe progress towards an affordable computational approach that provides the electronic stopping power for arbitrary trajectories of ions through a target material without compromising accuracy. To achieve that, cutting-edge descriptors of atomic geometries are extracted from real-time time-dependent density functional theory simulations and machine-learning models are trained on the corresponding electronic stopping data. This shows very low error bars and very high accuracy at million-fold reduced computational cost of the trained model for proton irradiated aluminum. Results presented here include predicted velocity dependent electronic stopping and entire Bragg peak simulations.

New aspects of electronic excitations in materials induced by keV light and heavy ions

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Accurate understanding of energy deposition by energetic charged particles in matter is mandatory for prediction of ion-induced materials modification, as in semiconductor doping or extreme environments, e.g. fusion devices. Such knowledge also forms the basis for analytical tools based on beams of energetic ions and yields well-defined test scenarios for models. Commonly energy deposition is described as an average value along the ion trajectory despite its origin from discrete excitation events, which can be quite distinct in their nature.

We present experiments investigating energy deposition phenomena and exit charge states using the Time-of-Flight Medium Energy Ion Scattering System at Uppsala University [1] employing self-supporting Si(100) & SiC(100) nanomembranes. Primary ion species from H to Ar in beams with fA current in the energy range of 5 – 200 keV were employed.

We compared spatial and energy distributions as a function of projectile type and energy for both axially channeled projectiles and particles transmitted off from low-index crystal axes ('pseudo'-random) [2][3][4][5][6]. A clear energy dependence of energy loss ratios (channeling vs. random) with characteristic behavior for different ion species is observed. We analyze the origin of different energy loss contributions, their statistics [6] and their impact parameter dependence inducing differences in the mean charge state for different trajectories [7], e.g. due to formation of molecular orbitals and charge transfer, and consider their relevance for applications [8].

References

- [1] M. Sortica et al., *NimB* 463 (2020) 16
- [2] S. Lohmann et al., *PRL* 124 (2020) 096601
- [3] S. Lohmann et al., *PRA* 102 (2020) 062803
- [4] R. Holeňák et al., *Ultramicroscopy* 217 (2021) 113051
- [5] E. Ntemou et al., *Rad. Phys. & Chem.* 194 (2022) 110033
- [6] E. Ntemou et al., *Phys. Rev. B* 107 (2023) 155145
- [7] S. Lohmann et al., *PRB* 107 (2023) 085110
- [8] R. Holeňák et al., *Phys. Rev. Applied* 21 (2024) 024048

Highly enriched ^{28}Si by ion beam modification for donor spin quantum computer devices

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We have developed a simple method to enrich silicon in which the rare ^{29}Si non-zero nuclear spin isotope ($I=1/2$, natural abundance 4.67%) is depleted in favour of the zero nuclear spin ^{28}Si isotope ($I=0$, 92.2%). Our method employs high fluence ^{28}Si ion implantation, from either a standard ion implantation system found in university laboratories and semiconductor foundries or a highly focused ion beam system. We seek to configure robust, long-lived coherent donor atom spin states in the highly enriched material thanks to depletion of the ^{29}Si nuclear magnetic moments. Guided by ion-solid computer simulations that predict one-for-one sputtering with 45 keV ^{28}Si ion beams, we have produced ^{28}Si enriched with fluences above $1\text{E}18$ $^{28}\text{Si}/\text{cm}^2$ in a broad beam implanter over 6×6 square mm and above $1\text{E}19$ $^{28}\text{Si}/\text{cm}^2$ for focused beams over an area of $\sim 20\times 20$ square microns. Secondary Ion Mass Spectrometry (SIMS) measurements confirm ^{29}Si depletion below 150 ppm for the broad beam samples and an unprecedented 2.3 ppm for the focused beam samples, both of which are free from isobar contamination (CO , N_2) to the limit of detection. Post-irradiation annealing restores the crystallinity of the samples resulting in a ~ 200 nm layer of high purity ^{28}Si on both bulk and 220 nm silicon-on-insulator substrates. We employ high sensitivity Electrically Detected Magnetic Resonance (EDMR) for lifetime measurements of implanted donor spins in our localised enriched volumes.

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Diamond-defect engineering of NV- Centres using ion beam irradiation

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Diamond, renowned for its exceptional material properties, has emerged as a leading candidate for various quantum technologies, particularly in quantum sensing applications. The creation and manipulation of nitrogen-vacancy (NV-) centres within diamond lattice structures offer unprecedented capabilities in optical initialization, readout, and microwave coherent control, rendering them highly promising for applications in quantum sensing, imaging, and information processing.

In this study, we investigate the synergistic interplay between ion beam modification techniques and the generation of NV- centres in nitrogen-doped synthetic diamond crystals. Our experimental approach involves differentiating between light (H^+) and heavy (Br^{+6}) ions irradiation to understand their respective impacts on NV centre creation. By varying ion energies and fluences, we investigate the influence of vacancy formation on NV centre generation. Moreover, to mitigate irradiation damage, samples underwent annealing at temperatures of 800 and 900 °C for 1 hour, effectively healing the lattice damage without inducing graphitization. The raise in vacancy mobility during the temperature annealing process seems to promote the formation of the desired nitrogen-vacancy pairs. Finally, we have characterized the creation of NV centres by photoluminescence and Raman spectroscopy.

Our findings not only highlight the versatility of ion beam techniques in diamond defect engineering but also offer insights into the development of next-generation quantum technologies for advanced sensing applications.

Formation and annealing of implanted group-IV vacancy quantum emitters in diamond

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Group-IV vacancy defects in diamond have emerged as an interesting platform for quantum nanophotonic applications due to their inversion symmetry and high Debye-Waller factor. A substantial amount of research has been devoted to studying the optical activation after ion implantation and annealing. However, knowledge of the structural formation of such defects is limited. To study these structural formation processes, we determined the lattice site of group-IV elements implanted into diamond using the β^- emission channeling (EC) technique with radioactive isotopes (^{75}Ge , ^{121}Sn , ^{209}Pb) produced at the ISOLDE/CERN facility [1,2]. These experiments covered an energy range of 30-60 keV, fluences from 2×10^{12} to $2 \times 10^{13} \text{ cm}^{-2}$, as well as implantation and annealing temperature ranges from room temperature up to 900°C.

For all 3 elements, substantial fractions (20-40%) of bond-centered (BC) sites, the lattice position corresponding to the split-vacancy configuration, are found upon room-temperature implantation. However, while the SnV and PbV defects are fairly stable up to 900°C, for Ge, annealing or implanting at moderate temperatures (300°C) already significantly reduces the amount of GeV defects in favour of substitutional sites, which we assign to a reaction with mobile carbon interstitials. Since thermal annealing thus reduces the amount of GeV, while at the same time photoluminescence of GeV is only observed after annealing at 800°C or above [3], we conclude that optical activation is not related to an increase in the number of GeV centers but rather required to adjust their electronic environment. Fully understanding these formation processes of the group-IV vacancy centers is crucial to advance the development of quantum technologies based on these defects in diamond.

References

[1] U. Wahl et al., Phys. Rev. Lett. 125 (2020) 045301

[2] U. Wahl et al., Structural formation yield of GeV centers from implanted Ge in diamond, submitted

[3] T. Iwasaki et al., Sci. Rep. 5 (2015) 12882

Spin Defects and Blue Quantum Emitters Generated by High Energy Ion Irradiations in hBN

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Recently the negatively charged boron vacancies (V_B^-) in hexagonal boron nitride (hBN) have been shown as spin defects that have great potential in quantum sensing. However, so far the sensitivity is limited by either photoluminescence (PL) brightness or the optically detected magnetic resonance (ODMR) contrast, and linewidth. In this work, we demonstrate the generation of these spin defects using high energy helium ion beams and perform ODMR measurements with different laser and microwave powers. The spin defects generated by high energy helium ions exhibit a high PL brightness and ODMR contrast while keeping a small linewidth, hence a good sensitivity. By comparing different fluences of helium irradiations, we determine an optimal fluence which is sufficient in creating spin defects without damaging the overall crystal lattice structure. With this optimal fluence, we can obtain a high signal-to-noise ratio ODMR spectrum with an accurate measurement of zero field splitting frequency, and a best sensitivity as $\sim 2.55 \mu\text{T/VHz}$. Moreover, with a focused beam, we can deterministically create such spin defects with nanometer precision.

Hexagonal boron nitride (hBN) has been a centre of interest due to its ability to host several bright quantum emitters at room temperature. However, the identification of the observed emitters remains challenging due to spectral variability as well as the lack of atomic defect structure information. In this work, we report two new blue quantum emitters with zero phonon line (ZPL) centred around 460 nm and 490 nm in hBN powders. We further demonstrate that the new emissions can be created by high temperature annealing or high energy ion irradiation in exfoliated hBN flakes. Scanning transmission electron microscopy (STEM) reveals that the dominant defect structures present in ion irradiated sample are vacancy-type ($V-x$) and adatom(interacalant)-type ($A-x$). Through first principle GW-BSE (Bethe-Salpeter equation) calculation, we attribute the observed emissions at 460nm and 490nm to originate from boron intercalant ($B\text{---}int$) and nitrogen intercalant ($N\text{---}int$) respectively. Our results not only discover a new group of blue quantum emissions in hBN, but also provide an insight on the physical origin of the emissions by correlating the emission wavelength with local atomic structures in hBN.

Truncated cone Janus microparticles for research in micro/nanoplastics

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Microplastics (MPs) < 5 mm and nanoplastics (NPs) < 1 μm [1] are considered a troublesome worldwide pollutant. A problem for laboratory research into understanding the effects of MPs and NPs on the biosphere is that the oceanic concentrations are very small (typically, << few per L). For small-scale experiments, a source of artificial well-characterized MPs and NPs is needed.

Janus microparticles have surfaces with two or more heterogeneous regions with different physics and/or chemical properties (e.g., a dielectric and a metal). These microparticles have found wide applications in nanotechnology, surface chemistry, and biomedicine. The Janus microparticles are generally fabricated with regular shapes, viz. disc, cube, and sphere. Other shapes are challenging to fabricate. In this work, we propose truncated cone Janus microparticles defined by the penetration depth of protons through a resist material followed by a metallic coating. The truncated cone dielectric (an epoxy-based photoresist SU-8) microstructures were generated by a 1 MeV proton beam writing at Shibaura Institute of Technology. Utilizing a proton penetration depth smaller than the resist thickness [2], the dielectric microstructures were detached from the substrates in the developing process. The detached dielectric microstructures were subsequently rotated at 90 degrees, enabling a metal deposition on one side to form truncated cone Janus microparticles. Here, we will present the Janus microparticles of different aspect ratios by varying diameters while keeping the same height. Moreover, the application of the Janus microparticles, especially in micro/nanoplastics, will be highlighted.

References:

[1] H. Cai et al., Chemical Engineering Journal 410 (2021) 128208.

[2] N. Puttaraksa et al., Japanese Journal of Applied Physics 63 (2024) 03SP49.

Strained Auxetic Nano-silicon Structures Created by Multi-step Focused Ion Beam Processing

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We introduce an ion-beam-based approach for generating substantial strains in group-IV semiconductor membranes, offering a straightforward and highly scalable single-step process [1]. This technique employs ion implantation to control amorphisation-induced contraction, producing significant tensile strains in the neighbouring crystalline region in a process analogous to the tightening of a drumskin. By employing conventional focused ion beam (FIB) microscopes, approximately 1×10^{15} Xe⁺ ions per square centimetre have been implanted (at 30 keV) into silicon single-crystal membranes. This implanted "tensioner" region "contracts", leading to substantial strains in the adjacent unimplanted crystal portion, referred to as the "tympanum. For instance, micro-Raman spectroscopy reveals that when an unexposed 8 μm diameter "tympanum" (within a membrane window of dimensions $L = 136 \mu\text{m}$) is examined, a redshift ($\Delta\omega$) of 6.8 cm^{-1} relative to bulk Si is observed. This corresponds to an estimated 0.8% biaxial tensile strain in a substantial active region of approximately 50 μm^2 . Recent direct measurements employing micro-XRD have corroborated these strain values. Furthermore, we exploit the tympanum geometry and Si crystal anisotropy to optimize the achieved strain, demonstrating maximum values of up to 3.1% biaxial and 8.5% uniaxial tensile strains. Additional experiments allowed us to understand the importance of a bilayer structure comprised of a top amorphous silicon on the top of a still crystalline material, and to discard micro-Raman laser heat artefacts.

To provide a visual representation of the ion beam induced strain, we used the FIB to create, rotate and expand micro-squares connected by sub-100 nm hinges straining the structure in an incredibly precise manner. These units will thereby be called auxetic structures since their elongation (opening) also results in transversal expansion. In this work, it is highlighted that full expansion of the auxetic structures are achieved followed by implantation of the tensioner region only, much larger than previously reported in the literature, and are only be achieved due to the gentle pulling forces applied at the tensioner/tympanum interface by the developed ion implantation methodology.

References

[1] Masteghin, Mateus G., et al. Physical review materials 5.12 (2021): 124603.

Ion beam-assisted H loading and materials modification for energy storage

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Solving the challenges of effective hydrogen storage is an important step towards a hydrogen economy [1]. Metal hydrides are considered potential storage materials as they feature higher volumetric hydrogen density in comparison with the conventional gaseous and liquid H storage options. Formation of metal hydrides is typically done from a gas phase, i.e. by exposing metals to H₂ often at elevated temperatures with subsequent rapid cooling. While this approach is well established and captivates with its simplicity, the amount of absorbed H is limited by the thermodynamics of the process. Besides, the short-range repulsive force between H atoms affects their arrangement within the metallic host lattice and thus imposes a limitation on achievable H concentrations.

Ion implantation, a technique widely used for many industrial applications, is an alternative route for delivering hydrogen into solids. The process of ion implantation is not constrained by considerations of classical thermodynamics, thus opening the possibility of achieving concentrations higher than those predicted by equilibrium solubility. Moreover, the lattice of the target can be modified under ion bombardment which in turn might lead to changes in the H solubility.

In this contribution, we investigate ion-beam assisted H loading into V crystals, a system previously studied for H storage [2, 3], and compare this process with loading from the gas phase. Vanadium films were grown epitaxially on MgO (100) substrates using DC magnetron sputtering and additionally capped with ~ 3 nm of Pd and a thin Al₂O₃ layer to facilitate H uptake from H₂ and hinder H outgassing, respectively. The films were irradiated with 2.5 keV H⁺ ions to different fluences and subsequently measured by Medium Energy Ion Scattering (MEIS) in backscattering geometry to access crystal damage as well as H-induced lattice expansion. The H concentration and its depth profile in V films were determined by NRA employing the resonant ¹H(¹⁵N, αγ)¹²C nuclear reaction.

References

- [1] G. Marban et al., Int. J. Hydrogen Energy 32 (2007) 1625-1637.
- [2] J. Bloch et al., Phys. Rev. B 75 (2007), 165418.
- [3] K. Komander et al., PRL 127 (2021) 136102.

Degradation of CVD SiC during synergistic proton irradiation/aqueous corrosion tests

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The Fukushima Daiichi event in 2011 demonstrated the need for improved nuclear energy safety and became a major driving force for the development of accident-tolerant fuels (ATFs), which are called to overcome the inherent technical shortcomings of the standard zircaloy/UO₂ fuels currently used in Gen-II/III light water reactors (LWRs). SiC/SiC composites are a 'revolutionary' ATF cladding material concept that combines inherent refractoriness, pseudo-ductility, and a lack of accelerated steam oxidation during a loss-of-coolant scenario. Its potential in meeting the strict requirements of the ATF cladding application has already claimed large global investments, yielding different variants of this material concept. In this work, synergistic proton irradiation/aqueous corrosion tests were performed on monolithic SiC produced by chemical vapor deposition (CVD). CVD SiC coatings are deposited on the outer surface of SiC/SiC composite ATF claddings to minimize material losses in water, i.e., under nominal operation conditions for Gen-II/III LWRs. The proton irradiation/aqueous corrosion tests were performed on CVD β -SiC discs (3 mm, 50 μ m in thickness) in three different test conditions: (a) 320°C, standard PWR (pressurised water reactor) water with 3 ppm H₂, (b) 320°C, PWR water with 0.1 ppm H₂, and (c) 288°C, BWR (boiling water reactor) water with 2 ppm O₂. All CVD SiC discs were irradiated with a beam of 5.4 MeV protons for 48 h, yielding a total damage dose of 0.1 dpa. The CVD SiC discs underwent post-test analysis by means of scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDS), atomic force microscopy (AFM), focused ion beam (FIB), high-resolution (scanning) transmission electron microscopy (HR(S)TEM) and electron energy loss spectroscopy (EELS), shedding new light into the radiation-assisted degradation of CVD SiC in contact with water radiolysis species (esp. H⁺), and the dependence of this degradation on the exact water chemistry.

Time resolved ion induced photoelectron spectroscopy (tr-IIPS)

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The bombardment with ions is a widely used tool to tailor material properties, perform structural modifications and for analysis on the nanoscale. The dynamic response of the material to the ion impact occurs on the atomic level and since these interactions occur on ultrafast time scales, only computer simulations are available to investigate the underlying dynamics. Pump-probe schemes have faced limitations due to the inability to generate and precisely time short, monoenergetic ion pulses, which are crucial for observing these ultrafast phenomena, especially in the keV regime.

With a novel approach that overcomes these challenges, we generated the world's shortest monoenergetic ion pulses in the keV regime [1], and even pushed the limit by creating an ion pulse with a precision of approximately 5 ps. These ion pulses are produced by utilizing femtosecond photoionization of a geometrically cooled gas jet coupled with a miniaturized buncher system. With the prospect of further reduction of the pulse duration to 1.2 ps for neon [2] and 500 fs for argon, as our simulations suggest.

In a proof-of-principle experiment, using graphene membrane targets, we conduct the first ion-based pump-probe experiment at a picosecond time scale, observing the emission of hot electrons post-ion impact, like the scheme of two-photon photoemission (2PPE) experiments. Our findings not only demonstrate the feasibility of our approach but also provide a direct measure of the ion pulse characteristics, and will in the future offer insights into the non-equilibrium dynamics of electronic excitation in solids following an ion impact.

This research paves the way for new methodology in understanding the fundamental processes underlying ion-solid interactions, with significant implications for semiconductor manufacturing and material science. Our work not only sets a new standard for temporal resolution in the study of ion-induced phenomena but also lays the groundwork for future innovations in the field.

References

[1] L. Kalkhoff et al. Phys. Rev. Research 5, 033106 (2023)

[2] P. Kucharczyk et al. New J. Phys. 25, 123015 (2023)

Highly bond-specific fragmentation of biomolecules induced by swift heavy ions

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Single swift heavy ions (SHI) are known to uniquely alter the properties of solid materials by means of bond breaking and defect creation. In organic materials, in particular in the case of complex molecules with a variety of different chemical bonds, the question arises whether fragmentation induced by SHI can be bond-specific and which parameters influence the cleavage probability for a given bond. Oligopeptides with their peptide backbone and a multitude of functional groups in the side chains are predestinated to study such bond-specific fragmentation in organic molecules. Using soft cluster-induced desorption/ionization mass spectrometry as an analytical tool [1,2], we find that SHI-irradiated peptide samples show a high abundance of specific fragments, i.e., cleavage took place at the peptide bonds of the peptide backbone. This is in clear contrast to previous experiments with keV-ions, for which the majority of fragments was observed to be non-specific [3]. It indicates that the fragmentation process is largely influenced by the respective energy loss mechanism, i.e., nuclear stopping in the case of keV-ions versus electronic stopping in the case of SHI. keV-ions interact directly with the nuclear subsystem, which implies a stronger local correlation between the interaction site and the breaking bond, thus leading to non-specific fragments. In the case of electronic stopping, first the electronic subsystem is excited on the (sub-)femtosecond timescale, followed by spreading of the energy through the electronic subsystem and excitation of the nuclear subsystem via electron-vibrational coupling. As a consequence, excitation of the nuclear subsystem is more evenly distributed over the whole molecule, leading to preferential breaking of weaker bonds, i.e., specific fragmentation of the peptide backbone. However, the amount of different fragment species observed, as well as the sensitivity of the intact molecules to the SHI irradiation, are strongly dependent on the oligopeptide investigated. These observations are discussed with respect to possible fragmentation mechanisms and means of control.

References

- [1] C. R. Gebhardt, A. Tomsic, H. Schröder, M. Dürr, K.-L. Kompa, *Ang. Chem. Int. Ed.* 48, 4162 (2009).
- [2] M. Baur, C. R. Gebhardt, M. Dürr, *Rapid Commun. Mass Spectrom.* 28, 290 (2014).
- [3] P. Schneider, F. Verloh, A. Portz, S. Aoyagi, M. Rohnke, M. Dürr, *Anal. Chem.* 92, 15604 (2020).

Quest for Subsurface Amorphization in Topological Bi-Sb Materials via Swift Heavy Ions

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Bismuth, a strongly diamagnetic semimetal, possesses intriguing and unconventional properties that have garnered significant attention over the years. Approximately 70 years ago, it was observed that amorphous bismuth exhibits superconductivity with a critical temperature (T_c) of about 6 K, contrasting with crystalline bismuth at ambient pressure, which does not display superconductivity. Shortly thereafter, alloys of bismuth with antimony (and with other similar elements) were also found to be superconductors with critical temperatures T_c ranging between 6.0 and 6.4 K.

More recently, bismuth-antimony alloys have attracted great interest due to their behaviour as topological insulators. The possibility of combining this behaviour with that of the superconducting state renders amorphous Bi-Sb alloys potential candidates for topological superconductivity. However, a significant challenge arises as both pure bismuth and bismuth-antimony alloys tend to crystallize when exposed to temperatures above those of liquid helium. Currently, we are exploring various hypotheses and strategies to overcome this limitation.

Last but not least, Bi-Sb alloys, both in crystalline and amorphous states, present promising thermoelectric properties for technological applications, which is an additional reason to exhaustively study these materials and learn how to modify their properties.

In this study, we have fabricated various polycrystalline films of Bi_{100-x}Sb_x ($x = 0, 5, 10, 15$) using either thermal evaporation or the melt-spinning technique. Subsequently, we induced significant internal structural damage in these films through ion beam irradiation with swift heavy ions, typically Bi ions in the 10-30 MeV range, aiming to amorphize the material. We have conducted a series of characterization experiments, both before and after irradiation, to assess the impact of the preparation method and degree of disorder. These experiments encompassed X-ray diffraction, Scanning Electron Microscopy imaging, and low-temperature measurements of electrical conductivity spanning from room temperature to nearly 2 K.

Defect Control for Enhancing Acetone Sensing in Graphene Gas Sensors

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Human respiratory gases primarily consist of oxygen, nitrogen, carbon dioxide, and trace amounts of volatile organic compounds (VOCs) such as ammonia, acetone, etc. Although VOCs are present in small quantities, they reflect the metabolic state of the human body, as they are byproducts of human metabolism. For instance, a diabetic patient exhales acetone gas at a concentration of 1.8 ppm, whereas a normal individual typically exhales acetone gas at levels ranging from 0.3 to 0.9 ppm. Therefore, detecting acetone gas can be utilized for diagnosing diabetes patients. In this presentation, we introduce a defective graphene gas sensor capable of detecting acetone gas, with the sensitivity influenced by both the quantity and type of defects present. To induce various defects on the graphene gas sensors, we utilized hydrogen ions, the smallest ion, and krypton ions, one of the heavier ions, while controlling the irradiation energy and dose. The quantity of defects was evaluated using Raman spectroscopy, and the sensitivity of the graphene gas sensors was measured using a simple 4-probe method. Interestingly, despite similar defect quantities, the sensitivity exhibited different behaviors. We discuss potential mechanisms of these defects based on the performance of the graphene gas sensors.

In situ monitoring of monolayer graphene self-healing following very low-energy ion beam bombardment

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Due to the two-dimensional (2D) nature of graphene, defects in its lattice are bound to induce significant changes in its properties. Experiments carried out on a setup specifically designed to examine plasma-surface interactions [1] shed light on defect recombination kinetics. In situ Raman spectrometry is used to monitor the evolution of Raman peaks of a monolayer graphene sheet evolution during and immediately after ion bombardment. The ratio of the D peak's intensity over the G peak's intensity is known to be proportional to defect concentration in graphene such as vacancies [2]. A sudden decrease is observed right after 13 eV ions bombardment, which is not observed at higher energy. While 90 eV ions generate sputtering, subthreshold ions (transferred energy below 18 eV [3]) are expected to create vacancies and adatoms on graphene's surface [4,5]. Self-healing can be attributed to adatoms' swift diffusion and recombination with vacancies. Furthermore, a comparison of experimental results with a kinetic model shows that self-healing efficiency is limited by adatom dimerization. To properly simulate the progress of defect concentration decrease over time, adatoms interplay with Stone-Wales defects must be considered. The latter acts as a temporary trap for adatoms, releasing them at a low rate and prompting vacancies' healing. Such phenomena are to be considered in any process containing sub-threshold ions interacting with graphene and, more generally, with any 2D materials.

References

- [1] Vinchon, P. et al. In-plasma analysis of plasma-surface interactions. *Review of Scientific Instruments* 94, (2023).
- [2] Lucchese, M. M. et al. Quantifying ion-induced defects and Raman relaxation length in graphene. *Carbon N Y* 48, 1592–1597 (2010).
- [3] Banhart, F., Kotakoski, J. & Krasheninnikov, A. V. Structural Defects in Graphene. *ACS Nano* 5, 26–41 (2011).
- [4] Vinchon, P., Glad, X., Robert Bigras, G., Martel, R. & Stafford, L. Preferential self-healing at grain boundaries in plasma-treated graphene. *Nat Mater* 20, 49–54 (2021).
- [5] Chen, J. et al. Self healing of defected graphene. *Appl Phys Lett* 102, 103–107 (2013).

A contactless single-step process for simultaneous nanoscale patterning and cleaning of large-area graphene

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Nanoscale patterning of 2-dimensional (2D) materials is crucial for various emerging applications such as nanoelectronics, 2D photonic metasurfaces, and chemical separation. Current methods, including focused ion beams (FIB) and extreme UV (EUV) lithography, have scalability limitations and may introduce contamination to the materials.

In this presentation, we introduce a contactless, chemical-free approach for simultaneous patterning and cleaning of self-supporting graphene membranes in a single step [1]. The approach relies on a broad beam of energetic ions passing through a self-supporting mask with predefined nanoscale patterns. The patterning of self-supporting graphene membranes achieves a spatial resolution of 15 nm, approaching the performance of small-area FIB and EUV lithography methods. However, our approach requires only a broad beam, eliminating the need for nanoscale beam positioning and enabling large-area patterning.

Furthermore, synthetic graphene is often heavily contaminated with hydrocarbon molecules during the transfer process, significantly affecting its properties. We demonstrate that our approach can simultaneously clean the graphene membranes from initial contamination. The cleaning mechanism is attributed to the coupling of surface diffusion and electronic and nuclear sputtering effects on surface contaminants.

Finally, utilizing high-resolution transmission electron microscopy and selective area electron diffraction, we investigate the extended propagation of defects from irradiated to non-irradiated areas at room temperature. These extended defects induce mosaicity in the graphene lattices, and the mobile contaminants appear to stabilize the material against defect propagation.

References

[1] T. T. Tran, H. Bruce, N. H. Pham, and D. Primetzhofer, 2D Materials 10, 025017 (2023).

Determination of the elastic constants of ion implanted Gallium Arsenide using Surface Brillouin Scattering

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Despite GaAs being at the frontiers in radiation detection technologies, the attendant radiation effects such as structural transitions have not been widely investigated. In this work, single crystal (100) gallium arsenide has been implanted with argon and silicon ions to investigate the physical properties of an amorphous surface layer overlying the crystalline (100) GaAs substrate. The implantations have been performed whilst varying the ion energies to obtain disordered layers with varying film thicknesses and degrees of disorder. The amorphous layer thicknesses have been determined by calculations using the stopping and range of ions in matter (SRIM) software. We will present Raman spectroscopy results showing the transitions from a single crystal to an amorphous layer. Further to this, we have also used the Surface Brillouin scattering (SBS) technique to determine the elastic properties of the disordered layer. SBS is an optical technique that uses a (3+3) pass Fabry-Perot interferometer to measure the frequencies of surface acoustic waves. The measurements are taken as a function of scattering angle and amorphous layer thickness to derive phonon dispersion curves. Thereafter, a least squares fitting approach has been used to fit simulations to the measured data and thereby determine elastic constants of the disordered layer. Preliminary results show that the two components of elastic constant tensor (C_{11} , C_{44}) for a-GaAs after ion implantation are $C_{11} = 94.5$ GPa and $C_{44} = 18.5$ GPa for argon ions and $C_{11} = 115.2$ GPa and $C_{44} = 27.5$ GPa for silicon ions. Raman spectroscopy was used to study the structural properties of amorphous GaAs and the transition from crystalline to amorphous has been observed.

Nanopatterning Si surface by ion beam irradiation with sub-sputter-threshold energies, revisited

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Ion beam irradiation (IBI) has been extensively utilized to induce self-assembly of nanoscale patterns on surfaces. The underlying mechanism has been attributed to the counteracting effects of destabilizing ion sputtering and stabilizing mass diffusion. About a decade ago, it was predicted that sputter effects would be negligible, while irradiation-driven mass redistribution would play a predominant role in destabilizing surfaces, as per the crater function theory (CFT). To assess this hypothesis, IBI experiments were conducted on various surfaces with ion energies (E_{ion}) below the sputter threshold energy (E_{th}), revealing pattern formation on diverse semiconductor surfaces, strongly corroborating CFT predictions. Furthermore, these patterns closely resemble those generated by IBI with $E_{\text{ion}} \gg E_{\text{th}}$, thus affirming that sputtering effects not only minimally contribute to surface destabilization but also play a minor role in shaping surfaces.

Previous studies have been deficient in crucial information, such as the ion energy distribution of the beam. Given the potentially broad energy distribution of ion sources and the presence of doubly ionized ions, conducting IBI with precisely defined E_{ion} is imperative to ensure the exclusion of ions with $E_{\text{ion}} > E_{\text{th}}$. To address this, we utilize a Faraday cup as a retarding field energy analyzer to ascertain the energy distribution of our ion source. Consequently, performing Kr IBI with $E_{\text{ion}} = 9$ eV, we could safely avoid the impact of ions on Si surfaces with $E_{\text{ion}} > E_{\text{th}}$.

IBI of Si with E_{ion} of 9 eV generates ripple patterns, robustly corroborating the prediction of CFT that mass redistribution can destabilize the surface. However, these ripple patterns differ significantly from those formed with an E_{ion} of 2 keV in several aspects: triangular structures do not emerge, and both the local slope distribution and coarsening kinetics deviate from cases involving ion sputtering. Furthermore, the angular dependence of the ripple wavelength, $\lambda(\theta)$, for $E_{\text{ion}} = 9$ eV does not align with CFT predictions, while reasonable reproduction is observed for $E_{\text{ion}} = 2$ keV. We tentatively attribute this difference to the very surface, short-range mass redistribution induced by IBI with an E_{ion} of 9 eV.

References

- [1] R. M. Bradley and J. M. E. Harper, J. Vac. Sci. Technol. A 6, 2390 (1988).
- [2] S. A. Norris, J. Samela, L. Bukonte, M. Backman, F. Djurabekova, K. Nordlund, C. S. Madi, M. P. Brenner, and M. J. Aziz, Nat. Comm. 2, 276 (2011).
- [3] A. Metya and D. Ghose, Appl. Phys. Lett. 103, 161602 (2013).

Advances in the prediction of ion-induced surface nanopatterning by continuum equations

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The properties of thin films, be they electrical, magnetic or catalytic, depend significantly on the surface and interfaces topography (roughness) on the nanometer scale. Ion irradiation can be used to engineer the surface roughness and induce the formation of self-organized nanoscale patterns [1]. Depending on the irradiation conditions, hexagonally ordered dot or pit patterns, checkerboard patterns, as well as periodic ripple patterns are formed spontaneously on the surfaces driven out of equilibrium by continuous ion irradiation.

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

If the temperature during ion irradiation is above the recrystallization temperature of the material, ion induced defects are dynamically annealed and amorphization is prevented. The diffusion of ion-induced vacancies and ad-atoms is now additionally affected by the Ehrlich-Schwoebel barrier on the crystalline surface: vacancies and ad-atoms are trapped on terraces and can nucleate to form pits or mounds, respectively. Patterns formed in this “reverse epitaxy” regime exhibit crystalline facets and the symmetry of the patterns is determined by the crystal structure of the irradiated surface [2]. However, also on crystalline surfaces ballistic effects can play a role and shape the resulting morphology. This has been observed for irradiations at high temperature and off-normal angle of incidence [3] as well as for high temperature and normal incidence in the intermediate regime between checkerboard and isotropic patterns [4].

The fundamental understanding of the formation of surface patterns at these non-equilibrium conditions is already quite advanced. Simulations based on atomistic methods, such as molecular dynamics (MD) and Monte-Carlo (kMC), or by continuum equations can describe in most cases the observations. In recent years, continuum equations have been further extended in order to achieved predictive power on both amorphous as well as crystalline surfaces.

References

- [1] Cuerno, R. & Kim, J.-S., J Appl Phys 128, 180902 (2020).
- [2] X. Ou, K.-H. Heinig, R. Hübner, J. Grenzer, X. Wang, M. Helm, J. Fassbender, and S. Facsko, Nanoscale 7, 18928 (2015).
- [3] D. Erb, R. de Schultz, A. Ilinov, K. Nordlund, R. M. Bradley, and S. Facsko, , Phys Rev B 102, 165422 (2020).
- [4] D. J. Erb, D. A. Pearson, T. Škřeň, M. Engler, R. M. Bradley, and S. Facsko, Phys. Rev. B 109, 045439 (2024).

Advancing Ion-Induced Surface Patterning Through Physics-Informed Neural Networks

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In the evolving landscape of 2D structures and surface-based technologies, ranging from nanofabrication to biology, ion radiation-induced surface patterning emerges as a key nanofabrication technique. Despite its relevance, the physics underlying the pattern formation remains under discussion due to the challenges in modelling these complex and unstable dynamics. The most successful models in describing the interaction, based on the non-linear partial differential Kuramoto-Sivashinsky (KS) equation, remain under debate. Not only the variation of the KS-based model is yet to be asserted, but also the equation parameters are hard to predict for the ion radiation and material under study. Such constraints arise from the traditional partial differential equation solvers, such as finite difference or finite element methods, being inadequate to solve the KS inverse problem.

Here, we introduce a novel approach using Physics-Informed Neural Networks (PINNs) to overcome these obstacles. By including physical laws in the neural network training, PINNs promise a breakthrough in estimating the terms and parameters of the KS equation, even from scarce and noisy experimental data obtained with techniques such as Atomic Force Microscopy. We also demonstrate how PINNs successfully handle, predict and correct large experimental uncertainties, such as sample misalignment and radiation fluence errors, that typically complicate the analysis of ion-induced patterning. Moreover, PINNs offer a way to reverse-engineer the process, allowing us to deduce the initial conditions necessary to achieve desired surface patterns.

This study highlights the potential of PINNs in advancing our understanding and application of ion-induced surface patterning. By joining the analytical capabilities of PINNs with experimental insights, we can improve the theoretical understanding of ion-solid interactions and open new routes for patterning design and control.

Can we study radiation damage from energetic charged particles during space travel using small ion accelerators?

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A challenge for future long-duration manned space missions is managing the effects of charged particle radiation on astronauts. The energetic charged particles originate from Galactic Cosmic Rays (GCR) and Solar Energetic Particles (SEP). Conventional animal model studies are expensive, long duration and require the use of expensive large high ion energy facilities. This presentation explores the viability of using an alternative and more economic approach using small ion accelerators with few MeV energy to irradiate thin ($<300\text{ }\mu\text{m}$) tissue samples.

The ISO standard GCR flux and standard flux models for SEP from Coronal Mass Ejections was used to predict the isotopic flux impinging on a spacecraft. The HZETRN code was used to predict the flux inside the spacecraft assuming 10 g cm^{-2} Al to be an equivalent spacecraft wall. Range, energy loss distributions and mean doses were calculated using the SRIM code. Microscopic dose distributions within ion tracks were investigated using the Spohr ion track model.

The internal spacecraft GCR flux has a continuous distribution which is dominated by H^+ in 5 – 500 MeV energy whereas the SEP flux is dominated by $< 100\text{ MeV H}^+$. The ^{56}Fe flux is a factor $10^{-5} - 10^{-6}$ smaller than for protons. Consequently, even though the mean doses (Gy per nucleon) to the skin for ^{56}Fe were about 50 $\times$ greater than from ^1H , the dominating mean dose contributions to an astronaut comes from low energy H^+ fluxes from GCR and SEP. The microscopic dose is a factor $\sim 10^4$ greater than for ^{56}Fe compared to ^1H out to the track radius (40 nm, 1.2 μm and 70 μm for 0.3, 3 and 30 MeV/u ions, respectively). However, a simple hit model implies the greater flux from low energy protons creates more double strand DNA breaks than ^{56}Fe . Taken together, the mean doses and radiation are completely dominated by $< 10\text{ MeV}$ protons and ^4He . The implication is that irradiation of thin tissue cultures with few-MeV light ions can be an effective, economic, ethical and rapid alternative to irradiation with animal models.

Developing a machine learning interatomic potential to study radiation-induced damage in 3C-SiC

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Silicon carbide (SiC) has been a long-standing subject of study for its application in harsh environments. Theoretically, the nano-structural state of irradiation-induced defects in cubic SiC (3C-SiC) has been extensively studied with molecular dynamics (MD) using various empirical interatomic potentials [1]. However, these potentials show significant discrepancy in predicting some of the properties, e.g. threshold displacement energies and defect formation and migration energies that are crucial in describing the evolution of defects generated in collision cascades [2]. We present a Gaussian approximation machine learning potential (GAP) [3], trained over the data collected from density functional theory (DFT) calculations. We build the dataset with representative perfect and defective crystalline, liquid and amorphous structures, with which we train our potential using a two-body and the turbo-SOAP [4] many-body descriptor. The elastic properties of 3C-SiC are captured by the inclusion of elastically deformed unit- and supercells; the thermal and vibrational properties are accounted for by including supercells thermalized at different volumes and temperatures; and the defects are represented by adding manually constructed defective configurations. The defect types include antisites, single-, di-, and tri-vacancies, and six interstitial configurations. The initial configurations for the liquid and amorphous phases were collected by sampling the DFT-MD melting and quenching simulations, respectively. Then, the dataset was enriched for these phases with iteratively sampling the MD simulations using the early version of the potential. The high repulsion of the energetic atoms encountered in collision cascades is captured by appending the ZBL [5] repulsive potential. The potential shows excellent agreement with DFT in predicting bulk, thermal, vibrational, and defect properties and reproduces the radial distribution function of amorphous and liquid phases.

References

- [1] Yan, Zefan, et al. "Molecular dynamics simulation studies of properties, preparation, and performance of silicon carbide materials: a review." *Energies* 16.3 (2023): 1176.
- [2] Yu, Jiajie, et al. "Comparison and Assessment of Different Interatomic Potentials for Simulation of Silicon Carbide." *Materials* 17.1 (2023): 150.
- [3] Bartók, Albert P., et al. "Gaussian approximation potentials: The accuracy of quantum mechanics, without the electrons." *Physical review letters* 104.13 (2010): 136403.
- [4] Caro, Miguel A. "Optimizing many-body atomic descriptors for enhanced computational performance of machine learning based interatomic potentials." *Physical Review B* 100.2 (2019): 024112.
- [5] Ziegler J.F., Biersack J.P. and Littmark U., *The Stopping and Range of Ions in Matter* (Pergamon, New York) 1985.

Finite-range repulsive interatomic potentials for binary collision simulations

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Accurate interatomic potentials are crucial for predicting energy loss, range distributions, and sputtering yields caused by ion bombardment of matter. The most common choice for simulations based on the binary collision approximation (BCA) is the so-called "universal" ZBL potential, e.g., as implemented in TRIM. The somewhat weaker Kr-C potential is also often used, e.g., by SDTrimSP and TRIDYN. Both interatomic potentials are described by screening functions that are sums of exponentials.

We have recently shown that interatomic potentials calculated using the DMol97 all-electron quantum-chemistry approach are in excellent agreement with even more advanced quantum-chemistry calculations [1]. For the present contribution, we have fitted the repulsive parts of these potentials for every Z1-Z2 combination with a sum of exponentials and a potentially negative linear term, so that the radius of zero interaction energy matches that of the DMol potential. This approximation allows the robust and accurate evaluation of the scattering integral using 4-point Gauss-Legendre integration. Using several examples, we show that the new interatomic potentials lead to sputtering yields that are up to a factor of three larger than those obtained with the universal ZBL potential, and a factor of two larger than using the Kr-C potential. Moreover, the new potentials also yield significantly different results for channeling implantations and for grazing-incidence ion reflection, and somewhat more radiation damage, while the ion range in amorphous materials is hardly affected. We believe that the new interatomic potentials pave the way for more consistent parameter sets of BCA simulations.

References

[1] K. Nordlund, S. Lehtola, G. Hobler, Comparative study of repulsive interatomic potentials from different levels of quantum chemical calculations, accepted for presentation at COSIRES-2024.

Fundamental Quantities for Ion-Beam Modification of Materials at Low Energies Assessed by Low-Energy Ion Scattering

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A detailed and quantitative understanding of the interaction between ions and solids is essential for controlled material modification with ion beams. For slow ions, this interaction is complicated by dynamic processes and solid-state effects, which renders ab-initio predictions a complex task. Simultaneously, experimental reference data is scarce, due to experimental challenges.

Here, we use time-of-flight low-energy ion scattering (ToF-LEIS), a non-destructive surface analysis method, to experimentally study two key aspects of the ion-solid interaction: the interatomic potential and the electronic energy loss.

The interatomic potential is commonly described as a screened Coulomb potential. Often used models like the Thomas-Fermi-Molière (TFM) and the Ziegler-Biersack-Littmark models, are known to be inaccurate for slow ions and are generally adjusted by applying a correction factor (ca) to the screening length [1].

We aim to improve the knowledge of interatomic potentials at low energies for fusion-relevant ion-solid combinations (D_2^+/He^+ on W/Fe) by extracting ca for the TFM model from angular scans of single crystalline samples using ToF-LEIS. By adjusting ca in molecular dynamics simulations, we reproduce the width of crystal channels in our experimental angular scans [2], thus determining the correct values for ca .

Additionally, we present electronic energy loss measurements for slow H^+ and He^+ in Ti, which we chose as a system of interest due to its high technological relevance, particularly in compound systems [3]. Electronic energy loss data is largely lacking at low ion velocities, and semi-empirical models like SRIM can deviate significantly. New experimental data will thus further enhance the quality of compositional and morphological analysis of Ti systems performed with ion beam analysis methods.

References

- [1] O'Connor & Biersack, NIMB 15, 14 (1986)
- [2] Primetzhofer et al., Surf. Sci. 602, 2921 (2008)
- [3] Wolf et al., Appl. Surf. Sci. 638, 158076 (2023)

Structural stability of nanotwinned high entropy thin film under Helium ion radiation.

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Radiation effects in High Entropy Alloys (HEA) have intrigued researchers for decades, with their unique material properties challenging conventional understanding. With the introduction of nanotwin structure, the self-healing effect and increment of defect sinks will benefit the radiation resistance of HEA thin film. This study demonstrated the radiation resistance of high entropy alloy (HEA) thin films with a high density of nanotwinned (NT) structures, compared to the conventional metallic alloys and nanocrystalline thin films. Utilizing a pulsed direct current sputtering system, we deposited CoCrFeNi HEA NT thin films, and the radiation damage experiment was investigated at room temperature under 275keV Helium ion radiation. Remarkably, the presence of small-sized helium bubbles and their distribution showed significant radiation resistance within this system.

Moreover, transmission electron microscopy and x-ray diffraction analysis showed the retention of stable grain and twin microstructures after radiation damage. Notably, interactions between defects, grains, and nanotwinned boundaries were observed. The HEA-NT thin films exhibited a phase transformation from a face-centered cubic to a hexagonal closed-packed phase owing to radiation-induced local strain build-up, accompanied by substantial local strain-induced grain rotation within the thin film structure. Further explanation of the mechanism will be discussed comprehensively.

References

- [1] Chen, Y., K.Y. Yu, Y. Liu, S. Shao, H. Wang, M.A. Kirk, J. Wang, and X. Zhang, Damage-tolerant nanotwinned metals with nanovoids under radiation environments. *Nat Commun*, 2015. 6: p. 7036.
- [2] Chen, Y., J. Li, K.Y. Yu, H. Wang, M.A. Kirk, M. Li, and X. Zhang, In situ studies on radiation tolerance of nanotwinned Cu. *Acta Materialia*, 2016. 111: p. 148-156.
- [3] Han, W.Z., M.J. Demkowicz, E.G. Fu, Y.Q. Wang, and A. Misra, Effect of grain boundary character on sink efficiency. *Acta Materialia*, 2012. 60(18): p. 6341-6351.

In situ TEM with heavy-ion irradiation of the new CrNbTaVW refractory high entropy alloy

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One of the important issues on the divertor of a nuclear fusion reactor is the thermal mismatch between the low-working temperature heat sink material (CuCrZr) – which embrittles under irradiation – and the plasma facing component W. In this context a new material has been proposed to serve as a compliant layer in this system: a refractory high entropy alloys. The CrNbTaVW refractory high entropy alloy (RHEA) was produced by ball milling and consolidated by Field Assisted Sintering Technology (FAST) at a temperature of 1600 °C and under a pressure of 90 MPa. Since the proposal materials will be applied as interlayer between W and CuCrZr and can be affected by the plasma occurrences, the irradiation effects are crucial to understand the resistance of them inside the reactor. Electron-transparent samples of the CrNbTaVW were irradiated at the MIAMI-2 facility using 300 keV Xe ions at room and 800°C. The effects of radiation in the CrNbTaVW RHEA were quantified in terms of defects within the microstructure and its phase stability. The nucleation and growth of Xe bubbles were related with an interesting effect of intragranular fracture. The results provide insights on the further optimization of novel RHEAs to be applied in extreme environments.

Role of anion sublattice and coherent materials' response to irradiation before amorphization in fluorite-derivative oxides

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Disordering in ternary oxide systems derived from the parent fluorite structure have attracted significant attention with particular interest in correlating the crystal chemistry and ordering of metal cations and oxygen anions to their radiation tolerance, ionic and thermal conductivity. Radiation effects in these systems have been mainly focussed on the role of cations in the disordering and amorphization while the role of anion sublattice is not well understood due to the unavailability of model system which allow to deconvolute the effect of both cation and anion sublattices. The current presentation will summarise work on radiation effects in $\delta\text{-Sc}_4\text{Hf}_3\text{O}_{12}$ and $\text{Gd}_2\text{Ce}_2\text{O}_7$ systems that exhibit excellent resistance to radiation-induced amorphization [1-4] but show anomalous structural transformations under swift heavy ion irradiation (SHI) as well as damage recover under post irradiation heat treatment or electron beam irradiations. Using quantitative x-ray diffraction and electron microscopy, we show how topological disorder on the anion sub-lattice grows faster than that on the cation sub-lattice in $\text{Gd}_2\text{Ce}_2\text{O}_7$, and how SHI is first able to stabilize a phase transformation to metastable Bixbyite structure in $\delta\text{-Sc}_4\text{Hf}_3\text{O}_{12}$ while electron beam irradiation reverses this back to the parent Rhombohedral and Fluorite domains by rearrangement of the anion vacancies. In addition, radiation damage models in ceramics typically trace the relative proportions of the two phases i.e. amorphous or crystalline, at any time during irradiation. Here, we develop a different approach wherein we describe at the atomic scale the coherent materials' response to irradiation before amorphization takes place.

References

- [1] M. Iwasaki, M. K. Patel, G. Baldinozzi, K. E. Sickafus, and M. Ishimaru, J. European Ceramic Soc. 44 (2024) 3131.
- [2] M. Iwasaki, Y. Kanazawa, D. Manago, M. K. Patel, G. Baldinozzi, K. E. Sickafus, and M. Ishimaru, J. Appl. Phys. 132 (2022) 075901.
- [3] Maulik K. Patel, Jeffery Aguiar, Kurt E. Sickafus, and Gianguido Baldinozzi, Phys. Rev. Materials 6 (2022) 013610.
- [4] Maulik K. Patel, Kurt E. Sickafus, and Gianguido Baldinozzi, Phys. Rev. Materials 4 (2020) 093605.

Hydrogen irradiation impact on oxide dispersion strengthened steels containing Y₂O₃ and Y₂Ti₂O₇ nanoparticles at elevated-temperature.

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Supercritical water reactor (SCWR) and nuclear fusion reactors, propose the potential of a carbon-free energy future; in this connection, fuel claddings are a crucial material for satisfying this ideal requirement. Oxide dispersion strengthened (ODS) steel and its optimized alloys are well known for its enhanced resistance to radiation-induced damage and the creep mechanism, due to the fine distribution of metallic oxide particles. In current work, YO and YTO ODS steels were prepared by adding Y₂O₃ and Y₂Ti₂O₇ nanoparticles (NPs). Furthermore, a Chinese low-activation ferritic/martensitic steel (CLF) was also employed for a comparison study. Hydrogen irradiation was performed using 50 keV H²⁺ implantation at 320 kV at 550 °C with a beam flux of $2.0 \times 10^{12} \text{ H}^{2+} \text{ cm}^{-2} \text{ s}^{-1}$. These samples were subsequently implanted to fluences of 4.6×10^{16} , 1.5×10^{17} , and $4.6 \times 10^{17} \text{ H}^{+} \text{ cm}^{-2}$, respectively to achieve 0.3, 1 and 3 dpa. The penetration of hydrogen was observed by the TEM, number of bubbles and average bubble size were calculated with the help of under-focus and over-focus techniques. The result shows that the number of bubbles and average bubble size are higher in the CLF followed by YO and lowest is observed in the YTO steel. This shows that Y₂Ti₂O₇ NPs resist the formation of hydrogen bubbles and decrease the defects formation. HRTEM shows the size of NPs in YTO are 38 nm while in YO it is 58 nm, that shows that small NPs in YTO hinder the segregation process and reduces the influence of irradiation. HRTEM and corresponding FFT images of YO and YTO steel after the hydrogen irradiation at 3 dpa are shown in Fig.1 and Fig. 2, respectively. After irradiation, it can be observed that a disordered region is formed in Fig. 1(c) and Fig. 2(c), it could be due to the formation of a hydrogen bubble-shell, which is also supported by the calculated average bubble size for the YO and YTO. Y₂Ti₂O₇ NPs are more stable and shows semi-coherent orientation while Y-Al-O NPs shows incoherent orientation with the matrix. Y₂Ti₂O₇ NPs reduces the internal stresses and interface defects that are usually produced in the ODS steels due to hydrogen irradiation. According to this study, it is suggested to add Y₂Ti₂O₇ NPs to the ODS steels to improve the resistance towards defects that are produced by the irradiation in SCWR to improve the life span of these materials under extreme working conditions.

A novel methodology for assessing near-surface diffusion in nuclear materials

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The diffusion of gaseous fission products such as Xe and Kr in nuclear fuel represents a significant performance and safety parameter due to their high fission-yields, high neutron absorption cross-sections and the potential to create pressure build-up within fuel cladding [1]. The study of the diffusion behaviour of these noble gas species is, however, an experimental challenge, due to difficulties in adding gas species to the fuel matrix and also in accessing techniques which can monitor gas concentrations and diffusion on ultrashort-length scales. In the majority of cases, diffusion parameters are derived from irradiated material [2], either through measurements in the plenum, or by annealing in Materials Tests Reactors and Post Irradiation Examination facilities. Although effective, the use of irradiated material requires significant infrastructure and resources to operate, and thus limits sample throughput. Presented here, is an extension of previous work [3] to combine medium energy ion implantation with time-of-flight elastic recoil detection analysis, to investigate the diffusion of volatile elements in high-density sample matrices including nuclear fuels. ZrO₂ and UN samples are each implanted with Kr and Xe, and the depth-dependent distributions of these implants are studied before and after annealing. This work contributes towards providing benchmarking data for the validation of short-length scale atomistic models, such as density functional theory and molecular dynamics, which in turn contribute significantly to the Accelerated Fuel Qualification initiative [4]. The technique described here has the potential to significantly reduce the cost and timescale of new fuel qualification, when compared to traditional methods.

References

- [1] H. Bailly, D. Menissier, C. Prunier, *The Nuclear Fuel of Pressurized Water Reactors and Fast Reactors: Design and Behavior*, CEA, Eyrolles, 1996.
- [2] G. Lawrence, A review of the diffusion coefficient of fission-product rare gases in uranium dioxide, *Journal of Nuclear Materials* 71 (1978) 195–218.
- [3] R.J.W. Frost, D.A. Lopes, K.D. Johnson, S. Patnaik, J. Oscarsson, M. Sortica, P. Petersson, D. Primetzhofer, “Evaluating the diffusion of Kr in UO₂ and ADOPT™ using Time-of-Flight Elastic Recoil Detection Analysis (ToF-ERDA)”, *Journal of Nuclear Materials* (under review).
- [4] K. Terrani, N. Capps, M. Kerr, C. Back, A. Nelson, B. Wirth, S. Hayes, C. Stanek, “Accelerating nuclear fuel development and qualification: Modelling and simulation integrated with separate-effects testing”, *Journal of Nuclear Materials* (2020).

Impact of irradiation on the chemical durability of UO₂, UThO₂ and UNdO₂ sintered pellets

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The reprocessing of actinides from spent nuclear fuels is essential for maintaining a closed nuclear fuel cycle. To understand these mechanisms, it is crucial to investigate the characteristics of spent fuel post-exposure within a nuclear reactor and the associated dissolution processes in an acidic medium. This work focuses on two primary damage regimes inflicted on the fuel by fission fragments: atomic collisions and electronic energy loss. While both the reprocessing of irradiated UO₂ and doped UO₂ have been studied separately [1-2], the coupling of these two phenomena has not been thoroughly explored. To this goal, three distinct model systems of UO₂ pellets doped with 10% Th or 10% Nd have been synthesized and investigated, to serve, respectively, as a surrogate for Pu and to investigate the effect of incorporated trivalent elements into the crystalline structure of UO₂. SRIM calculations were performed to select the irradiation parameters. The samples were irradiated with Au ions at 1, 2, and 7 MeV, to achieve an almost constant depth distribution of atomic displacements over a depth of 1 μm and with Xe ions at 1 GeV, corresponding to a constant electronic stopping power on the first 20 μm. Surface characterizations were conducted using AFM and Raman spectroscopy to examine the effects of irradiation on roughness, grain reorganization and defects, as well as to determine the specific surface area of each sample. Chemical durability was assessed by identifying the effects of acidity and temperature. The speciation of the species was analyzed using Inductively Coupled Plasma Spectroscopy and Photon-Electron Rejecting Liquid Alpha Spectroscopy. In the early stages of lixiviation, doping is manifesting a stronger influence than irradiation, while the impact of Xe irradiation remains negligible compared to Au irradiation.

References

- [1] Bricout, M., et al. Journal of Nuclear Materials, 554, 153088.
- [2] Barral, T., et al. Corrosion Science, 222, 111380

Interstitial loop unfaulting and extended defect coalescence in uranium dioxide and other fluorite oxides

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Evolution of dislocation loops and lines as well as fission gas bubble play an important role in nuclear fuel behavior. Their evolution has significant implications on fission gas release and fuel restructuring. In this presentation, we discuss utilization of transmission electron microscopy (TEM) to image defects in irradiated UO₂ and ThO₂. TEM imaging is done under various conditions including in-situ characterization under ion beam irradiation and in-situ annealing of pre-irradiated sample, as well ex-situ counterparts. To interpret our experimental observations, we employ cluster dynamics simulations to describe evolution of extended defects. Our analysis reveals various evolution mechanisms including growth of interstitial dislocation loops by point defect absorption, unfaulting of Frank loops, as well as coalescence of dislocation loops and bubbles.

Post-irradiation characterization of proton irradiated sample indicates that at low irradiation doses faulted dislocation loops are homogeneously nucleated and grow via absorption of point defects. Irradiation with heavier krypton ions allows characterization of extended defects at higher dose, where results suggest that dislocation loops undergo unfaulting process and exhibits coalescence. While voids are not very common under proton irradiation, krypton ion irradiation produces gas bubbles. In general, post-irradiation annealing results in further evolution of extended defects where loops, voids, bubbles coarsen. While initial krypton ion irradiation experiments only provided an indication for coalescence of the extended defects as a coarsening mechanism. Most recent, in-situ annealing experiments provide further evidence for coalescence of extended defect. These results provide means for validating some of the assumptions made to describe microstructure evolution in irradiated nuclear fuels.

POSTER 1 ABSTRACTS

Optically Active Chalcogen Vacancies and Robust N-type Doping by Proton Irradiation in 2D TMDs

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Defect engineering of atomically thin semiconducting crystals is an attractive route to developing single photon sources and valleytronic devices. For these applications, defects with well-defined optical characteristics need to be generated in a precisely controlled manner. However, defect-induced optical features are often complicated by the presence of multiple defect species, hindering identification of their structural origin. Here, we report systematic generation of optically active atomic defects in monolayer MoS₂, WS₂, MoSe₂, and WSe₂ via proton beam irradiation. Defect-induced emissions are found to occur 100~200 meV below the neutral exciton peak, showing typical characteristics of localized excitons such as saturation at high excitation rate and long lifetime. Using scanning transmission electron microscopy, we show that freshly created chalcogen vacancies are responsible for the localized exciton emission. Density functional theory and GW-BSE calculations reveal that the observed emission can be attributed to transitions involving defect levels of chalcogen vacancy and the valence band edge state.

Besides the optically active property, the defects generated by proton irradiation also induce a robust n-type doping effect in 2D TMDs. For example, we demonstrated a reliable and long-time air stable n-type doping scheme with WSe₂ by proton irradiation. The irradiated WSe₂ remains an n-type semiconductor even after it is exposed to ambient conditions for a year. Localized ion irradiation with a focused beam can directly pattern on the sample to make high performance homogenous p-n junction diodes.

Exploring 2D graphene as atomic armor to protect uranium from ambient corrosion

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Uranium (U) is a nuclear material with tremendous technological importance. One outstanding challenge in preserving its intrinsic nuclear properties is its high susceptibility to ambient corrosion. The corrosion, initiates at surfaces and interfaces, can form different phases, alter the dimensions of components, and even cause surface spalling, thus degrade the nuclear performance. Protective coatings are effective means to prevent metals from corrosive environments. However, anticorrosion coatings, when applied to actinides including U, faces a unique challenge from self-irradiation, which can degrade coatings' integrity by radiation damage and thus compromise the long-term efficacy of the applied coatings for corrosion protection.

This research aims to explore the feasibility of 2D graphene coating as atomic armor to protect U from ambient corrosion. Compared with traditional vapor-deposited film coatings, the defect formation in 2D material coatings is randomly distributed across layers, thus drastically reducing gas permeation paths. This unique 2D characteristics enables us to use significantly thinner coatings to achieve required anticorrosion efficacy; thus, can better preserve nuclear properties of the U material by minimizing unwanted "impurities" from the anticorrosion coatings itself.

Ion beams are used to mimic U self-irradiation environments including high energy alpha particle ionizations and heavy daughter product recoil cascades; thus, the accelerated irradiation doses of years and decades equivalent U-shelf lifetime can be effectively evaluated at the laboratory scale. Raman spectroscopy is used to evaluate irradiation stability of our 2D graphene coatings. Sieverts corrosion techniques are used to evaluate anticorrosion efficacy of the 2D graphene coatings when uncoated and coated U surfaces are exposed to hydrogen gas environments.

Surface modification of diamond coatings through Ag ion implantation for antibacterial applications

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Microorganism-induced corrosion has resulted in significant losses in many industrial sectors including biomedical engineering and marine engineering. Antibacterial diamond coatings, grown using chemical vapor deposition technique, such as ultra-nano-crystalline diamond (UNCD), nano-crystalline diamond (NCD), and microcrystalline diamond (MCD), have shown promising performance as a solution to reduce microorganism-induced corrosion. These UNCD, NCD, and MCD coated surfaces exhibit varying hydrophobic/hydrophilic properties due to different sp³/sp² carbon bond ratios, influencing their anti-adhesion behavior against bacteria. Further surface engineering of these diamond coatings is introduced through low energy Ag ion implantation. This step is crucial for further improvement in their antibacterial effectiveness. These coatings are effective against both Gram-negative (*E. coli*) and Gram-positive (*B. subtilis*) bacteria within 1-6 hours of contact. Prolonged contact, especially with MCD coatings, significantly reduces bacterial colonies and enhances bacteriostatic rates for both *E. coli* and *B. subtilis*. The experimental antibacterial observation suggests that these surface engineered diamond coatings kill bacteria through a combination of mechanical effects and surface functional groups.

Synaptic transistor based on charge trapping in ion-implanted gate dielectrics

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Neuromorphic computing aims to emulate the human brain using parallel networks of solid state synapses and neurons[1]. Novel devices, including: memristors, ferroelectric transistors, synaptic transistors and memtransistors are currently being investigated for such applications [2, 3]. Here, we report the fabrication of a synaptic field effect transistor (FET) based on charge trapping and de-trapping in the gate dielectric.

Back-gated field-effect transistors (FETs) with ultra-thin indium-oxide channel layers were fabricated by squeezing a droplet of In between 300nm SiO₂/p++ Si substrates heated to 250 °C in air. After separation and cleaning, this produced a uniform area of InOx with a thickness ~5 nm that serves as the semiconducting channel of the transistor. Electron beam lithography was subsequently used to define Cr/Au Source/Drain electrodes. The synaptic response of the transistors was achieved by ion-implanting the gate-dielectric prior to InOx deposition, with the memory effect arising from the capture and emission of charge carriers. Details of these devices and the mechanisms underlying their synaptic response will be discussed.

References

- [1] M.K. Kim, Y. Park, I.J. Kim, J.S. Lee, 'Emerging Materials for Neuromorphic Devices and Systems', *iScience* 23(12) 101846 (2020).
- [2] S. Dai, Y. Zhao, Y. Wang, J. Zhang, L. Fang, S. Jin, Y. Shao, J. Huang, 'Recent Advances in Transistor-Based Artificial Synapses', *Adv Funct Mater* 29(42) (2019).
- [3] Z. Li, W. Tang, B. Zhang, R. Yang and X. Miao, 'Emerging memristive neurons for neuromorphic computing and sensing', *Sci Technol Adv Mater.* 24, 2188878 (2023)

Development status of the Low-Energy ION implanter (LEION) at the Tandem Laboratory

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Low-energy ions with sub-keV energies are becoming more frequently employed for near-surface modification of materials, the modification of thin films and, as the field expands, the modification of 2D materials. As examples: ultralow-energy ion implantation of dopants like boron is a feasible method for the manufacture of ultra-shallow MOSFET junctions [1]; low-energy ion implantation of hydrogen in silicon solar cells affects surface passivation and enhances conversion efficiency [2]; the electronic properties of 2D materials can be tailored by utilizing ultralow-energy ions to replace individual target atoms with dopants [3]; and high-flux low-energy ion irradiations are capable of simulating the effect of the fusion plasma on structural components of future fusion devices [4]. The present work details the development of the ultralow-energy ion implantation facility at the Tandem Laboratory [5], Uppsala University. This facility is intended for surface, thin-film and 2D materials modification. The ion source can produce beams from both solid and gaseous feed-sources, and implantations can be performed at energies from tens of eV to several keV, at currents up to several μA , over areas of $3 \times 3 \text{ cm}^2$. Homogeneous implantation profiles are achieved using an electrostatic X-Y deflection system. Verification of implanted depth, fluence and homogeneity are performed through a range of ion-beam based analysis techniques. The current status of the implanter, experimental verification of its performance, and further developments planned for the near future will be presented.

References

- [1] H. Yabuhara and A. Miyamoto, "Prediction of low-energy boron doping profile for ultrashallow junction formation by hybrid molecular dynamics method", *Japanese Journal of Applied Physics* 55 (2016) 016503 doi: 10.7567/JJAP.55.016503
- [2] B. Parida et al., "Hydrogen passivation effect on the conversion efficiency of Si solar cells by low-energy proton implantation", *Solar Energy*. 122 (2015) 486-96, doi: 10.1016/j.solener.2015.08.041
- [3] U. Bangert et al., "Ion Implantation of Graphene—Toward IC Compatible Technologies", *Nano lett.* 13, no. 10 (2013) 4902-4907, doi: 10.1021/nl402812y
- [4] P. Ström et al., "Sputtering of polished EUROFER97 steel: Surface structure modification and enrichment with tungsten and tantalum", *Journal of Nuclear Materials* 508 (2018) 139-146, doi: 10.1016/j.jnucmat.2018.05.031
- [5] P. Ström and D. Primetzhofer, "Ion beam tools for nondestructive in-situ and in-operando composition analysis and modification of materials at the Tandem Laboratory in Uppsala", *Journal of Instrumentation*, 17, P04011 (2022) doi: 10.1088/1748-0221/17/04/P04011

Design of an intense nanosecond pulse neutron generator

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The intense nanosecond pulse neutron generator is an accelerator-based neutron source that is widely used in research fields such as materials, fusion energy, and element analysis, et al. However, currently there are few intense nanosecond pulse neutron generators that can meet the requirements of relevant experimental research. Since the 1980s, Lanzhou University has been engaged in the research and development of various neutron generators[1-3]. Recently, an intense nanosecond pulse neutron generator is under development[4], and this article will introduce its design.

The intense nanosecond pulse neutron generator consists of a Cockcroft-Walton accelerator[5], a beam chopper, a beam buncher, a rotating target, control system, et al. In order to design the beam-line, a simulation program called IONB1.0 was developed. The deuteron beam is extracted from a duoplasmatron ion source and then accelerated to an energy of 400 kV by an accelerating column[6]. A magnetic quadrupole triplet lens used to focus the beam size to a horizontal radius is 2 cm. Subsequently, the beam is deflected by a switch magnet to a beam chopper, which cuts the continuous beam into long bunch and its full width at half maximum is of several tens ns, then the long bunch is focused into short bunch by the beam buncher and its full width at half maximum is of several ns. Finally, each short bunch bombards the target, the deuteron deuteron fusion reaction occurs, and intense nanosecond pulse neutrons are produced.

The Cockcroft-Walton accelerator has been built. The beam chopper and the beam buncher are under construction.

References

- [1] Tongling S U, Biehe S, Baotai Y, et al. An intense 14 MeV neutron source[J]. Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 1990, 287(3): 452-454.
- [2] Yao Z E, Su T L, Cheng S W, et al. Design status of an intense 14 MeV neutron source for cancer therapy[J]. Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2002, 490(3): 566-572.
- [3] Lu X, Wang J, Zhang Y, et al. Design of a high-current low-energy beam transport line for an intense DT/DD neutron generator[J]. Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2016, 811: 76-81.
- [4] Lu X. Simulation study on beam chopper for an intense nanosecond pulsed neutron generator[J]. Journal of Radiation Research and Applied Sciences, 2023, 16(2): 100578.
- [5] Lu X, Chen S, Zhang Y, et al. Development of a 400 kV 80 mA Cockcroft-Walton power supply and 12 kW isolation transformer systems for neutron generators[J]. Journal of Instrumentation, 2017, 12(06): P06006.
- [6] Lu X L, YAO Z E, ZHNAG Y, et al. Simulation of high-intense beam transport in electrostatic accelerating column[J]. Nucl. Sci. Tech., 2015, 26: 060201.

Long indirect hot cathode ion source with multi-slit electrodes for material modification process

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We have developed a long indirectly heated cathode (IHC) ion source with multi-slit electrodes. This ion source can stably extract a sheet beam with a height of 300mm. The beam current extracted from the ion source can reach a maximum of 220mA. The beam is extracted through slits in four electrodes, each called plasma, puller, suppressor, and ground, respectively. Each slit in the electrodes is three in number, with a height of over 300mm. The current density extracted from each slit is small, so the beam divergence due to space charge effects is small. However, since the extraction area is large, we can obtain a very high extraction current. This results in excellent beam transport efficiency. The first electrode assembly consists of a plasma and a puller electrode, while the second electrode assembly consists of suppression and ground electrodes. This ion source is equipped with a manipulator that allows for the adjustment of the alignment between the first and second electrode assemblies. Depending on the ion species, extraction energy and beam current density, we adjust this manipulator so that the beam efficiently passes through the electrodes. This ion source is installed in the implantation tool we developed for material modification process [1]. The beam currents of B⁺, C⁺, Si⁺, and P⁺ exceed 40mA, 35mA, 32mA, and 32mA, respectively, at an energy of 1keV.

Reference

[1] H. Kai et al., MRS Advances 7, 1248–1252 (2022).

Superconductivity in Ga-Doped Si_{0.3}Ge_{0.7} via Ion Implantation and flash lamp annealing

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The superconductivity in Si and Ge induced by p-type doping has attracted widespread attention due to its potential for developing low-temperature circuits, particularly scalable hybrid superconductor-semiconductor platforms. However, achieving hyperdoping in Si and Ge is challenging due to limited solid solubility of acceptors. Ion implantation emerges as a promising method to achieve hyperdoped semiconductors that are needed for superconductivity [1].

In this work, we present the formation of superconducting phases of Ga-precipitates in hyperdoped SiGe with different ratios of Si/Ge composition. Using ion implantation and flash lamp annealing (FLA) in the millisecond range, we explore the coherent coupling of Ga network within the bulk instead at the SiO₂/Si or SiO₂/Ge interfaces [2, 3]. As the Si concentration in the alloy increases, but with an identical Ga concentration, the samples show a transition from a superconducting to a non-superconducting phase due to an increase in film resistivity caused by a decrease in Ga solubility in the alloy. Hyperdoped Si_{0.3}Ge_{0.7} with 13 % of Ga shows superconducting transition temperature of 3.5 K, critical magnetic field of 1 T and a critical current of approximately 250 μ A. The use of strongly non-equilibrium processing allows to control the doping level and transition temperature in group IV semiconductors.

References

- [1] Prucnal, S., Heera, V., Hübner, R., Wang, M., Mazur, G. P., Grzybowski, M. J., Qin, X. F., Yuan, Y., Voelskow, M., Skorupa, W., Rebohle, L., Helm, M., Sawicki, M., & Zhou, S. (2019). Superconductivity in single-crystalline aluminum- and gallium-hyperdoped germanium. *Physical Review Materials*, 3(5).
- [2] Sardashti, K., Nguyen, T., Sarney, W. L., Leff, A. C., Hatefipour, M., Dartailh, M., Yuan, J., Mayer, W., & Shabani, J. (2021). Tuning superconductivity in Ge:Ga using Ga⁺ implantation energy. *Physical Review Materials*, 5(6).
- [3] Skrotzki, R., Fiedler, J., Herrmannsdörfer, T., Heera, V., Voelskow, M., Mücklich, A., Schmidt, B., Skorupa, W., Gobsch, G., Helm, M., & Wosnitza, J. (2010). On-chip superconductivity via gallium overdoping of silicon. *Applied Physics Letters*, 97(19).

Ion beam-assisted modification of resistive switching properties in bi-layered oxide films

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Ion beam-based methods are extensively studied as a tool that allows good precision and control over the modification of the structure and material properties. We are investigating ion beam-based methods for tuning the properties of bi-layered oxide thin films. Specifically, multi-layer structures of Pd/Al₂O₃/TiO₂/Pd/Ti are deposited on SiO₂/Si substrates using magnetron sputtering. Al₂O₃/TiO₂ bi-layer structures exhibit resistive switching (RS) properties, i.e., they modulate their resistance based on the magnitude and polarity of the voltage applied across them and retain their resistive state when the voltage is reset to zero. Pd layers are used as electrodes for electrical characterization. The preliminary results show bipolar RS with the SET process (switching from a high resistance state to a low resistance state) for a negative potential and the RESET process (switching from a low resistance state to a high resistance state) for a lower but positive potential. RS-based devices have plausible applications in, for example, non-volatile data storage, pattern recognition and neuromorphic computing [1]. Some of the properties being investigated are SET/RESET voltage, resistance ratio, retentivity, stability, reproducibility and power consumption. In this study, we are investigating the effects of two key factors on the RS properties of these multi-layered films: (i) ion irradiation using ions with energies of a few tens of MeV to study the effect of ion track formation and (ii) controlled ion implantation at various depths to study the effect of localized change in stoichiometry or creation of defects. This two-pronged approach will help us improve our understanding of the underlying mechanism behind the RS phenomenon and explore ion beam-based methods to tune the properties of these bi-layered oxide films for improved memristor functionality.

References:

1. Khan, R., Rehman, N. U., Iqbal, S., Abdullaev, S., Aldosari, H. M. ACS Appl. Electron. Mater., 2024, 6, 73–119.

Synthesis of graphene on SiO₂ substrate using plasma-based ion implantation

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In recent years, graphene, a two-dimensional molecule consisting of carbon atoms arranged hexagonally on a plane due to carbon sp² bonds, has attracted attention because of its unique mechanical and electrical properties. Several graphene synthesis methods have been proposed so far, and among them, the plasma ion implantation method, in which carbon ions are implanted into a Ni thin film deposited on a substrate and then annealed to precipitate graphene on the surface, has the advantage to form graphene in a large area and on a curved surface. Previous research has revealed a process in which Ni aggregates through annealing and graphene is directly formed on the exposed substrate, but the synthesized graphene still has a high defect ratio and it is difficult to control the number of layers. In this research, we synthesized graphene using a plasma-based ion implantation method using nickel film on a SiO₂ substrate. The Ni thickness and implantation parameters were optimized for direct synthesis of graphene on the substrate. We also aim to control the number of layers and defects in directly synthesized graphene. As a result, there is a positive correlation between the ion implantation time and the number of graphene layers synthesized. The optimum thickness of Ni exists to form graphene. When the film thickness of Ni is too thin, graphene is not synthesized due to nickel evaporation. For the thick Ni film, when the amount of carbon ions implanted is small, graphene is not synthesized because nickel aggregation does not occur due to a few nucleation sites for nickel aggregation. When the amount of implanted carbon ions is large enough, Ni aggregation occurs to synthesize graphene.

Effect of Composition on Radiation Induced Diffusion in UK Nuclear Waste Glasses

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The glass compositions used in the UK to immobilise highly radioactive waste arising from the reprocessing of spent nuclear fuel are termed MW [1] and CaZn [2]. In this work time-of-flight elastic recoil detection analysis (TOF-ERDA) has been employed to understand the radiation induced diffusion of elements in the glass network. Hardness testing was carried out using nanoindentation to correlate the diffusion of elements with hardness of the glasses. Monoliths of CaZn and MW base glasses have been prepared with varying lithium contents to evaluate the impact lithium concentration has on the radiation induced diffusion and the change in hardness of the glasses. The pristine glasses were irradiated with 8 MeV Au³⁺ ions to simulate alpha recoil damage in the network. TOF-ERDA was carried out on the pristine and irradiated samples, the results highlighted the inward diffusion of Li, Na and B and the outward diffusion of Si and O upon irradiation. The results also revealed the diffusion of species is greater in the MW composition compared to the CaZn suggesting that CaZn has a higher radiation tolerance. This correlates with the results from nanoindentation testing which revealed a decrease in hardness upon irradiation, the largest decrease in hardness was observed for the MW composition with the lowest lithium concentration. This suggests that a higher lithium content will help stabilise the glass network against radiation induced changes.

References

1. M.T. Harrison, Vitrification of High Level Waste in the UK, *Procedia Mater. Sci.* 7 (2014) 10–15.
2. R. Short, Phase Separation and Crystallisation in UK HLW Vitrified Products, *Procedia Mater. Sci.* 7 (2014) 93–100.

Pushing the Tellurium doping limit in Si by ion implantation for infrared optoelectronics

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Tellurium is one of the deep-level impurities in Si, leading to states of 200-400 meV below the conduction band. Non-equilibrium methods allow for doping deep-level impurities in Si well above the solubility limit, referred as hyperdoping, that can result in exotic properties, such as extrinsic photo-absorption well below the Si bandgap [1]. The hyperdoping is realized by ion implantation and pulsed laser melting. We will present the resulting optical and electrical properties as well as perspective applications for infrared photodetectors.

With increasing the Te concentration, the samples undergo an insulator to metal transition [2]. The electron concentration obtained in Te-hyperdoped Si is approaching 10^{21} cm^{-3} and does not show saturation [3]. It is even higher than that of P or As doped Si, and mid-infrared localized surface plasmon resonances (LSPR) are also observed [4]. Using Te-doped Si, we demonstrate the room-temperature operation of infrared photodetectors with both vertical and planar device geometries [5,6]. The key parameters, such as the detectivity, the bandwidth and the rise/fall time, show competitiveness with commercial products. To understand the microscopic picture, we have performed Rutherford backscattering/channeling angular scans and hard x-ray spectroscopies [4, 7]. The Te-dimer complex sitting on adjacent Si lattice sites is the most preferred configuration at high doping concentration. Those substitutional Te-dimers are effective donors, leading to the insulator-to-metal transition, the non-saturating carrier concentration as well as the sub-band photoresponse. Our results are promising for the integration of active and passive photonic elements on a single Si chip, leveraging the advantages of planar CMOS technology.

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References

- [1] J. M. Warrender, Appl. Phys. Rev. 3, 031104 (2016).
- [2] M. Wang, et al., Phys. Rev. Appl. 10, 024054 (2018).
- [3] M. Wang, et al., Phys. Rev. Appl. 11, 054039 (2019).
- [4] M. Wang, , Nanoscale 14, 2826-2836 (2022).
- [5] M. Wang, et al., Adv. Opt. Mater. 9, 2001546 (2020).
- [6] M. S. Shaikh, et al., Optics Express 31, 26451-26462 (2023).
- [7] M. Hoesch, et al., Appl. Phys. Lett. 122, 252108 (2023).

In-situ TEM ion irradiation studies of layered MAX phase materials

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Materials in the core of a nuclear reactor are exposed to severe environments, particularly in future Generation IV nuclear systems, which perform in environments with high temperatures and high fluxes of fast neutrons, causing hundreds of displacements per atom (dpa) as well as substantial helium (He) doping by nuclear transmutation. MAX phases have attracted attention for their potential in nuclear materials due to their demonstration of high stabilities [1]. This study investigates the impact of sequential irradiation with light and heavy ion irradiation of MAX phases, specifically comparing the irradiation induced changes in Ti_3SiC_2 and Ti_3AlC_2 . Cross sections of both MAX phases were prepared using focused ion beam milling. These were irradiated inside the MIAMI transmission electron microscopy (TEM), in situ TEM irradiation facility [2], first with 75 keV He⁺ ions at a dose of 2.6×10^{16} ions/cm² up to 3 dpa, and then with 600 keV Ar²⁺ ions with a total fluence of 9.2×10^{16} ions/cm² up to 50 dpa, at both room temperature and 350°C. TEM imaging and diffraction are used during in-situ ion irradiation for direct observation of the microstructural and unit cell evolution. In-situ TEM observations indicate that both materials retained their crystal structures for the full irradiation dose. There was no observation of significant amorphization, phase transformations, He bubbles, or decomposition. The helium irradiation-induced damage, manifested as point defects, increases with damage level (dpa), resulting in anisotropic changes in lattice parameters in both structures up to ~9% and at both room temperature and irradiated temperatures. Interestingly, a significant recovery towards the as-synthesized unit cell parameters was observed post-irradiation within a few days of ambient storage at room temperature. Subsequent irradiation then followed similar irradiation damage profiles as the original pristine MAX phase with lattice parameter changes up to ~8% without significant amorphization, followed by another room temperature structural recovery when the irradiation is stopped. This observation of exceptional irradiation stability combined with room temperature recovery provides new evidence of the potential of MAX phases in protective coatings for nuclear applications and for radiation sensing and detection.

Keywords

In-situ radiation, MAX phases, amorphization resistance, radiation damage

References

- [1] Barsoum, M. W. (2000). The MN+ 1AXN phases: A new class of solids: Thermodynamically stable nanolaminates. *Progress in solid state chemistry*, 201--281.
- [2] Greaves, G. M. (2019). New microscope and ion accelerators for materials investigations (MIAMI-2) system at the University of Huddersfield. *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*, 931, 37-43.

Reusable Electrospun Nanofiber Mat of Carbon Nitride Decorated with nanoparticles: Photocatalytic Remediation of Organic Contaminants

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A photocatalyst responsive to visible light, consisting of polyacrylonitrile-dispersed graphitic carbon nitride adorned with either Ag₃PO₄ or MoS₂ nanofibers (referred to as Ag₃PO₄-g-C₃N₄/PAN and MoS₂-g-C₃N₄/PAN nanofibers), was synthesized through electrospinning. The uniform dispersion of g-C₃N₄ within the nanofibers addresses issues like aggregation and recycling difficulties commonly associated with powdered catalysts. Various techniques including FTIR, XRD, TGA, XPS, FESEM and the mechanical properties were employed to investigate the resulting electrospun nanofibers. The model substrate, methylene blue (MB), was swiftly adsorbed into the PAN nanofibers and efficiently decomposed in situ under visible-light exposure in the presence of Ag₃PO₄-g-C₃N₄/PAN and MoS₂-g-C₃N₄/PAN over a wide pH range. Mechanical testing revealed significant enhancements in properties of the fabricated nanofibers. Moreover, as fibrous catalysts, these nanofibers were easily recyclable, maintaining high catalytic activity without significant decline after multiple uses. Nanofibers with higher concentrations of Ag₃PO₄ and MoS₂ exhibited impressive degradation rates of over 98% and 97% respectively of original MB solution after 120 minutes of visible-light exposure. These findings underscore the potential applications of these engineered nanofibers in diverse structural uses, notably in the purification of organic-contaminated water.

Development of Plasma Flood Gun for Low Energy and High Current Ion Implanter

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A plasma flood gun (PFG) has been developed for low energy and high current ion implanter. The irradiation of a high current ion beam to the wafer easily causes a positive charging voltage, which often results in damage to the devices on the wafer. Furthermore, the space charge effect of low energy ion beam gives rise to beam divergence and makes beam transportation difficult. Therefore, a PFG that can supply a high enough electron flux to neutralize the beam is required. In the newly developed PFG, Inductively Coupled Plasma (ICP) was adopted. The PFG configuration has been optimized to introduce a low gas flow into the PFG chamber and generate a high-density plasma using 2MHz radio frequency. This PFG was installed on the side of the beamline. Electrons in the ICP are extracted by lowering the potential in the PFG chamber, efficiently supplying electrons to the ion beam.

To investigate the performance of the developed PFG, plasma diagnosis was performed with an ion beam using an electrostatic probe. The probe was installed on the wafer scan position to confirm whether the beam space charge potential is sufficiently neutralized during ion implantation. As a result of probe measurements, it was found that the beam plasma potential decreased as the amount of electron extraction increased. In addition, TEG (Test Element Group) evaluation was performed with P⁺ ion beam irradiation for 30mA at 1 keV. Even at an antenna ratio of 1M, there was no electrostatic destruction of elements. This result confirms that this PFG can sufficiently neutralize the low energy and high current ion beam and suppress the positive charging voltage.

Stopping force of C,Si and Co ions in Pt foils by time of flight spectrometry

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The stopping force of energetic ions in matter is of importance in many aspects of materials research and development using ion beams. Common applications include ion implantation, ion beam modification of materials and ion beam analysis. In many instances stopping force data is obtained from semi-empirical and theoretical formulations. While the accuracy of these data sources is now generally acceptable for light ions (H, He), more work still needs to be done to improve their predictive accuracy for heavier ions ($Z > 6$). Heavy ion-matter interaction parameters that are not so well described by theory include charge exchange effects among others. In this presentation we describe a simple experimental method that may be used to account for charge-exchange effects in the energy loss rate of carbon ions through 78Pt foil. The measurement was carried out in a Time of Flight – Elastic Recoil Detection Analysis (ToF-ERDA). A 40 MeV $^{197}\text{Au}^{9+}$ beam were used to recoil ^{12}C , ^{28}Si and ^{59}Co ions from a thick carbon, silicon oxide and cobalt substrate towards the stopper foil. The energy loss of the incident recoils through the stopper foil was calculated from the measured ToF across a fixed path length, with and without the stopper foil, and the stopping force then calculated using the measured foil thickness [1]. The thickness of the used target was measured using Rutherford Backscattering Spectrometry (RBS). Given the simultaneity of the measurements for silicon, cobalt and carbon recoils, the observed relative deviations between experiment and theory in the stopping force of these ions can be attributed to charge exchange effects.

References

[1] M. Msimanga, C. M. Comrie, C. A. Pineda-Vargas, S. Murray, R. Bark, G. Dollinger, A Time of Flight-Energy spectrometer for stopping power measurements in Heavy Ion-ERD analysis at iThemba LABS, Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms 267 (16) (2009) 2671–2674.

Sputter deposition and characterisation of multilayers incorporated with Mn/Mg co-doped BiFeO₃ film

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BiFeO₃ (BF) is simultaneously ferroelectric and antiferromagnetic above room temperature and has therefore been studied extensively during past twenty years. Recently, it has also been studied as a potential material for photodegradation and photovoltaic applications [1,2]. In this work, BF was co-doped with Mn and Mg, i.e. BiFe_{0.9}(Mn_{0.5}Mg_{0.5})_{0.1}O₃ (BFMM), in order to reduce band gap, leading to a more efficient absorption of sunlight for these emerging applications. Various multilayers incorporated with BFMM as the functional layer were grown on glass substrates by RF magnetron sputter deposition, including Pt/BFMM/LaNiO₃ (LN), Pt/BFMM/WO₃/LN, and Pt/BFMM/TiO₂/LN. The conductive LN on the substrate served as bottom electrode, while Pt on BFMM was used as top electrode. The phase purity, texture and microstructure of the prepared multilayers were examined by X-ray diffraction and scanning electron microscopy. BFMM was revealed to have the n-type conductivity by the Mott-Schottky measurement. All the multilayers showed a rectifying J-V curve and exhibited photovoltaic effects under sunlight illumination. The highest photovoltaic effect was observed with the poled multilayers of Pt/BFMM/WO₃/LN, which had the short-circuit current density (J_{sc}) and open circuit voltage (V_{oc}) of -6.68 μA/cm² and 1.12 V, respectively. The J_{sc} and V_{oc} could be switched to 8.72 μA/cm² and -1.01 V by poling the sample in opposite field direction. The electronic band positions of BFMM, WO₃ and TiO₂ were determined by ultraviolet photoelectron spectroscopy, which indicated that the band alignment allowed the electron transport from BFMM to WO₃, leading to an efficient charge separation of photoexcited electrons and holes.

References

- [1] A. Haruna, I. Abdulkadir, S.O. Idris, Heliyon 6, e03237 (2020).
- [2] D.S. Knoche, M. Steimecke, Y. Yun, et al., Nat. Commun. 12, 282 (2021).

Microstructure and nanomechanical properties of medium-/high-entropy materials modified by ion irradiation

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The high-/medium- entropy materials (H/MEMs) are newly intriguing materials with outstanding properties [1-3]. Combined with specific compositions and structures, H/MEMs can show both remarkable mechanical properties and radiation resistance, as alloying can mitigate ion irradiation-induced heterogeneous damage [4]. Among them, CoCrNi-based materials seem to be the pioneers in these properties. Of particular interest is their incredible radiation resistance, which unfortunately remains open to debate. In this work, microstructure and nanomechanical properties of CoCrNi-based single crystal alloys, and nanocrystalline ceramics, modified by ion irradiation, were studied using HRTEM and nanoindentation. The materials were ion-radiated over a wide fluence range. The results show that, the H/MEMs show different hardening/softening mechanisms after modification by ion irradiation. The radiation damaged structures were studied using HRTEM. The current work reveals the potential of H/MEMs for applications in extreme environments.

References

- [1] W. Huo, F. Fang*, H. Zhou, Z. Xie, J.K. Shang, J. Jiang. Remarkable strength of CoCrFeNi highentropy alloy wires at cryogenic and elevated temperatures. *Scripta Materialia*, 141, 125-128 (2017).
- [2] Y. Li, Ł. Kurpaska, E. Lu, Z. Xie, H.S. Kim, W. Huo*. Body-centered cubic phase stability in cobalt-free refractory high-entropy alloys. *Results in Physics*, 60, 107688 (2024).
- [3] A. Naghdi, F.J. Domínguez-Gutiérrez, W. Huo, K. Karimi, and S. Papanikolaou*, Dynamic nanoindentation and short-range order in equiatomic NiCoCr medium-entropy alloy lead to novel density wave ordering. *Physical Review Letters* 132, 116101 (2024).
- [4] E. Wyszowska*, C. Mieszczynski, Ł. Kurpaska, A. Azarov, I. Jóźwik, A. Kosińska, W. Chromiński, R. Diduszko, W. Huo*, I. Cieřlik and J. Jagielski, Tuning heterogeneous ion-radiation damage by composition in NixFe1-x binary single crystals. *Nanoscale* 10, 4870-4881 (2023).

Time-of-Flight Elastic Recoil Detection Analysis for Simulated Radiation Induced Diffusion Effects on Nuclear Waste Glasses

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Borosilicate glasses, such as Calcium Zinc (CaZn) [1] and Mixed Windscale (MW) [2] are of interest for nuclear waste glass due to low processing temperatures and durability, with the capability to incorporate a wide range of radionuclides. With a high capacity of waste loading into the glass structure, the glasses can retain radionuclides for thousands of years. The radiation produced by the nuclear waste does affect the glass structure causing defects, which may impact its suitability.

To mimic the effect of the nuclear waste, the various glass samples were irradiated with 8 MeV Au³⁺ for a total fluence of $1 \times 10^{16} \text{ cm}^{-2}$. The Au simulates the effect of damage on the glasses caused by the alpha decay process where an actinide, for example ²³⁹Pu, converts to ²³⁵U by releasing an alpha particle and acting as an energetic recoil causes displacements within the glass. Various CaZn and MW glasses with a differing amount of Li present were studied, with a pristine and irradiated region to determine which were most stable to damage caused by the Au irradiation.

To analyse the displacements and measure the compositions with respect to depth, time-of-flight elastic recoil detection analysis (ToF-ERDA) was used [3]. For the ToF-ERDA measurements an 16 MeV ¹²⁷I⁸⁺ ion source was used to enable analysis of the many elements present within the glasses including H, Li, B, O, Na, Si, Ca and Zn due to the enhanced mass separation from measuring the recoiled atoms velocity as well as the energy. The measurement was also able to separately analyse the Li isotopes 6 and 7, B isotopes 10 and 11 along with O isotopes 16 and 18. From ToF-ERDA compositional depth profiles were compared for the pristine and Au irradiated regions in the glasses. With the lighter elements present within the glasses, especially Li and B showing the larger degree of radiation induced diffusion, with MW glasses showing greater displacement compared to the CaZn glasses.

References

- [1] M.T. Harrison, Vitrification of High Level Waste in the UK, *Procedia Mater. Sci.*, 7 (2014) 10–15.
- [2] R. Short, Phase Separation and Crystallisation in UK HLW Vitrified Products, *Procedia Mater. Sci.* 7 (2014) 93–100.
- [3] Y. Shi, et al., Characterization of solar cell passivating contacts using time-of-flight elastic recoil detection analysis, *Appl. Phys. Lett.*, 123 (2023) 261106

Medium Energy Ions & In-Situ Synthesis: A Compelling Tool for Materials Research

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Ion beams form the basis for unique tools for thin film characterization in terms of composition and structure on nm to μm length scales. In parallel, the ongoing miniaturization of nanoelectronic devices makes it necessary to study the continuously shrinking structures, challenging the analytical methods employed, and, in the case of ion beams, requiring a reduction of the ion energies. With surfaces coming more into the focus for keV-beams, details in sample preparation protocols and materials processing procedures of the highest standards in terms of cleanliness become of increased importance. Thus, in-situ preparation of materials is a logical next step for detailed studies of material properties and their controlled modification.

The Medium-Energy Ion scattering (MEIS) system at the Tandem laboratory research infrastructure at Uppsala University incorporates a wide spectrum of ion-beam-based methods including backscattering, crystal cartography, forward recoils analysis, surface desorption/sputtering analysis and electron and photon spectroscopy. The newly developed equipment for sample preparation complements the MEIS system with tools for in-situ materials synthesis and modification.

In this contribution, we showcase the expanded capabilities of the combined instrumentation with examples from a number of relevant research topics:

- I) Phase transitions in ultrathin metal-silicide layers
- II) Synthesis pathways and photo-resistive behaviour of yttrium oxyhydrides
- III) Hydrogen and deuterium retention in sputter-cleaned tungsten surfaces
- IV) Mapping of projectile trajectories during ion implantations into crystalline materials
- V) Hydrogen site location and lattice expansion in crystalline materials
- VI) Surface conditioning of self-supporting membranes used for fundamental research on ion-solid interaction

Radiation induced hardening of Fe-Mn-Ni-Cu model alloys under irradiation

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The neutron irradiation of Fe based model alloys and steels leads to an increase in the ductile-to-brittle transition temperature (DBTT) with a decrease in the upper shelf energy. It is well known that the Cu content has a strong influence on the embrittlement phenomena; especially, the Cu-rich precipitates have been thought to be directly responsible for the embrittlement. In contrast, mechanical property studies for the steels with different Cu levels have shown that so-called matrix defects are dominant in the embrittlement of low-Cu steels as well as in that of high-Cu steels at high fluences. To study the effect of dislocation loop formation at high fluencies and high flux on radiation hardening in those steels, ion irradiation have been conducted for Fe-based model alloys with different Ni and Mn levels. The neutron irradiation was also performed in BR2 (BAMI and CALLIST) . Hardness tests were conducted before and after the irradiation at room temperature. After the irradiations, microstructure was observed by Cs-corrected microscope (ARM200FC).

The hardness increases with irradiation dose. STEM-EDS observation revealed that this is due to the formation of very high density of interstitial type dislocation loops at lower temperature. On the other hand, at 563K, small loops and solute clusters of about 2nm were formed in matrix and also in the vicinity of dislocation. The recovery behaviour of the hardness by post-irradiation annealing at 723K was related with disappearance of these loops.

In-situ elastic recoil detection analysis for graphene oxide and nanoporous alumina analysis

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Ion beam analysis techniques (such as the most commonly used RBS and PIXE) are generally considered non-destructive. However, ERDA (elastic recoil detection analysis) as a technique for elemental depth profiling of thin films, can induce changes to studied samples due to usage of high-energy heavy ion beams. These ion beams can modify sensitive materials easily and are capable of producing ion tracks in some of the studied materials. However, this “disadvantage” can be taken advantage of, in a manner that the same high-energy heavy ion beam which modifies the material, can simultaneously be used for the analysis (in-situ ERDA). Previously, we have used this approach to monitor loss of nitrogen from GaN and loss of oxygen from TiO₂ [1,2]. In this contribution, we present ERDA results on stoichiometry changes when graphene oxide is exposed to iodine ion beams in the range of 12-23 MeV, and also analyse ion irradiation effects in nanoporous alumina by ERDA and GISAXS (grazing incidence X-ray scattering).

References

- [1] M. Karlušić, R. Kozubek, H. Lebius, B. Ban-d’Etat, R.A. Wilhelm, M. Buljan, Z. Siketić, F. Scholz, T. Meisch, M. Jakšić, S. Bernstorff, M. Schleberger, B. Šantić, Response of GaN to energetic ion irradiation: conditions for ion track formation, *J. Phys. D: Appl. Phys.* 48 (2015) 325304.
- [2] M. Karlušić, S. Bernstorff, Z. Siketić, B. Šantić, I. Bogdanović-Radović, M. Jakšić, M. Schleberger, M. Buljan, Formation of swift heavy ion tracks on rutile TiO₂ (001) surface, *J. Appl. Cryst.* 49 (2016) 1704.

Novel deposition method for nanoparticles on silicon substrates utilizing Poly (ethylene glycol) for MEIS analysis

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The use of nanoparticles has increased significantly in many areas, such as biomedical research, being highly useful as nanoprobe for imaging and as nanocarriers for drug delivery applications. Nevertheless, this potential can only be achieved with the correct characterization of the nanoparticles, since their size and shape can directly affect their biological behavior. In this study, we propose a novel approach for a monolayer deposition of gold and platinum nanoparticles on Si substrates suitable for Medium Energy Ion Scattering (MEIS) analysis. The samples were prepared using PEG 6000 as a coating agent for the substrates, utilizing a spin coater, a versatile, cost-effective and practical technique. The samples were first analyzed with the RBS technique to assess the adhesion and overlapping of the nanoparticles on substrates coated with PEG 6000 and then characterized through the MEIS technique. The analysis through MEIS allowed the determination of the shape, size, and coverage area of the nanoparticles. Scanning and transmission electron microscopy were also performed on the samples, with the results corroborating the findings of the MEIS experiment. Together, the data obtained with microscopy and the MEIS technique suggest the effectiveness of the method in the production of monolayer samples.

Improved electrochemical properties of Mn₃O₄ nanorod networks low-energy nitrogen ion irradiation.

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Manganese oxide has been researched as a potential electrode material in hybrid with other materials for supercapacitor applications because of its high capacitance, improved electrical conductivity, low cost, and environmental friendliness [1]. Supercapacitors based on Mn₃O₄ nanorods offer enormous potential for high energy density per unit volume and hold significant promise for the advancement of energy storage technologies [2]. To improve charge storage capacity, the current work shows how to join manganese oxide nanorods which in turn forming network like structure on a large scale by using an ion beam to create defects in the surface. Ion irradiation is a suitable technique for modifying the various nanostructured materials to form clusters [3], nano networks [4] etc.

Mn₃O₄ nanorods produced hydrothermally then spin-coated on a silicon wafer, were exposed to a low energy 5 keV N⁺ ion beam by varying the ion fluences. The morphology, crystallinity and vibrational characteristics have been characterized using FESEM, XRD and Raman measurements before and after irradiation. Furthermore, electrochemical measurement was carried out to check capacity for storing the charge. At a mass normalised current of 10 A/g, pristine and irradiated Mn₃O₄ nanorods demonstrated respective areal capacitances of 45 mF/cm² and 132 mF/cm² (3 times higher) [5]. Irradiated nanorods shows better charge transport than pristine. Moreover, after 5000 measurement cycles, the irradiation sample maintains 90% of its initial capacitance. Additionally, simulations from SRIM, IRADINA, and TRI3DYN [6] support this study work. The irradiation sample's enhanced charge storage capacity, increased surface area, and induced oxygen vacancy all contribute to the increase in the areal capacitance value. This work adds to the growing body of evidence showing that ion beam irradiation can modify the surface area, conductivity, and charge storage capacity of the supercapacitor electrode.

References:

- [1] Raj, B.G.S., Asiri, A.M., Wu, J.J. and Anandan, S., 2015. Synthesis of Mn₃O₄ nanoparticles via chemical precipitation approach for supercapacitor application. *Journal of Alloys and Compounds*, 636, pp.234-240.
- [2] Bose, V.C. and Biju, V., 2015. Mixed valence nanostructured Mn₃O₄ for supercapacitor applications. *Bulletin of Materials Science*, 38, pp.865-873.
- [3] Patro, A., Nayak, S.R., Rajbhar, M., Chatterjee, S. and Dhal, S., 2023. Cluster formation by the precise joining of iron oxide nanoparticles on low energy nitrogen ion irradiation. *Radiation Effects and Defects in Solids*, 178(7-8), pp.976-989.
- [4] Dhal, S., Das, P., Rajbhar, M.K., Möller, W., Chatterjee, S., Ramgir, N. and Chatterjee, S., 2018. Superior electrical conduction of a water repelling 3D interconnected nano-network. *Journal of Materials Chemistry C*, 6(8), pp.1951-1958.
- [5] Patro, A., Rajbhar, M.K., Chatterjee, S., Patra, A., Rout, C.S. and Dhal, S., 2023. Augmented electrochemical properties of manganese oxide nanorods on low energy nitrogen ion irradiation. *Journal of Alloys and Compounds*, 960, p.170441.
- [6] Stadlmayr, R., Szabo, P.S., Mayer, D., Cupak, C., Dittmar, T., Bischoff, L., Möller, S., Rasiński, M., Wilhelm, R.A., Möller, W. and Aumayr, F., 2020. Sputtering of nanostructured tungsten and comparison to modelling with TRI3DYN. *Journal of Nuclear Materials*, 532, p.152019.

Helium ion irradiation effects on microstructure and magnetism of BCC iron-based alloys

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Iron-chromium alloys with a body-centered cubic (BCC) structure, such as low-activation ferritic steel for fusion reactor blankets, are structural materials used in harsh irradiation environments. An assessment of the electromagnetic forces acting on the blanket during plasma disruptions is needed. In numerical analysis, the magnetic properties of unirradiated materials are used because irradiated data is lacking. There is limited research on the magnetic properties of heavily irradiated iron alloys. Some reports suggest a significant increase in the saturation magnetization of iron after ion irradiation of 10 dpa or more [1], but the mechanism remain unclear. On the other hand, there are no reports on the relationship between helium cavities formed during neutron irradiation due to nuclear transmutation and magnetic properties. In this study, we report on the magnetic properties of BCC iron-based alloys heavily irradiated with helium ions.

Iron-based alloy films containing Cr and/or Ni were deposited via ultra-high vacuum on MgO substrates, reaching thicknesses of about 200 nm. Helium ions at 30 keV were irradiated from room temperature to 500°C using a light ion accelerator, resulting in a damage level of approximately 20 dpa. The structures before and after irradiation were examined using EBSD, XRD, TEM, and APT, and the magnetization curves were measured using a VSM. As for pure iron containing helium atoms, first-principles calculations were conducted.

Epitaxial growth of the BCC(001) films with a 45-degree rotation on MgO(001) was confirmed in all samples before irradiation. XRD measurements and TEM observations revealed lattice expansion in the film's normal direction and the formation of high-density cavities after irradiation. No changes were observed in the magnetization curves of Fe and Fe-Ni films. The saturation magnetization behavior of pure iron was consistent with the results of first-principles calculations. In contrast, significant changes were observed in the magnetization curves after irradiation in Fe-Cr and Fe-Cr-Ni films, confirming an increase in the magnetic field required for saturation magnetization. It is believed that the rearrangement of chromium atomic positions due to irradiation caused changes in the magnetic properties.

References

[1] K. Papamihail et al., Phys. Rev. B93, (2016) 100404(R).

Cross-sectional observation of magnetic domain structures of Fe³⁺ irradiated iron-chromium alloys

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Iron-chromium alloys have shown potential as materials for fusion reactor blankets; however, they face a significant issue of degradation of material properties due to neutron irradiation. Changes in magnetism can also lead to adverse consequences. Ion irradiation is essential for studying the high-dose irradiation effects in a fusion reactor environment. We have been studying ion-irradiated thin films, which are advantageous for evaluating magnetic properties [1]. In order to understand the effects on practical materials, it is important to investigate bulk materials. However, evaluating their magnetic properties is challenging due to the presence of both damaged and undamaged regions, caused by the short penetration depth of ions. One possible approach to address this issue is to conduct cross-sectional observations of magnetic domain structures. In this study, we investigated the magnetic properties of ion-irradiated iron-chromium alloys using this method.

Fe-x%Cr (x=0, 16, 36) model alloys were irradiated with 10.5MeV Fe³⁺ using a tandem accelerator. The irradiation temperatures were 300°C and 500°C, the damage level was 12 dpa at a depth of 1 μm. After irradiation, thin plates were cut using EBSD and FIB devices along the <100> bcc direction, which is the easy magnetization direction. Static and dynamic magnetic domain observations were conducted using a Lorentz TEM capable of applying a magnetic field, and the distribution of elements was examined using STEM-EDS.

In the case of the Fe-36%Cr specimen irradiated at 300°C, white and black lines were observed in the under-focused image of the cross-section, representing magnetic domain walls. In regions deeper than 2.5 μm (undamaged region), typical large closure domains were observed, while in near-surface regions (damaged region), ripple domains were observed, and in intermediate regions, fine closure domains were observed. Elemental mappings showed a uniform distribution of chromium in the undamaged region, whereas variations were observed in the damaged region. These results indicate that ion irradiation accelerated the phase separation of Fe-Cr alloy and altered the magnetic domain structure.

Acknowledgments:

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References:

[1] Y. Kamada et al., Metals., 13 (2023) 1905

Multi-channeling characterization of radiation-induced effects and defects by Yb in the β -Ga₂O₃

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Rare earth (RE) doped gallium oxide, especially in its stable beta form (β -Ga₂O₃), has great potential for future use in optoelectronic devices. This is because, with the addition of RE ions into wide bandgap oxide materials, the base-light emission of the matrix can be optically tuned to the visible spectral range. Hence, the β -Ga₂O₃:RE systems seem attractive in applications such as phosphors, displays, and LEDs, that can operate even in harsh environments. A crucial task in this field today is the development of controlled methods for doping this material.

One of the attractive ways to produce β -Ga₂O₃:RE systems is the ion implantation technique. However, due to the ballistic nature of the process, crystal lattice defects are formed. Created damage quenches the luminescence and makes a shorter lifetime of devices based on defected material. Thus, the annealing leading to the crystal recovery is required. The type of thermal treatment highly influences the structural and optical properties of the material.

In the current research, we paid particular attention to the issue of Yb-ion radiation-induced defects in the differently oriented β -Ga₂O₃:RE crystals, the structure recovery after different thermal treatments, and the optical response of Yb ions to these structural changes as well. To understand the nature of the defects and other observed effects, complementary analytical techniques such as HRXRD, HRTEM, and RBS/c were used, supported by Monte Carlo-based computer simulations by McChasy¹. Our studies reveal the strong structural anisotropy in damage, with a significantly lower damage level for (010) oriented β -Ga₂O₃ crystals compared to (-201) and (001), and also in radiation-induced strain^{2,3}. These differences mainly concern the number of extended defects, which affects the level of crystal recovery achieved after thermal annealing and is reflected in the Yb optical response. Moreover, a complicated evolution of the defect structures is observed for all the cases studied, suggesting the co-existence of at least two crystal channel blocker types of defects created in the implanted zone, with their different sensitivity to both, radiation and annealing. One of them is associated with Ga₂O₃ phase transition^{1,4,5}. The Yb ions, after implantation, occupy interstitial positions in the matrix for all orientations and are optically inactive. The lattice site positions of Yb in β -Ga₂O₃ remain unchanged after annealing. During certain thermal treatments, the Yb charge state transitions to 3+, resulting in its emission observed in the PL spectra. So far, the highest optical efficiency of Yb has been achieved after annealing in oxygen.

Structural and mechanical responses of (ZrTiNbTa)₄C and ZrC ceramics under energetic He-ions

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High entropy carbide ceramics (HECCs) are potential structural materials for advanced reactor concepts where numerous helium atoms would be produced due to the (n, α) nuclear transmutation reaction. However, the irradiation behaviors of high entropy ceramics are not well understood until now. In present work, the responses of high entropy (ZrTiNbTa)₄C and its binary constituent ZrC ceramics to energetic He-ions irradiation have been studied. X-ray diffraction analysis showed that He-ions irradiation resulted in peak shift and broadening of diffraction peaks in both (ZrTiNbTa)₄C and ZrC, which denotes lattice expansion and structural damages induced by the irradiation. Transmission electron microscope observation revealed that nano-sized spherical helium bubbles distribute uniformly in the grain interiors of (ZrTiNbTa)₄C while string-like bubbles with a preferred orientation are observed in ZrC grains. The accumulation and coarsening of He bubbles at grain boundaries are confirmed for both (ZrTiNbTa)₄C and ZrC, but no grain boundaries tearing was observed. Nanoindentation characterization gives that the irradiation induced hardening of (ZrTiNbTa)₄C is less definite than that of ZrC, which is attributed to irradiation induced bubbles and defect clusters act as obstacles during the deformation upon nanoindentation. Based on the experimental results, it can be concluded that the high entropy (ZrTiNbTa)₄C exhibits a less microstructural damage and reduced hardening than ZrC under identical irradiation conditions, suggesting the HECCs may possess a better irradiation resistance than the binary carbides.

Radiation-Induced Degradation Effects on Si and SiC Devices

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Semiconductor devices are now an integral component of modern life, having a variety of low- to high-tech applications. Sometimes, these devices are subject to exposure to radiation while working in radiation abundant environments such as space or during the devices' processing (ion implantation, lithographic processes), which can result in defects' introduction in a device. Consequently, it is of utmost importance to comprehend the effects of radiation on these devices and to develop radiation-hard solutions to circumvent any associated degradation. Usually, the radiation effects are detached in ionization and displacement damage on the basis of the type of radiation-solid interaction.

In this contribution, we focus on the displacement damage effects on Si and SiC devices (650 V and 1200 V) by depositing the incoming ions (radiation in the lab environment) with 2 and 6 MeV. The devices of both technologies used for the study are of commercial grade with similar ratings. The effects are then compared through electrical measurements. The results show that the SiC diodes are ~4.5 times more tolerant than Si diodes in the forward mode, despite the SiC has higher carrier removal rate than Si. This tolerance can be attributed to two factors: (i) the base region doping concentration in Si diodes is approximately ~2 orders of magnitude higher than that of SiC diodes, and (ii) the bipolar nature of Si PiN diodes makes them prone to severe recombination lifetime degradation, which leads to a reduction in on-state resistance. Similarly, SiC diodes demonstrate superior radiation hardness in the reverse mode due to their wider bandgap. Furthermore, the leakage current in SiC diodes is even lower than that measured before irradiation measured after a few hours of irradiation, possibly due to a proton irradiation-induced "self-healing" effect.

To generalize the study to practical space energies, typically in hundreds of MeVs, a methodology is developed for the experimental results of low energy to higher energies, using the hypothesis of displacement damage. This eliminates the need of additional experiments at high energies. The Non-Ionizing Energy Loss (NIEL) concept is also used to develop a TCAD-based framework which can simulate the displacement damage effects in planar semiconductor devices without relying on any previous irradiation experiments. The simulation results are in good agreement with the experimental data for both the Si and SiC diodes.

An attempt to predict oligomer sputtering using binary collision approximation simulations

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The binary collision approximation (BCA) program IMINTDYN [1] allows a prediction of ion solid interactions. For sputtering of carbon and SiO₂ experimental sputter yields are significantly higher than yields from BCA simulations. SDTrimSP simulations [2] reproduce experimental sputter yields by adjusting the surface binding energies. For O atoms 1 eV instead of the elemental sublimation energy of 2.58 eV and for carbon 4.5 eV instead of 7.4 eV is used. For sputtering of carbon it was shown [3] that sputtering of oligomers and clusters is relevant. We introduce a model to simulate oligomer sputtering using the IMINTDYN program based solely on thermodynamic formation enthalpies. In particular sputtering of O₂ and SiO dimers and carbon oligomers is energetically favorable. To predict the oligomer sputter fraction, we use Boltzmann factors based on the ratios of oligomer and monomer formation enthalpies. We show that we can quantitatively predict the carbon and SiO₂ experimental sputter yields.

References

- [1] H. Hofsäss, A. Stegmaier, Nucl. Instr. Meth B 517 (2022) 49
- [2] A. Mutzke, R. Schneider, W. Eckstein, R. Dohmen, K. Schmid, U. von Toussaint, G. Bandelow, SDTrimSP Version 6.00, MPI Plasma Physics, report IPP 2019-02 (2019)
- [3] E. Oyarzabal, R.P. Doerner, M. Shimada, G.R. Tynan, J. Appl. Phys. 104 (2008) 043304

Lithium depth profiling with proton beam NRA

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Lithium is one of the most important elements for energy storage. There are several methods available for detection - one of which is nuclear reaction analysis (NRA). The nuclear reaction ${}^7\text{Li}(p,\alpha){}^4\text{He}$ with a Q value of 17 MeV is suitable for lithium detection [1]. Two alpha particles with 7.5 MeV each are generated, which are detected using PIN diodes. We use our Pelletron accelerator to generate a proton beam with an energy of 2.5 MeV. The aim of the investigations is to make a statement about the depth profile of the lithium which is not dominated by the statistical energy distribution of the alpha particles. For this purpose, ta-C coated silicon wafers are implanted with 30 keV lithium, measured, covered with an additional carbon layer using sputter deposition and measured again. This leads to a shift in the alpha spectrum to lower energies due to the additional energy loss in the deposited carbon. Furthermore, the experiments are simulated using the binary collision approximation (BCA) Monte Carlo program IMINTDYN [2,3]. Additionally to the aspects of ion-solid interactions, IMINTDYN offers the option of generating the NRA for a specific isotope and projectile after simulating an implantation, taking into account energy loss and deflection of the projectiles and the generated alpha particles.

References

- [1] F. Junge, P. Kirscht, H. Hofsäss, Quantitative light element analysis: Complementary IBA methods for H to O detection using an external proton beam, Nuclear Instruments and Methods in Physics Research Section B (517) (2022), 16-23
- [2] H. Hofsäss, A. Stegmaier, Binary collision approximation simulations of ion solid interaction without the concept of surface binding energies, Nuclear Instruments and Methods in Physics Research Section B (517) (2022), 49-62
- [3] H. Hofsäss, F. Junge, P. Kirscht, K. Van Stiphout, Low energy ion-solid interactions: a quantitative experimental verification of binary collision approximation simulations, Materials Research Express (2023), DOI 10.1088/2053-1591/ace41c

Fast simulation of ion beam analysis spectra using binary collision approximation

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The dynamic binary collision approximation program IMINTDYN [1,2] allows a reliable prediction of ion solid interaction. We have extended the IMINTDYN program to efficiently simulate high energy ion scattering as well as ion induced nuclear reaction spectra. This includes RBS, LEIS, ERDA, coincidence ERDA, ERCS, NRA and SIMS. The optimization includes (i) adjustable mean free path of high energetic ions (ii) enforced large angle scattering with scattering cross sections stored in weight factors, and (iii) enhanced data handling to identify coincident scattering events. The program runs on a AMD Ryzen Threadripper PRO 5965WX workstation. Typical simulations with millions of projectiles are finished within 2-20 minutes, faster than the duration of the experiment. The simulations provide details of the spectra, like single, dual and multiple scattering events, energy versus depth information, isotope information etc. We present selected examples for He ion RBS [1], Low energy He ion scattering (LEIS) as well as non-Rutherford backscattering of MeV H ions.

References

- [1] H. Hofsäss, F. Junge, P. Kirscht and K. van Stiphout, Material Research Express (2023) DOI 10.1088/2053-1591/ace41c
- [2] H. Hofsäss, A. Stegmaier, Nucl. Instr. Meth B 517 (2022) 49

Low energy ion-solid interactions: a quantitative experimental verification of binary collision approximation simulations

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Ultra-low energy ion implantation has become an attractive method for doping of 2D materials. The dynamic binary collision approximation Monte Carlo program IMINTDYN [1,2] allows a reliable prediction of low energy implantation profiles and target compositional changes, as well as efficient simulation of high energy light ion scattering. To demonstrate the quality of these simulations, we present implantation of W ions into tetrahedral amorphous carbon with low (10 keV) and ultra-low (20 eV) energies and high resolution Rutherford backscattering spectrometry (HR-RBS) to analyze the W implantation profiles with [1]. The experiment is compared with a complete simulation of all aspects of ion-solid-interactions of the experiment using the IMINTDYN. A unique novel simulation option is the inclusion of the vacancy as target species with dynamic vacancy generation and annihilation. We find excellent agreement between simulated and measured HR-RBS spectra if vacancy formation is included.

References

- [1] H. Hofsäss, F. Junge, P. Kirscht and K. van Stiphout, Material Research Express (2023) DOI 10.1088/2053-1591/ace41c
- [2] H. Hofsäss and A. Stegmaier, Nucl. Instr. Meth B 517 (2022) 49-62

Insights on molecular P implantation in Si for scalable spin qubit arrays.

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Future quantum computing technologies require an implantation precision which is higher than any focused ion beam technology existing currently. Towards improving the placement precision of P donors in a Si diamond lattice, the use of a PF₂ molecular ion instead of a single atom P ion has significantly improved the detection confidence of the implant while preserving a low straggling in its placement [1].

Although the overall results seem promising, the deviations from the intended placement of a P donor in Si are expected due to the highly stochastic nature of ion implantation. Computer simulations using the molecular dynamics method can provide more additional details on the process. In my presentation, I will discuss the physics of the energy deposited by the ions moving in the material via electronic stopping power which translates into an electric signal used in experiment for detection of the ion's placement position. Said signal is different in channeling and off-channeling directions.

In this work, we are investigating the synergies in energy deposition due to simultaneous impact of three ions during a molecular ion implantation. To mitigate this, we will explore the effect of a 5 nm amorphous SiO₂ layer which grows naturally on the pure Si wafer's surface. I will also describe in detail the damage caused by the highly energetic particles in the lattice and I will delve into the long-term damage evolution processes and how the annealing conditions can be improved in such a way that the post-implantation diffusion of the P atom is minimum while guaranteeing a total recovery of the substrate.

References

[1] Holmes, D., Wilhelm, B., Jakob, A. M., Yu, X., Hudson, F. E., Itoh, K. M., Dzurak, A. S., Jamieson, D. N., & Morello, A. (2024). Improved Placement Precision of Donor Spin Qubits in Silicon using Molecule Ion Implantation. *Advanced Quantum Technologies*.
<https://doi.org/10.1002/qute.202300316>

The French Research Federation of Accelerators for Irradiation and Analysis of Molecules and Materials

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This contribution aims at presenting the French EMIR&A research infrastructure (Federation of Accelerators for Irradiation and Analysis of Molecules and Materials). EMIR&A is built around several structuring and innovative facilities, that are shared to provide access to ion and electron beams to the largest scientific community at the national and international scale. EMIR&A includes a total of 15 ion and electron accelerators installed on 11 platforms distributed over 6 sites in the northern half of France (Caen, Orléans) and near Paris (Paris, Palaiseau, Orsay, Saclay). Those facilities are owned by Higher Education institutions, CNRS (National Scientific Research Centre), Universities, Grandes Ecoles and CEA (French Alternative Energies and Atomic Energy Commission), making this structure a worldwide unique portal for such research.

The facilities are complementary in terms of the nature and energy of the particles accelerated and the associated in situ characterization instruments for irradiation and analysis of materials (such as Transmission Electron Microscopy, Raman spectroscopy, X-Ray Diffraction, infrared spectroscopy, optical absorption, ion beam analysis...) or studies of radiolysis processes. Once a year, this set of accelerators and instrumentations is made available to users after evaluation by an international scientific committee. There is also the possibility of proposing pump priming experiments all year long.

It is a recent step towards an overall national structure for ion and electron beam science and applications like those set up in neighboring countries (e.g. the UK National Ion Beam Centre, Surrey, or the Helmholtz-Zentrum at Dresden-Rossendorf in Germany). It contributes to connecting the scientific communities studying condensed matter with ion or electron accelerators, to establish new collaborations through the pooling of these instruments and the associated expertise.

More information can be found at <https://emira.in2p3.fr/>

Glass Corrosion Study Using Time of Flight Elastic Recoil Detection Analysis

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The generation of radioactive waste material is a significant environmental concern from nuclear power, with spent fuels remaining active for over thousands of years even after disposal. The storage of waste in a vitrified form within glasses is a potential solution to this issue, with radioisotopes immobilised for safe storage and disposal [1]. Stability of these glasses is paramount, especially in a corrosive environment for the duration that the waste material remains active.

To better understand the mechanisms involved along with the long-term durability in geological disposal conditions, the longevity of glasses in aqueous conditions were investigated. This was carried out using several standard borosilicate glasses corroded in multiple pH solutions for varying time periods.

To characterise the corrosion effect on the various glass samples, the technique time-of-flight elastic recoil detection analysis (ToF-ERDA) was used [2]. The ToF-ERDA measurements were undertaken using an incident beam of 16 MeV $^{127}\text{I}^{8+}$. The simultaneous measurement of velocity and energy of recoiled atoms allows for an enhanced mass separation. This allows for individual characterisation of elements of interest, in this case Na and B, including the two B isotopes, ^{10}B and ^{11}B . The composition depth profiles from ToF-ERDA were used to compare the different samples, which showed the near surface leaching of both B and Na and allowed the calculation of corrosion rates. From these rates, the diffusion coefficients of B, Na and H_2O could be determined for each pH value.

References

- [1] H. Liu, et al., Effects of surface initial condition on aqueous corrosion of glass —A study with a model nuclear waste glass, *J. Am. Ceram. Soc.*, 102, 1652–1664 (2019)
- [2] Y. Shi, et al., Characterization of solar cell passivating contacts using time-of-flight elastic recoil detection analysis, *Appl. Phys. Lett.*, 123 (2023) 261106

An intermediate morphology in the ion beam induced patterning of the crystalline Ge(001) surface

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We investigate the nanoscale self-organized pattern formation of the Ge(001) surface induced by ion beam bombardment at sample temperatures above the recrystallization temperature, i.e., in the reverse epitaxy regime. Two previously-observed kinds of topographies are seen: anisotropic patterns consisting of upright and inverted rectangular pyramids, as well as isotropic patterns composed of shallow basins [1]. In addition, we observe the formation of an unexpected third type of pattern. In this intermediate morphology, isolated pyramidal peaks with rectangular cross sections are surrounded by shallow, rounded basins, i.e. characteristics of the other two morphologies coexist. Which morphology is observed depends on the ion energy and flux and on the surface temperature. An anisotropic pattern is replaced by an intermediate pattern and then by an isotropic pattern as the sample temperature is increased. The same sequence of transitions is observed as the ion energy or flux is reduced.

To model the observed pattern morphologies, we extend past theoretical work on the equation of motion to include a second order correction term resulting from the curvature dependence of the sputter yield [2]. This term produces the isolated peaks in the intermediate patterns and would result in the formation of spike singularities if this were not averted by the Ehrlich-Schwoebel effect. For a range of parameter values, the resulting continuum model of the surface dynamics produces patterns that are remarkably similar to the morphologies we observe in our experiments [3]. This shows that the role of erosion in reverse epitaxy is more than the provision of mobile species as previously thought, since it also contributes directly to the actual pattern morphology.

References

[1] X. Ou et al., Phys. Rev. Lett. 111, 016101 (2013)

[2] R.M. Bradley and G. Hobler, J. Appl. Phys. 129, 194301 (2021)

[3] D.J. Erb, D.A. Pearson, T. Skeren, M. Engler, R.M. Bradley, S. Facsko, Phys. Rev. B 109, 045439 (2024)

Formation of nanomagnets and modification of matrix magnetic properties via sequential ion implantation

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The possibility to locally introduce ferromagnetism in a paramagnetic matrix via ion implantation opens possibilities both for practical applications and studies of emergent physics. Previous work has demonstrated the methodology [1,2], but complex systems involving 3D arrays of implanted structures have not been investigated in this context. Furthermore, the complexities enabled by ion implantation, for example nanoscale patterns implanted into a matrix that is either unmodified or implanted with a different dopant to a different concentration, have not been thoroughly explored. In the present contribution we aim to investigate nanoscale magnetic implantations into a paramagnetic Pd matrix. A commercial, self-supporting Au mask, featuring 290 nm wide circular openings, 600 nm apart will be employed to imprint a pattern where size-scale effects on the magnetic properties of the resulting system are expected. The pattern will be realized through implantation of ferromagnetic materials (Co, Fe, Ni, Gd) at tens of keV restricting the affected sample area to the mask openings, as well as higher energies to implant through the mask. The latter approach is intended to generate a matrix featuring a relatively low dopant concentration into which the structures of interest can be embedded, modifying their interactions. Thus, the studied parameter space comprises the ion type and concentration implanted both in the active structures and the surrounding matrix. Combinations of elements may also be implanted, possibly generating structures that feature several transition temperatures associated with the Curie temperatures of the different implanted regions.

References:

1. P. Ström et al., J. Magn. Magn. Mater. 552 (2022), 169207.
2. P. Ström et al., Phys. Stat. Sol. RRL, in press, <https://doi.org/10.1002/pssr.202400053>

MeV ion irradiation with charge state flexibility employing a new end-station at Uppsala University

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The irradiation beamline at the Tandem Laboratory in Uppsala has recently been upgraded with a new sample chamber. This contribution aims to present the upgrade as well as the possibilities it opens to carry out irradiation experiments for users. In short, the new chamber improves reliability and throughput due to more robust sample handling compared to the previous set-up, enables active current monitoring for improved control of ion fluence and provides vacuum conditions such that the residual gas pressure during irradiation is decreased by one order of magnitude. It further enables relatively simple installation of systems for sample annealing (contact or radiative heating along with a thermocouple for temperature feedback), optical characterization and electrical contacts for in-operando irradiations of electronic components. In addition to presenting the chamber itself, we also address the fact that the projectile ion charge state has been identified as a parameter of interest both for ion beam assisted nanostructure formation [1,2] and fundamental studies concerning ion-solid interactions [3]. In that light, we look at the opportunities and pitfalls arising when one attempts to generate a beam of MeV ions far from charge state equilibrium in a tandem accelerator by adding a stripping foil before the analysing magnet. Potential application cases for such ions are discussed, including surface nanopatterning and nanopore shape control.

References:

1. K. Tomić Luketić et al., Crystals 12 (2022), 865.
2. R. Kaur et al., Nucl. Instr. Meth. Phys. Res. B 551 (2024), 165335.
3. P. Ström et al., Phys. Rev. A 103 (2021), 022803.

ReMade@ARI: a hub for materials research for the circular economy

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ReMade@ARI (REcyclable MAterials DEvelopment at Analytical Research Infrastructures) is a Horizon Europe project, which offers comprehensive analytical services for research focusing on the development of new materials for the circular economy [1]. In contrast to the currently dominating linear economy, in which materials are taken from the Earth, turned into products and thrown away as waste at the end of their life, the circular economy aims to design products that are more durable, reusable, repairable and recyclable.

In order to address this challenge, the most significant European analytical research infrastructures have joined forces in the ReMade@ARI project to provide a support hub for materials research focused on exploring the properties and structures of recyclable materials.

ReMade@ARI offers coordinated access to over 50 research infrastructures across Europe, including electron microscopy facilities, synchrotrons, free electron lasers, neutron sources, high magnetic field laboratories and ion or positron beam facilities. An application for complementary measurements at various facilities is possible within one proposal, providing a simplified path for access in the form of interdisciplinary and correlative research. For proposal submission, an easy-to-use application portal is used for proposals from both academic and industrial users.

Assistance provided by the project ReMade@ARI goes far beyond infrastructure access. ReMade@ARI also offers advanced scientific support for users throughout their entire projects – and beyond! Senior scientists, facility experts and young researchers contribute scientific knowledge and extensive support to provide user services [2]. Particular attention is given to the implementation of comprehensive support mechanisms for researchers and developers from industry [3]. For industrial users, ReMade@ARI also provides grants, as well as fast-track experiments (dedicated for small and medium enterprises) to provide them with technical expertise from research and technology organisations for challenging problems.

The offer of ReMade@ARI is complemented by a series of workshops and training events to help circular economy researchers, aiming to develop and improve their skills in instruments and techniques offered within the project.

ReMade@ARI releases calls for standard access (ReMade-TNA) twice a year. The next call for TNA proposals opens in summer and closes on 9 October 2024. Separate calls for additional modes of access dedicated to industry are released separately. The call for small and medium enterprises (ReMade-SME) is through rolling access and will remain open until 16 December 2024, while the call for industry in collaboration with a knowledge provider (academic or RTO) has a final deadline of 30 August 2024 [4].

References:

- [1] info@remade-project.eu (for general information)
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RIANA: Research Infrastructure Access in Nanoscience & Nanotechnology

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Research in the fields of nanoscience and nanotechnology is vital for a global sustainability. As the advancement in nanoscience and nanotechnology cannot be achieved without using research infrastructures (RI), the EU-funded RIANA project joined 7 European networks of top-level RIs providing access to the most advanced techniques relevant for nanofabrication, processing/synthesis, characterization and analytic as well as simulation capacity [1].

Highly customized and efficient access to 69 infrastructures, spread across 22 European countries is coordinated via a single-entry point and enabled through comprehensive scientific and innovation service by senior scientists, facility experts and highly trained junior scientists. This core of RIANA is aligned to attract experienced and new users from academia or industry and will be prioritized for researchers with the brightest ideas and approach to make best use of the RI for nanoscience and nanotechnology in view of sustainability [2].

The excellence of user projects will be upheld by an independent review panel applying sharp evaluation criteria, in particular:

- scientific excellence,
- potential to technology readiness level increase
- level of cross-disciplinarity
- impact on safety for environment
- impact on nanoscience or nanotechnology.

RIANA will accept user proposals based on a “continuous call” that will be launched soon.

References:

[1] RIANA proposal - grant agreement No. 101130652

[2] RIANA-project.eu



POSTER 2 ABSTRACTS

Quantifying structural evolution of germanium and germanium nanomembranes under self irradiation

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Under ion irradiation, germanium (Ge) undergoes a transformation into highly dense networks of nanoscale pores, the mechanism of which is still under discussion. In this study, we investigate the structural evolution of Ge under self-irradiation with 330 keV and 2.5 MeV ions using transmission electron microscopy (TEM), microbeam Rutherford backscattering spectrometry (μ RBS), and a unique Ge-on-Si sample design. This combination of characterization methods and sample structure facilitates unprecedented quantification of properties, such as sputtering yield and mass density, during porosity evolution.

We find the mass density of the amorphous and porous phases of Ge to remain constant at $\approx 95\%$ and $\approx 50\%$ of bulk density, respectively, regardless of irradiation doses. Experimental evidence challenges vacancy clustering as a commonly cited mechanism for pore formation. Instead, relaxation in structurally weakened volumes, particularly near the material surface due to micro-explosions, can explain most observations.

From an applied perspective, we demonstrate that the porous structures are highly customizable for specific applications through controlled ion doses and energies. Unlike Ge irradiated with keV ions, which features large openings and long channels, Ge irradiated with MeV ions exhibits significantly smaller pores interconnected by ultra-small channels. Experimental results indicate that atmospheric water vapor can permeate homogeneously through the entire thickness of the porous material, suggesting efficient gas transport through the porous structure. As an inorganic material, Ge with such porous structures exhibits greater durability than polymer or hybrid polymer/inorganic membranes for filtering applications in high-temperature and strong pH environments.

Finally, we present preliminary results on the fabrication of self-supporting Ge nanomembranes and their behaviours under ion irradiation.

TRI3DYN Modelling of Neon Irradiated Embedded Silver Nanoparticles in Silicon Nitride

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Nanoscale structures, and nanoparticles (NPs) in general, have properties that can be used in modern electronics [1]. As such, synthesis of these NPs is important and factors such as their shape and distribution impact on their applicability heavily. Synthesis and characterisation of these materials is challenging and the use of ion beams hoped to aid in tailoring and analysing these materials.

The use of a 200keV, 60° Ne ion beam incident on Ag nanoparticles buried within Si₃N₄ substrate was hoped to decompose the nanoparticles. Medium Energy Ion Scattering (MEIS) was used to characterise the NPs post irradiation and provide quantitative data on size and composition. However this leaves ambiguity in the physical processes taking place in the coarsening of the NPs.

In this work we have used the Monte Carlo binary collision approximation code TRI3DYN [2] to inform future MEIS analysis and provide further information. TRI3DYN uses voxels to simulate 3D structures. This can be used to extract topographical information about the evolution of the substrate and describe the decomposition of the NPs. The code also accounts for dynamic alterations and evolution of the surfaces due to the ion implantation and atomic mixing.

The TRI3DYN analysis was calibrated to the MEIS analysis with experimental conditions. In this work we have used this calibration to predict results for variation in the angle and energy of the incident beam. The presented results will give information about the topographical development of the NP under differing conditions.

References

[1] Temple, T.L. et. al., 2009. Solar Energy Materials and Solar Cells, 93(11), pp.1978-1985.

[2] Möller, W., 2014. Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, 322, pp.23-33.

Passive air quality investigation of leaves, moss and trees using Ion Beam Analysis techniques

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Environmental conditions are of growing concern as large population are affected by climate change and pollution, an estimation of millions of people worldwide are dying from lower air quality [1]. Projects including living wall plant studied have been investigated to limit and improve air quality indoor and outdoor [1,2,3,4]. This project aims to explore the potential of plants, moss and trees as bio-indicators of environmental pollution. Quantification pollution indicator measured using Ion Beam Analysis (IBA) techniques; Rutherford backscattering (RBS), particle induced x-ray emission (PIXE). PTFE Air filters are used as supplementary samples to corroborate the findings from plant samples. This comprehensive approach also includes identifying potential pollution sources, thereby contributing to a broader understanding of environmental pollution dynamics in Guildford. The collection site locations were chosen to provide complementary information as NO_x collection site are present along the motorway passing in the middle of Guildford. Sites along the railways were also chosen to have a wider representation of the possible pollution source in town. Other location sites were selected to function as controlled environment, location expected to have low level of pollution. In this presentation, we will show the latest results of qualitative and quantitative analysis of pollution indicators.

- [1] Weerakkody U, Dover JW, Mitchell P, Reiling K. Particulate matter pollution capture by leaves of seventeen living wall species with special reference to rail-traffic at a metropolitan station. Urban forestry & urban greening. 2017 Oct 1;27:173-86.
- [2] Weerakkody U, Dover JW, Mitchell P, Reiling K. Quantification of the traffic-generated particulate matter capture by plant species in a living wall and evaluation of the important leaf characteristics. Science of the Total Environment. 2018 Sep 1;635:1012-24.
- [3] Sheweka S, Magdy AN. The living walls as an approach for a healthy urban environment. Energy Procedia. 2011 Jan 1;6:592-9
- [4] Mannan M, Al-Ghamdi SG. Investigating environmental life cycle impacts of active living wall for improved indoor air quality. Building and Environment. 2022 Jan 15;208:108595.

Materials radiation damage research at the University of Manchester Dalton Cumbrian Facility

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The University of Manchester Dalton Cumbrian Facility has established itself as a key research facility for radiation related studies within the UK, with a user community of over 70 universities and companies. It hosts a suite of radiation sources (ions, gammas and x-rays) and analytical equipment, carrying out research in sectors as diverse as nuclear (e.g. decommissioning, radiation tolerance of materials for existing and future nuclear technologies), space and healthcare.

Accelerated materials radiation damage research with the use of energetic ions, focused on materials of interest for the nuclear industry, is one of the key activities at the Dalton Cumbrian Facility and enabled by its two ion accelerators, eight beam lines and associated end stations. Our ion accelerators can generate proton beams up to 10 MeV, helium/alpha up to 15 MeV, and heavy ions up to 35 MeV. Standard radiation damage experiments can be conducted at temperatures up to 800°C, soon to be expanded to above 1000°C and cryogenic temperatures. Recent expansion of materials radiation damage capabilities includes developments in dual-beam irradiation and in-situ tensile testing. Full range of capabilities and exemplary research topics will be presented.

Effect of He-ion irradiation on the microstructural evolution of a titanium aluminium alloy

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TiAl alloys due to their low density and high temperature oxidation, corrosion, and creep resistance has been proposed as a candidate material for nuclear applications particularly as a structural material for Generation IV high temperature gas cooled fission reactors as well as a first-wall and blanket material for fusion reactors. In this project, the radiation response of a dual-phased (α_2 and γ) fully lamellar TiAl alloy was investigated. Results from in situ TEM annealing and in situ heating XRD confirmed the lamellar microstructure to be thermally stable up to 800°C. Samples were irradiated in situ TEM with 10 keV and 100 keV He⁺ ions at room temperature, 350°C, 500°C, and 700°C, up to a fluence of 1×10^{17} ions/cm². Different temperatures were chosen to represent a range of reactor operating temperatures. The 10 keV and 100 keV energies were chosen to compare the effect of different helium dose to damage ratios, replicating the neutron-induced transmutation reaction in reactors materials. Irradiation-induced microstructures were investigated by TEM. No cavities were observed at room temperature for both energies which was expected since the vacancy mobility temperature for TiAl is approximately 300°C. Cavities were visible at 1×10^{16} ion/cm² and 5×10^{15} ions/cm² for the 10 keV and 100 keV, respectively. Cavities were uniformly distributed on the lamellae initially for all fluences and energies up to 350°C. At 500°C and 700°C, the distribution of cavities varied with fluence and were preferentially distributed along lamellar interfaces for the 10 keV as opposed to cavity denuded zones along lamellar interfaces for the 100 keV. In all, the size of the cavities increased with fluence.

Ferroelectric inversion layer created by ion implantation and annealing in single crystals LiTaO₃

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Single crystal LiTaO₃ (LT) is widely used for its good ferro- and piezoelectric properties, as well as for its optical properties. Applications range from second harmonic generation to acoustic resonators and filters.

In particular, LiTaO₃ is used as a substrate for Surface Acoustic Waves (SAW) resonators. To improve the temperature coefficient of frequency of SAW filters, most designs require a thin single crystal layer on an insulator. This structure (LT/insulator/substrates) is called Piezoelectric on Insulator (POI) [1][2].

Here, hydrogen ion implantations were performed at various energies and fluencies in single crystals bulk monodomain LiTaO₃ and in POI monodomain LiTaO₃ structures. After controlled annealing, damage and lattice deformations induced by the implantations have healed, as assessed by x-ray diffraction. Piezoresponse force microscopy observations reveal the appearance of a monodomain inverted layer starting from the implantation depth and growing towards the surface. This inversion takes place only when the surface of the implanted samples has a positive polarity.

References

- [1] : Yang, Yansong, et al. "4.5 GHz lithium niobate MEMS filters with 10% fractional bandwidth for 5G front-ends." *Journal of Microelectromechanical Systems* 28.4 (2019): 575-577.
- [2] : Eric Butaud;Brice Tavel;Sylvain Ballandras;Marie Bousquet;Alexis Drouin;Isabelle Huyet;Emilie Courjon;Aymen Ghorbel;Alexandre Reinhardt;Alexandre Clairet;Florent Bernard;Isabelle Bertrand; (2020). Smart Cut™ Piezo On Insulator (POI) substrates for high performances SAW components . 2020 IEEE International Ultrasonics Symposium (IUS), (), -. doi:10.1109/IUS46767.2020.9251517

Insights to the Effects of Ion/Host Matrix Choice on Nanoparticle Elongation During Energetic Ion Irradiation

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Swift heavy ions can be used to permanently modify the shape of metal nanoparticles embedded in suitable host materials such as Silicon dioxide or Silicon Nitride. Multiple parameters in the irradiation conditions and the quality of the dielectric host materials vary at the same time between different experiments, making it difficult to pinpoint the effects of individual components.

We explore how the differences between materials, the quality of the same material, and the ion used in the irradiation affect the ion track dynamics on the atomic level. Using the inelastic thermal spike model combined with molecular dynamics, we gain an understanding of processes, unreachable with continuum methods alone, such as pressure effects, density fluctuations, and different amorphous phases created by the irradiation.

Characterizing irradiation effects in silver nanoparticles exposed to a 200 keV neon ion beam

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Room temperature 200 keV Ne⁺ ion irradiation effects on Ag nanoparticles embedded in silicon nitride films were investigated using Medium Energy Ion Scattering (MEIS) and Scanning Transmission Electron Microscopy (STEM), and the results were discussed in comparison with Monte Carlo binary collision approximation TRI3DYN simulations [1]. The study aimed to elucidate irradiation-induced microstructure evolution mechanisms at both individual nanoparticle and system levels. The samples were prepared via magnetron sputtering, depositing Ag and silicon nitride layers (about 3 and 10 nm thick, respectively) on Silicon Nitride/Si wafers. We present an innovative MEIS approach capable of quantitatively determining Ag atomic dispersion and nanoparticles spatial distribution for a planar system of nanoparticles exposed to ion irradiation. STEM observations revealed nucleation of smaller Ag satellite-like nanoparticles within the solute field around the original distribution. The TRI3DYN simulations suggest that a fraction of the solute content is reincorporated within the original nanoparticles. These results are discussed considering that thermal diffusion processes at room temperature are significantly retarded on silicon nitride substrates, which leads to an interpretation based mainly on atomic displacements induced by irradiation [2]. The study demonstrates quantifying atomic dispersion and coalescence from ion irradiation, with implications for nanoparticle ensemble manipulation using ion beams.

References

- [1] W. Möller, TRI3DYN – collisional computer simulation of the dynamic evolution of 3-dimensional nanostructures under ion irradiation. Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, 322, 2014.
- [2] M. Mousley, et al. Structural and chemical evolution of Au-silica core-shell nanoparticles during 20 keV helium ion irradiation: a comparison between experiment and simulation. Scientific Reports, 10, 2020.

PALS and nanoindentation analysis of high fluence helium ion irradiated Eurofer97 and ODS Eurofer steels

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Addressing the challenge posed by elevated levels of transmutation helium in materials for use in advanced nuclear reactors, both fusion and fission, is crucial due to the formation of helium bubbles causing embrittlement and swelling. While current research primarily examines fundamental aspects such as defect evolution and void swelling at the nanoscale, our study particularly investigates the bulk properties of these materials and their practical engineering applications. We irradiated Eurofer97 and its ODS variant, along with SIMP, PM2000, OSD Eurofer, SS 310S, and 800H structural steels, designed for demanding radiation environments, using a helium ion beam ranging from 17 MeV to 1 MeV. By gradually decreasing energy levels, we achieved a uniform "box-profile" with a helium concentration of 1000 appm, resulting in a consistently irradiated layer approximately 65 μm thick. This enabled subsequent micromechanical testing and assessment of engineering-relevant material properties. Our contribution presents initial findings, particularly in the areas of positron annihilation lifetime spectroscopy (PALS) and nanoindentation analysis of the irradiated steel properties.

Charge Collection Efficiency and Radiation Resistance of GaN Core–Shell Microwire Radiation Sensors

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Gallium nitride nano- and microwires have garnered increasing interest due to their unique geometry and flexibility, and have already been successfully applied in optoelectronics. One important advantage is their superior crystalline quality compared to their thin-film counterparts. Additionally, GaN is known for its high radiation resistance, attributed to the large displacement energy of the atoms in its crystal lattice and efficient dynamic annealing properties.

In this study, single GaN core-shell p-n junction microwires were processed into radiation detectors [1]. We determined an average charge collection efficiency (CCE) of approximately 25% using high-precision ion-beam-induced charge (IBIC) measurements with 1 MeV Si ions. CCE maps coupled with three-dimensional Monte Carlo simulations suggest that this average CCE is limited by geometrical effects in the 3D structure and the small active region of the device. In fact, the CCE within the space charge region is estimated to be significantly better than the average value since a large fraction of energy deposition occurs outside the active region of the device [2]. With increasing ion fluence, the CCE deteriorates. Nevertheless, the devices exhibit impressive radiation resistance. The effects of ion irradiation on the electrical and optoelectrical characteristics were further studied with 1 and 2 MeV protons. By measuring the dark and photocurrent as a function of the proton fluence, we show that for fluences up to 10^{14} protons/cm², there is no significant modification of any of these parameters, and that serious degradation only occurs for fluences above 10^{15} protons/cm².

References

[1] D. Verheij et al., Appl. Phys. Lett. 118 (2021) 193501

[2] D. Verheij et al., ACS Appl. Electron. Mater. 6 (2024) 1682

A Study of Radiation Damage in AlFeMnNiCu₂ Using Ar-300 keV In-Situ Ion Irradiation at MIAMI-2

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The MIAMI (Microscopes and Ion Accelerators for Materials Investigation) facilities [1] are a unique group of instruments combining ion irradiation with transmission electron microscopy (in-situ TEM). TEM with in-situ ion irradiation can give significant insight into the effect of radiation on materials, including the HEAs (High Entropy Alloys) of interest to this report. This allows us to study the real-time response of the materials to ion beam and direct observation. Our interest in HEAs is due to their unique properties like wear, fatigue, and fracture resistance, excellent strength, stability at elevated temperatures, and high elongation as compared to new classes of stainless steel [2].

A high Entropy Alloy with composition AlFeMnNiCu₂ was formed using vacuum arc melting. The four elements Al, Fe, Mn, and Ni were taken in equal percentages making 98% and copper was taken 2%. X-ray Fluorescence analysis reports showed that the composition was remarkably close to what was planned with Al, Fe, Ni, and Mn being in near equiatomic composition and Cu being 2.5 at% in the bulk sample. XRD indicates the sample dual phased. This addition phase can be accredited to the addition and precipitation of Cu. The sample morphology is uniform under TEM (Transmission Electron Microscopy) with Cu precipitation. The sample was annealed in-situ and ex-situ at 350°C and 500°C but there was negligible change in the shape and size of these precipitates which proves that they are thermally stable [3].

The performance of AlFeMnNiCu₂ Compared with compositionally complex alloy AlFeMnNi, both alloys were irradiated with medium energy Ar-300 keV ion beam in situ using the MIAMI facility at the University of Huddersfield. Three irradiations were conducted the first at 350°C, 500°C, and the last one at room temperature. The irradiation steps were zero dpa, 1 dpa, 3 dpa, 7.5 dpa, and 10 dpa respectively in all the irradiation. The electron diffraction indicated both alloys had a crystalline structure as prepared but after 10 dpa the polycrystalline ring started to form in AlFeMnNi which indicates stability of AlFeMnNiCu₂ due to the addition of Cu in minor quantity.

This project aims to explore the response of HEAs to extreme conditions of irradiation and temperature relevant to applications such as extra-terrestrial deployment with high flux of radiation and nuclear power systems at extremely elevated temperatures and radiation [4].

References

- [1] Hinks, J.A., J.A.v.d. Berg, and S.E. Donnelly, MIAMI: Microscope and ion accelerator for materials investigations. *Journal of Vacuum Science & Technology A*, 2011. 29(2): p. 021003.
- [2] Tsai, M.-H. and J.-W. Yeh, High-Entropy Alloys: A Critical Review. *Materials Research Letters*, 2014. 2(3): p. 107-123.
- [3] Nordin, N.H.B., Phase transformation in High Entropy Bulk Metallic Glass (HE-BMG) and Lamellar Structured-High Entropy Alloy (HEA), in Department of Materials Science and Engineering. 2018, The University of Sheffield.
- [4] Yvon, P. and F. Carré, Structural materials challenges for advanced reactor systems. *Journal of Nuclear Materials*, 2009. 385(2): p. 217-222.

Determining the optimal conditions for a quantum-grade SnGe thin film.

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The SnGe binary alloy is a recently developed group IV material that demonstrates a direct bandgap when the tin (Sn) content exceeds 6% [1], opening up the possibility of optical interactions with a qubit system. An intriguing phenomenon known as layer exchange (LE) occurs during heat treatment, wherein metal and semiconductor layers undergo exchange. Depending on the combination of materials involved in LE and the growth conditions, the resulting semiconductor layer displays various characteristics, including low-temperature crystallization, controlled grain size, and crystal orientation control to (100) or (111) [2].

The primary objective of this research is to achieve the growth of smooth tin (Sn) films on various substrates at different temperatures, followed by the deposition of germanium (Ge) on top. Subsequently, the SnGe samples undergo annealing to initiate the layer exchange process. By systematically varying the growth temperature and examining the resulting SnGe films, this study aims to determine the optimal conditions for obtaining quantum-grade SnGe films. The resulting SnGe films were characterized using various analytical techniques to assess their structural and morphological properties.

References

- [1] Jun Zheng^{1,2}, Zhi Liu, Chunlai Xue, Chuanbo Li, Yuhua Zuo, Buwen Cheng, and Qiming Wang, "Recent progress in GeSn growth and GeSn-based photonic devices," *Journal of Semiconductors*, vol. 39, 2018.
- [2] Kaoru Toko and Takashi Suemasu, "Metal-induced layer exchange of group IV materials," *Journal of Physics D: Applied Physics*, vol. 53, no. 373002, 29 June 2020.

Atomistic Modeling of the Isotopic Enrichment via Ion Irradiation of Silicon-28 Layers for Quantum Architectures

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High fluence ion implantation with silicon-28 into natural silicon substrates has been shown to result in the depletion of the nuclear spin 1/2 silicon-29 isotope to below 3 ppm resulting in a close to spin-free matrix for donor-based quantum computer architectures. Optimisation of this enrichment process requires a detailed understanding of the atomic dynamics during the deposition process. Given that previous binary collision Monte Carlo simulations, employed to model experimental settings, lack the mechanistic detail needed for process optimisation, a more exhaustive description of the ion implantation process remains to be addressed. In this context, we employ molecular dynamics (MD) simulations, to examine the enrichment process by performing overlapping depositions of silicon-28 ions across a wide range of energies followed by a post-irradiation annealing, resulting in the overall enrichment of the sample with silicon-28, and reduced silicon-29 and silicon-30 isotopes. Our results show how the key variables, such as the deposition energy and angle of impact can influence factors including the enrichment depth and sputtering yield. By comparing with experimental outcomes, we aim to validate and enhance the understanding of the silicon-28 enrichment process for future quantum computing architectures.

Ion Beam Amorphisation Effects in Bulk Silicon Measured Using Rutherford Backscattering Spectrometry Channelling

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While Silicon is a widely used material it is still not fully understood what effects the fluence and flux of an incident beam have on its structure. This study aimed to quantify the effects these variables have on the crystal structure of the material and whether it is possible to accurately control the degree of amorphisation. An accurate method to determine the amorphisation rate is essential to be able to control this.

To study the amorphisation of Si, multiple bulk Si samples were prepared and implanted using an ion beam to change the crystallinity of the first 100nm of the samples. Several fluences around the expected onset of amorphisation along with two different flux rates were used, to examine heating effects.

Rutherford Backscattering Spectrometry / Channelling (RBS/C) is a useful technique for the determination of amorphous regions in crystalline materials, due to the change in ion yield as the sample is rotated around the crystallographic directions. The Si samples were compared along both the growth direction and one of the other major axial channels to examine the amount of amorphisation caused by the different ion implantation conditions.

To corroborate the results Electron Backscatter Diffraction (EBSD) was used, with this technique being surface sensitive. Whereas RBS/C needs to travel through roughly the first 20nm of the material before channelling occurs. The full comparison of the results for the different fluences and fluxes and their effect on the Si structure, will be discussed in detail.

Focussed Ion Beam Profile Characterisation with Nanoapertures

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The potential of single ion implantation using a focussed ion beams for quantum technology, requires a good measure of the spot size and beam profile outside of imaging resolution is becoming ever more important. The extended tails outside of the central beam spot are a problem in sensitive quantum systems where the positioning of single atoms is key. This means that an understanding the shape of the beam spot profile outside of image resolution is needed to create reproducible and scalable quantum devices. Prior unpublished work has shown that the beams tails extend beyond what is generally considered the spot resolution of the ion beam, with the potential of lattice damage extending for several microns. In this study we have adopted new techniques for accurate determination of the beam spot profile of focussed ion beams in both low and high current regimes.

One method used is the creation of nanoapertures, where the beam is aligned central to an aperture with a detector aligned directly beneath. At low current, ions are deterministically counted in as the ions pass through the aperture or hit the material outside of it creating secondary electrons, and at high current a clean membrane is irradiated until a hole first appears, which is determined through measuring the current beneath the membrane, and then the size is measured and compared to the dose. Changing doses should allow for mapping of the beam core. Another way of profiling the spot size is by checking with Ion Beam Induced Charge (IBIC) measurements, to find out the effects of these tails during a typical alignment procedure, as IBIC will record if an ion will land in the channel. IBIC was also used to measure the profile with holes in the channel much like in the apertures.

These techniques have been used to find the cause of the tails and spread in ion beams, with experimental and computational data to understand further what limits spot size and implantation accuracy of a single ion. We believe we have created a good method to profile a beam in a reasonably quick and quantifiable way for any given species, hopefully allowing for better analysis of problems and improvements for optics design and tuning for these single ion implanters.

Isotopically Pure Ion Deposition System for Quantum Grade Substrates

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Isotopically-pure substrates are critical for preventing decoherence in spin qubit quantum computing, but such substrates cannot be grown with conventional techniques. Multiple techniques involving electromagnetic separation of ion beams for generating such substrates are currently under investigation, including layer exchange mechanisms [1] and direct ion implantation [2]. The University of Surrey Ion Beam Centre is currently developing an ion implantation tool with a system for high fidelity deceleration of the ion beam to achieve deposition, or “soft landing,” of the electromagnetically separated ions onto the surface of commercially available wafers and substrates. Using low energy ions is expected to reduce contamination from layer mixing, whilst eliminating sputtering that limits growth rate, but it does require broad area deposition.

The materials IPIDS will primarily explore are ²⁸Si, as well as the direct-bandgap ⁷⁴Ge¹²⁰Sn alloy, which may be produced by a subsequent layer-exchange process being developed at the IBC (see Poster "Determining the optimal conditions for a quantum grade tin-germanium thin film"). This poster discusses the development and achievements of the IPIDS tool, as well as the applications and limitations of isotopically pure deposition.

References

[1] E. Schneider et al, ACS Applied Materials and Interfaces 2023 15 (17), 21609-21617

[2] D. Holmes et al, Phys. Rev. Materials 5, 01460

Influence of Ar Ion Implantation on Precipitation Behavior of FCC-based Al_{0.2}Co_{1.5}CrFeNi_{1.5}Ti_{0.3} High Entropy Alloys

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Compared to BCC-structured HEAs, FCC-structured HEAs could suffer the weakness of lower hardness at elevated temperature. Previous studies have showed that the addition of precipitation strengthening phases into alloy can enhance the hardness. This age hardening enables HEAs to possess favorable mechanical properties over a wide temperature range. However, so far it is still unclear whether the precipitation behavior would be affected by irradiation. For this reason, this study aims to clarify the effects of radiation damage on precipitation-strengthened HEAs under various aging temperatures. The FCC-structured Al_{0.2}Co_{1.5}CrFeNi_{1.5}Ti_{0.3} samples with varying precipitate sizes were employed in this study. Two different aging temperatures were utilized to obtain distinct microstructures. Coherent precipitates of L12 structure were observed within the matrix. In addition, a separate set of cold-rolled samples was also prepared to serve as the control group. In order to evaluate the radiation tolerance of the samples underwent different aging temperatures, the samples were irradiated by 190 keV Ar ions to a fluence of 8.5E15 cm⁻². A comparison of the mechanical properties, component distribution, and microstructures was made between the pristine and irradiated samples. The results revealed that the sample with higher aging temperature has better radiation resistance. A detailed discussion will be also done to clarify the ordering-disordering mechanism of nanoprecipitates.

Roadmap for Focused Ion Beam Technologies

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This roadmap document comprises a review of the current state-of-the-art of advanced focused ion beam (FIB) processing and technology followed by an outlook on required future developments curated by a diverse group of stakeholders.

FIBs play an important role in scientific research in fields ranging from health and biology to quantum technology and nuclear fusion research. However, usually FIBs are perceived as tools for the preparation of samples for other methods such as transmission electron microscopy or atom probe tomography. The intention of this document is to show that this is a clear underestimation of the method by showcasing current and past applications as well as providing a guideline for academia, industry and funding agencies on necessary future developments. The roadmap starts with presenting the state-of-the-art of the FIB technology and instrumentation. The working principle of the FIB is described and an overview of additional instrumentation and detectors who widen the applicability of the method is given. In the second section the available instruments for the simulation and prediction of the focused ion implantation and milling process is given.

This includes advanced simulation techniques such as DFT and MD but also computational efficient methods like BCA which can be used in the every day lab work by FIB users. The core part of the review describes the various applications which go beyond the preparation of TEM samples and include in addition to the above mentioned applications also the fields of spintronic and magnonics super conductivity, photonics, micromechanics, MEMS/NEMS and many more.

In the last part the authors comprising the relevant stake holders give an overview of the required future development which will enable FIB technology to stay at the forefront of research in the discussed fields. This outlook part is partly based on a survey conducted within the European COST Action CA19140 FIT4-NANO which unites more than 200 users, developers and manufacturers of FIB technology. The intention of this part is to act as a guideline for academic and commercial developers as well as funding agencies to steer the future developments in a direction agreed upon by the community. It is this aim supported by the diverse group of contributors to the review which makes this roadmap relevant and timely for many fields of research.

Acknowledgement

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References:

[1] K. Höflich et al., "Roadmap for focused ion beam technologies," Applied Physics Reviews, vol. 10, no. 4, 041311 Dec. 2023, doi: 10.1063/5.0162597.

Migration behavior of silver in SiO₂–SiC double layer

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In nuclear fuels, thin film diffusion barriers are necessary to prevent the release of radioactive waste products. The combination of chemically stable silicon carbide (SiC) and silicon oxide (SiO₂) layers was considered to be beneficial in preventing the release of silver from TRISO particle fuel, at normal reactor operating temperatures (between 800 and 1000 °C). However, it is important to investigate the efficiency of the SiO₂–SiC double layer at higher temperatures, similar to temperatures under accident conditions. In this study, 300 keV silver (Ag) ions were implanted into polycrystalline SiC to a fluence of 1×10^{16} ions/cm² in vacuum at room temperature and 600 °C. The as-implanted SiC samples were coated with SiO₂ layers to a thickness of about 100 nm, using DC magnetron sputtering. After SiO₂ deposition, the samples were subjected to sequential isochronal annealing at temperatures ranging from 1100 to 1400 °C in steps of 100 °C for 5 hours, using a vacuum tube furnace. The thickness of the SiO₂ layers before and after annealing as well as and the migration behavior of Ag in the SiO₂–SiC double layer were investigated using Rutherford backscattering spectrometry (RBS) and annular bright-field scanning transmission electron microscopy (ABF-STEM). Our investigations show that the diffusion of Ag in SiC was not observed after annealing at 1100, 1200 and 1300 °C. However, annealing at temperatures from 1100 to 1300 °C caused partial sublimation of SiO₂ layer and thermal etching of SiC surface. Moreover, RBS results showed that annealing at 1400 °C resulted in the complete sublimation of SiO₂ layer from the surface of SiC, while thermal etching of SiC caused a shift in the Ag depth profile towards the surface. This was accompanied by a huge loss of Ag from SiC.

The Benchmarking of Stopping Power Models

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The slowing down of energetic charged ions in matter involves two contributions: the nuclear and electronic stopping powers. Although the nuclear stopping power can now be predicted with high accuracy [1], substantial uncertainties remain in the calculation of the electronic stopping power, especially below the Bohr velocity. These uncertainties are exacerbated for ions moving in crystal channel directions, where the encountered atomic and electronic densities are significantly below the average [2]. This presents challenges in predicting the effects of ion irradiation in nuclear, space, materials science, and microelectronics industries.

In this work, we present a simulation framework designed to benchmark electronic stopping power models against direct observables from ion beam irradiation experiments. We present the exemplary case of the irradiation of a silicon foil with silicon ions, as conducted experimentally in [3]. We utilize a molecular dynamics (MD) framework to compare widely used velocity-dependent scalar stopping power models with a model that is dependent on the local electron density experienced by the ion [4]. This latter model is parameter-free and inherently trajectory-dependent. We discuss how this model can mitigate the uncertainties in predicting energy losses, particularly in crystal channels, and how it provides genuine predictive capability in modelling the electronic stopping power.

This work enhances the modelling accuracy of electronic energy losses in ion-material interactions and presents an opportunity to significantly improve the fidelity of ion irradiation simulations.

References

- [1] Peltola, J., et al. *Radiat. Eff. Defects Solids* 161.9 (2006): 511-521.
- [2] Sillanpää, J., et al. *Phys. Rev. B* 62.5 (2000): 3109-3116.
- [3] Lohmann, S., et al. *Phys. Rev. A* 102.6 (2020): 062803.
- [4] Tamm, A., et al. *Phys. Rev. Lett.* 120.18 (2018): 185501.

Fundamental Mechanisms the Moderate on Irradiation Dislocation focused the Channel of Microvoids and Cracks

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The Scientific study to review intends to officer an overview of the fundamental mechanism in the field at moderate irradiation conditions.. With the development of numerical simulation capability and advanced experimental equipment. This mysterious veil covering the fundamental mechanism of irradiation - hardening and embrittlement has been gradually unveiled in recent years.The irradiation -hardening and embrittlement have been widely observed in nuclear structures materials. The formation of irradiation-induced defects is discussed, covering the influence of both irradiation conditions and materials propertics. To findings out the current irradiation-hardening, aims to help design next generation irradiation-resistant materials. The evolution mechanism of defects and dislocation are focused formation of defect-free channels and generation of microvoids and cracks.

Keywords: Mechanism, Irradiation.Study, Structure and Materials.

Scientific Application on ion Beam processing Device.

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For ion beam processing microelectronics to focused electron beams, which initially to employed diagnostic test. Development technology of microelectronics application of security monitoring medical sciences. The advanced on integrated circuit. The valves achievable by photolithography. The advancement features of ion implantation doping and limitations of beams processes imposed by fundamental optical effect and tomography scan High electromagnetic The high-quality mesoscale structure from materials that grown in thin- film form and the experimentally physical phenomena. Prototype device can also be processed in silicon chip environmental to investigate directly the materials application potential for future electronics. The ion beam shaping of the matter and extent of surface damage and materials disorders inherent to these techniques. The ion beam processing as given an overview of recent experiments on FIB- structured crystal.

Nuclear Materials: Research and Technology in Current Trends.

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The special nuclear materials Plutonium -239, Uranium -233, and Radium -226 , Thorium -233 and Uranium enriched in the isotopes of 235 and 233 and any material containing one or more of the foregoing. It already has in possession and those it may acquire subsequently. The State also declared the application of nuclear Fuel cycle and energy ionizes to which these materials will be possible. The design of the facilities where work carried out, identified the flow of the nuclear Uranium ore has to be processed in a series of steps before making it fit for use as a fuel in nuclear reactor. Then the spent fuel has to be processed and the radioactive waste properly disposed . All these steps are collectively referred to as the nuclear fuel cycle. Uranium, as it occurs in nature consists primarily of the two isotopes like U-235 and U-238.

The relative concentration of the two isotopes nature Uranium are about 0.7% and 99.3% respectively. Pu-239, other isotopes of Plutonium and fission products . The relative proportion of these depends on the nuclear fuel cycle type of components and reactors type the original fuel, power level, duration of operation. Recovered Plutonium -239 can be converted to its oxide and mixed with Uranium oxide to a form known as a mixed oxide (MOX).

From Roadmap to Reality – Shaping Focused Ion Beam Implantation with P-NAME

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The 2023 Roadmap for Focused Ion Beam (FIB) Technologies laid out a series of challenges which need addressing in order for FIBs to be used as a method of materials modification, particularly for nanoscale and quantum applications. Amongst these are novel ion sources which allow access to individual isotopes, fast blanking and single ion detection to facilitate deterministic implantation, and chicane blanking with ultra-high vacuum systems to avoid contamination while doping.

The Platform for Nanoscale Advanced Materials Engineering (P-NAME) is a multi-beam tool which is designed for low dose and single ion implantation, with high-sensitivity secondary electron detectors enabling deterministic implantation. Electrical feedthroughs also enable use of in situ detection through avalanche and ion beam induced charge detectors. Operation of the tool in DC mode allows implantation across a wide variety of doses, from single ion implantation to $>10^{19}$ ion/cm², with <10 nm spatial resolution achievable in low-dose mode.

We have demonstrated the ability to isolate individual isotopes from the vast range of liquid metal alloy ion sources of the P-NAME system which results in a high-purity mono-isotopic beam, avoiding any contamination of the implanted substrate. The coincident SEM imaging in the P-NAME system has enabled alignment procedures which ensure sub-micron precision of implantation targeting without the need to image at or around the site of interest with the FIB beforehand, further reducing contamination.

These capabilities have enabled a variety of applications including localised silicon enrichment (<2 ppm ^{29}Si), generation of colour centres in diamond, and telecoms compatible photon emission in lithium niobate. The ever-expanding user-base of the P-NAME system demonstrates the applicability and necessity of advanced FIB technologies as outlined in the Roadmap.

Development of Imprint Mold with F⁺ Ion Implantation for Detachability.

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Metasurface has been the focus because their microstructure enables the design of unconventional optical properties. Hundreds of nanometer patterning is required to realize this structure.

Photolithography technology is not enough to develop metasurface technology, electron-beam (EB) lithography and deep-ultraviolet lithography are used. But electron-beam lithography has the problem of low productivity, while deep-ultraviolet lithography has the problem of extremely high equipment. Therefore, nanoimprint lithography technology (NIL), which is inexpensive to implement, is featured. One of the problems with nanoimprinting is peeling during imprinting. Conventionally, a dry or wet coating is applied to the mold surface to improve peelability. However, most wet coating requires coating each time before use. In addition, the dry coating layer is covered about 100 nm, which may affect the accuracy of the mold when processing patterns of 10 ~ 100 nm. This study investigated the use of ion implantation to improve the peelability. Ion implantation does not cause dimensional changes because ionized ion species are implanted into the surface. Therefore, it is considered to be the most suitable method for processing patterns of 10~100 nm. In our previous study, The Si mold was fabricated with a 100 nm fine line pattern using EB lithography and DeepRIE, and transferred the Au pattern using the transfer imprinting method, one of the nanoimprinting methods. The results showed that the ion-implanted molds showed improved peelability. In this study, we analyzed the surface wettability, surface roughness, and coefficient of friction to evaluate the effect of ion implantation on the peelability of the nanoimprinted molds. The results will be presented.

Cluster Ion Beam Irradiation at Low Energy and Surface Pattern Formation

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Ion beam sputtering is a solid-surface nanostructuring procedure. In this study, we are interested in the bombardment of a metallic Co(110) surface bombarded with clusters at oblique incidence. Cluster bombardment accentuates the effect of surface ripple formation. Two processes explain the pattern formation effect at the collisional level when diffusion phenomena can be neglected: sputtering and atomic redistribution: sputtering erosion and surface atomic redistribution. In this work, the importance of both is analyzed for different angles of incidence. It is found that in this type of substrate the weight of sputtering is greater for grazing angles and the weight of redistribution is greater for intermediate angles.

Thermal stability of latent tracks in β -Ga₂O₃ induced by swift heavy ions

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β -Ga₂O₃ is a promising material for high power electronics, deep-ultra-violet photodetectors, and gas sensors due to its ultra-wide energy bandgap (~4.8 eV) and high critical electric field (breakdown field of ~8 MV/cm). Due to its high bond energy, β -Ga₂O₃ is also considered to have high radiation hardness to the displacement damage induced by nonionizing radiation. However, β -Ga₂O₃ materials have been proven to be sensitive to the swift heavy ions. Our previous study found that the electronic energy loss (Se) threshold of latent track formation in β -Ga₂O₃ was about 17 keV/nm for 5-10 MeV/u heavy ions, which was much lower than the Se threshold of SiC and GaN. Therefore, these permanent damages (latent tracks) could significantly affect the performance of β -Ga₂O₃ devices in the space radiation environment. In this work, the β -Ga₂O₃ samples were irradiated with 2.4 GeV and 2.9 GeV ¹⁸¹Ta ions at 5×10¹⁰ ions/cm². After that, the irradiated β -Ga₂O₃ were annealed at different temperatures from 473 to 773 K in vacuum. The microstructures of irradiation damages were characterized by transmission electron microscopy. The changes of average diameter and morphology about latent tracks were observed as a function of annealing temperature. The reduction of latent tracks areal density after annealing at 773 K indicates that most latent tracks have been recovered. We suggest that the lower activation energy of thermal recovery processes in β -Ga₂O₃ was the main reason for latent track recovery, compared with SiC, GaN, AlN and diamond. This study could help estimate the service capability of β -Ga₂O₃-based devices under extreme high-temperature irradiation environments.

Probing non-isothermal annealing of Sn/Ti thin films using Rutherford Backscattering Spectrometry as a probing tool

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Metallic multilayer thin films have become increasingly important in modern nanotechnology, finding applications in various industries. Their relevance stems from their unique properties that can be easily controlled and modified at the nanoscale. This study investigates the effects of annealing epitaxially deposited thin films on silicon dioxide substrate. The thin films were composed of Sn and Ti with two different layer configurations: 15 nm bilayers (15 nm uncapped), and 25 nm bilayers with a 5 nm Si capping layer (25 nm capped). Non-isothermal annealing was achieved by a femtosecond laser with a wavelength of 1030 nm, 300 fs pulse duration, and 500 kHz repetition rate at laser fluences of 0.08 J/cm², 0.16 J/cm², 0.24 J/cm², 0.32 J/cm². The surface morphology, atomic depth profile, and compositional analysis of the bilayer samples were investigated using a scanning electron microscope, atomic force microscope, and Rutherford backscattering spectrometry. The as-deposited samples indicated irregular nanodroplet-like surface morphology. Following annealing, the surface morphology indicated the formation of subsurface voids and randomly distributed nanostructures, which increased as a function of laser fluence. Moreover, the 25 nm capped bilayers indicated the existence of laser-induced periodic surface structures. The atomic depth profile indicated that laser annealing induced surface roughness which increased as a function of laser fluence. The average surface roughness increased from 3.75 nm to 46.3 nm for the 15 nm uncapped bilayers and 8.28 nm to 79.88 nm for the 25 nm capped bilayers. Compositional analysis obtained by Rutherford backscattering spectrometry indicated the formation of a thin oxide layer whose thickness increased upon femtosecond laser annealing. In addition to the top oxide layer, a second layer was formed beneath, which comprised the two bimetals, attributed to the intermixing of the two metals with an estimated activation energy of $E_a = 0.35 \pm 0.020 \text{ eV/atom}$.

Irradiation effects of two-dimensional material heterojunction phototransistors

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Two-dimensional (2D) materials such as graphene, h-BN, transition metal dichalcogenides (TMDCs), black phosphorus, et al., have exceptional electronic and photoelectric properties. Van der Waals heterostructures (vdWH) constructed with various 2D materials are expected to develop a new-generation of ultrathin, high efficiency, broadband and flexible photodetectors, which have a broad application prospect towards outer space exploration. However, due to the ultrathin structure, the defects and impurities induced by irradiation would significantly influence the properties of 2D materials. In this work, we fabricated molybdenum sulfide and graphene vdWH field effect transistors (MoS₂/G FETs) and investigated the evolution of electronic and photoelectric properties induced by swift heavy ions (SHIs) irradiation.

MoS₂/G FETs fabricated in this work had excellent carrier mobility which was comparable to GFETs and much stronger optoelectronic response to pure graphene. The MoS₂/G FETs were irradiated by 2.76 GeV Ta, and the evolution of electronic and photoelectric properties with increasing ion fluence were investigated. At lower ion fluence, SHIs irradiation can optimize the device properties. The decreased resistance R and increased carrier mobilities, total photocurrent I_p and photoelectric responsivity R_p were detected after irradiation. The significant enhancement of I_p and R_p was observed at a fluence of 10^9 ions/cm², while when the fluence surpasses 1×10^{10} ions/cm², I_p and R_p were slightly changed. At high fluence (1×10^{11} ions/cm²), the devices properties were deteriorated by SHIs irradiation. What's exciting is that the device can still operate under such harsh irradiation conditions. Defects in MoS₂, graphene and SiO₂ were investigated by Raman spectrum, photoluminescence microscopy and atomic force microscope (AFM). The optimized and degraded properties of the devices could be ascribed to competition among doping, local annealing and defect scattering. Our work provides experimental basis for the design and development of future ultrathin, flexible low-dimensional photodetectors with strong irradiation tolerance.

Electrical Properties of Heavy Ion Irradiated TMDC Based Devices

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With current mainstream silicon technology reaching its limits, various emerging materials have been proposed to replace silicon as channel materials. In particular, transition metal dichalcogenides (TMDCs)-layered materials have been attracting intense research efforts with totally changed physical scenario. Tunable of the layer thickness, bandgap and charge transferring affords TMDCs the opportunity to engineer many properties for a variety of applications. Heavy ion irradiation technology is a common method to simulate the influences of radiation ions on the electronic devices in space environment. In our work, heavy ion irradiation technology under different conditions was utilized to produce complex defects in TMDC-based devices. Defects with amorphous structure in the core, called latent tracks, were observed averagely distributed in the irradiated TMDCs. Morphology of the tracks varies from nearly circle shape to be cylindrical as the incident direction of heavy ions change from normal to oblique. Visible ellipsoid ends were found in the oblique irradiated samples. Electrical transport and optoelectronic properties were concerned. Degradation mechanism related to trap localization in the channel and Schottky barrier at the interface was explored. We believe that our work serves as a foundation for radiation aerospace application of all-in-one devices.

Study on the crystallization of amorphous HfO₂ thin films by swift heavy ion irradiation

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The cubic and tetragonal phases of HfO₂ could have larger dielectric constant of 29 and 70 compared to the amorphous one, which is usually deposited in CMOS devices. This suggests that the dielectric constant of the HfO₂ thin films can be further increased in a way without changing materials. It was reported that the introduction of the dopant and impurities to the crystal lattice is one of the effective ways to stabilize the high permittivity phase. However, it is almost inevitable to change the physicochemical properties of HfO₂ resulting from the change in the binding energy, bond length and local cation distribution around the oxygen atom after doping. Besides, it was reported that the pure cubic and tetragonal phases of HfO₂ are high temperature phase and can be obtained by thermal annealing above 1700°C and 2700°C, respectively. However, high temperature thermal annealing may cause the deformation in morphologies and the formation of agglomerated structures of HfO₂. The formation of pure cubic or tetragonal phase of HfO₂ at room temperature is challenging and attractive. Heavy ion irradiation is one of the state-of-art means for material modification. The swift heavy ions (SHIs) can result in amorphous-to-crystalline or crystalline-to-crystalline phase transformation when the electronic energy loss ((dE/dx)_e) of SHIs exceeds a threshold value. Some of the phase transformation induced by SHIs is unique and cannot be achieved by other means. In this work, the swift heavy ion irradiation effects on the HfO₂ thin films were investigated. HfO₂ thin films were deposited by an atomic layer deposition (ALD) system at a substrate temperature of 250 °C on p-type Si wafers with (100) orientation. The samples were fabricated by the Laboratory of Microfabrication, Institute of Physics, Chinese Academic of Sciences (CAS). Irradiation experiments were performed in the Institute of Modern Physics (IMP), Chinese Academy of Sciences (CAS). The specimens were irradiated by 6.3 MeV/u 56Fe ions up to fluence 2×10¹⁴ ions/cm² at room temperature. The electronic energy loss ((dE/dx)_e) and the nuclear energy loss ((dE/dx)_n) of 6.3 MeV/u 56Fe ions in HfO₂ are 13.0 keV/nm and 7.3×10⁻² keV/nm respectively. The amorphous HfO₂ films crystallized after SHIs irradiation and undergone a transformation of monoclinic to cubic/tetragonal phase with the increase of the ion fluences. The as-deposited HfO₂ films take on nonstoichiometric state, and became close to the stoichiometric one under SHIs irradiation. This work provides an approach to stabilize the higher-k phase HfO₂ and optimize the interface between HfO₂ and Si by SHIs irradiation.

The influence of Aluminum Grain Size on the Uniformity of Isotopically Enriched ^{28}Si Substrates

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This poster presentation describes the initial results of a process to manipulate the grain size of aluminum to influence the uniformity of enriched ^{28}Si layers that uses ion implantation and layer exchange.

The implanted layer exchange process involves depositing Al on a native oxide free silicon substrate and then implanting it with ^{28}Si . The implanted layer is then annealed at low temperature to initiate layer exchange where the ^{28}Si diffuses into the Al and then either nucleates at a grain boundary or epitaxially grows on the substrate, displacing the Al until the layers have exchanged places.

The experiment to achieve different Al films with different grain sizes involves depositing ~150nm thick Al layers via thermal disposition at different temperatures. As implanted ^{28}Si atoms diffuse along the Al grain boundaries, we believe certain grain sizes may affect the uniformity of ^{28}Si layer exchange. The uniformity of the ^{28}Si layer exchange has proven to be an obstacle in previous experiments in producing isotopically enriched ^{28}Si substrates [1].

Through S/TEM-EDX and AFM analysis, this poster presentation will investigate whether the grain size of the aluminum layer will impact the layer-exchanged ^{28}Si 's uniformity and help meet the purity and crystal requirements of 'quantum-grade' silicon needed for quantum computers. These requirements consist of a purity of ~99.9%, perfect single crystals, and a surface uniformity of ± 0.2 nm.

References

[1] Schneider, E. and England, J. (2023) 'Isotopically Enriched Layers for Quantum Computers Formed by ^{28}Si Implantation and Layer Exchange', ACS applied materials & interfaces, 15(17)

Secondary Ions produced by Protons Passing Through Shielding & Packaging and Induced SEU in Nano-Devices

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With integrated circuit feature sizes shrinking and the commercial aerospace industry flourishing, single-event upsets (SEUs) triggered by protons have emerged as a critical threat to on-orbit spacecraft anomalies. Recent studies reveal that low-Z secondary ions generated from proton-device material nuclear reactions are progressively dominating the contribution to SEU cross-sections. However, software tools like CRÈME and SPACERAD employed for predicting on-orbit error rates solely account for the shielding effects of spacecraft shielding and device packaging against primary protons, neglecting the impacts of secondary heavy ions produced as protons traverse these shielding layers on device SEUs. This work conducted simulation research based on Geant4 for this situation. The simulated results demonstrate that as device feature sizes shrink and incident proton energies rise, the quantity of secondary ions collected within device sensitive volumes originating from spacecraft shielding and packaging correspondingly increases. Once incident proton energies above 1 GeV, the contributions from secondary ions emanating from shielding layers and packaging to SEU cross-sections in devices with sub-65nm feature sizes become non-negligible. Furthermore, above 5 GeV incident proton energies, these secondary ions and their induced SEU cross-sections even dominate as the primary sources of SEUs.

Unveiling microstructural damage for leakage current degradation in SiC Schottky diode after heavy ions irradiation

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Single-event burnout and single-event leakage current (SELC) in SiC power devices induced by heavy ions severely limit their space application, and the underlying mechanism is still unclear. Material damage is widely presumed to be the origin of permanent SELC degradation in SiC power device. However, the nature of material damage responsible for SELC degradation is still under debate. To solve this fundamental and long-standing problem, high-resolution and direct characterization of radiation damage in SELC degraded SiC device is crucial.

In this work, high-resolution transmission electron microscopy (TEM) was used to characterize the radiation damage in the 1437.6 MeV Ta-irradiated SiC junction barrier Schottky diode under 200 V. The irradiation experiments were performed at the Heavy Ion Research Facility in Lanzhou (HIRFL) in the Institute of Modern Physics, Chinese Academy of Sciences. The amorphous radiation damage with about 52 nm in diameter and 121 nm in length at the Schottky metal (Ti)-semiconductor (SiC) interface was observed. More importantly, it is the first time that the atomic mixing of Ti, Si, and C in the damage site was identified by electron energy loss spectroscopy and high-angle annular dark-field scanning TEM. It indicates that the melting of the Ti-SiC interface induced by localized Joule heating is responsible for the amorphization and the formation of titanium silicide, titanium carbide, or ternary phases. These modifications at nanoscale in turn cause the localized degradation of the Schottky contact, resulting in the permanent increase in leakage current. This experimental study provides very valuable clues to thorough understanding of the SELC mechanism in SiC diode.

Investigation of Radiation Effects Induced by Heavy Ions in Spin Transfer Torque MRAM

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NON-VOLATILE MEMORIES (NVMs) are essential for a variety of space applications, for data or code storage. As process nodes scale down, traditional silicon-based memories like PROM and Flash encounter challenges with increasing leakage currents and capacity bottlenecks. Magnetic Random Access Memory (MRAM) is considered one of the most promising storage solutions for space missions due to its high storage density, low power consumption and superior radiation tolerance. In MRAM, the basic storage unit is the magnetic tunnel junctions (MTJ) which consist of two ferromagnetic layers sandwiching a tunnel barrier. Depending on whether the magnetization directions of two ferromagnetic layers are parallel or antiparallel, MTJ exhibit two distinct resistance states: low or high. In this work, we irradiated commercial STT-MRAM with 16 MeV/u Ta ions to study its radiation effects. During the irradiation experiments, we conducted both dynamic and static tests on the devices. Experimental results indicate that the linear energy transfer (LET) and the irradiation angle of heavy ions can affect the single event upset cross-section. We believe that single-event upsets in MRAM are caused by the magnetization reversal of ferromagnetic layers, induced by a localized temperature increase resulting from a single heavy ion strike. It is significant that the two resistance states of MTJ show distinct sensitivities to heavy ion irradiation, resulting in different single event upset cross sections. This difference may stem from the different thermal stabilities of the two resistance states of MTJ. The results also show that the peripheral circuit of MRAM exhibits single event functional interrupt during ion irradiation. We further analyzed and identified that the sensitive regions responsible for single event functional interruptions is digital power supply control module. In summary, these experimental results help us understand the mechanism of radiation effects in MRAM.

Combining ion beam heating, ion irradiation, and infrared imaging for remote characterization of thermal properties

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This study explores an approach for in situ and remote characterization of the thermal properties of materials during ion irradiation experiments. The method involves using a focused proton beam as a localized heating source, generating a distinct hot spot on the sample surface. Subsequent deactivation of the proton beam allows the analysis of lateral heat dissipation patterns using an infrared (IR) camera. The heat dissipation pattern, in conjunction with finite element analysis, provides a method to characterize the thermal properties of the target. Unlike other energy deposition methods such as lasers, the penetration volume and power density of beam heating are precisely known. Additionally, this method can be combined with ion irradiation by alternating between beam irradiation (using a large beam spot) and beam heating (using a small collimated beam spot). By doing so, the systematic dependence of thermal property changes as a function of damage levels can be obtained from a single specimen. Utilizing 2 MeV proton irradiation/beam heating, IR imaging, and finite element analysis, we studied the thermal property changes in quartz as a function of both temperature and radiation damage. Interestingly, the study shows that thermal diffusivity first increases, then decreases as a function of damage during room temperature irradiation.

Irradiation-induced formation of G-phase precipitates and M₂X carbides in self-ion irradiated HT-9

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Ferritic-martensitic steels with high chromium content (9-12 wt%) are a promising material group for advanced nuclear systems due to their high temperature strength and good irradiation tolerance. HT9 is one optimized alloy in this group and is a primary material choice for the fuel cladding of liquid metal-cooled fast reactors. However, although limited reactor testing data exist, there is a lack of systematic data on the radiation response of HT-9 at extremely high damage levels. Here, we report the irradiation response of HT-9 after self-ion irradiation by 5 MeV Fe ions at temperatures ranging from 450°C to 700°C. Transmission electron microscopy and atom probe tomography are combined for structural and compositional analysis. M₂₃C₆ carbides, pre-existing prior to irradiation, remain stable under all irradiation conditions. At 450°C and 500°C, the formation of spherical-like G-phase precipitations and needle-like M₂X carbides is observed. G-phase precipitation is enriched in Ni, Si, Fe and shows no interface segregation, whereas needle-like M₂X carbide, rich in Cr, Mo, and Mn, displays clear interface segregation of Ni and Si. Both G-phase precipitates and M₂X carbides do not appear at temperatures of 600°C and above. The study provides nanometer-scale details of the structural evolution of HT-9, influencing both its radiation response and mechanical properties.

Ion irradiation studies on C₆₀ film

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C₆₀, also known as fullerene or buckminsterfullerene, has a variety of applications across different fields due to its unique molecular structure. Notably, C₆₀ can be used as photodetectors, sensors, lubricants, and coatings. Owing to its high surface area, C₆₀ film is ideal as chemical and biological sensors. Towards the sensor applications, ion beams can be utilized to introduce dangling bonds and vacancies to increase efficiency in trapping molecules. Here, the irradiation response of C₆₀ films is studied as a function of fluences of 100 keV helium ion beam. The C₆₀ film is deposited on a Mica substrate via thermal evaporation of C₆₀ powders. The as-deposited film exhibits a periodic topographical pattern formation which was analyzed using atomic force microscopy. Upon ion irradiation, Raman spectra show an increase in the D/G mode intensity with increase fluences, consistent with previous studies on low-dimensional carbon systems. The D/G mode intensity, however, begins to decrease when damage levels are high enough to reduce the number of six-fold rings, corresponding to amorphization. The threshold amorphization fluence was measured.

Finite element analysis of beam heating in simultaneous ion irradiation and molten salt corrosion experiments

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Ion irradiation is widely accepted as an emulation of neutron irradiation in nuclear materials studies due to its capability to introduce damage levels orders of magnitude higher than those inside a reactor. There has recently been rising interest in combining ion irradiation with molten salt corrosion to evaluate the synergistic effects of radiation damage and corrosion in molten salts, a key issue in molten salt reactors. Such experiments utilize a proton beam to penetrate a thin foil of the test material, which also serves as a window for a molten salt corrosion cell. The irradiation introduces damage into the foil and affects the salt-specimen interface region. In the present study, a digital twin of a typical target setup and finite element analysis are used to simulate the temperature evolution of the corrosion cell during the initial melting stage and when the ion beam is turned on. Two representative cases, a rastered beam and a focused beam, are compared. The foil is a 25-micron thick 316L stainless steel, and the salt is FLiNaK. The study shows that: (1) the molten salt corrosion cell needs to be heated to a temperature at least 100°C higher than the salt's melting point to ensure the salt within the container melts uniformly, due to an observed underheating zone adjacent to the foil specimen. (2) A focused proton beam with typical energy of 2 MeV and a current of 1 microamp creates a superheated zone on the foil sample. The central temperature of a 316 stainless steel foil is about 300°C higher than at the edges. (3) Beam heating also introduces a significant stress field due to differences in thermal expansion. (4) Both beam heating and heterogeneous stress fields can be largely avoided using a rastered beam covering the whole specimen. This study provides useful information for the experimental design of similar experiments and highlights several pitfalls if an inappropriate beam mode is selected.

Ni self-ion implantation using an isotopic beam obtained from a 3 MV NEC tandem accelerator

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Self-ion irradiation has been widely used in studying radiation damage of nuclear materials, avoiding composition changes and doping effects introduced by implanted ions. One issue with such irradiations is the accuracy of the implant profiles, which affects the determination of local damage levels. Experimental validation of ion penetration depth requires ion implantation of isotopes that are significantly low in natural abundance. Such isotopic beams are often obtained using expensive isotope-pure sputtering cathode materials. Alternatively, a cathode material of natural abundance can be used, but requires a 90-degree bending magnet for better isotopic separation. We demonstrate that an isotopically pure beam can be obtained using natural cathode materials with traditional bending magnets, equipped as standard components in commercial NEC tandem accelerators, to separate isotope peaks. The key is to use the beam collector after the acceleration tank for mass scanning and selection, with the additional resolution of separation gained from the long distance between the low-energy and high-energy magnets. As a demonstration, we obtain distinct peaks corresponding to Ni-58, Ni-60, Ni-61, and Ni-62 from a Ni cathode. Ni-62 is selectively implanted into Ni. The depth profiles of Ni-62, obtained at various beam energies, are analyzed using secondary ion mass spectrometry, showing dramatic differences in comparison with SRIM predictions. Ni ion irradiation has been widely used in early studies on void swelling of alloys as a method to emulate neutron damage. The inaccuracy in Ni stopping power, as observed in the present study, points to the need to reevaluate early literature data.

Effect of Epitaxial Buffer Layer on Single-Event Burnout in Silicon Carbide Junction Barrier Schottky Diode

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Silicon carbide (SiC) materials are known for their band gap width, which is approximately three times wider than that of silicon, as well as their higher breakdown electric field and thermal conductivity, making them a good power semiconductor material [1,2]. In comparison to silicon and gallium nitride (GaN) devices, SiC devices can operate at higher power and voltage, making them theoretically ideal for aerospace applications [3-6]. However, in practical applications, it has been observed that SiC devices can only operate at less than half the rated voltage in space environments due to their susceptibility to radiation. Space is a high-radiation environment with numerous high-energy particles [7], and the combination of these particles with the high voltage of the device can cause single event leakage current (SELC) degradation or even single event burnout (SEB) of the device [8]. Prior research has demonstrated that heavy ion irradiation of SiC power devices such as Schottky diodes and metal oxide semiconductor field effect transistors (MOSFETs) can lead to Joule heat accumulation, resulting in lattice temperatures exceeding the melting point of SiC and causing the formation of leakage channels [9-12]. However, despite previous studies, there remains a lack of effective radiation-hardened methods to ensure the safety of SiC power devices in space applications. Recently, Li et al. used Technology Computer Aided Design (TCAD) simulations to demonstrate that adding multiple buffer layers with varying concentrations in the drift region of SiC Schottky diodes can effectively improve their radiation resistance [13]. However, no radiation testing has been conducted on actual devices that employ this type of reinforcement.

To evaluate its radiation resistance, we conducted radiation testing on the device using three heavy ions, namely Bi, Kr, and Ta. The degree of improvement in the device's radiation resistance was then determined. We compared and analyzed the effects of the different heavy ions on the device, and conducted simulation-assisted theoretical analysis. The experimental equipment and simulation parameters are described in the second section, while the experimental and simulation results are presented in the third section. Finally, the conclusions of this study are summarized in the fourth section. These findings provide useful insights for developing reliable radiation-hardening methods for SiC power devices.

The ruggedized SiC JBS devices in the form of the TO247 package used in this study provided by the 55th CETC Research Institute. Keithley 2657A was used to supply the reverse bias voltage (VR) and to monitor the leakage current (I) during irradiation.

SiC JBS diodes with a rating of 1200V-15A was selected as the device under test (DUT). The diode is made of 4H-SiC with an epitaxial layer thickness of about 10 μ m. The single event effect hardening (SEEH) device adds a 10 μ m epitaxial buffer layer structure. The device structure is shown in Fig. 1.

The heavy ion irradiation experiments were conducted at the Heavy Ion Research Facility in Lanzhou (HIRFL), in the Institute of Modern Physics, Chinese Academy of Sciences. Table 1. shows the heavy-ion parameters at the surface of DUTs.

The experimental results of Bi ions are shown in Fig. 2. The results show that the SELC degradation threshold voltage and the SEB threshold voltage of the ruggedized device increase by about 200 V, and the SEB threshold voltage increases to more than half of the rated threshold voltage.

In this study, Kr and Ta ions were used to irradiate both the device without epitaxial buffer layer at reverse bias voltages of 350 V and 425 V, and the reinforced device at a reverse bias voltage of 575 V. The irradiation results are presented in Figures 3, 4, and 5, respectively.

The experiment found that there was no significant change in the device leakage current when using Kr ion irradiation at 350 V voltage, while using Ta ion irradiation, the device leakage current significantly increased.

At the voltage of 425 V, using Kr ion irradiation increases the device leakage current. Using Ta ion irradiation, the device leakage current quickly reaches the current limit, resulting in SEB. At the voltage of 575 V, using Kr ion irradiation, the device leakage current gradually increases to the current limit. Using Ta ion irradiation, the device leakage current rapidly increases to the current limit, resulting in SEB. The experimental results show that this reinforcement method can effectively improve the radiation resistance of the device, but with the increase of incident particle LET, the radiation resistance of the device will weaken, making it more prone to SELC degradation and SEB.

The charge collection process and device lattice temperature evolution of heavy ion impact in reverse biased SiC JBS devices were simulated by TCAD. As shown in Fig. 6(a)(b), comparing the unstiffened and SEEH DUTs under the same bias voltage conditions, one of the electric field peaks occurs at the SiC side of the Schottky contact. Another peak of the electric field appears at the interface between the epitaxial layer and the substrate of the unreinforced device, and for the SEEH device, the doping concentration of the five-layer MBL gradually increases with depth. Hence, the gradient doping suppresses the displacement current and consequently the electrons will not move to the N-/N+ junction for a long time.

This paper investigates the effects of adding multiple buffer layers with different concentrations in the drift region of SiC JBS devices for radiation-hardening, through both experiments and simulations. The effects of different heavy ions on the device are also compared. This reinforcement method improves the SEB threshold voltage of the device to a certain extent, but as the Linear Energy Transfer LET of the incident particle increases, the SEB threshold voltage of the device decreases. The effectiveness of this reinforcement method is also demonstrated by the electric field and lattice temperature simulated by TCAD. The experimental results, combined with the TCAD simulation, provide further insights into the reinforcement principle. Overall, this research will facilitate the development of radiation-hardened SiC power devices.

References

- [1] P. Roussel, "SiC Market and Industry Update", International SiC Power Electronics Applications Workshop, ISiCPEAW, Kista, Sweden, 2011.
- [2] K. Ino, M. Miura, Y. Nakano, et al., 2019 IEEE International Conference on Electron Devices and Solid-State Circuits
- [3] Advanced Technology Materials, Inc., 7 Commerce Drive, Danbury, CT 06810-4169.
- [4] Cree Research, Inc., 2810 Meridian Parkway, Durham, NC 27713.
- [5] Casady J B, Johnson R W 1996 Solid-State Electron. 39 1409.
- [6] J. Millán, P. Godignon, Xavier Perpiñà, A. Pérez-Tomás and J. Rebollo, "A survey of wide bandgap power semiconductor devices," IEEE Trans. Power Elec., vol.29, no. 5, pp. 2155-2163, May 2014.
- [7] M. Xapsos, IEEE Transactions on Nuclear Science, 2019, 66 (1), 17-37.
- [8] Lichtenwalner D J, Akturk A, McGarrity J, et al. Reliability of SiC power devices against cosmic ray neutron single-event burnout[J]. Materials Science Forum, 2018, 924: 559–562.
- [9] S. Kuboyama, C. Kamezawa, N. Ikeda, et al., IEEE Trans. Nucl. Sci., 53 (2006) 3343-3348
- [10] A. F. Witulski, R. Arslanbekov, A. Raman, et al., IEEE Trans. Nucl. Sci., 65 (2018) 256-261
- [11] Javanainen Arto, et al. "Molecular Dynamics Simulations of Heavy Ion Induced Defects in SiC Schottky Diodes." IEEE Transactions on Device and Materials Reliability 18.3 (2018).
- [12] C. Abbate, et al. "Thermal damage in SiC Schottky diodes induced by SE heavy ions." Microelectronics Reliability 54.9-10(2014). doi:10.1016/j.microrel.2014.07.081.
- [13] Li, M. B. , et al. "High Single-Event Burnout Resistance 4H-SiC Junction Barrier Schottky Diode." IEEE Journal of the Electron Devices Society 9 (2021).

Heavy ion energy influence on multiple-cell upsets in small sensitive volumes

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Multiple-cell upsets (MCUs) have become the primary physical mechanism behind single-event upsets (SEUs) in advanced nanometer node devices. The range of ionization track effects increases with higher ion energies, and spacecraft in orbit primarily experience SEUs caused by high-energy ions. However, ground accelerator experiments have mainly obtained low-energy ion irradiation data. Therefore, the impact of ion energy on the SEU cross-section, charge collection mechanisms, and MCU patterns and quantities in advanced nanometer devices remains unclear.

In this work, based on the experimental platform of the Heavy Ion Research Facility in Lanzhou (HIRFL), low- and high-energy heavy-ion beams were used to study the SEUs of 28nm SRAM devices. The influence of ion energy on the charge collection processes of small-sensitive-volume devices, MCU patterns, and upset cross-sections was obtained, and the applicable range of the inverse-cosine law was clarified. The results revealed that low-energy ions induce higher MCU ratios and SEU cross-sections in low- and medium-LET regions, whereas at high-LETs, MCU ratios become similar. The discrepancies in MCUs are attributed to the varied influence of ion energy on the charge collection mechanism. Low-energy ions displayed superior direct charge collection and bipolar amplification gains in the low- and medium-LET regions. At a high LET, the well potential perturbations induced by heavy ions of different energies are similar.

In tilted testing in the medium-LET region, we clarified the applicable range of the inverse-cosine law for effective LET methods. This law applies only if both the dominant charge collection mechanism and occupancy of the sensitive region remain constant as the incidence angle changes. The trend in SEU cross-section resulting from high-energy ions at tilted incidences resembles that of vertical incidence, whereas the distinction between the SEU cross-sections of low-energy ions and zero-angle incident ions tends to initially increase and subsequently decrease. This is because the dominated charge collection mechanism for high-energy ions shifts only at approximately 45° and stabilizes to be dominated by the parasitic bipolar effect at 60°. In contrast, the dominated charge collection mechanism for the low-energy heavy ions undergoes an abrupt shift immediately upon the initiation of the tilt angle. The findings of this study are an important guide for the accurate evaluation of SEUs in advanced nanometer devices and for the development of radiation-hardening techniques.

Review of research progress on single particle effects in SiC MOSFETs

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With the rapid development of space technology, SiC MOSFETs have been increasingly applied due to their unique advantages. However, the single particle effects caused by high-energy particle radiation in the environment (such as SEB and SEGR) have gradually become prominent. Mizuta et al. first studied the single particle effect of SiC MOSFETs in 2014 [1]. In 2016, Wang Jingxuan et al. studied the physical mechanisms of SEB and SEGR induced by Br, I, and Au heavy ion irradiation on SiC MOSFETs. They found that the SEGR threshold decreased continuously with the increase of LET value, and proposed methods to increase the thickness of the gate oxide layer or replace high K materials to improve its radiation resistance [2]. In 2017, Liu Zhongyong et al. used TCAD simulation research to believe that 4H-SiC is more radiation resistant than 6H-SiC [3]. In 2018, Witulski et al. found that the SEB damage threshold is closely related to the particle incident position, and the entire process of electrical performance degradation is mainly related to the opening mechanism of parasitic BJT [4]. In the same year, Ikpe et al. found that parasitic BJTs did not participate in the SEB induction mechanism of SiC MOSFETs because compared to Si based MOSFETs, SiC MOSFETs require higher voltage to activate parasitic BJTs [5]. In 2019, Yu Qingkui et al. found that when the rated voltage is below half, heavy ions can cause permanent damage to the interior of the device, and radiation damage can lead to significant leakage and even SEB [6]. In the same year, Martinella et al. found that when the VDS was low, the leakage current path caused by heavy ion irradiation was from the drain to the gate. When VDS is high, the leakage current path is from the drain to the source [7]. In 2020, the team used microbeam research to demonstrate that the main contribution area of leakage current will gradually shift from the JFET region below the gate oxide layer to the pn junction region as VDS increases [8]. In the same year, Ball et al. found that under the localized high-energy effect induced by ions, as well as the larger electric field at the epitaxial/substrate interface, collision ionization significantly enhanced the SEB degradation phenomenon in heavy ion irradiated MOSFETs and diodes [9]. In 2023, Yu Qingkui's team conducted a study on SEGR in SiC MOSFETs and found that the gate oxide in SiC MOSFETs is the most sensitive to SEE, and gate oxide damage is positively correlated with bias voltage, LET, and flux[10]. For cases where the gate bias during irradiation is less than half of the rated voltage and no gate breakdown occurs, post gate stress testing should be conducted after the experiment to determine whether potential defects have occurred. At present, research mainly faces the following problems: the evolution process and physical mechanism of SiC MOSFET SEE are unclear. Difficulty in finding critical conditions for current degradation, burning, and grid breakdown. Lack of research on the synergistic effects of TID and SEE on devices. Lack of radiation resistant reinforcement technology for SiC MOSFETs. The radiation resistance evaluation system for SiC MOSFETs is not mature.

Keywords: SiC MOSFET, single particle effect, SEB, SEGR, radiation hardened

References

- [1] Mizuta E, Kuboyama S, Abe H, et al., IEEE Trans on Nuclear Science, 2014, 61 (4), 1924-1928
- [2] WANG Jingxuan, WU Hao, WANG Yongwei, et al., Smart Grid, 2016, 4 (11) : 1078 – 1081
- [3] LIU Zhongyong, CAI Li, LIU Xiaoqiang, et al., Micronanoelectronic Technology, 2017, 54 (2), 80 – 85
- [4] Witulski A F, Ball D R, Galloway K F, et al., IEEE Trans on Nuclear Science, 2018, 65 (8), 1951 – 1955.
- [5] Ikpe S A, Lauenstein J M, Carr G A, et al., 2016 IEEE Int Reliability Physics Symposium (IRPS) .
- [6] YU Qingkui, et al., Atomic Energy Science and Technology, 2019, 53 (10) : 2114 – 2119.
- [7] Martinella C, Stark R, Ziemann T, et al., IEEE Trans on Nuclear Science, 2019, 66 (7) : 1702 – 1709.
- [8] Martinella C, Ziemann T, Stark R, et al., IEEE Trans on Nuclear Science, 2020, 67 (7) : 1381 – 1389.
- [9] Ball D R, Galloway K F, Johnson R A, et al., IEEE Trans on Nuclear Science, 2020, 67 (1) : 22 – 28.
- [10] YU Qingkui, et al., ICREED 2023.

Irradiation response of SiOC under simultaneous helium and silicon ion irradiation

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SiOC is an amorphous ceramic that has been intensively studied recently due to its potential applications in harsh environments requiring extreme radiation tolerance. For example, SiOC could be used in reactors and spent fuel storage if the materials can sustain their amorphous phases. In amorphous materials, the concept of point defects does not apply. The effects of radiation damage and displacement creation do not change the overall dimensions and structures. The lack of grain boundaries also makes it superior in corrosion environments. Although SiOC has been intensively studied using ion irradiation, so far there has been no experimentation involving simultaneous helium ion irradiation and self-ion irradiation. Hence, the potential synergistic effects from gas atom introduction and damage production are unclear. In this study, amorphous SiOC is irradiated using a 150 keV helium ion beam and a 1.5 MeV silicon ion beam simultaneously, at room temperature, 300°C, and 500°C. A focused ion beam is used to lift out specimens for transmission electron microscopy characterization. Cross-sectional TEM and selected area electron diffraction both show that SiOC retain its amorphous phase under all these irradiation conditions. Nanometer-sized Si-enriched precipitations, however, appear at all irradiation temperatures. Surface scanning electron microscopy characterization shows periodic patterning appearing on the surfaces of room temperature and 300°C irradiated samples, but not in 500°C irradiated samples.

Ion irradiation and finite element analysis to assess the effect of swelling on Cr-coated cladding

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By combining ion irradiation and finite element analysis, the effect of irradiation-induced swelling on the structural integrity of nuclear reactor components can be assessed. In this study, ion irradiation is used to obtain the void swelling as a function of damage level in pure chromium (Cr). Compared to other pure metals such as iron, Cr swells easily and exhibits almost no incubation period for swelling. The experimentally obtained swelling curve is then used as input in finite element analysis to evaluate the interfacial stress buildup in Cr-coated zircaloy tubes at reactor operation temperatures. As one accident-tolerant fuel design currently under evaluation by the nuclear industry, Cr coating can improve the oxidation resistance of zircaloy fuel cladding under abnormal conditions. However, the debonding likelihood of the Cr coating from Zircaloy tubes needs to be evaluated. Without irradiation, the interface stress between Cr and the fuel cladding is primarily caused by differences in thermal expansion coefficients between Cr and Zircaloy. With irradiation, the stress becomes much more complex as Cr exhibits void swelling, while the Zircaloy tube does not. This void swelling effect can be modeled by modifying the thermal expansion coefficients of Cr. The methodology reported in this study can be applied to other coating systems to evaluate their radiation tolerance.

Self-ion irradiation of ZrC up to 300 displacements per atom

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ZrC is a candidate as fuel matrix in high-temperature gas-cooled reactors and as first wall materials for fusion reactors, owing to its high melting point, low neutron capture cross-section, and good mechanical properties. The radiation tolerance of ZrC is critical in such applications. Due to the excessive vacancies that naturally form in ZrC, it is expected that ZrC has excellent defect recombination efficiencies. In this study, ZrC is manufactured using plasma sintering techniques. Self-ion irradiation by carbon ions of 5 MeV is carried out at room temperature, 300°C, and 600°C, with ion fluences up to 300 displacements per atom (dpa). Transmission electron microscopy characterization shows that ZrC does not exhibit amorphization under any of these irradiation conditions. No phase changes are observed. Raman spectra display well-separated acoustic and optical bands in the wavenumber region less than 800 cm⁻¹. These bands show gradual broadening with increasing damage levels. For wavenumbers higher than 800 cm⁻¹, D and G modes, absent in the virgin sample, appear after irradiation. The increasing D/G mode intensity with rising damage levels suggests localized graphitization. Overall, the study demonstrates the excellent amorphization tolerance of ZrC under extreme conditions.

Defects and structural modifications in MgF₂ with high energy heavy ion irradiation aiming at improving UV optical applications

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MgF₂ is widely used as an optical material for multilayer coatings for far UV optical space^[1,2] and laser applications^[3]. The far ultraviolet (FUV, wavelengths shorter than 200 nm) spectral range contains fundamental spectral lines for astrophysics and solar physics communities, who require efficient optics and coatings tuned at such wavelengths. Multilayers (MLs) based on two fluorides are the only available coatings to provide narrowband FUV reflectors. The most common materials to make these MLs alternate either AlF₃ or MgF₂ with LaF₃^[1,2]. MLs based on these materials are proposed for LUMOS (LUVOIR Ultraviolet Multi-object Spectrograph) instrument for future space observations. The interest has been recently renewed on alkali halides^[3,4] and, particularly, in nanostructured MgF₂, due to their important properties, applications and possible new light emission features^[5,6].

Ion irradiation is a well-known method to modify most of the physical properties of the near surface region of materials. This can be addressed using both, high energies (several MeVs, i.e. using the electronic damage), or lower energies (i.e. using the nuclear damage). We have studied for this broad project the physical and optical changes induced in MgF₂ (both in bulk samples and in ultrathin evaporated films) irradiated with a broad set of ions (He, C, F, Si, I), energies (1-50 MeV) and fluences, aiming at devising strategies to improve UV optics or to find new optical properties in the high emission capabilities.

We have used several complementary characterization methods:

- Simultaneous in-situ optical measurements such as Ionoluminescence [7] and Absorbance for obtaining a detailed kinetics of the defects and damage creation and accumulation. However, these techniques provide integral information of the whole ion range, including both electronic and nuclear damage. In order to characterize the in-depth defects/damage profiles we have also addressed other methods:
- Optical reflectance measurements have been used since provides direct surface information.
- Irradiation at external heavy ion beam so as to use the energy degradation due to ion propagation in air to record a “spectroscopic” stripe of damage, to be combined with measurements of IL, OD, Photoluminescence (PL) excited with UV and micro Raman spectroscopy.
- RBS/C has also been performed to obtained in-depth damage profiles for high fluences
- Using thin film MgF₂ samples,
- Optical waveguide fabrication & characterization using high energy ions such as 20-40 MeV C, F, Si.

References:

- [1] S. Schröder et al., "Nanostructure and optical properties of fluoride films for high-quality DUV / VUV optical components," Proc. SPIE 5963, 59630R (2005).
- [2] P. López-Reyes, et al., Opt. Mater. Express 11 (2021) 1678-1691.
- [3] A. Gatto et al., “Towards resistant vacuum-ultraviolet coatings for free-electron lasers down to 150 nm,” Appl. Opt. 45, 7317 (2006).
- [4] K. Schwartz, C. Trautmann, R. Neumann, Nuc. Instrum. Methods in Physics Research B 209 (2003) 73-84.
- [5] A.N. Novikova, et al., Journal of Luminescence 209 (2019) 244–250
- [6] A.P. Voitovich et al., Journal of Luminescence 201 (2018) 57–64
- [7] M.L. Crespillo, J.T. Graham, F. Agulló-López, Y. Zhang, W.J. Weber, Crystals, 11 (2021) 315.

Submicro patterning in LiNbO₃ by Fe ion implantation for the assessment of novel type of photovoltaic optoelectronic tweezers

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In the last years, photovoltaic optoelectronic tweezers (PVOT) have emerged as a versatile multifunctional tool for a large variety of applications in different fields, such as optical manipulation and trapping of nano-objects [1], optofluidics [2], plasmonics [3] or biotechnology/biomedicine [8], to cite a few. The technique is based on the bulk photovoltaic effect. It is a singular phenomenon that appears in a few crystalline ferroelectric materials (LiNbO₃ clearly standing out) when properly doped (mainly Fe). By default, the available iron doped LiNbO₃ crystals (Fe:LN) are homogeneously doped in bulk format. In addition, these crystals are much more expensive than the nominally pure LN.

The required optimum Fe atomic concentration for good PVOT performance is of the order of 1/1000. 24 MeV Fe implantation at the CMAM, UAM have been used to obtain such moderate concentrations, locally in a submicro pattern format to be exploited, in the implanted layer. We have used here in-situ annealing during irradiation to prevent damage/disorder accumulation taking place at the first few microns beneath the surface [4]. Successful PV trapping, along the implanted Fe line, of silver nanoparticles diluted in solvent is shown in the photograph.

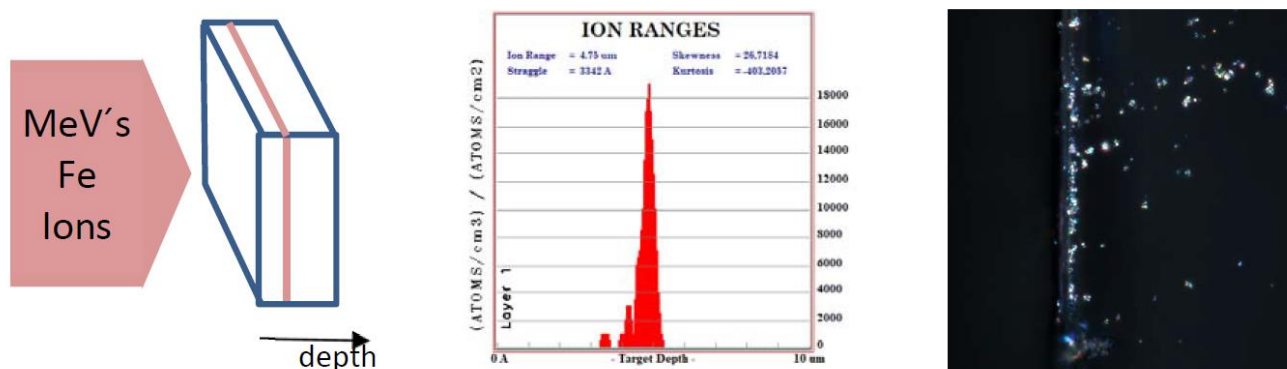


Figure 1 Left: Schematic 3D drawing, not to scale, of the proposal for generating Fe doped lines (of mm-cm length) of submicron thickness by Fe implantation in a standard pure LN sample; and then using the polished perpendicular surface to the ion implanted surface to study the PVOT performance. **Middle:** SRIM calculations showing the depth profile of the implanted Fe ions for the case of 24 MeV Fe ions. Most ions are implanted and concentrated in a thin layer of < 500 nm thickness. **Right:** Micro-photograph of Ag nanoparticles trapped along the Fe implanted line position.

References:

- [1] M. Carrascosa, A. García-Cabañes, M. Jubera, J.B. Ramiro, F. Agulló-López, Appl. Phys. Rev. 2, 040605 (2015)
- [2] L. Chen, S. Li, B. Fan, W. Yan, D. Wang, L. Shi, H. Chen, D. Ban, S. Sun, Sci. Rep. 6, 29166 (2016)
- [3] I. Elvira, J.F. Muñoz-Martínez, M. Jubera, A. García-Cabañes, J.L. Bella, P. Haro-González, M.A. Díaz-García, F. Agulló-López, M. Carrascosa, Adv. Mater. Technol. 2, 1700024 (2017)
- [4] A. Blázquez-Castro, J.C. Stockert, B. López-Arias, A. Juarraz, F. Agulló-López, A. García-Cabañes, M. Carrascosa, Photochem. Photobiol. Sci. 10, 956–963 (2011)
- [5] M. L. Crespillo, O. Caballero-Calero, V. Joco, A. Rivera, P. Herrero, J. Olivares and F. Agulló-López. Appl. Phys. A. (2011).

Utilising Boron-Oxygen Complexes for Monitoring of Ion Implant Fluence and Uniformity

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The Ion Beam Centre at the University of Surrey has run an in-house QA program for over 10 years, both for quality purposes and as part of the ISO9001 accreditation. For the technical aspects of the ion implantation service, the QA program is concerned with...

1. The uniformity of the implanted dose across the wafer
2. The repeatability of the implanted dose
3. The absolute accuracy of the dosimetry system
4. The sensitivity of the dosimetry system

Typically, implant QA has been performed using ion implantation of an appropriate electrical dopant species into silicon wafers; this is then followed by an activation anneal followed by Four-Point-Probe (4PP) analysis and Rutherford Backscattering Spectroscopy (RBS) analysis.

For the new 1.25MV implanter recently installed at the University of Surrey Ion Beam Centre, performing a “traditional” implant (i.e., an electrically active dopant species into silicon) is not possible due to the nature of the ion source technology that the tool employs. Therefore, a new technique has had to be developed whereby a p-type silicon wafer pre-doped with boron is implanted with oxygen and subsequently annealed. The implanted oxygen combines with the boron to form a complex defect that degrades the carrier lifetime; this is a process that has been widely studied and investigated and is well understood by the semiconductor community. The degradation of carrier lifetime results in an increase in the sheet resistivity of the wafer from the initial pre-doped value and allows 4PP analysis to be performed as a function of implanted dose without having to directly implant an electrically-active dopant.