

# Program

Komitee Forschung mit nuklearen Sonden und S ╲ Ionenstrahlen









Liebe Ionenstrahler,

herzlich willkommen an der Universität Duisburg-Essen! Mitten in der Metropolregion Ruhrgebiet gelegen, zählt unsere Universität mit rund 40.000 Studierenden zu den größten und zugleich jüngsten Universitäten Deutschlands. Seit ihrer Gründung im Jahr 2003 hat sie sich zu einer international anerkannten Forschungsuniversität entwickelt und ist an zahlreichen Sonderforschungsbereichen beteiligt. Besonders hervorheben möchte ich den SFB 1242 – "Non-Equilibrium Dynamics of Condensed Matter in the Time Domain", dessen großzügige finanzielle Unterstützung diesen Workshop erst ermöglicht hat.

Ich wünsche allen Teilnehmern einen inspirierenden Workshop mit exzellenten Vorträgen und anregenden Diskussionen.

Lars Breuer

Dear Ion Beam Users,

welcome to the University of Duisburg-Essen! Located in the heart of the Ruhr metropolitan region, our university, with approximately 40,000 students, is one of the largest and also one of the youngest universities in Germany. Since its founding in 2003, it has developed into an internationally recognized research institution and is involved in numerous Collaborative Research Centers (SFBs). I would especially like to highlight SFB 1242 – "Non-Equilibrium Dynamics of Condensed Matter in the Time Domain", whose generous financial support has made this workshop possible. I wish all participants an inspiring workshop with excellent presentations and stimulating discussions.

Lars Breuer



# Proton Beam Based Production of a Positron Emitter by Exploiting the  $27$ Al(p,x)<sup>22</sup>Na Reaction

### C. Hugenschmidt, L.-M. Krug, L. Chryssos

Compact setups for defect spectroscopy based on positron annihilation conventionally comprise a  $\beta^*$  emitter as positron source. We produced <sup>22</sup>Na sources by irradiating aluminum targets with a 68 MeV proton beam available at the cyclotron at the Helmholtz-Zentrum Berlin (HZB). The design of the target allowed the production of multiple positron sources at once as well as the analysis of the depth dependent activity of  $^{22}$ Na, which was found to be in agreement with the simulated depth profile. In total, a <sup>22</sup>Na activity of 140(23) kBq was produced, which is spread over 50 individual Al discs whereby the highest activity achieved amounts to 4.62(23) kBq. Using the activated Al discs as positron emitters intrinsically avoids wet chemical processes. The production of stronger sources is desired for positron annihilation spectroscopy experiments can easily be achieved by irradiating the target for a longer period of time. Other radionuclides among <sup>7</sup>Be, <sup>48</sup>Sc, <sup>54</sup>Mn and <sup>56</sup>Co were produced with a total activity of 70(5) kBq, but can be avoided aside from 7Be by using aluminum of a higher purity.

# Status of the low-energy ion beam facility and of the EU projects ReMade@ARI and RIANA

### $S.$  Facsko<sup>1</sup>, D. Erb<sup>1</sup>, R. Heller<sup>1</sup>, G. Hllawacek<sup>1</sup>, N. Klinger<sup>1</sup>

#### *<sup>1</sup>Helmholtz-Zentrum* Dresden*-Rossendorf*

At the Ion Beam Center (IBC) of HZDR a Low Energy Ion Nano-Engineering Facility (LEINEF) is currently being commissioned. The aim of this facility is to broaden and advance experiments with ions of low (10 eV) to medium (< 500 keV) energy and to enable new experiments with cluster and highly charged ions beams. Combined with in-situ preparation and characterisation in UHV by chemical and structural analysis before, during, and after ion processing, the study of ion doping, ion implantation and modifications of thin films and novel 2D materials becomes possible without deterioration.

The facility comprises a 100 keV accelerator platform equipped with several ion sources including a duoplasmatron, a liquid metal ion source, an electron beam ion source (EBIT), and a cluster ion source. In addition, separate irradiation chambers for highly charged ions and for surface nanopatterning by ion erosion are included in the new facility. Connected by a UHV linear transfer system, different characterisation tools are also available: Medium Energy Ion Scattering (MEIS), a variable temperature Scanning Probe Microscopy (AFM/STM), a Scanning Electron Microscope (SEM), Auger Electron (AES) and X-Ray Photoelectron Spectroscopy (XPS). For the preparation of surfaces and thin films a Pulsed Laser Deposition and a preparation chamber are planned. An additional chamber will allow the flexible modular extension for in-situ optical, electric, and magnetic properties.

Finally, I will also report on the status of the two running EU-projects ReMade@ARI and RIANA, which offer trans-national access to European infrastructures from the ARIE network (including European Ion Beam Centers) for the development of materials for the circular economy and for research in nanoscience and nanotechnology, respectively.

# Hyperfine parameters of  $181$ Ta implanted into TiO<sub>2</sub> from density functional theory simulations

## <u>J. Siqi<sup>1</sup></u>, J. Schell<sup>1</sup>

### *<sup>1</sup>CERN*

The electric field gradient (EFG) of the  $181$ Ta impurities doped in the rutile TiO<sub>2</sub> single crystals (denoted <sup>181</sup>Ta(TiO<sub>2</sub>)) was measured using the time differential e<sup>-</sup>γ perturbed angular correlation (e<sup>-</sup>γ TDPAC) spectroscopy by the ion-implanted <sup>181</sup>Hf tracers that decays to  $181$ Ta. The main parameters include largest component of the electric field gradient tensor ( $V_{\rm z}$ ), asymmetry parameter (*n*) which characterize the interstitial  $^{181}$ Ta trace impurities surrounded by the octahedral-like TiO<sub>2</sub> host matrix surroundings. This study aims at investigating the temperature dependence of the hyperfine parameters in  $^{181}$ Ta(TiO<sub>2</sub>) though Density Functional Theory (DFT) simulation. The challenges lie in that introducing the effect of finite temperature on atomic electric field gradient (EFG) since DFT could only calculate the properties at the ground state of the system. Secondly, in the doped supercell system, the local symmetry could not represent the global symmetry. Hence three approaches were tested at different levels. As a classical starter, the frozen phonon method is tested where only harmonics is considered. Secondly, *ab initio* Molecular Dynamics (AIMD) was performed trying to statistically yield the expected EFG at specific temperatures in the NPT ensemble but failed due to the inaccuracy of calculating EFG at the atomic coordinates that is far away from its ground state. Lastly, quasi-harmonic approximation is under testing where the thermal expansion of the lattice is considered. Currently, a decent combination of functional + basis set is under investigation.

### Rare nuclide target production (short talk)

### J. Franke $1$

#### *<sup>1</sup> Max-Planck-Institut für Kernphysik Heidelberg*

The high-precision Penning trap mass spectrometer PENTATRAP located at the Max-Planck-Institute for nuclear physics in Heidelberg is able to measure mass ratios of highly-charged ions with a relative uncertainty of  $10^{-11}$  or better. PENTATRAPs setup features five synchronously operated traps and access to external ion sources. The production of highly-charged ions is realized in an electron beam ion trap (EBIT). So far the measurements are restricted to stable or long-lived ions. The goal of this thesis is to investigate the feasibility of using ion implantation as a technique to prepare laser targets of rare nuclides. This is of interest because it would give PENTATRAP access to nuclides with lifetimes down to several weeks and which are only available in small quantities. The ions of interest, especially  $7B$ e, can be produced and implanted at ISOLDE, a radioactive beam facility.

Ion implantation is a process where ions of one element are accelerated into a solid target and thereby implanted. If the resulting impurity concentration is high enough and close to the surface, the modified target could be put in the EBIT where it would then be irradiated by a laser which would cause ablation of the target material as well as the implanted species.

As the first task of the project the mean implantation depth and depth distribution for different target materials and a singly-charged <sup>7</sup>Be beam of energies up to 30 keV will be investigated through a simulation software (SRIM). A test setup for the implantation of  $7$ Li (as a temporary replacement for  $7$ Be) into various target materials will be developed, which includes the design of a low-energy ion gun. Then the interaction of lasers with the different target materials needs to be studied theoretically as well as in an experimental setup to ensure stable evaporation of the implanted species. Finally the prepared targets will be placed in the EBIT where a time-of-flight spectrum can be measured.

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

## M. Dürr<sup>1</sup>, P. Schneider<sup>1</sup>, P. Keller<sup>1</sup>, I. Schubert<sup>2</sup>, M. Bender<sup>2,3</sup>, C. Trautmann<sup>2,4</sup>

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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. Here we investigate fragmentation of oligopeptides induced by SHI using soft cluster-induced desorption/ionization mass spectrometry as an analytical tool [1]. Mass spectra of SHIirradiated samples show a high abundance of specific fragments, i.e., cleavage took place at the peptide bonds of the peptide backbone [2]. 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 thus pointing towards a clear influence of the molecular structure on the fragmentation process.

### **References**:

[1] M. Baur, et al., Rapid Commun. Mass Spectrom. 28, 290 (2014).

- [2] P. Schneider, et al., Sci. Rep. 12, 17975 (2022).
- [3] P. Schneider, et al., Anal. Chem. 92, 15604 (2020).

# Efficient production routes of  $129$ m, $131$ m, $133$ m $Xe$  for a novel medical imaging technique, gamma-MRI

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The future gamma-MRI imaging modality will allow the simultaneous exploitation the advantages of SPECT –sensitivity of gamma-ray detection, and MRI –spatial resolution and flexibility. The combination of these technique requires use gamma-emitting nuclei (like in SPECT) with highly polarized spins, leading to anisotropic emission of gammaray, and allowing spin manipulation with rf pulses (like in MRI).

An efficient production of 11/2 spin isomers  $129mXe$  (T<sub>1/2</sub>=8.9days),  $131mXe$  $(T_{1/2}=11.8$ days) and  $^{133m}$ Xe (T<sub>1/2</sub>=2.2days) is an important aspect of the gamma-MRI project. This contribution will present results of systematic studies of two production routes: at ISOLDE and in nuclear reactors. At ISOLDE, during four beamtimes in 2022 and 2023, we investigated the best production and implantation conditions. We used a UC<sub>x</sub> with plasma ion source and a cooled transfer line and implanted beams of different Xe isotopes inside the GLM chamber into aluminium and gold foils with and without beam sweeping for seconds and hours. We then compared the number of implanted ions and the activity of the samples determined with ISOLDE gamma detectors to our simulations based on the ISOLDE in-target yields. As a result, we could determine the isomeric ratio for 11/2 to 3/2 states and the total efficiency of xenon extraction from the target. The study will allow us to determine the best conditions to collect high-activity samples (>10MBq) of  $129$ m, $131$ m, $133$ m $Xe$ .

The second method production of  $129mXe$  and  $131mXe$ , which we investigated in several campaigns between 2020 and 2024, is based on neutron irradiation of highly enriched stable  $^{128}$ Xe and  $^{130}$ Xe samples in the high-flux nuclear reactors: RHF reactor at Institute Laue-Langevin (ILL, Grenoble, France) and MARIA reactor in the National Centre for Nuclear Research (NCBJ, Swierk, Poland). We developed and optimised experimental setups for efficient enclosure of stable Xe, extraction and characterisation of the produced xenon isomers. The results show that both reactors provide isomer activities sufficient for the project (>50 MBq) with few unstable contaminants. The presentation will give a brief introduction to the gamma-MRI technique and will provide experimental details as well as results of xenon-isomer production at ISOLDE and at ILL and MARIA reactors.

### Current status of MINIBEE – Minibeam beamline for preclinical experiments

A. Rousseti<sup>1</sup>, J. Bundesmann<sup>2</sup>, A. Denker<sup>2</sup>, A. Dittwald<sup>2</sup>, G. Dollinger<sup>1</sup>, M. Kang<sup>2</sup>, G. Kourkafas<sup>2</sup>, J. Neubauer<sup>1</sup>, . Reindl<sup>1</sup>

*<sup>1</sup>Universität der Bundeswehr München <sup>2</sup>Helmholtz-Zentrum Berlin*

Radiotherapy aims to broaden the therapeutic window while protecting healthy tissues. Novel techniques, like proton minibeam radiotherapy (pMBT) can contribute to this goal. pMBT exploits the benefits of proton beams combined with spatial fractionation. Preclinical studies have already highlighted the potential of pMBT in sparing healthy tissues while better tumor control is also possible. Constructing a minibeam beamline for preclinical experiments (MINIBEE) at the Helmholtz Zentrum Berlin (HZB) will offer the possibility of doing systematic research in the field. HZB has a proton beam of 68 MeV, which is appropriate for studies in small animals. Dipoles and quadrupole triplets transport the beam to the experimental room where a high gradient quadrupole triplet generates the minibeam by magnetic focusing. Also, a pair of scanning magnets will be used for raster scan applications. If necessary, the beam's energy can be modulated by a degrader right after the cyclotron, defining the highest energy, and a range shifter close to the target can create a Spread-out Bragg peak (SOBP) to fully cover the tumor. A small animal radiation research platform will be used for animal imaging and positioning and a microscope will offer the option for in vitro studies. A simulation study has been conducted showing that the proposed facility can generate minibeams with σ=50μm, center-to-center (ctc) distance in the mm range and beam current up to 1nA. The facility can intensify the research in pMBT to fully understand the underlying mechanisms.

# IBEX: A blood flow simulation system for advanced proton therapy research (short talk)

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*<sup>1</sup>Universität der Bundeswehr München <sup>2</sup>Helmholtz-Zentrum Dresden-Rossendorf*

Radiotherapy aims to broaden the therapeutic window while protecting healthy tissues. Novel techniques, like proton minibeam radiotherapy (pMBT) can contribute to this goal. pMBT exploits the benefits of proton beams combined with spatial fractionation. Preclinical studies have already highlighted the potential of pMBT in sparing healthy tissues while better tumor control is also possible. Constructing a minibeam beamline for preclinical experiments (MINIBEE) at the Helmholtz Zentrum Berlin (HZB) will offer the possibility of doing systematic research in the field. HZB has a proton beam of 68 MeV, which is appropriate for studies in small animals. Dipoles and quadrupole triplets transport the beam to the experimental room where a high gradient quadrupole triplet generates the minibeam by magnetic focusing. Also, a pair of scanning magnets will be used for raster scan applications. If necessary, the beam's energy can be modulated by a degrader right after the cyclotron, defining the highest energy, and a range shifter close to the target can create a Spread-out Bragg peak (SOBP) to fully cover the tumor. A small animal radiation research platform will be used for animal imaging and positioning and a microscope will offer the option for in vitro studies. A simulation study has been conducted showing that the proposed facility can generate minibeams with σ=50μm, center-to-center (ctc) distance in the mm range and beam current up to 1nA. The facility can intensify the research in pMBT to fully understand the underlying mechanisms.



### News from ISOLDE

### $H.Heylen<sup>1</sup>$

#### *<sup>1</sup>CERN*

The scientific programme at ISOLDE-CERN covers a broad spectrum of research with radioactive beams. This includes studying the structure of exotic nuclei and astrophysics through precision measurements, decay experiments, and nuclear reactions using post-accelerated beams. Another distinct area of research involves leveraging radioactive isotopes as powerful probes for applications in condensed matter physics and life sciences.

With almost six decades of expertise and continuous advancements in target and ion source technologies, the ISOLDE facility provides access to around 1300 isotopes of 75 chemical elements. Serving a diverse community of over 1000 users from across Europe and beyond, ISOLDE conducts 45 to 55 experiments annually using one of its 15 experimental stations.

In this presentation, I will offer an overview of the facility and highlight recent developments. Following that, I will outline strategies to address current challenges and discuss plans to expand scientific opportunities beyond the current capabilities of the facility.

### Solid State Physics at ISOLDE-CERN

### J. Schell $^{1,2}$

#### *<sup>1</sup>CERN <sup>2</sup>Universität Duisburg-Essen*

ISOLDE-CERN is the worldwide reference facility for the production and delivery of radioactive ion beams of high purity. The produced beam is dedicated to many different purposes for, e.g., atomic and nuclear physics, astrophysics, material science, biophysics, and medical research. Since the late 70s the laboratory is pioneer in the use of nuclear techniques for studying local properties of materials using hightechnology equipment [1]. For instance, the brand-new ultra-high-vacuum implantation chamber called ASPIC's Ion Implantation chamber (ASCII) [2] decelerates the radioactive ion beam delivered at ISOLDE-CERN allowing to perform ultra-low energy ion implantations, and local measurements on the surface and interface of materials. The new MULTIPAC setup for Perturbed Angular Correlation Experiments in Multiferroic (and Magnetic) Materials [3] consists of a unique cryogenic magnetic system that simultaneously allows to measure local magnetic and ferroelectric properties of materials in magnetic fields up to 8.5 T. Last, but not least, the eMIL-Setup [4] is an advanced emission Mössbauer spectrometer for measurements in versatile conditions of several classes of materials, thanks to the emission Magnetic Mössbauer Analyzer (eMMA) extension [5]. This presentation introduces the new setups as powerful tools and discuss the possibilities of investigations on the frontiers of solid-state physics research [5].

#### **References:**

- [1] https://doi.org/10.1088/1361-6471/aa81ac
- [2] https://doi.org/10.3390/cryst12050626
- [3] https://cds.cern.ch/record/2845935/files/INTC-I-249.pdf
- [4] https://doi.org/10.1016/j.nima.2020.163973
- [5] http://cds.cern.ch/record/2705975/files/INTC-I-211.pdf

# Diffusion in HCP high-entropy alloys: intricate interplay of chemical complexity and lattice distortions

S. Sen, X. Zhang, L. Rogal, J. Schell<sup>1,2</sup>, G. Wilde, B. Grabowski, S. Divinski<sup>3</sup>

*<sup>1</sup>CERN <sup>2</sup>Universität Duisburg-Essen <sup>2</sup>University of Münster*

Self-diffusion of Ti, Zr, Sc and Zn in hexagonal close-packed (HCP) Al-Sc-Hf-Ti-Zr multiprincipal element alloys is measured using the radiotracer technique and utilizing the CERN facility for implantation of the <sup>46</sup>Sc isotope. In the investigated temperature interval, no systematic deviations from linear Arrhenius temperature dependencies are observed. Alloying equiatomic HfTiZr with Al and Sc enhances self-diffusion rates and the effect becomes more pronounced with increasing Al content. The selfdiffusivities in the present multi-principal element alloys are found to exceed the values predicted by simple geometric means of the corresponding diffusion coefficients in the pure metals by orders of magnitude, a phenomenon which we refer to as 'anti-sluggish' diffusion. Lattice distortions are speculated to dominate the relative enhancement of self-diffusion in these HCP high-entropy alloys, inducing the 'anti-sluggish' behaviour. The interplay of chemical complexity and local atomic strains is quantified using ab initio-informed calculations. The mean-square atomic displacements are shown to contribute to the observed "anti-sluggish" diffusion behavior in these high-entropy alloys.

### Bismuth Ferrite, the Drosophila in Multiferroics Research

### D. Lupascu $<sup>1</sup>$ </sup>

#### *<sup>1</sup>Universität Duisburg-Essen*

Bismuth Ferrite is a type-I multiferroic, meaning that the same crystal incorporates two a priori independent ordering phenomena. Below the polar ordering temperature,  $T_c$ =1100 K, the lone pair electrons of the Bi<sup>2+</sup>-ions drive the crystal into a polar crystal phase which exhibits high temperature ferroelectricity and yields the best ceramic piezoelectric material at high temperatures. This phase is not only polar, but the polar domains can be switched by external electric fields making the material a classical ferroelectric. Below the Néel temperature,  $T_N = 643$  K, the material additionally exhibits antiferromagnetic ordering. This fact has driven the inherent dream to partly alter the crystal such that the anti-order turns into an effective magnetization that can be influenced by the outside, namely external fields. The search for such a system is ongoing, because it would offer the possibility to generate magnetoelectric coupling for a multitude of technological applications. On-top of these properties, BiFeO<sub>3</sub> also exhibits a fairly small bandgap making it susceptible to the influences of light. Nanoparticles have proven to be outstanding photocatalysts. This presentation will outline all these interesting features of this material and their real and potential applications, before the details of material investigations using nuclear techniques will be presented in the following presentations.

# Independent characterization of electric and magnetic sublattices in bismuth ferrite

 $\underline{\text{T}}$ . T. Dang<sup>1</sup>, M. Escobar Castillo<sup>1</sup>, A. Dubey<sup>1</sup>, S. M. Fathabad<sup>1</sup>, A. M. Gerami<sup>2</sup>, J. N. Gonçalves<sup>3</sup>, J. Heiniger-Schell<sup>1,4</sup>, D. Lewin<sup>1</sup>, D. C. Lupascu<sup>1</sup>, I. C. Jie Yap<sup>1</sup>, D. Zyabkin<sup>5</sup>

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The time differential perturbed angular correlation (TDPAC), a nuclear solid-state technique, has been demonstrated to be an effective approach for characterizing ferroic materials at the unit- cell scale, employing a radioactive probe as a tracer ion. Proper use of the tracer ion can be instrumental in investigating ferroic materials at both the ferroelectric and magnetic sublattices independently, whereas Mössbauer probes, another nuclear solid-state technique, are limited to exploring the magnetic sublattice only. This talk will discuss the importance of TDPAC in comparison to other microscopic and macroscopic approaches to probe multiferroic bismuth ferrite at both Bi and Fe sublattices using different tracer ions. Our data show that a very large coupling of magnetic moment and electrical distortions arises on the magnetic sublattice (Fe site). The oxygen octahedra around the iron site experience a large tilt due to the onset of magnetic ordering. Nevertheless, the Bi-containing complementary sub-lattice carrying the ferroelectric order is practically unaffected by this large structural change in its direct vicinity. The magnetoelectric coupling thus vanishes already at the unit cell level. These experimental results agree well with an ab-initio density functional theory (DFT) calculation.

### AMS at HZDR - Status of DREAMS and update on the new HAMSTER facility

 $G. Rugel<sup>1</sup>$  A. Wieser<sup>1,2</sup>, A. Rolofs<sup>1</sup>, A. Wallner<sup>1,3</sup>, D. Koll<sup>1</sup>, J. Wolf<sup>1</sup>, J. Lachner<sup>1</sup>, K. Stuebner<sup>1</sup>, R. Ziegenrücker<sup>1</sup>, S. Fichter<sup>1</sup>, S. Zwickel<sup>1,3</sup>, S. Winkler<sup>1</sup>, T. Döring<sup>1</sup>

*<sup>1</sup>Helmholtz-Zentrum Dresden-Rossendorf <sup>2</sup>University of Vienna <sup>3</sup>TU Dresden*

Accelerator Mass Spectrometry (AMS) is an ultrasensitive method for detection of naturally or anthropogenically produced long-lived radionuclides in our environment. Up to now we use the DREsden AMS-facility (DREAMS) at the Helmholtz-Zentrum Dresden-Rossendorf (HZDR). In operation since 2011 and based on a 6 MV Tandetron (manufactured by High Voltage Engineering Europa), this accelerator facility is shared with other research groups. A focus of DREAMS is the measurement of the cosmogenic radionuclides Be and Al. Over the years, we have improved the DREAMS measurement capabilities in various aspects. One example is an improvement in the Be measurement efficiency by a factor of 1.4 [1].

Currently a second, dedicated AMS facility, HAMSTER (Helmholtz Accelerator Mass Spectrometer Tracing Environmental Radionuclides), is being set up at the Department of Accelerator Mass Spectrometry and Isotope Research. HAMSTER is based on a 1-MV tandem accelerator from NEC (National Electronics Corp.) and will have enhanced actinide measurement capabilities. In addition, it is featuring a new ion cooler we develop in cooperation with the University of Vienna [see talk of A. Wieser] allowing laser-based isobar separation. In this presentation, I will highlight present and future AMS capabilities at HZDR.

#### **References:**

[1] Lachner, J., et al. (2023) Nucl. Inst. Meth. B 535, 29.

### Ion-Laser Interaction in Accelerator Mass Spectrometry

### A. Wiesner<sup>1,2</sup>, J. Lachner<sup>1</sup>, O. Marchhart<sup>2</sup>, M. Martschini<sup>2</sup>, S. Merchel<sup>2</sup>, R. Golser<sup>2</sup>, A. Wallner<sup>1</sup>

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Accelerator mass spectrometry (AMS) is a highly sensitive method for detecting longlived radionuclides in the environment. However, large accelerators with terminal voltages > 10 MV are required to efficiently measure radionuclides in the mass range 60-200 amu, with few exceptions. In this region of the nuclide table are radionuclides important in astrophysics ( $182$ Hf) and environmental sciences ( $135$ Cs,  $90$ Sr), which cannot be detected with necessary sensitivity using conventional AMS.

To overcome this problem, an ion-laser interaction setup (ILIAMS) has been coupled to the Vienna Environmental Research Accelerator (VERA) AMS facility, which is based on a 3 MV tandem accelerator. ILIAMS suppresses interfering isobars by laser photodetachment and molecular dissociation processes. This method is independent of the relative nuclear charge difference between the isotope of interest and the interfering isobar. Consequently, it can be employed for isotopes across the entire range of the nuclide chart [1]. For many radionuclides, ILIAMS is so efficient that no additional element separation is required in the detection system. In extreme cases, no chemical preparation of samples is required. It has been demonstrated for stony meteorites that the ratios  $^{26}$ Al/<sup>27</sup>Al and  $^{41}$ Ca/<sup>40</sup>Ca could be measured directly by suppressing the isobars  $^{26}$ Mg and  $^{41}$ K by 14 and 11 orders of magnitude, respectively [2]. This way, measurements are performed with only a few mg of meteorite material without any chemical pre-treatment.

ILIAMS has been further developed into a new ion-laser interaction setup (ILTIS), which was designed and built at the Helmholtz-Zentrum Dresden-Rossendorf (HZDR) in cooperation with the University of Vienna. This setup is coupled to the new dedicated AMS facility HAMSTER (Helmholtz Accelerator Mass Spectrometry for Tracing Environmental Radionuclides) at HZDR based on a 1 MV tandem accelerator.

Part of this project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101008324 (ChETEC-INFRA) and grant agreement No 824096 (RADIATE).

[1] Martschini et al. 2021, 5 years of Ion-Laser Interaction Mass Spectrometry – Status and prospects of isobar suppression in AMS by lasers

[2] Bischoff et al. 2024, Cosmic pears from the Havelland (Germany): Ribbeck, the twelfth recorded aubrite fall in history

# Independent characterization of electric and magnetic sublattices in bismuth ferrite

### R. Dohmen<sup>1</sup>, T. Bissbort<sup>1</sup>, S. Chakraborty<sup>1</sup>, D. Rogalla<sup>1</sup>

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The main focus of studies in Mineralogy that apply ion beam analysis are the determination of diffusion coefficients for a variety of elements in minerals. Solid-state diffusion controls a variety of processes, for example dislocation and diffusion creep, the closure of radiogenic isotope systems or thermometers based on element exchange between minerals. In addition, in the last two decades diffusion modeling became a powerful tool to determine time scales of geological and planetary processes. All these applications rely on the accurate determination of the relevant diffusion coefficients.

The main approach of our group to measure diffusion coefficients for minerals is based on thin-film diffusion couples that were produced by pulsed laser deposition. Before and after the diffusion anneal concentration depth profiles of the elements of interest were determined by Rutherford-Back scattering, Nuclear Reaction Resonance analysis or Secondary Ion Mass Spectrometry. With this approach we determined diffusion coefficients for example for Cr-Al interdiffusion in spinel, Fe-Mg interdiffusion in various silicates or H diffusion in glasses. In this presentation we will give examples on these three cases of our data and discuss their applications.

# Electron doped double-layered perovskite manganite  $Ca<sub>2.8</sub>Nd<sub>0.2</sub>Mn<sub>2</sub>O<sub>7</sub>$ : Crystal structure, magnetism and local probing

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Oxygen octahedral distortions, including tilts/rotations, deformations, and offcentering in naturally layered perovskites, can result in ferroelectric polarisation known as hybrid improper ferroelectricity [1], paving the way for a possible route for the development of room temperature ferroic and multiferroic compounds.  $Ca_3Mn_2O_7$ , a Ruddlesden-Popper structure-based naturally bilayer manganite, is a hybrid improper ferroelectric compound with tremendous interest due to potential multiferroicity. The crystal structure of  $Ca_3Mn_2O_7$  consists of two-layer  $CaMnO_3$  perovskite blocks separated along the perovskite axis by an extra CaO rock-salt layer to form a natural superlattice with alternating bilayer perovskite blocks displaced by a half unit cell in the in-plane direction. Similar to the 3D perovskite analogue  $Ln_{1-x}A_xMnO_3$  [2], the bilayer manganites are expected to show complex evolution of crystal structure, magnetism and transport properties as a function of composition. Electron/hole doping induces manganese valence state fluctuation, which plays a core role in tailoring the magnetism and transport properties of manganite. Here we report the evolution of structure, magnetic behaviour and local probing studies on bilayer manganite Ca<sub>2-x</sub>Nd<sub>x</sub>Mn<sub>2</sub>O<sub>7</sub> ( $x = 0 - 0.5$ ). Doping with trivalent Nd ion (electron doping) induces manganese valence state fluctuation  $(Mn^{4+}/Mn^{3+})$ , thereby introducing a ferromagnetic component  $(Mn^{4+}-O-Mn^{3+})$ : double exchange) in the antiferromagnetic matrix  $(Mn^{4+}-O-Mn^{4+})$ : super exchange) resulting in competing magnetic interactions and low temperature frozen spin states. Atomic scale study has been carried out using the local probe technique, Perturbed γ-γ angular correlation (PAC spectroscopy), which confirms phase pure low symmetric polar structure at 300 K, high symmetric non-polar structure at 1200 K and the evidence for magneto-electric coupling below 100 K.

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ISOLDE-CERN:  $111 \text{m}$ Cd beam time and IS647 research proposal for the study of Perovskites.

### Swift heavy ion induced cratering and track formation in Bi nanomaterials

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In recent decades, extensive research has focused on interaction processes of various materials with swift heavy ions. Despite the increasing prominence of nanomaterials in applications such as sensors and electronics, their behavior under swift heavy ion exposure remains poorly understood. The unique characteristics of nanomaterials, including their high surface-to-volume ratio and reduced dimensionality affecting e.g. thermal conductivity, can significantly influence their response to irradiation. Conducting detailed, size-dependent studies is crucial for a better understanding of the unique ion-nanostructure interactions.

At GSI, we currently combine our expertise in the production of tailored nanostructures by ion-track nanotechnology and electrodeposition, with the capability to analyze insitu as well as ex-situ material modification produced by swift heavy ion irradiation.

In this contribution, we will present recent experiments on swift heavy ion irradiation of Bi nanowires and films with diameters and thicknesses systematically adjusted between 30 and 1500 nm. The nanowires were fabricated by electrodeposition in iontrack etched polymer foils, Bi films were produced by thermal evaporation. Both, wires and films were exposed to Au ions (energies between 950 and 2200 MeV) of the GSI UNILAC accelerator, and the morphological, compositional and crystallographic changes were investigated by scanning and transmission electron microscopy (SEM and TEM) as a function of the ion fluence. In-situ resistivity measurements were performed on ion-irradiated Bi films. We will discuss the observed size-dependent effects such as roughness increase, and crater and track formation in the nanomaterials.

### Time Resolved Ion Induced Photoelectron Emission Spectroscopy (tr-IIPES)

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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 occur 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 photo ionization of a geometrically cooled gas jet coupled with a miniaturized buncher system. With the prospect of further reduction of the pulse duration to 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.

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### Additive Manufacturing of S-Band RF Cavities

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Globally, approximately 30,000 linear particle accelerators (linacs) are in operation, serving a range of functions, including basic research. A linac's fundamental components are radiofrequency (RF) cavities, which, due to their complex geometry and stringent vacuum requirements, are conventionally assembled from several parts joined through methods like brazing. This process is costly and often requires compromises in cavity design.

In contrast, additive manufacturing (AM) allows for one-piece production, potentially reducing costs while enhancing cavity performance. Our research focuses on exploitation this potential for S- and C-band RF cavities made from pure copper. We demonstrate a manufacturing approach that employs laser powder bed fusion (L-PBF/SLM) combined with chemical post-processing to enhance the electrical surface conductivity.

Prototypes of a 5-cell S-band drift tube resonator and side-coupled cavity cells, commonly used in linac systems for medical and industrial applications, have been successfully additively manufactured. Evaluation of these prototypes reveals that AM cavities perform comparably to conventionally manufactured in terms of e.g. vacuum tightness, geometric accuracy and surface conductivity. Simultaneously, AM allows for a major cost reductions and increased shunt impedance.

Our results highlight the potential of AM in RF cavity fabrication and, consequently, performance improvements for linacs.

# Exploring lattice sites and charge states of Fe following  $57$ Mn<sup>+</sup> implantation in InGaN

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 $In_xGa_{x-1}N$  is a versatile and tuneable key material in modern optoelectronics [1-3]. Iron (Fe) doping opens up additional avenues for engineering its properties, leading to potentially new and improved applications in electronics, optoelectronics, and spintronics. <sup>57</sup>Fe emission Mössbauer Spectroscopy (eMS) was employed to probe the lattice site, charge state and magnetic behaviour of Fe in InGaN. Temperaturedependent eMS measurements were conducted at ISOLDE/CERN using radioactive  $57$ Mn<sup>+</sup> ( $t_{1/2}$  = 1.5 min) ions which decay to  $57$ Fe. Our data analysis revealed ferrous iron  $(Fe<sup>2+</sup>)$  in a cation site (In/Ga) near a nitrogen vacancy, along with iron in a 3+ charge state exhibiting paramagnetism. The results obtained for temperatures ranging from 140 - 831 K showed the evolution of ferrous Fe from high-spin at 140 K to low-spin at 830 K. This is a result of the charge distribution of *3d* orbitals adopting symmetry at higher temperatures<sup>4</sup>. The Fe<sup>3+</sup> ions showed slow spin-lattice relaxation over the temperature range. Moreover, a  $T^2$  temperature relation of the relaxation rates was observed, akin to a two-phonon Raman process.

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# Irradiation with highly charged ions: Impact of the kinetic and potential energy on particle emission

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Ion beams are a strong tool for tailored modification of various solid properties, e.g. for manipulating a surface structurally on the nanometer scale as well as chemically regarding its stoichiometry. Since these modifications are relevant for applications such as for fabrication of membranes by pore creation [1], the investigation of ion-solidinteraction and understanding of its underlying fundamental effects are crucial for technological progress.

It is well known that both the kinetic energy and the potential energy of an ion have an influence on created defects regarding e.g. pore diameters. There are various models in literature describing kinetic and potential sputtering of the sample due to ion impacts in accordance with experimental data such as the linear cascade theory [2]. However, there is no generally admitted universal model considering all experimental observations especially for the influence of the potential energy. A founded analysis of an ion's energy deposition in a solid requires a separate analysis of the influence of the ion's kinetic and potential energy, respectively.

Our HICS setup located at the university of Duisburg-Essen is designed to vary the kinetic energy and the potential energy independently over a broad range. The highly charged ions are provided from an EBIS (Dresden EBIS-A, DREEBIT) and their potential energy i.e. charge state is selected via a magnetic sector magnet followed by an acceleration/deceleration unit [3].

We present time-of-flight secondary neutral mass spectrometry (ToF-SNMS) studies on the influence of the potential and kinetic energy on the sputter yield of  $WS<sub>2</sub>$ . In our studies we used highly charged Xe ions with potential energies between 12 keV and 40 keV and kinetic energies spanning from 20 keV to 260 keV. Our experiments show a linear dependence of the W sputter yield on both the kinetic and potential energy in these ranges. Nevertheless, the influence of the potential energy is stronger than the influence of the kinetic energy.

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# Influence of the substrate on pore creation in single-layer  $MoS<sub>2</sub>$  using highly charged ion irradiation

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Ion irradiation serves as a versatile tool for modifying 2D materials and surfaces, enabling the creation of defects, pores, and incisions. However, characterizing the nanometer-sized structural changes induced by ion irradiation has proven challenging, often necessitating high-resolution TEM. Notably, direct characterization of such defects has primarily focused on suspended 2D materials, neglecting the substrate's influence on defect formation during irradiation. To address this issue, we irradiated single-layer MoS<sub>2</sub> on a Si/SiO<sub>2</sub> substrate using highly charged ions (HCIs) at 20 keV and 180 keV and different charge states. Subsequently, the material was transferred to a TEM-grid and analyzed using scanning transmission electron microscopy (STEM). Welldefined, round pores were observed for all kinetic and potential energies, indicating a rather small influence of sputtered substrate material. In contrast to suspended MoS<sub>2</sub>, significant differences in both pore size and pore creation efficiency were evident. These observations hold particular significance for 2D material applications that utilize ion irradiation as a mean to create pores and catalytically active sites, as they allow for a precise control of pore density and defective area by choosing appropriate irradiation parameters.

### EBIS & ECRIS Applications - from Supernovae to Next Generation Transistors

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#### *<sup>1</sup>Dreebit GmbH | Pfeiffer Vacuum*

The Dresden EBIS-A is a table-top sized facility for ion production and acceleration with multiple application areas ranging from astrophysics to materials science and information technology. In this presentation, we give an overview of recent Dresden EBIS-A installations at various institutions worldwide to demonstrate their capabilities and inspire future projects.

Using colinear laser spectroscopy like it is done at the COALA apparatus at TU Darmstadt, it is possible to determine transition frequencies and fine-structure splitting in He-like low-Z Atoms, which are highly charged (e.g. C<sup>4+</sup>-Atoms 1). To reach the highest possible accuracy, the line shape of the fluorescence response function was studied for pulsed and continuous ion extraction modes, as the Dresden EBIS-A can provide both. Thus, the symmetry and linewidth could be optimized, and a high accuracy could be reached.

Moreover, EBIS-A machines can be used to study the interior of stars and supernovae by means of x-ray and optical spectroscopy, measuring characteristic x-rays form highly charged metal ions. The challenge here is the production of highly charged ions from rare earth elements. The solution provided by Dreebit is the technique of Metal Ions from Volatile Compounds (MIVOC) [3] in combination with a Metal Alloy Ion Source with the possibility to inject ions produced by both methods into the EBIS-A.

For materials research in solid state physics, highly charged ions (HCI) can be used to obtain permanent modifications of surfaces and to obtain next generation transistors [4,5] Those modifications range from isolated point defects to phase transitions. Ion induced surface features are widely studied, but the theoretical understanding of the mechanisms is difficult. Since the EBIS allows for production of ions with different charge states and a tunable kinetic energy, contributions from potential and kinetic energy deposition can be studied independently, gaining a deeper understanding of the interaction details.

In contrast to the highly charge low current EBIS systems, Electron Cyclotron Resonance Ion Sources (ECRIS) can provide much high current of single or double charged ions for various applications like particle therapy and fundamental research.

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# Materials science with radioactive isotopes - highlights from emission Mössbauer spectroscopy

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Intentionally incorporating foreign atoms in semiconductors to realize new and/or novel functionalities gives rise to structural changes that profoundly affect their electronic, magnetic and optical properties. Consequently, information on material properties and dynamic processes such as dopant diffusion and relaxation processes are necessary and can be determined using various techniques. A particular class are techniques employing radioactive isotopes implanted in materials as probes. These combine a two-fold approach: (a) material modification and (b) material characterization at the atomic level, the latter achieved through utilizing the isotopes mainly as "spies" via the radiation/particles emitted during decay. This provides knowledge on lattice sites of desired daughter dopants, lattice location changes with thermal annealing, and the defects/complexes formed with host atoms.

Mössbauer Spectroscopy is a very sensitive technique capable of detecting minor shifts in energy levels that emanate from hyperfine interactions between the nuclear moments of the probe/dopant and any local electric and magnetic fields in their immediate environment. A novel extension is emission Mössbauer Spectroscopy (eMS) employing short-lived radioactive isotopes developed at ISOLDE, CERN. eMS studies have been undertaken mainly using  $57$ Mn\* ( $t_{1/2}$  = 1.5 min) produced via proton-induced fission in a UC<sub>2</sub> target followed by multistage laser ionization [1], mass separation and acceleration to 40-60 keV. In addition, other precursor isotopes, such as  $57$ Co (t<sub>1/2</sub> = 272 days) and  $119$ In (t<sub>1/2</sub> = 2.4 min), have also been used.

Over the years, eMS has been applied in several different material systems at ISOLDE, with investigations initially on the role of Fe in silicon to recent studies on the nature and origin of magnetic effects observed in transition metal doped semiconductors [2-5] envisaged for spintronic applications. Special features of the technique will be presented and discussed, together with highlights. These will focus mainly on the probe's lattice sites, charge and spin states, and magnetic interactions.

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# Influence of highly charged ion irradiation on the electrical and memory properties of black phosphorus field-effect transistor

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Black phosphorus (bP) is one of the more recently discovered layered materials. In particular its high hole mobility and finite, thickness dependent, direct bandgap may pave its way to new applications as optoelectronic devices. Utilizing the hysteresis in the transfer characteristics of bP field-effect transistors (FETs), several approaches to realize non-volatile memory devices have been successfully put forward. This hysteresis is commonly attributed to charge trapping and detrapping in defects and impurities either in the underlying substrate, or in the bP itself. In this work we deliberately introduce additional defects into bP FETs by irradiating the devices with highly charged Xe<sup>30+</sup> at a kinetic energy of 180 keV to manipulate the electrical and memory properties of the devices. We find an increase of conductivity and p-doping with increasing ion fluence, while other device parameters, like i.e. charge carrier mobility, degrade for the higher irradiation fluences. Most importantly, we find an increase in the width of the hysteresis and the memory window due to the irradiation. By controlling the kinetic energy of the ions, we can demonstrate, that this increase is caused by additional defects in the underlying  $SiO<sub>2</sub>$  substrate and not in the bP itself.

# Applications of Perturbed Angular Correlation (PAC) of γ-rays Spectroscopy in Biology

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PAC spectroscopy was first applied in biology in 1968, in a study of serum albumin [1]. Over the following decades a number of applications have appeared, demonstrating that PAC spectroscopy is useful tool for the study of local structure and dynamics at metal ion binding sites in biomolecules [2]. Selected examples of applications of PAC spectroscopy to metal ion binding proteins will be presented [3]

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# Enhanced Control System for Negative Ion Photodetachment Experiments Utilizing Beckhoff Automation

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Precise control of negative ion sources and beam parameters is critical for optimizing the performance of photodetachment experiments used in Accelerator Mass Spectrometry (AMS). In this work, we present a state-of-the-art control system designed to improve the stability and efficiency of a negative ion beam setup. The system leverages Beckhoff Automation's EtherCAT technology and TwinCAT software for real-time monitoring, data acquisition, and control.

Key operational parameters—such as voltage, current, vacuum pressure, and temperature—are continuously monitored using Beckhoff industrial hardware. Realtime data acquisition is integrated with Python scripts to extract live metrics, enabling dynamic adjustments to ensure stable ion beam performance and improve system reliability during operation.

To further enhance system management, we developed a custom graphical user interface (GUI) that provides real-time visualization of critical ion source parameters, including heater temperature, line heater temperature, power consumption, and resistance. This intuitive interface allows operators to monitor system performance and make immediate adjustments, improving usability, safety, and operational efficiency.

This control system represents a significant advancement in ion beam automation, offering a scalable and adaptable solution for controlling ion beam setups. By integrating Beckhoff technology with custom software, we deliver a flexible and reliable control environment capable of meeting the evolving demands of modern ion beam research. The system is also designed to accommodate more complex ion source configurations for future applications.

# Structural Transitions in metavanadates with  $111 \text{ m}$ Cd-TDPAC at ISOLDE (short talk)

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In this work, we investigated structural transitions in a series of metavanadates of Ca, Cd, Mn, and Zn as a function of temperature using TDPAC spectroscopy. At ISOLDE,  $111 \text{ m}$ Cd was produced and implanted into the vanadate samples, enabling the tracking of local modulations in charge density distributions through the analysis of evolving hyperfine parameters. We propose a strategy for identifying hyperfine interactions based on characteristic 'fingerprint' transitions within the metavanadate series. Additionally, we explore the influence of various factors on the temperaturedependent behavior of hyperfine parameters, including the relaxation of the nearest coordination sphere and ionic contributions.

# MULTIPAC/PACBIT: The 3rd Generation Time Differential Perturbed Angular Correlation (TDPAC) spectrometers in ISOLDE-CERN

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MULTIPAC and PACBIT are the next generation of digital spectrometers at ISOLDE-CERN that use the Time Differential Perturbed Angular Correlation (TDPAC) technique in versatile measurement conditions, such as the application of high-magnetic fields combined with low temperature measurements T >3.5 K.

TDPAC is a sensitive nuclear condensed matter physics technique used to investigate the hyperfine interactions of a studied material. By incorporating radioactive probes into particular sites of the crystal lattice, the local magnetic and electric fields, are characteristic of the studied material, and are determined via the Larmor frequency and/or via the electric field gradient. The hyperfine interactions occur in the intermediate state of the double gamma-ray (γ-γ) cascade of the radioactive probe.

MULTIPAC and PACBIT aim to bring more experimental capabilities and superior computing prowess as compared to the previous two generations. MULTIPAC incorporates a cryogen-free superconducting magnet, and a vibrating sample magnetometer (VSM). The all-in-one package allows users to explore simultaneously the local properties of magnetic or multiferroic materials and the external influences from the applied magnetic field.

PACBIT is the TDPAC hardware architecture of MULTIPAC and is being designed for ease of maintenance and for superior data acquisition. The PACBIT project also includes 1) software updates that include techniques of machine learning for data analysis and fitting, 2) modular instruments such as a cryostat for temperature measurements.

## Cage motion of Iron (Fe) in Silicon (Si)

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Due to its negative impact on semiconductor devices, iron (Fe) is one of the most thoroughly investigated impurities in silicon. It is a usual unintended impurity in silicon manufacturing, functioning as a fast diffuser and severely lowering carrier lifetimes, especially harmful for solar cells applications. It is still unclear how defects or other impurities interact with substitutional and interstitial Fe under implantation conditions.

Obtaining an understanding of the behaviour of metal impurities, such as Fe, in silicon can result in methods for improving gettering procedures, which transfer metallic impurities to less hazardous areas of devices.

This motivates investigation of the fundamental properties and behaviour of Fe in silicon at the atomic scale. Techniques such as emission Mössbauer spectroscopy and emission channelling provide valuable insights into the behaviour of dilute probe atoms in these contexts.

We demonstrate, using  $57$ Fe Mössbauer spectroscopy following implantation of  $57$ Mn  $(T<sub>2</sub> = 1.5)$  min. that substitutional Fe in silicon is not located on the ideal substitutional site, but exhibits cage motion or jumps via saddle sites, located 0.17(3) Å from the ideal substitutional site. In the temperature range from 300 K to 500 K, the jump rates follow an Arrhenius behaviour, with rates in the vicinity of  $10<sup>7</sup>$ -10<sup>8</sup> Hz and an activation energy of 0.18(3) eV. Our data also suggest compressive strain on substitutional sites and relaxing strain on interstitial sites when the implantation is below ~450 K. These findings provide new insights into the atomic-scale behaviour of Fe in silicon, which is essential for improving material processing and device performance.

### The M-branch at the GSI UNILAC: Status and applications in astrochemistry

### F. Koch<sup>1</sup>, I. Schubert<sup>1</sup>, D. Severin<sup>1</sup>, P. Simon<sup>1</sup>, M. E. Toimil-Molares<sup>1,2</sup>, C. Trautmann<sup>1,2</sup>

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The M-branch at the universal linear ion accelerator UNILAC of the GSI/FAIR facility in Darmstadt provides three end stations dedicated to international users from materials science and other cross-disciplinary research fields. Ion beams up to uranium of kinetic energy between 3.6 – 11.4 MeV per nucleon are available. In this energy regime, heavy ions induce complex structural modifications in the materials within a highly localized nanoscale damage zone. The M-branch beamlines are equipped with a large variety of in-situ and on-line characterization methods. In particular, the multiuse irradiation chamber at M3 is designed to easily adapt the in-situ analysis techniques and sample environments to new experiments and systems under investigation.

In this contribution we will provide an overview of the currently available analysis techniques, which include SEM, FTIR, UV-vis, XRD, SIMS/SNMS, Raman spectroscopy and a cryo- and high temperature stage, as well as an outlook of planned upgrades. Special emphasis will be put on recent astrochemistry experiments, where the ion beam is used to irradiate samples like ices to simulate the effect of cosmic radiation in astrophysical. Heavy ions, although only a small fraction of cosmic radiation, play a key role in the chemical processes occurring in interstellar clouds due to their large energy deposition.

In collaboration with international user groups from France, Slovakia and Germany, we apply in-situ IR spectroscopy at M-Branch to study the evolution of organic molecules, such as polyaromatic hydrocarbons or amino acids at temperatures as low as those of the clouds (~20 K), under irradiation. This yields destruction and creation crosssections, which are essential for astrochemical models aiming to explain the emergence and evolution of complex molecules in space, which are thought to be the precursors of life.

# Swift heavy ion irradiation of bismuth nanowires pressurized in diamond anvil cells

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The simultaneous exposure of materials to multiple extreme conditions is a field of increasing interest in modern high pressure research [1]. Applying concomitantly high pressures and irradiation with swift heavy ions (SHI) of GeV energies has demonstrated its potential in creating new phases and stabilizing high pressure phases down to ambient conditions [2,3].

In the present study, bismuth nanowire networks (Bi-NWNWs) were compressed to high static pressures and subsequently exposed to uranium ions provided by the GSI heavy ion synchrotron SIS18 in order to investigate the impact of ion irradiation on structure and high pressure phase transitions of nanomaterials. The experiments were performed using Bi-NWNWs with diameters between 35 and 85 nm fabricated by electrodeposition in etched ion-track membranes [4]. High pressure was applied by mounting the miniaturized samples in diamond anvil cells (DACs) followed by ion irradiation with relativistic heavy ions of typically several tens of GeV kinetic energy.

Preliminary results will be presented on the structural changes in compressed Bi-NWNWs observed using a newly installed experimental setup that enables in-situ characterization during ion irradiation through Raman spectroscopy. Additionally, highpressure x-ray diffraction studies on both irradiated and pristine Bi-NWNWs will be discussed. The aim of this project is to investigate to what extent size effects can be utilized in order to promote SHI-induced high p-T phase transitions and to provide insight into the mechanisms underlying the combined effects of pressure and ion irradiation.

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### Local effects in vanadia-based compounds (short talk)

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The current study focuses on the temperature-dependent structural modulation of the local environment of  $M^{2+}$  ions in vanadium bronzes  $M_xV_2O_5$  and vanadates  $xMnO-V<sub>2</sub>O<sub>5</sub>$ . The growing interest in  $V<sub>2</sub>O<sub>5</sub>$ -based materials is in view of their potential for cathodes in M ion batteries, as highlighted in recent research [1]. Although the (de)intercalation mechanism of M ions is considered fundamental to charge transfer [2], a detailed description of this process is still lacking. In this regard, it becomes interesting to investigate vanadia-based materials with local methods, such as Time-Differential Perturbed Angular Correlation (TDPAC) spectroscopy to gain deeper insights into the structural dynamics involved. Samples were synthesized using incipient wetness impregnation method and the standard Pechini route. The X-ray diffraction method was employed to control over sample quality. For TDPAC measurements, the radioactive probes were introduced either through ion implantation of  $111 \text{mC}$ d beam at ISOLDE or directly during synthesis using  $111$ InCl<sub>3</sub> sourced from IPEN-Brazil. The behavior of hyperfine parameters indicates a temperature-dependent modulation of the local environment of the Cd probes in both V<sub>2</sub>O<sub>5</sub>:Cd and xMnO-V<sub>2</sub>O<sub>5</sub>:Cd systems. The observed effect can be associated to either distortions induce by the probe atom; or to intrinsic local structural variation. The two possibilities will be discussed in this presentation.

# Nano-strain induced ferromagnetism in epitaxial thin films of bismuth ferrite (short talk)

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The existence of an uncompensated magnetic order in epitaxial thin films of multiferroic bismuth ferrite (BiFeO<sub>3</sub> or BFO) is still the subject of intense debate. The Time Differential Perturbed Angular Correlation (TDPAC) technique monitors local fields at the atomic scale without altering the structure of the investigated materials. Using such an approach, we observed that BFO epitaxial thin films exhibit local ferromagnetic order at the unit cell level. TDPAC data obtained at room temperature with the  $111 \text{mC}$ d probe show that the strong magnetic field (~ 5 Tesla) exists at the nonmagnetic sublattice (Bi site). It is assumed that the nano-strain resulting from the mismatch between the substrate and the BFO thin film produces a non-zero net local magnetisation of the sample.

# The study of silver diffusion in hard coatings by means of Ion Beam Analysis techniques

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Hard coatings of a few micrometre thickness are often used to extend the lifespan of machining tools and components for, e.g., automotive and aerospace applications [1]. A further increase of the lifespan of these tools and components can be achieved by making so-called self-lubricant coatings. They make use of self-adaptive mechanisms that can lead to a protective tribolayer as a solid lubricant [2]. Self-lubrication can be achieved by the incorporation of noble metals like silver in hard matrices. When applied in this way, silver can diffuse to the surface and act as a solid lubricant. However, these benefits are limited in time as the silver is released and is quickly depleted from the coating.

The fast depletion of silver can be reduced by encapsulating it in a dense barrier sandwich layer [3]. In this presentation, the diffusion of silver in two hard matrices (TiN and TiSiN) is studied during annealing by in-situ Rutherford Backscattering Spectrometry (RBS) using the cluster tool at HZDR [4]. Samples were annealed at 600°C and 800°C for two hours with continuous monitoring by RBS measurements. These show changes in the elemental distribution during and after annealing as a function of sandwich type and microstructure. The results are part of a larger study to understand the effect of microstructure of hard coatings on the diffusion behaviour of silver, which also includes Transmission Election Microscopy measurements [5].

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# ASCII: The Ultra-Low Energy Ion Implantation of Radioisotopes for Surface Characterization at ISOLDE-CERN (short talk)

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Over the past four decades, the Apparatus for Surface Physics and Interfaces at CERN (ASPIC) has been an ultra-high vacuum (UHV ≤10−8 mbar) setup installed in the ISOLDE experimental hall. It was dedicated to the study of metallic surfaces [1], the magnetic behavior of thin films [2], an interface evolution [3], among other systems, employing radioactive isotopes, and a variety of surface and thin film fabrication and modification techniques [4].

Recently, the installation has been upgraded with the creation of a brand-new UHV chamber known as the ASPIC's Ion Implantation Chamber (ASCII) [5]. Thus, the ASCII chamber's purpose is to implant radioactive ions at various energies, including ultralow (> 20 eV) values.

This allows to implant several probes, including  $(^{111m}Cd,^{204m}Pb)$  in two-dimensional materials (graphene, MoS2), (multi)ferroic materials, nanoparticles and topological insulators [5, 6]. Similar to the initial ASPIC chamber, it is kept at an extremely high vacuum of ≤10−9 mbar. The chamber was successfully tested at the University of Göttingen for implanting  $111$ Ag, including the beam sweep.

Currently, the setup is being finished at ISOLDE to become operational. Once the commissioning finishes, the setup will be available for the wide community of collaborators. In particular, ASCII will play an important role in nuclear condensed matter physics for the local study of surfaces and interfaces.

