O 31: Focus Session: Ion Beam Interaction with Surfaces and 2D Materials III

Time: Tuesday 10:30–12:45 Location: GER 38

Topical Talk O 31.1 Tue 10:30 GER 38

Ultra-low energy ion implantation of two-dimensional materials — •Hans Hofsäss[1], Felix Junge[1], Manuel Auge[1], Beata Kardynal[2], Ursel Bangert[3], Martin Wenderoth[4], and Lino Pereira[5] — [1]2nd Institute of Physics, University of Göttingen, Germany — [2]Peter Grünberg Institute, Forschungszentrum Jülich, Germany — [3]Department of Physics, University of Limerick, Ireland — [4]4th Institute of Physics, University of Göttingen, Germany — [5]Department of Physics, KU Leuven, 3001 Leuven, Belgium

Doping of two-dimensional (2D) materials by ion implantation requires unique requirements regarding ion energy, ion beam optics and sample preparation. Efficient substitutional incorporation of low energy ions into the 2D lattice requires energies around 20 eV. We use a low energy mass selected ion beam system with UHV implantation chamber. A 30 keV mass selected ion beam is guided through differential pumping stages and homogenized using a beam sweep. An area of about 1-2 cm^2 can be uniformly irradiated with these ultra-low-energy (ULE) ions with a beam current up to several microAmp. Results for doping of monolayer graphene with B^+, N^+ an P^+ ions and doping of 2D MoS_2 with Se^+ and Cr^+ ions will be presented. We discuss challenges for ULE ion implantation, such as non-flat substrates, ion sources and lateral selective doping. Results for analyses of the implantation efficiency and lateral doping are presented. The simulation of ULE ion implantation using novel Monte Carlo Binary Collision Approximation programs is also discussed.

O 31.2 Tue 11:00 GER 38

Low-Energy Ion Implantation with an electron beam evaporator — •Tom Weinert, Denise Jennifer Erb, Stefan Facsko, René Heller, and Ulrich Kentsch — Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Deutschland

For ion implantation of thin films and in particular of two-dimensional materials, it is necessary to reduce the ion energy down to 10eV. For this purpose, we develop a a simple and robust setup via a new approach. We use an electron beam evaporator to generate the desired ions. This has the advantage of a relatively small energy distribution of the ions, and in addition numerous different metal ions can be generated. An electrostatic analyzer is used to filter out the neutral atoms and to improve the energy distribution of the ion beam to below 5eV. The used ion energy is below 1keV and is suitable for the implantation of very thin surface layers or, after further energy reduction, for implantation in two-dimensional materials. Ion implantation can change the properties of two-dimensional materials, enabling, for example, new electrical, magnetic or catalytic applications.

O 31.3 Tue 11:15 GER 38

Fabrication of 2D magnets by ion implantation of phyllosilicates — Muhammad Zubair Khan[1], Nico Klingner[2], Gregor Hlawacek[2], Aleksandar Matković[1], and •Christian Teichert[1] — [1]Institute of Physics, Montanuniversität Leoben, 8700 Leoben, Austria — [2]Helmholtz-Zentrum Dresden-Rossendorf e.V., 01328 Dresden, Germany

Since the first reports on intrinsically magnetic two-dimensional (2D) materials in 2017 [1,2], the price-to-pay for accessing their monolayers is still the lack of ambient stability. Recently, we demonstrated weak ferromagnetism in 2D Fe:talc at room temperature and proposed iron-rich phyllosilicates as a promising platform for air-stable magnetic monolayers [3]. Since these minerals are rather rare and since phyllosilicates are hard to synthesize, we suggest here as an alternative ion implantation to tailor the magnetic properties of the phyllosilicates. Nonmagnetic, single-crystalline bulk talc crystals [4] were implanted with 50 keV iron and cobalt ion beams at different substrate temperatures. In all cases, ultra-thin layers could be exfoliated indicating that the layered crystal structure is maintained after ion irradiation. For both ion species, the Mg-OH Raman peak showed a triplet formation implying a successful substitution of Mg by Fe or Co in the talc layers.
[1] Gong, C., et al., Nature 546, 265 (2017). [2] Huang, B., et al., Nature 546, 270 (2017). [3] A. Matković, et al., npj 2D Mat. Appl. 5, 94 (2021). [4] B. Vasić, et al., Nanotechnology 32, 265701 (2021).

O 31.4 Tue 11:30 GER 38

Charge exchange of highly charged ions scattered under grazing incidence — •Matthias Werl, Anna Niggas, Friedrich Aumayr, and Richard A. Wilhelm — TU Wien, Institute of Applied Physics, Vienna, Austria

When a highly charged ion approaches a surface, electrons are resonantly captured from the material, starting at distances of $\approx 10-25$ Å above the surface. The electrons are captured into shells with $n \approx q_{in}$ (q_{in}: incident charge state), forming a hollow atom (HA) - a state where (mostly) high-n shells are populated. In the free case, these excited HAs would then decay via a combination of auto-ionization and radiative pathways, recharging the projectile in the process. At very close distances from a surface ($d_I \leq 3$ Å), another process, known as Interatomic Coulombic Decay (ICD), can take place. Here, the HA quickly decays to its ground state due to electron-electron scattering with electrons from the material.
To study the HAs and their free decay, neutralization via ICD is to be prevented. This can be achieved if the distance of closest approach is larger than d_I, which happens at very grazing angles. Previous experiments showed that only a minor fraction of charged particles survive up to the detector under an incident angle of $\alpha_{inc} = 1.6°$. Decreasing the incident angle even further ($0.1° \leq \alpha_{inc} \leq 1.0°$), more charged particles are expected to arrive at the detector.
Here, we present our setup to achieve these small incident angles with an accuracy of $\approx \pm 0.2°$ as well as first experimental results for the charge state distribution of the scattered projectiles.

O 31.5 Tue 11:45 GER 38

Green functions simulation of the energy and charge transfer between highly charged ions and 2D materials — •Michael Bonitz[1], Karsten Balzer[2], Hannes Ohldag[1], Jan-Philip Joost[1], Anna Niggas[3], and Richard Arthur Wilhelm[3] — [1]CAU Kiel, Institute for Theoretical Physics and Astrophysics — [2]CAU Kiel, Computing Center — [3]TU Wien, Institute of Applied Physics, Vienna, Austria

We have developed Nonequilibrium Greenfunctions (NEGF) - Ehrenfest dynamics simulations for the energy loss of ions that impact correlated 2D materials. An interesting prediction was an ion-induced increase of the doublon number [1]. Recently, these simulations were extended to highly charged ions and to the associated charge transfer and electron emission. We find reasonable agreement with the experimental predictions [2]. Here we discuss how these simulations can be extended to longer times and improved selfenergies via our G1-G2 scheme [3], combined with an embedding selfenergy approach [4].

[1] K. Balzer et al., Phys. Rev. Lett. 121, 267602 (2018); [2] A. Niggas et al., Phys. Rev. Lett. 129, 086802 (2022); [3] N. Schluenzen et al., Phys. Rev. Lett. 124, 076601 (2020); [4] N. Schluenzen et al., submitted for publication, arXiv:2211.09615

O 31.6 Tue 12:00 GER 38

Particle emission from 2d materials induced by highly charged ion impact — •Lucia Skopinski[1], Lars Breuer[1], Silvan Kretschmer[2], Arkady V. Krasheninnikov[2], and Marika Schleberger[1] — [1]Universität Duisburg-Essen, Duisburg, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Two-dimensional (2d) materials such as graphene or transition metal dichalcogenides are expected to be key materials for novel applications. Defect engineering by highly charged ion (HCI) beams could be a way to modify their unique properties even further. An ion carries energy in the form of kinetic energy E_{kin} and potential energy E_{pot}, the latter corresponding to the energy required to create its respective charge state. Once the ion impinges on the surface, its energy is deposited into the solid and can lead to modifications and sputtering. However, the fundamental mechanisms of defect formation due to HCI-surface interaction are still under investigation.
Here, we discuss the emission of secondary ions and atoms as well as their velocity distribution from a substrate supported 2d material under HCI irradiation. The measured distributions allow a distinction between sputtering driven by the potential and the kinetic energy of the primary ion. The potential sputtering yield of MoS_2 has a similar dependence on the potential energy as the pore formation found in freestanding MoS_2 after irradiation with HCIs. The low velocities of the emitted particles indicate an interaction mechanism connected to electron-phonon coupling.

O 31.7 Tue 12:15 GER 38

Highly charged ion-induced electron emission from atomically thin materials — •Anna Niggas[1], Karsten Balzer[2], Matthias Werl[1], Friedrich Aumayr[1], Michael Bonitz[3], and Richard Arthur Wilhelm[1] — [1]TU Wien, Institute of Applied Physics, Vienna, Austria — [2]Computing Center of Kiel University, Kiel, Germany — [3]Kiel University, Institute for Theoretical Physics and Astrophysics, Kiel, Germany

When a highly charged ion impacts on a material surface, its potential energy, i.e., the sum of the binding energies of all missing electrons, is deposited within the very first surface layers. This, in turn, triggers many processes such as the emission of electrons. While both the electron yield and energy distribution of bulk samples have been extensively studied in the past, data for 2D materials is rather scarce. This is due to the challenging task of separating signals of the 2D material itself from its support structure. Therefore, we developed a coincidence setup correlating ions after transmission with electrons emitted from the material. This allows us to discriminate signals from the support via the ion energy loss in the sample and, consequently, to access the emission from the 2D material alone.

In this contribution we will present our recent studies on the electron emission induced by highly charged ion impact on monolayers of graphene and MoS_2 and their 3D counterparts. We find a 6-fold higher emission yield for graphene compared to MoS_2 and a vanishing contribution of $< 10\,\mathrm{eV}$ electrons for MoS_2. These findings are supported by simulations of the ion-induced surface charge dynamics.

O 31.8 Tue 12:30 GER 38

Light ion transmission through atomically thin material: insights from non-adiabatic first-principles simulations — •Silvan Kretschmer[1], Arkady V. Krasheninnikov[1], Anna Niggas[2], Lukas Fischer[2], and Richard A. Wilhelm[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden, Germany — [2]TU Wien, Institute of Applied Physics, Vienna, Austria

Two-dimensional materials, as surface-only targets, are ideally suited to study the neutralization and deexcitation of charged particles. Using atomistic Ehrenfest dynamics simulations we rationalize the experimental findings obtained for transmission of H^+ and He^+ through graphene and 2D-MoS_2. Here semi-metal and semi-conductor are chosen exemplary to explore potentially different neutralization behaviour. Changes in the electronic structure are calculated along with the energy loss and the charge transfer from the target to the projectile during the transmission and compared to the experiment. Furthermore, low-charge state ions represent a suitable model system to validate the framework of Ehrenfest dynamics to be extended to their highly charged counter parts.