DS 49: Ion Interactions with Nano Scale Materials IV (Focused Session – Organisers: Diesing, Facsko)

Time: Thursday 17:45–19:15 Location: GER 37

Topical Talk DS 49.1 Thu 17:45 GER 37

Nano-scale surface modifications produced by highly charged ion impact — •Friedrich Aumayr — TU Wien, Inst. für Angewandte Physik

The large amount of potential energy stored in highly charged ions (HCI) is liberated during the interaction with a solid surface within a few femtoseconds into a nanometer size volume close to the surface. It is therefore not astonishing that severe surface modifications with nanometer dimensions have been demonstrated for the impact of individual slow HCI on various surfaces, similar to the impact of individual swift heavy ions. Depending on the type of material, nano-hillocks, nano-pits or caldera-like nano-craters have been found at the ion impact site.

Present research tries to control the production of material modifications on surfaces and thin films (including 2D carbon-nanosheets and graphene) with well-defined size in the nanometer region by a variation of the HCI potential energy. The current status of this rather new field will be presented.

DS 49.2 Thu 18:15 GER 37

Nanostructures induced by slow highly charged ions on KBr(001) surfaces — •Richard Wilhelm, René Heller, and Stefan Facsko — Helmholtz-Zentrum Dresden - Rossendorf – Institut für Ionenstrahlphysik und Materialforschung – Bautzner Landstraße 400 - 01328 Dresden

Highly charged ions carry a large amount of potential energy (up to 100 keV) which is defined as the sum of all binding energies of all missing electrons. This energy can be used to modify surfaces on the nano-scale and due to very low kinetic energies (less than 100 eV) significant bulk damage can be avoided. The production of nanometer sized pit-like structures on KBr(001) surfaces by the impact of single highly charged ions was studied in detail previously. The investigation of high fluence effects of highly and lowly charged ions is important to clearly identify the mechanism of defect mediated desorption as the driving force for the creation of pit-like nanostructures on ionic crystals like KBr. Results of high fluence compared to low fluence irradiations will be shown and kinetic and potential energy effects will be discussed.

DS 49.3 Thu 18:30 GER 37

Surface patterning by ion bombardment: predictions of large-scale atomistic simulations — •Bartosz Liedke, Karl-Heinz Heinig, Stefan Facsko, and Wolfhard Möller — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Germany

Despite of intense studies in recent years, atomistic understanding of surface evolution during ion irradiation is still under discussion. Continuum models, like the Bradley and Harper theory, cannot explain microscopic processes during ion irradiation. So far, atomistic simulations could not describe pattern dynamics on spatiotemporal scales of experiments.

We present a novel program package that unifies the simulation of collision cascades with kinetic Monte-Carlo simulations. The 3D atom relocations were calculated in the Binary Collision Approximation (BCA), whereas the thermally activated relaxation of energetically unstable atomic configurations as well as diffusive processes were simulated by a very efficient bit-coded kinetic 3D Monte Carlo code.

Our studies show that: (i) bulk defects continuously created within the collision cascade are responsible for local surface topography fluctuations and induce surface mass currents. These currents smooth the surface from normal incidence up to $\theta = 40°$, whereas at $\theta > 40°$ ripple patterns appear; (ii) sputtering is not the dominant driving force for the ripple formation at non-grazing incidence angles. Surface patterning is caused by processes like bulk and surface defect migration, recombination, bulk and surface diffusion and ion induced diffusion.

DS 49.4 Thu 18:45 GER 37

Temporally resolved track creation in dielectrics after swift heavy ion irradiation. Part I: Monte-Carlo simulation — •Nikita Medvedev[1,2], Orkhan Osmani[1,3], Marika Schleberger[3], and Baerbel Rethfeld[1] — [1]Technical University of Kaiserslautern, Germany — [2]CFEL at DESY, Hamburg, Germany — [3]University of Duisburg-Essen, Germany

The dynamics of structural modifications of dielectrics irradiated with swift heavy ions (SHI, with energies E > 1 MeV/u and masses M > 20 proton mass) are investigated theoretically. We developed a combination of Monte-Carlo method (MC), used to describe SHI penetration and following excitation and relaxation of the electronic subsystem, with Two Temperature Model (TTM) describing the heating of the lattice [1,2].

In part I of this report we describe the MC method and its main results: the thermalization time of electrons in track, the distribution of energies of electrons, holes, and lattice. That gives a physical background, limits of validity, initial conditions and parameters necessary for the subsequent TTM calculations, presented in the part II.

[1] N.Medvedev, A.E.Volkov, N.Stcheblanov, B.Rethfeld, Phys. Rev. B **82**, 125425 (2010)

[2] N.Medvedev, O.Osmani, B.Rethfeld, M.Schleberger, Nucl. Instrum. and Meth. B **268**, 3160 (2010)

DS 49.5 Thu 19:00 GER 37

Temporally resolved track creation in dielectrics after swift heavy ion irradiation. Part II: Two Temperature Model — •Orkhan Osmani[1,2], Nikita Medvedev[1], Bärbel Rethfeld[1], and Marika Schleberger[2] — [1]University of Duisburg-Essen, Germany — [2]Technical University of Kaiserslautern, Germany

The dynamics of structural modfications of dielectrics irradiated with swift heavy ions (E>1MeV/u and masses M>20 proton mass) are investigated theoretically. In part II of this report on our combined Monte Carlo–Two Temperature description we show that the results obtained from the MC calculations determine the conditions at which the TTM can be applied. Out of these results material parameters for the electron system, such as the specific heat capacity and the electron-phonon coupling, can be extracted. These parameters are necessary for the final track radii calculations within the TTM [1] and are often not accessible by experiments. It will be demonstrated how to couple the (kinetic) MC results with the (continuum) TTM simulation. Finally the computed track radius will be compared with experimental observations [2].

[1] O. Osmani, A. Duvenbeck, E. Akcöltekin, R. Meyer, H. Lebius and M. Schleberger, New J. Phys. 10, 053007 (2008)

[2] P. Kluth, C. S. Schnohr, O. H. Pakarinen, F. Djurabekova, D. J. Sprouster, R. Giulian, M. C. Ridgway, A. P. Byrne, C. Trautmann, D. J. Cookson, K. Nordlund, and M. Toulemonde, Phys. Rev. Lett., 101 175503 (2008)