MM 34: Computational Materials Modelling - Matter-Particle Interaction

Time: Wednesday 10:15–11:15 Location: IFW D

MM 34.1 Wed 10:15 IFW D

Structural evolution in a heavily irradiated BCC metal. — •Peter Derlet[1] and Sergei Dudarev[2] — [1]Condensed Matter Theory Group, Paul Scherrer Institute, Switzerland — [2]Department of Physics and Thomas Young Centre, Imperial College London, United Kingdom

Using atomistic simulations and a simplified and computationally highly efficient defect-creation protocol, we study the micro-structure emerging under high-dosage neutron and ion irradiation conditions. The so-called Creation Relaxation Algorithm (CRA) simulations exhibit the gradual transition from isolated defects to a micro-structure characterized by an extended dislocation network and a population of vacancy and interstitials. The corresponding internal stress/strain structure characterizes a spatially correlated and multi-scale potential energy-landscape whose material descriptors remain largely insensitive to further irradiation exposure. With full atomic resolution, the CRA rapidly produces a complex microstructure with strong experimental analogues in BCC materials experiencing doses relevant for the ITER fusion reactor project. Examples are given for both BCC Fe and W.

MM 34.2 Wed 10:30 IFW D

Post-ionization dynamics in proton-irradiated ice — •Daniel Muñoz-Santiburcio — CIC nanoGUNE, San Sebastián, Spain

Ion irradiation of water systems is receiving an increasing attention due to many important applications. In the case of liquid ice the main interests are the radiation damage of biological tissues and radiation treatment of tumors, while for water ice the interest concerns astrophysical/chemical processes taking place in interstellar dust, comets, asteroids and satellites.

Here I will show, in a first step, how it is possible to use the results of Ehrenfest MD simulations of the irradiation of ice with highly energetic protons to define plausible single- and double-ionized ice configurations; and in a second step, how these can be propagated via remarkably challenging ab initio MD simulations in order to observe different chemical reactions: *i*) the ultrafast conversion of the water cation H_2O^+ into the hydroxy radical $HO^\cdot$ plus the solvated H^+ which undergoes fast Grotthuss diffusion, and *ii*) the formation of H_2O_2 after the fragmentation of two neighboring H_2O^+.

MM 34.3 Wed 10:45 IFW D

Improved Stopping in the Binary Collision Approximation — •Alrik Stegmaier and Hans Hofsäss — 2. Physikalisches Institut, Universität Göttingen

Stopping of ions in materials is an important process in implantation physics, radiation safety, nuclear medicine, sputtering, proton beam writing and many more. As such, precise simulations of stopping are required, where typically a balance between accuracy and speed of the simulation is struck.

Due to the simplicity and relative accuracy, the binary collision approximation (BCA) is one of the most important models used for stopping today. In BCA stopping is treated as a series two body collisions.

Here we present an improved binary collision approximation model for ion stopping that is based on velocity dependent interatomic potentials. Both a new model for stopping of ions in an inhomogeneous electron gas and an approximate bond breaking/relaxation model for electronic stopping allow predictions over a large projectile velocity range and target structure.

The free parameters of the model are almost entirely constrained by density functional theory simulations and the properties of the (in-)homogeneous electron gas.

MM 34.4 Wed 11:00 IFW D

Quantum mechanical modelling of light-matter interactions — •Mark Kamper Svendsen and Kristian Sommer Thygesen — Technical University of Denmark, Kgs. Lyngby, Denmark

First-principles calculations based on density functional theory (DFT) have been pivotal for our understanding of the chemical, thermodynamic, and electronic properties of materials close to their ground state. However, when it comes to interaction with light such calculations are challenged in two important ways: First, the description of the electronic excited states is much more involved than the description of the ground state. In particular, collective excited states such as excitons or plasmons are challenging and not well described by standard DFT. Secondly, the light field is usually treated classically, and the quantum description is retained only for the electrons. This approximation can be justified in situations where the photon number is very large. However, in cases where the photon number is low and the field amplitude large, e.g. in cavities or near plasmonic structures, the quantum nature of the light field cannot be ignored.
We present a fully quantum mechanical model of the coupling between confined optical modes such as graphene plasmons and transitions in solid state systems. The model uses existing ab-inito methods to calculate the material properties and then uses those as input for accurate models of the light-matter interaction based on Macroscopic quantum electrodynamics.