Title

Atomistic modeling of irradiation-driven chemistry for 3D nano-printing of metals

Description and objectives

The Low Dimensional Materials group (https://www.empa.ch/web/s206/low-dimensional-materials) of the Laboratory for Mechanics of Materials (https://www.empa.ch/web/s206/overview) is developing novel nanostructures & nano-materials using various combinations of state of the art deposition techniques. This comprises the investigation of focused electron and ion beam induced chemical vapor deposition (FEBID, FIBID) as a specific selective deposition technique with the highest spatial resolution and potential as a 3D nano printing platform among other state-of-the-art nanomaterial fabrication methods.

Atomistic simulations are proven to be a useful tool for investigating the dynamics of atomic and molecular systems at the nanoscale. Using recent developments in modeling irradiation-driven chemistry, we would like to explore the dynamics of metal deposition induced by electron and ion beams at the nanoscale. This Master project aims to facilitate competence development in atomistic modeling of irradiation-driven chemistry by using top-notch computing infrastructure, recently acquired and managed by our modeling expert, Dr. Vladyslav Turlo (https://www.empa.ch/web/s204/modeling-simulations) from the Laboratory for Advanced Materials Processing, whose team of experts in atomistic modeling will provide extensive support during the project execution.

Workplan

As a part of an interdisciplinary team, you will first get in touch with the advanced simulation tool called LAMMPS (https://www.lammps.org/) and will learn the basics of molecular dynamics and mechanics methods. After that, you will learn the key aspects of irradiation-driven chemistry using FEBID and FIBID and will work closely with experimentalists to fine-tune the model to study the evolution of deposited atoms, forming metal clusters and nanoribbons on the free surface. Please check the following paper (https://www.nature.com/articles/s41598-020-77120-z) for more details. The goal of this project is to incorporate the irradiation-driven chemistry model into the open-source LAMMPS software to enable the large-scale simulations on Swiss National Supercomputing facilities, allowing for modeling millions or even billions of molecules simultaneously.

Required skills

General understanding of physics and chemistry (atomic and molecular structure, different types of bonding in materials, etc.). Prior experience with atomistic and molecular simulations would be an advantage.

Languages

English (Advanced)

Location

Empa Thun

Remark

The technical details of the project can be discussed with Dr. Vladyslav Turlo (vladyslav.turlo@empa.ch).

Related masters

Physics
Applied physics
Electrical and electronic engineering
Mechanical engineering
Microengineering
Robotics
Materials science and engineering
Computer science
Mathematics
Applied mathematics
Computational science and engineering