Contribution ID: **36** Type: **Oral**

#2011287 Cu Surface Diffusion Bias under Electric Field Gradient - Accelerated Molecular Dynamics, Finite Elements Method, and Density Functional Theory

Thursday, 22 September 2022 10:00 (30 minutes)

Vacuum-facing metal surfaces are exposed to strong electric fields in many devices, such as particle accelerators, free-electron lasers and fusion reactors. Under sufficiently strong fields, current can arc through the vacuum, disrupting and damaging these devices. Despite decades of research, the precise mechanisms of the vacuum arc breakdowns are still unknown. The interplay of different physical phenomena, as well as their associated length and time scales, pose numerous challenges in experiments and simulations.

In our earlier study [1], we showed in simulation that a runaway process of Cu nanotip melting and evaporation can produce the necessary material for the formation of plasma that will conduct the electric current through vacuum. An open question remains of the growth of these nanotips, as well as their sharpening for enhanced field emission and heating.

A proposed mechanism of biased diffusion under electric field gradient could contribute to mass transfer toward the extremities of any initial protrusions or roughness on the surface [2]. In the study at hand [3], we simulated Cu surface diffusion directly in these conditions using molecular dynamics (MD). The implementation of the electric field involves concurrently solving the Laplace equation of macroscopic electric field on a finite elements method (FEM) mesh that follows the discrete atomic system and extends beyond it. Furthermore, we extended the time scale of our simulations by the collective variable -driven hyperdynamics (CVHD) method for better collection of diffusion statistics. Finally, we estimated the surface polarization characteristics from our MD simulations, and compared them directly to density functional theory (DFT) calculations, finding good agreement.

In this talk, we will discuss the evidence we found for biased diffusion on Cu surface, as well as the practicalities of coupling CVHD-accelerated MD with FEM.

[1] Kyritsakis, Andreas, et al. Journal of Physics D: Applied Physics 51.22 (2018): 225203.
[2] Kyritsakis, Andreas, et al. Physical Review B 99.20 (2019): 205418.
[3] Kimari, Jyri, et al. In preparation.

Topic

Modeling and Simulations

Primary author: KIMARI, Jyri

Co-authors: KYRITSAKIS, Andreas; DJURABEKOVA, Flyura (University of Helsinki); Prof. ZADIN, Veronika (University of Tartu (EE)); WANG, Ye (University of Tartu (EE))

Presenter: KIMARI, Jyri

Session Classification: Modelling & Simulation

Track Classification: Simulations