MULTISCALE MODELLING OF NANO-PROTRUSION GROWTH ON METAL SURFACES UNDER ELECTRIC FIELD

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Recent experiments showed that femtosecond laser irradiation of a sharp 250 nm tungsten tip exposed to strong DC electric field leads to gradual and reproducible surface modifications [1]. Asymmetric surface faceting mainly on the laser-exposed side along with the formation of a few nanometers high nano-protrusion in the corner between the facets were observed. A metallic nano-protrusion with sharpness of a few nanometers, can be highly beneficial for many applications such as electron diffraction, microscopy, and holography. Therefore, investigation of the influence of electric field on surface evolution of metals may be an important input for finding technological solutions of nano-tip fabrication process.

The growth of nano-tips under intense fields is also of potential importance to the particle accelerator community. Strong rf-field, such as planned to use in the Compact Linear Collider (CLIC) at CERN, Switzerland [2], may induce the formation of nano-protrusions on the surface of copper accelerating structures. Shortlived nano-protrusions are believed to cause vacuum arcs, which significantly decrease the efficiency of the accelerator.

We first investigated the effect of laser heating on modifications of a W tip surface with the finite element analysis and Molecular Dynamics simulations. The formation of well pronounced asymmetric faceting was linked to the surface stress introduced by the ultrafast laser pulses exposed on one side of a W tip.

In order to research the mechanism of nano-protrusion growth , the electric field effect on the surface diffusion should be investigated. We used DFT nudged elastic band (NEB) simulations to find the minimum energy paths of the diffusion processes on W and Cu surfaces. DFT calculations were also used to find dipole moments and polarisabilities of W and Cu adatoms. The obtained results of the DFT calculations were then used to implement the effect of the electric field on the atomic energy barriers into the recently developed Kinetic Monte Carlo (KMC) model of surface diffusion for fcc and bcc metals [3]. We have parametrised the KMC model for W diffusion on W and investigated the mechanism of the nano-protrusion growth on faceted W surface under electric field.

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[2] The CLIC, et al. CERN Yellow Reports (2016).
[3] V. Jansson, E. Baibuz, F. Djurabekova Nanotechnology 27 (2016) 265708.