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Growth mechanism of a nano-protrusion on tungsten tip under electric field

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Understanding the mechanisms behind the growth of nano-protrusions on metal surfaces exposed to electric field is particularly interesting to the wide range of applications. Nano-protrusions growing on the electrode surfaces under the strong rf-field are proposed to cause vacuum arcs formations in Cu accelerating structures of CLIC. Recent experiments have shown that the femtosecond laser irradiation of a sharp tungsten tip exposed to the strong DC electric field leads to an asymmetric surface faceting mainly on the laser-exposed side along with the formation of a nano-protrusion few nanometers high. [1]

In order to research the mechanism of nano-protrusion growth, the long-term atomic diffusion should be taken into account. We have recently developed a Kinetic Monte Carlo (KMC) model of the surface diffusion for fcc and bcc metals[2]. This KMC model has to be parameterized for a material under study in terms of migration energy barriers and attempt frequencies for all possible diffusion jumps. In order to extend the KMC model with electric field, its effect on the energy barriers of the migrating atoms should be researched.

In the current work, we have used the DFT nudged elastic band (NEB) simulations to find the minimum energy paths of the diffusion processes on W surface under electric field. We have also used the DFT calculations to find dipole moments and polarisabilities of adatoms on W and Cu surfaces. We have explored the conditions of nano-protrusion growth on W tip under the laser irradiation and the field emission conditions within the scope of Molecular Dynamics and Kinetic Monte Carlo simulations.

[1] H. Yanagisawa, V. Zadin et al., APL Photonics 1 (2016) 091305.
[2] V. Jansson, E. Baibuz, F. Djurabekova, Nanotechnology 27 (2016) 265708.

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Modelling and Simulations

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