Parameterization of the Kinetic Monte Carlo model of the long-term evolution of metal surfaces

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Surface evolution of metals operated under high electric fields is of particular interest for wide range of applications. In the presence of high gradient electric field, such as in the accelerating structures of the Compact Linear Collider (CLIC) at CERN, Switzerland, defects on the Cu surface become of prime interest. Defects, such as short-lived nano-protrusions, are believed to cause vacuum arcs, which significantly decrease the efficiency of the accelerator. It is proposed that such protrusions grow when high electric field is applied, enhance the electric field enough to initiate an arc, and flatten down when the electric field is removed. The formation of the nanotips among with other defects as faceting are also observed in tungsten in the presence of electric field. Tungsten is widely used for operation under high electric fields and the prediction of its behaviour under field emission conditions is crucial for various applications.

A Kinetic Monte Carlo (KMC) model of surface diffusion has been developed in our group for fcc and bcc metals to access the long time-scale evolution of the surfaces. The model is extended to include the electric field effects on the diffusion of surface atoms. This KMC model has to be parameterized for every material in terms of migration energy barriers and attempt frequencies for all possible diffusion jumps.

We have developed a parameterization algorithm for calculating the migration energy barriers for the atom jumps using the Nudged Elastic Band (NEB) method. In order to reduce the barriers calculations, we characterize diffusion jumps with the number of nearest and next-nearest neighbour atoms of the initial and final sites only. The NEB calculations exhibit issues since some of the processes include atoms in unstable or metastable positions, making it impossible to find the minimum energy path with any of the minimisation techniques. We have developed methods to approach these problematic cases. The same attempt frequency, fitted to Molecular Dynamics data, was used for all jump processes. Our KMC model has been parameterized for Cu, Fe, W, and Au and validated by comparing with experimental and MD results with a good agreement.

We have studied the behaviour of Cu and W nanotips in the absence and presence of the electric field. The stability of W and Cu nanotips have been compared. The shape evolution of W nanotips in the presence of electric field has been simulated with KMC and the results have been compared with the experiments.

[1] M. Aicheler, P. Burrows,etc., CLIC Conceptual Design Report, CERN (2012).
[2] V. Jansson, E. Baibuz, F. Djurabekova F. Submitted.