SIMULATIONS OF METAL SURFACES UNDER HIGH ELECTRIC FIELDS IN CLIC VACUUM BREAKDOWN STUDIES

Simon Vigonski[1,2], Ekaterina Baibuz[2], Ville Jansson[2],
Alvo Aabloo[1], Flyura Djurabekova[2], Vahur Zadin[1]

[1]Institute of Technology, University of Tartu, Nooruse 1, 50411 Tartu, Estonia
[2]Helsinki Institute of Physics and Department of Physics, P.O. Box 43 (Pietari Kalmin Katu 2), FI-00014 University of Helsinki, Finland
Corresponding author: simon.vigonski@ut.ee

The Compact Linear Collider (CLIC) [1] is a new planned particle accelerator at CERN to study electron-positron collisions at energies up to 3 GeV. The collider uses high-frequency electric fields to accelerate particles in a vacuum at room temperature. The use of high electric fields results in vacuum breakdowns, which lead to disruption of the beam and damage to the structures.

The detailed mechanism of vacuum breakdown is not known, but nanoscale surface defects are thought to play an important role. Field enhancement near the surface leads to increased field emission, atom evaporation, and eventually arcing. Atomic scale simulations are very useful in studying dislocation behaviour and surface defects and can provide important information to complement experimental findings.

We use a Kinetic Monte Carlo (KMC) method combined with Molecular Dynamics (MD) to simulate diffusion and relaxation processes on gold and copper surfaces. To characterize the diffusion of adatoms, we have developed an improved migration barrier calculation method. This tethered Nudged Elastic Band (NEB) method is better at describing unstable atomic configurations, which occur frequently around surface protrusions. We use the MD simulations, as well as KMC with tethered NEB, to study defect formation and stability on metal surfaces under high external electric fields.

References

[1] Updated baseline for a staged Compact Linear Collider, edited by P.N. Burrows, P. Lebrun, L. Linssen, D. Schulte, E. Sickling, S. Stapnes, M.A. Thomson, CERN-2016-004 (CERN, Geneva, 2016), DOI: 10.5170/CERN-2016-004

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