ATOMISTIC MODELING OF METAL SURFACES UNDER HIGH ELECTRIC FIELDS: DIRECT COUPLING OF ELECTRIC FIELDS TO THE ATOMISTIC SIMULATIONS

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With the aim to challenge the frontiers of high energy physics, the European Organization for Nuclear Research (CERN) has initiated a new compact electron-positron linear collider (CLIC) project. The collision energies of leptons in CLIC are planned in the range of 0.5-5 TeV. To achieve such energies cost-efficiently, the particles must be accelerated by electric fields up to 300 MV/m near the surface of the accelerating structures. Using such high fields leads to vacuum breakdowns in the system. To ensure the proper behavior of the accelerator, the probability of those breakdowns must be held below 3×10^{-7} pulse^{-1}m^{-1}.

The actual triggering mechanism of vacuum breakdowns is not entirely clear yet, but experiments have shown a significant field enhancement near copper surfaces. This could lead to breakdown events via positive feedback effect. Such an enhancement could be caused by nanotips with aspect ratio of 30-140, although they have not been observed directly. According to current hypothesis, the lack of observation of such protrusions is caused by their tendency to collapse without external force acting on them. Depending on the mechanism behind the collapse the process may be too fast to be observable with conventional experimental methods.

To enhance the pace of research, experimental techniques are complemented by the computational ones. In 2011 the hybrid electrodynamics – molecular dynamics code HELMOD [1] was developed to study the effect of electric field to the stability of metal surface. That code has been successfully used in several projects. However, to cope with the forthcoming challenges the efficiency of the software must be enhanced. This can be done by transferring the electric field solver from the finite difference basis into the finite element framework and by adding the parallel computations capability. The code will be entirely open-source and will be shared with all the interested colleagues.

The code has the tools to generate the finite element mesh around the atomistic simulation domain, to dynamically solve the Laplace's equation in 3D domain, and to calculate the charges and electrostatic forces for surface atoms. It also has the interface to be coupled with classical molecular dynamics and kinetic Monte Carlo codes.

[1] F. Djurabekova, S. Parviainen *et al*, Phys. Rev. E 83, 026704 (2011)