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Mechanistic understanding of material evolution under electric fields during Rf breakdown

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High-gradient electric-fields are inevitably encountered in technologies ranging from accelerating structures to miniaturized electronic devices. It is now well understood that material functionality under extreme field conditions can heavily depend on the coupling between electro-thermal loading and microstructural deformation, but the fundamental mechanisms underpinning this coupling remain poorly understood. While they are difficult to explicitly access experimentally, relevant nanoscale deformation mechanisms can in principle be directly probed by atomistic simulations. We include electric-field-induced Lorentz forces using a charge-equilibration molecular dynamics framework that allows for the dynamical evolution of atomic charges. Using this tool, we explore the joint effect of electric-fields-induced stresses and thermo-mechanical stresses on the plastic deformation of fcc metals. We explore the motion and multiplication of dislocations in both the bulk and at free surfaces and discuss the various regimes of electric fields and pulsed heating as they couple with the plastic deformation and surface diffusion. These results inform possible mechanisms of breakdown precursor formation in accelerating structures.

Topic

Modeling and Simulations

Primary authors: Dr PEREZ, Danny (Los Alamos National Laboratory); Dr BAGCHI, Soumendu

Presenter: Dr BAGCHI, Soumendu

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