Contribution ID: **47** Type: **not specified**

Atomistic modeling of the coupling between electric fields and bulk plastic deformation in RF structures

Wednesday, 21 April 2021 08:00 (30 minutes)

A notable bottleneck in achieving high-gradient RF technology is dictated by the onset of RF breakdown. While the bulk mechanical properties are known to significantly affect the breakdown propensity, the underlying mechanisms coupling EM fields to bulk plastic deformation in experimentally relevant thermal and electrical loading conditions remain to be identified at the atomic scale. Here, we present the results of large-scale molecular dynamics simulations (MD) to investigate possible modes of coupling. Specifically, we consider the activation of Frank-Read
sources, which leads to dislocation multiplication, under the action of bi-axial thermal stresses and surface electric-field. With the help of a charge-equilibration formalism incorporated in a classical MD model, we show that a surface electric field acting on an either preexisting or dislocation-induced surface step, can generate a long-range resolved shear stress field inside the bulk of the sample. We investigate the feedback between step growth following dislocation emission and
subsequent activations of Frank-Read sources and discuss the conditions where such a mechanism could promote breakdown precursor formation.

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Session Classification: Session 6