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Multiscale material design of robust semiconductor photocathodes under strong fields

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Unprecedented electron beam brightness can potentially be achieved by exploiting high gradients in cryo-cooled RF cavities functionalized with high QE semiconductor photocathode materials. However, strong electric fields and thermal stresses from associated emission currents could potentially affect material stability, leading to breakdown events which may shorten device lifetime or degrade performance. To ensure robust performance and long operational lifetimes, the underlying processes leading to microstructural evolution in such semiconductor photocathodes needs to be explored under strong fields. Here, we present a suite of multiscale modeling tools specially tailored to probe the electro-thermo-mechanical behavior of semiconductor photocathodes. We first parameterize a machine learning interatomic potential suitable for classical charge equilibration molecular dynamics (MD) using density functional theory (DFT) calculations of CsTe. DFT and MD informed material properties are further incorporated into a meso-scale finite element (FE) model to predict morphological evolution of cathode surfaces under fields and thermal stresses due to emission currents.

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

Co-authors: HUANG, Chengkun (Los Alamos National Laboratory); SIMAKOV, Evgenya (Los Alamos National Laboratory); WANG, Gaoxue (Los Alamos National Laboratory)

Presenter: BAGCHI, Soumendu (Los Alamos National Laboratory)

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