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Simulations of material surface modifications due to combined influence of femtosecond laser irradiation and applied electric fields

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Extreme field enhancement factor of 50-100 is commonly measured in CLIC accelerator design. Such field enhancement values are often associated with high aspect ratio surface irregularities appearing under applied electric fields. Recently, femtosecond laser experiments with tungsten tip under applied electric field demonstrated spontaneous formation of such field emitting modification in time range of minutes due to repeated laser pulsing [1].
Under such conditions, several time and length scales are combined, starting form the application of single laser pulse, towards formation of steady state thermal profile in tip in tens of nanoseconds while incorporating atomic diffusion time scales in order of magnitude of microseconds and finally, ending with formation of the tip in range of minutes. Thus, application of conventional simulation methods becomes extremely challenging, as available tools like molecular dynamics or atomistic kinetic Monte-Carlo succeed in capturing accurately only up to microsecond scale, while standard finite element analysis tools tend to introduce excessive homogenization and either lose the accuracy at the nanoscale or expendability to macroscopic time scales.
In current study we present the outcomes of extensive multi-physics and multi scale simulations, including reproduction of femtosecond laser pulsing using two-temperature model and nanoscale electro-mechanical material response analyses.
To overcome the limitations of extendability of models with the respect of time scales, we utilize the surface stress model [2] in the framework of topology optimization, coupled with electric field and two-temperature approach motivated tip temperature calculations. The topology optimization relies on Lagrangian formalism and moving mesh approaches, leading to continuous surface changes of the system in every optimization step. Thus, allowing successful relaxation of structure the due to combined influence of femtosecond laser heating, applied electric field and nanoscale surface stresses. As a result, we successfully overstep the time scale limitations accurate atomistic scale stress calculations while being able to observe physics motivated surface modifications. In combined simulations, we observe significant influence of applied electric field to the surface behavior. For example, tested Cu tip successfully relaxed to {111} dominated pyramidal shape of minimal surface energy, often observed in kMC simulations as well. However, in case of applied electric field, fast flattening of the top of tip similarly to the results in [1] was observed. Moreover, the simulation setup, relying on the energy minimization of the sample and combining the influence of surface stress, thermal stress and electric field caused stress opens several possible mechanisms for explaining observed spontaneous surface modifications.

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[2] V. Zadin, M. Veske, S. Vigonski, V. Jansson, J. Muszinsky, S. Parviainen, A. Aabloo, F. Djurabekova, Simulations of surface stress effects in nanoscale single crystals, Model. Simul. Mater. Sci. Eng. 26 (2018) 035006. doi:10.1088/1361-651X/aaa928.

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