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Atomistic modeling of the generation of crystal defects and microstructure development in short pulse laser processing of metals

Wu, Chengping, cw5xj@virginia.edu; Zhigilei, Leonid, University of Virginia, United States

ABSTRACT

Because of the extremely fast and localized energy deposition, short-pulse (pico- and femtosecond) laser irradiation of a metal target can induce ultrafast heating (1013-1014 K/s) and melting within a surface layer of the irradiated target as thin as tens of nanometers. The shallow melt depth produced by the short-pulse laser irradiation and the high thermal conductivity of metals then lead to very high cooling rates (1011-1012 K/s), strong undercooling and rapid resolidification. In this study, the melting and resolidification processes occurring under conditions of extreme heating and cooling rates are investigated in large-scale atomistic simulations performed with a computational model that combines the classical molecular dynamic method with a continuum description of the laser excitation of conduction band electrons, electron-phonon coupling and electron heat conduction. The fast melting and resolidification cycle is found to be responsible for the generation of crystal defects, nonequilibrium phases and unusual microstructure in the surface region of the irradiated target. The kinetics of the resolidification process and the microstructure of the surface region are found to be defined by a competition between the epitaxial regrowth of the substrate and nucleation of crystallites within the undercooled melted region. The dependence of the final microstructure of the surface region on the irradiation conditions is discussed based on the results of the atomistic simulations. A special consideration is given to the conditions that result in the massive homogeneous nucleation and growth of the crystallites in a strongly undercooled surface region of the target. The generation of thin nanocrystalline surface layer with a high density of the grain boundaries, twins, and stacking faults suggests an effective method for highly localized surface hardening. In addition, the possibility of metastable phase generation is illustrated by an example in which the generation of metastable BCC-Cu structure and the following collapse into a close-packed structure through BCC-HCP transformation are observed.