Generation and stabilization of crystal defects in short pulse laser processing of copper

Chaobo Chen,[1] Andrius Žemaitis,[2] Julian H. Keophanboua,[1] Kory Burns,[1] Iaroslav Gnilitskyi,[3] Paulius Gečys,[2] and Leonid V. Zhigilei[1,*]

[1] University of Virginia, Charlottesville, USA
[2] Center for Physical Sciences and Technology (FTMC), Vilnius, Lithuania
[3] Lviv Polytechnic National University (LPNU), Lviv, Ukraine
*Corresponding author email: lz2n@virginia.edu

Short pulse laser processing of metal surfaces combined with simultaneous nanoalloying offers an attractive non-contact approach for the generation of thermally stable nanostructured gradient surface layers exhibiting a combination of high strength and hardness, fatigue resistance, and enhanced catalytic activity. The mechanisms of laser-induced surface nanostructuring are investigated in atomistic simulations performed with a hybrid atomistic-continuum model combining molecular dynamics method with a continuum two-temperature model. Simulations are performed for single-crystal Cu targets and are focused on the exploration the effect of laser pulse duration and nanoalloying on the defect structures generated be laser irradiation. The conditions of the simulations are mapped to those realized in laser processing experiments, and the computational predictions are verified in a detailed experimental characterization of surface regions modified by short pulse laser irradiation.

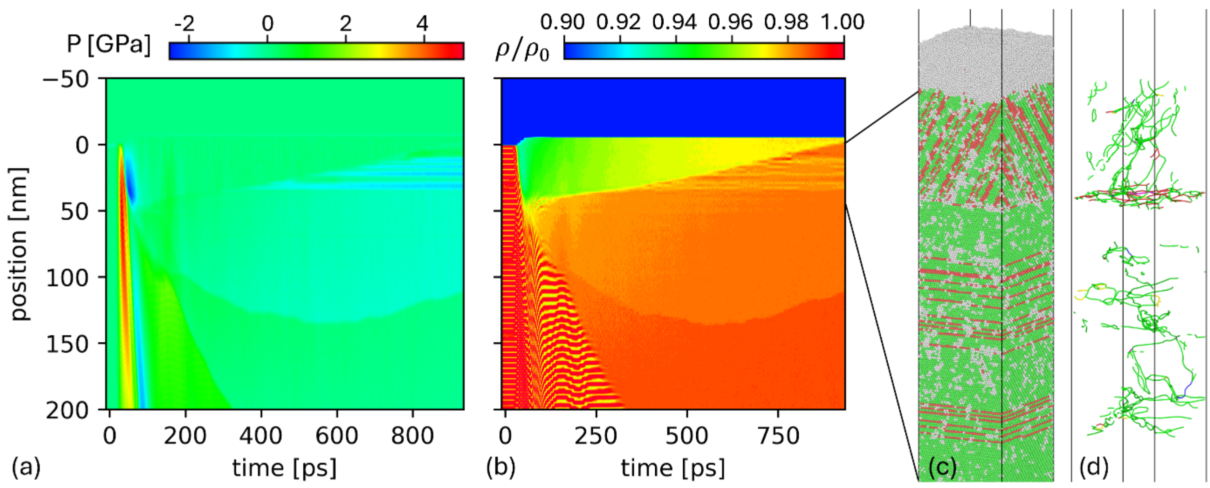

Figure: Results of preliminary simulations of laser-induced melting and resolidification of a Cu single crystal target irradiated by 10 ps laser pulse at an absorbed laser fluence of 1000 J/m^2. The spatial and time evolution of pressure and density in the surface region of the target is shown in (a) and (b), respectively. The defect structure in the resolidified part of the target is shown in (c) and (d). In (c), red planes on green background correspond to twin boundaries. In (d), dislocations lines are shown and colored by type, *e.g.*, green for 1/6 ⟨112⟩, blue for 1/2 ⟨110⟩, yellow for 1/3 ⟨100⟩, magenta for 1/6 ⟨110⟩.

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