Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Generation of point defects in femtosecond laser interactions with Cr targets EAMAN TAHIR, University of Baghdad, Iraq, ZHIBIN LIN, Texas A&M University, USA, LEONID ZHIGILEI , University of Virginia, USA — The mechanisms and driving forces responsible for the generation of point defects (vacancies and interstitials) in femtosecond laser interactions with Cr target are investigated in atomic-scale simulations. Two series of simulations are performed. In the first set of simulations, the processes induced by 200 fs laser pulse irradiation of a bulk Cr target are studied 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 distribution of point defects in the surface regions of irradiated targets is analyzed for a broad range of laser fluences, covering the regimes of surface melting, photomechanical spallation, and ablation. To investigate the relative contributions of the thermally-activated generation of vacancy-interstitial pairs and the production of the vacancies during the solidification process, the second series of simulations of solidification at fixed temperatures below the melting point is performed. The densities of vacancies generated under different undercooling conditions are related to the distributions observed in laser-irradiated targets. The implications of the computational predictions for atomic mixing and damage accumulation in multi-pulse irradiation regime are discussed.

Leonid Zhigilei
University of Virginia, USA

Date submitted: 29 Nov 2008 Electronic form version 1.4