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Atomic-level simulations of structural transformations in layered Au-Cu and Ag-Cu metal targets irradiated by a femtosecond laser pulse[1]

CHENGPING WU, University of Virginia, DEREK THOMAS, University of Tokyo, Japan, ZHIBIN LIN, Colorado School of Mines, LEONID ZHIGILEI, University of Virginia — The structural transformations in Ag/Au film - Cu substrate systems irradiated by femtosecond laser pulses are investigated in simulations performed with a model that couples the molecular dynamics method with a continuum-level description of the laser excitation and subsequent relaxation of the excited electrons. The higher strength of the electron-phonon coupling in Cu compared to Ag and Au results in a preferential sub-surface heating and melting of the Cu substrate. The melting is followed by rapid cooling and resolidification. In the case of Cu-Ag system, the rapid resolidification results in a complex structure of the interfacial region, where the lattice-mismatched interface is separated from the Ag-Cu mixing region by an intermediate pseudomorphic bcc Cu layer that grows epitaxially on the (001) face of the fcc Ag film during the final stage of the resolidification process. The new lattice-mismatched interface consists of a periodic array of stacking fault pyramids outlined by stair-rod partial dislocations. The intermediate bcc layer and the stacking fault pyramid structure of the mismatched interface present a barrier for dislocation propagation, resulting in the effective hardening of the layered structure treated by laser irradiation.

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