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Molecular Dynamic Simulation of Laser Melting of Nanocrystalline Gold ZHIBIN LIN, REMRSEC and Dept. of Physics, Colorado School of Mines, ELODIE LEVEUGLE, Thales Group, France, EDUARDO BRINGA, Dept. of Physics, Universidad Nacional de Cuyo, Argentina, LEONID ZHIGILEI, Dept. of Materials Science and Engineering, Univ. of Virginia — We present the mechanisms and kinetics of short pulse laser melting of single crystal and nanocrystalline Au films based on the results of atomic-scale simulations. The simulations are performed for a broad range of laser fluences with a computational approach that combines the molecular dynamics method with a continuum-level description of laser excitation and subsequent relaxation of conduction band electrons. At high fluences, grain boundary melting in nanocrystalline films results in a decrease of the size of crystalline grains at the initial stage of the laser heating and is followed by a rapid (within 1-3 ps) collapse of remaining crystalline parts of the film as soon as the lattice temperature exceeds the limit of the crystal stability against the onset of homogeneous melting. At low laser fluences, the initiation of melting at grain boundaries can steer the melting process along the path where the melting continues below the equilibrium melting temperature and the crystalline regions shrink and disappear under conditions of substantial undercooling. This unusual melting behavior is explained based on thermodynamic analysis of the stability of small crystalline clusters surrounded by undercooled liquid.

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