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High Strain Rate and Shock-Induced Deformation in Metals[1]

RAMON RAVELO[2], University of Texas-El Paso

Large-scale non-equilibrium molecular Dynamics (MD) simulations are now commonly used to study material deformation at high strain rates (10^9-10^{12} s^{-1}). They can provide detailed information– such as defect morphology, dislocation densities, and temperature and stress profiles, unavailable or hard to measure experimentally. Computational studies of shock-induced plasticity and melting in fcc and bcc single, mono-crystal metals, exhibit generic characteristics: high elastic limits, large directional anisotropies in the yield stress and pre-melting much below the equilibrium melt temperature for shock wave propagation along specific crystallographic directions. These generic features in the response of single crystals subjected to high strain rates of deformation can be explained from the changes in the energy landscape of the uniaxially compressed crystal lattice. For time scales relevant to dynamic shock loading, the directional-dependence of the yield strength in single crystals is shown to be due to the onset of instabilities in elastic-wave propagation velocities. The elastic-plastic transition threshold can accurately be predicted by a wave-propagation stability analysis. These strain-induced instabilities create incipient defect structures, which can be quite different from the ones, which characterize the long-time, asymptotic state of the compressed solid. With increase compression and strain rate, plastic deformation via extended defects gives way to amorphization associated with the loss in shear rigidity along specific deformation paths. The hot amorphous or (super-cooled liquid) metal re-crystallizes at rates, which depend on the temperature difference between the amorphous solid and the equilibrium melt line. This plastic-amorphous transition threshold can be computed from shear-waves stability analyses. Examples from selected fcc and bcc metals will be presented employing semi-empirical potentials of the embedded atom method (EAM) type as well as results from density functional theory calculations.

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[2]Computational Physics Division, Los Alamos National Laboratory