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Large-Scale Classical Molecular Dynamics Simulations of Shock-Induced Plasticity in bcc Niobium TIMOTHY GERMANN, Los Alamos National Laboratory — Large-scale classical molecular dynamics simulations are used to study the response of bcc Nb to shock compression, for perfect crystals in the [100] and [110] orientations. An embedded atom method (EAM) potential due to Johnson and Oh is used to describe the interatomic forces. Both orientations appear to plastically deform primarily by twinning, and we observe a bcc-hcp phase transformation at shock pressures above $\sim$75 GPa. There is no experimental evidence for any such transformation in Nb, although a similar transformation occurs in Fe and other bcc metals, so it is likely that this is an artifact of the EAM potential.

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