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Pressure Induce Phonon Instabilities in BCC Tantalum Single crystals OSCAR GUERRERO, UTSA — Large-scale atomistic simulations of shock-wave propagation in single crystals exhibit large anisotropies in the elastic-plastic and solid-liquid transitions. Characteristic of this type of simulations are the large strains at which the crystal yields plastically, regardless of crystal orientation. At these large strains, uniaxial deformations, such as those produced in planar shock loading generate phonon instabilities. Using non equilibrium molecular dynamics simulatsion (NEMD), We have investigated the directional anisotropy of the elastic limit in body-centered-cubic Tantalum (bcc) crystals, under quasi-isentropic compression, and using the embedded atom method (EAM) to model the atomic interactions. We show that the elastic-plastic transition in BCC defect-free crystals is caused by the appearance of soft-phonon modes and not via homogenous nucleation of extended defects.

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