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Solid-solid phase transformation in shocked Cs and Ce using molecular dynamics VIRGINIE DUPONT, TIMOTHY C. GERMANN, Los Alamos National Laboratory — Cesium (Cs) and cerium (Ce) both undergo a significant (>10%) volume collapse associated with an isomorphic fcc-fcc phase transformation when subject to compressive loading. Molecular dynamics (MD) simulations provide significant insight into the atomic mechanisms of plasticity and phase transformation. We report here the results of MD simulations of Cs and Ce samples subjected to shocks with pressures ranging from 0.5 to 30 GPa. An Embedded Atom Method (EAM) potential is used to model the interaction between atoms in Ce, and an EAM-like two-band second moment model potential by Ackland and Reed is used for Cs. A split wave structure is observed, with up to 3 waves: an elastic precursor followed by two plastic waves. The latter plastic wave causes the expected fcc-fcc phase transformation. An analysis of crystallography and orientation is conducted, which shows that reorientation of the lattice depends upon the original orientation of the sample.

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