Large-Scale Molecular Dynamics Simulations of the fcc-fcc Volume Collapse Transition in Shocked Cesium

KAI KADAU, TIMOTHY GERMMANN, Los Alamos National Laboratory — We have utilized large-scale classical molecular dynamics simulations to study the isomorphic fcc-fcc transformation in shocked cesium perfect crystals. Ackland and Reed [1] developed an interatomic potential to describe the similar volume collapse transition in Cs, adding an internal variable for the relative occupation of two \( s \) and \( d \) electronic bands on each atom to an embedded atom method (EAM)-like model. Using an orientation imaging map algorithm, we find a significant dependence upon initial crystallographic orientation: shock compression in the [001] direction leads to a product with a predominantly [011]-like texture, while [111] loading accomplishes the volume collapse transition without any crystallographic rotation. A three-wave (elastic-plastic-product phase) structure is also observed for shock pressures around 5 GPa in the [111] case, while the [001] plastic wave is overdriven prior to the onset of transformation.