Abstract Submitted
for the SHOCK09 Meeting of
The American Physical Society

Large-Scale Molecular Dynamics Simulations of the fcc-fcc Volume Collapse Transition in Shocked Cesium KAI KADAU, TIMOTHY GERMANN, 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.

[1] G. J. Ackland and S. K. Reed, *Two-band second moment model and an interatomic potential for caesium*, Phys. Rev. B **67**, 174108 (2003).

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Date submitted: 19 Feb 2009 Electronic form version 1.4