Abstract Submitted
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Atomistic Simulations of Shock Waves in Polycrystalline Iron Compared to Experiments[1] KAI KADAU, T.C. GERMANN, P.S. LOMDAHL, R.C. ALBERS, LANL, J.S. WARK, A. HIGGINBOTHAM, University of Oxford, B.L. HOLIAN, LANL — The propagation of shock waves through a polycrystalline iron sample is explored by large-scale atomistic simulations. For large enough shock strengths the passage of the wave causes the body-centered-cubic (bcc) structure to transform into a close-packed structure with most structure being isotropic hexagonal-close-packed (hcp) and, depending on shock strength and grain orientation, some fraction of face-centered-cubic (fcc) structure. The simulated shock state as represented by the Hugoniot is compared to experimental data. By calculating the extended x-ray absorption fine structure (EXAFS) directly from the atomic configurations obtained by our simulations, a comparison to recent experimental EXAFS measurements of nanosecond-laser shocks in polycrystalline iron shows that the experimental data is consistent with a phase transformation. However, the atomistically simulated EXAFS spectra also show that an experimental distinction between a product hcp or fcc phase is not possible based on the EXAFS spectra alone.

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Kai Kadau
LANL

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