Abstract Submitted
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**Shock induced alpha-epsilon phase transition in iron: Analysis of MD simulations and experimental data**[1] JAMES HAWRELIAK, K. ROSOLANKOVA, J. SHEPPARD, J.S. WARK, Univ. of Oxford, J.F. BELAK, G.W. COLLINS, J.D. COLVIN, J.H. EGGERT, D.H. KALANTAR, H.E. LORENZANA, J.S. STOLKEN, LLNL, H.M. DAVIES, AWE, T.C. GERMANN, K. KADAU, P.S. LOMDAHL, LANL, M.A. MEYERS, M.S. SCHNEIDER, UCSD
— Multi-million atom non-equilibrium molecular dynamics (MD) simulations for shock compressed iron are analyzed using Fourier methods to determine the long scale ordering of the crystal. By analyzing the location of the maxima in k-space we can determine the crystal structure and compression due to the shock. This poster will present results from different shock pressures and compare them to recent experiments of shock compressed iron where the crystal structure was determined using in-situ wide angle x-ray diffraction.

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