Abstract Submitted
for the SHOCK19 Meeting of
The American Physical Society

Shock-induced alpha-epsilon phase transformation in nanocrystalline iron: Plastic deformation and phase transitions HOANG-THIEN LUU, Computational Material Sciences/Engineering, Institute of Applied Mechanics, Clausthal University of Technology, 38678 Clausthal-Zellerfeld, Germany, RAMON J. RAVELO, Physics Department and Materials Research Institute, University of Texas, El Paso, TX, 79968, USA , EDUARDO M. BRINGA, CONICET and Faculty of Engineering, University of Mendoza, Mendoza, 5500, Argentina, TIMOTHY C. GERMANN, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM, 87545, USA, NINA GUNKELMANN, Computational Material Sciences/Engineering, Institute of Applied Mechanics, Clausthal University of Technology, 38678 Clausthal-Zellerfeld, Germany — Shock compression is widely used to examine the mechanical responses of iron under dynamic loading. It has been long known that α-iron transforms to ε-iron under high pressure. Recently, molecular dynamics simulations have shown that plasticity occurs just before the parent phase transforms into ε-iron. However, due to computational reasons, only small grain sizes have been studied where dislocation emission will be partially accommodated by grain boundary sliding. To provide insights into elastic and plastic activities of shocked iron, we performed atomistic simulations of shock compression of nanocrystalline iron with a mean grain size of 20 nm comprising a total number of 267.5 million atoms. We observe elastic and plastic deformation before the phase transformation takes place. Dislocations nucleate and pile-up at grain boundaries. The results are in good agreement with experiments of similar time and length scales.

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Date submitted: 28 Feb 2019 Electronic form version 1.4