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Molecular dynamics study of shock waves in iron-carbon single crystals HOANG-THIEN LUU, NINA GUNKELMANN, Computational Material Sciences/Engineering, Institute of Applied Mechanics, Clausthal University of Technology, 38678 Clausthal-Zellerfeld, Germany — Shock compression experiments in pure iron show a three-wave structure: an elastic wave, a plastic wave and the phase-transformation from α- to ε-iron. This three-wave structure has been confirmed by both experiments and molecular dynamics (MD) simulations. Large-scale MD studies provide insights into the transformation kinetics of iron including the transformation mechanisms, stacking faults and twins in ε-iron and the orientation dependence of iron single crystals. However, the influence of carbon on the transformation process remains an open topic. By atomistic simulations of high-strain rate compression of iron-carbon, we show that carbon decreases the elastic limit, but strongly increases the transformation pressure. We examine the role of carbon in the material transformation process under intense shock wave loading in Fe and Fe-C single crystals.

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