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Molecular dynamics simulations of steady shock waves in nickel BRIAN DEMASKE, VASILY ZHAKHOVSKY, University of South Florida, CARTER WHITE, Naval Research Laboratory, IVAN OLEYNIK, University of South Florida — Shock waves in single-crystal nickel samples were investigated by molecular dynamics (MD) simulations. Standard piston simulations were used to investigate the elastic-plastic split-shock-wave regime, whereas regimes having a single steady shock-wave structure were studied by a novel moving window (MW-MD) technique. Two distinct regimes were investigated, including the regimes of split elastic and plastic shock waves and the steady two-zone elastic-plastic single wave. Split shock waves were shown to form at moderate piston velocities out of a metastable high-pressure elastic state that decays into a two-wave structure consisting of a slow plastic wave and fast elastic precursor. At higher piston velocities, the plastic wave overtakes the elastic precursor but does not overrun it. Instead, both waves were found to move in tandem with the same average speed while maintaining a finite, and in some cases strongly fluctuating, separation width that may extend to several microns. The dependence of shock wave structure on crystallographic orientation and concentration of defects was investigated.

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