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Shock wave propagation in semi-crystalline polyethylene: An atomic-scale investigation ROBERT M. ELDER, U.S. Army Research Laboratory, THOMAS C. O'CONNOR, Johns Hopkins University, Physics and Astronomy, IN-CHUL YEH, TANYA L. CHANTAWANSRI, TIMOTHY W. SIRK, U.S. Army Research Laboratory, MARK O. ROBBINS, Johns Hopkins University, Physics and Astronomy, JAN W. ANDZELM, U.S. Army Research Laboratory — Highly oriented polyethylene (PE) fibers are used in protection applications, therefore elucidation of their response under high strain-rate impact events is vital. Although PE fibers can have high crystallinity (>95%), they also contain defects such as amorphous domains. Using molecular dynamics simulations, we investigate shock propagation through crystalline, amorphous, and semi-crystalline PE. We generate compressive shock waves of varying strength, quantify their dynamics, and characterize their effect on material properties at the atomic scale. In the semi-crystalline PE model, the differing density and molecular order of amorphous PE and crystalline PE result in differing shock impedances, which causes reflection and refraction of shock waves at interfaces between the phases. We quantify the properties (e.g. pressure, velocity) of the reflected and refracted waves, which differ from those of the incident wave, and compare with results from impedance matching. We also examine the reflection, absorption, and transmission of energy at the crystalline-amorphous interface. Depending on shock strength, amorphous defects can dissipate shock energy, which attenuates the shock and leads to effects such as localized heating.

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