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Simulation studies of shock wave propagation and reflection in semi-crystalline polyethylene ROBERT M. ELDER, TANYA L. CHANTAWANSRI, YELENA R. SLIOZBERG, TIMOTHY W. SIRK, IN-CHUL YEH, U.S. Army Research Laboratory, THOMAS C. O'CONNOR, MARK O. ROBBINS, Johns Hopkins University, JAN W. ANDZELM, U.S. Army Research Laboratory — Polyethylene (PE) fibers are used in many applications where high-strain-rate impacts occur, so understanding their response to such events is vital. Although PE fibers often have high crystallinity, they also contain defects such as amorphous domains. Using molecular dynamics simulations, we generate compressive shock waves of varying strength in crystalline, amorphous, and semi-crystalline PE models. The differing properties of amorphous and crystalline PE result in an impedance mismatch, which causes partial reflection/refraction of shock waves at interfaces between the phases. We quantify the properties (e.g., pressure) of these waves and the reflection/transmission of energy at interfaces, and we compare with a simple continuum-level theory. The theory and simulations agree that amorphous domains attenuate weak shocks more effectively than strong shocks. However, the simulations unexpectedly show that small amorphous domains reflect less energy than theoretically predicted. We identify nanoscale mechanisms that reduce the impedance mismatch, and thus reflection, at thin amorphous domains, including confinement-induced stiffness, chain ordering, and density. The significance of these results emerges as a design choice, in that processing techniques can be used to tune the size of amorphous inclusions for the requirements of a particular application.

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