

Abstract Submitted
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Shock compression of dense polymer and foam systems using molecular dynamics and DFT J. MATTHEW D. LANE, GARY S. GREY, AIDAN P. THOMPSON, KYLE R. COCHRANE, MICHAEL P. DESJARLAIS, THOMAS R. MATTSSON, Sandia National Laboratories — Organic polymers and nanocomposites are increasingly being subjected to extreme environments. Molecular scale modeling of these materials offers insight into failure mechanisms and response. Classical molecular dynamics (MD) and density functional theory (DFT) MD simulations of the principal shock Hugoniot will be presented for two hydrocarbon polymers, polyethylene (PE) and poly(4-methyl-1-pentene) (PMP). We studied two reactive and two non-reactive classical MD interaction potentials. We will show the exp-6 interaction of Borodin et al. has much better agreement with experiment than OPLS. Further, that ReaxFF displayed decidedly better agreement than AIREBO. DFT were in excellent agreement with experiment. NEMD studies of low-density foam materials will be discussed. Qualitative response will be characterized. Quantitative comparison will be made with experiment.

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