Abstract Submitted
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Molecular Dynamics Simulations of Shock Wave Propagation across the Nitromethane Crystal-Melt Interface[1] SHAN JIANG, THOMAS D. SEWELL, DONALD L. THOMPSON, Department of Chemistry, University of Missouri-Columbia, Columbia, MO 65211 — We are interested in understanding the fundamental processes that occur during propagation of shock waves across the crystal-melt interface in molecular substances. We have carried out molecular dynamics simulations of shock passage from the nitromethane (100)-oriented crystal into the melt and *vice versa* using the fully flexible, non-reactive Sorescu, Rice, and Thompson force field. A stable interface was established for a temperature near the melting point by using a combination of isobaric-isothermal (NPT) and isochoric-isothermal (NVT) simulations. The equilibrium bulk and interfacial regions were characterized using spatial-temporal distributions of molecular number density, kinetic and potential energy, and C-N bond orientations. Those same properties were calculated as functions of time during shock propagation. As expected, the local temperatures (intermolecular, intramolecular, and total) and stress states differed significantly between the liquid and crystal regions and depending on the direction of shock propagation. Substantial differences in the spatial distribution of shock-induced defect structures in the crystalline region were observed depending on the direction of shock propagation.

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