MOLECULAR DYNAMICS SIMULATIONS OF PRESSURE SHOCKS IN LIQUID PHASE NITROMETHANE

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Abstract

The dynamic energy transfer processes present in liquid nitromethane (NM) under pressure shock loading conditions have been investigated by nonequilibrium molecular dynamics methods using a previously developed, fully flexible NM force field (Sorescu, D. C.; Rice, B. M.; Thompson, D. L. J. Phys. Chem. B 2000, 104, 8406). Generally good qualitative agreement with the corresponding experimental values was found for sound speeds (C) as a function of temperature. This is true as well for the PVT Hugoniot data calculated for the shock compressed zones behind our simulated shock fronts. But from equipartition theory we found that T is not equilibrated behind these fronts within the maximum timeframe of our simulations (< 10 ps). The predicted C(T) are ~13 – 30% higher than experiment (Lysne, P. C.; Hardesty, D. R. J. Chem. Phys. 1973, 59, 6512) and our predicted densities are consistently 4 – 10% lower than experiment (Winey, J. M.; Duvall, G. E.; Knudson, M. D.; Gupta, Y. M. J. Chem. Phys. 2000, 113, 7492). Accurate Hugoniot pressures are predicted at all three initial temperatures (255, 300, 350 K) studied which span the experimental ambient pressure temperature range of liquid NM (~ 244 – 373 K).