

Abstract Submitted
for the SHOCK09 Meeting of
The American Physical Society

Eckart-Sayvetz Alignment: A Useful Tool for the Analysis of Molecular-Scale Simulation Data for Studies of Material Under Extreme Thermodynamic Conditions THOMAS D. SEWELL, RICHARD DAWES, ALI SIAVOSH-HAGHIGHI, DONALD L. THOMPSON, Department of Chemistry, University of Missouri-Columbia, Columbia, MO 65211-7600 — Molecules subjected to shock wave loading will, in general, be highly distorted and arbitrarily displaced compared to their (0 K, 0 GPa) structures. This complicates the analysis for such systems, particularly when the goal is to express dynamic molecular-scale properties in a frame indexed to the static equilibrium geometry. The Eckart-Sayvetz condition (ESC) provides a rigorous approach by which the optimal alignment between frames for such analyses can be achieved. We illustrate the use of the ESC in a MD study of shocked nitromethane crystal, for initial temperatures of 50 and 200 K and impact velocities ranging from 0.5 to 3.0 km/s. The results provide clear evidence of melting for impacts of at least 2 km/s and provide insights into the fundamental events associated with its onset. Energy redistribution in the shocked crystal was studied by monitoring the time dependence of the molecular normal mode kinetic energies. The energy-transfer results are sensitive to shock strength and initial temperature, but are generally consistent with the notion of vibrational up-pumping.

Thomas D. Sewell
Department of Chemistry, University of Missouri-Columbia, Columbia, MO 65211-7600

Date submitted: 19 Feb 2009

Electronic form version 1.4