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Classical and Quantum Dynamics of Energy Transfer under Shock Conditions[1] R.C. MOWREY, NRL, M.L. ELERT, U. S. Naval Academy, C.T. WHITE, NRL — Classical molecular dynamics (MD) simulations of shocks in molecular solids predict rapid excitation of bond motion indicating efficient translational to vibrational coupling. The validity of the MD description of collisional energy transfer near shock fronts has not been carefully tested. The importance of quantum effects under shock conditions is explored in classical MD and quantum mechanical (QM) simulations of a molecular lattice model consisting of three collinear diatomic molecules and a stationary wall. A fast-moving diatom collides with its neighbor initiating a collision cascade. The multiplicity of collisions precludes *a priori* prediction of the detailed collision dynamics. The time-dependence of the six degrees-of-freedom wave function describing the system is determined using QM time-dependent wave packet methods. The intra- and inter-molecular interactions are described using nearest-neighbor potentials. Predicted vibrational and translational energy changes and bond breaking and formation from QM and MD calculations are compared. The dependence of the dynamics on the characteristics of the model (e.g., heavy vs. light atoms, homonuclear vs. heteronuclear diatoms, intra- and inter-molecular bond strengths) is investigated.

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