

Non-Equilibrium Molecular Dynamics Simulations of Temperature Profiles at the Front of a Shock Wave

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Using Non-Equilibrium Molecular Dynamics Simulations (NEMD), we determined profiles of kinetic and configurational temperatures at the front of two-dimensional, stationary, plane shock waves. Shock waves travelled through (1) a crystal and (2) through a gas. In both cases the particles in the systems interacted by short-range, repulsive, smooth and finite pair potential. In spite of shear stress and heat flow, which were present in both cases, the equivalence between kinetic and configurational temperatures appeared only in the second case, which is not too far from equilibrium.