Entropy Production in Shock Waves

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Shock waves have been used as examples of physical processes that violate the assumption of local thermodynamic equilibrium [1] and thus exclude analysis in terms of linear non-equilibrium thermodynamics (NET). We show in this work that shock waves may indeed be described by NET. Based on recent progress on NET for surfaces [2], we treat a shock wave as a moving surface and set up the balance- and conservation equations for the shock. The central property is the entropy production, which is used to derive expressions for the coupled heat- and mass fluxes in the system in terms of thermodynamic forces. The assumption of local equilibrium was examined by non-equilibrium molecular dynamics simulations for a Lennard-Jones model system. A 256,000-particle model for a dense gas at equilibrium was perturbed by suddenly switching on a local heat source. This led to propagation of a supersonic shock wave and an accompanying heat wave. The formal expressions from NET were used to analyse the fluxes, forces, and the entropy production. The data did not show signs of violation of the assumption of local equilibrium, even in the shock front. This is in contrast with earlier simulations at lower densities [3], but in agreement with recent results at higher densities [4].

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