Argon-Argon Cross-Sections for Supersonic and Hypersonic Flows

R. J. Magyar, M.A. Gallis

Multi-Scale Science, Org. 1444 Sandia National Laboratories Albuquerque, NM 87185 USA rjmagya@sandia.gov
Thermal/Fluid Component Sci., Org. 1513 Sandia National Laboratories Albuquerque, NM 87185 USA magalli@sandia.gov

In supersonic and hypersonic flows, the mean free path of a molecule is of the same order as the representative physical length scale, and Navier-Stokes equations can be inaccurate. For these flows, Direct Simulation Monte Carlo (DSMC) provides accurate results. One of the critical parameters in DSMC, the mean-free path, is inversely related to the scattering cross-section. We present calculations of the differential scattering cross-section for Argon with Argon near thermal velocities and at atomic scale impact parameters. The computational results can be compared to experimental and theoretical data and can be used to inform the predictions of viscosity at a range of temperatures that might not be readily accessed experimentally. The calculations are based on the time-dependent density functional theory (TDDFT) with coupled electron-ion dynamics in the Ehrenfest approximation. TDDFT does not rely on material specific parameters and provides a general model including many-body quantum mechanics, charge transfer, and inelastic scattering. We will compare this methodology with the quantum-classical trajectory approach.

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Security Administration under contract DE-AC04-94AL85000.