
COLLISION FREQUENCY OF LENNARD-JONES FLUIDS AT HIGH DENSITIES BY EQUILIBRIUM MOLECULAR DYNAMICS SIMULATION.

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Abstract

Detailed classical molecular dynamics simulation of transport coefficients and collision frequencies at high densities in rare gases are presented in this paper with a view to investigate the likely cause of discrepancy between theory and experiments. The results, when compared with experiments, showed an underestimation of the viscosity calculated through the Green-Kubo formalism, but the results are in agreement with some other calculations performed by other groups. The origin of the underestimation was considered in the present work. Analyses of the transport coefficients showed a very high collision frequency which suggested that an atom might spend much less time in the neighbourhood of the fields of force of another atom. The distribution of atoms in the systems adjusts itself to a nearly Maxwellian type that resulted in a locally and temporarily slowly varying temperature. We showed that during collision, the time spent by an atom in the fields of force of other atoms is so small compared with its relaxation time, leading to a possible reduction in local velocity autocorrelation between atoms.