Microscopic origins of the viscosity of a Lennard-Jones liquid

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In contrast with crystalline solids or ideal gases, transport properties remain difficult to describe from a microscopic point of view in liquids, whose dynamics results from complex energetic and entropic contributions at the atomic scale. Two scenarii are generally proposed: one pictures dynamics in a fluid as a series of energy barrier crossings, leading to Arrhenius-like laws, while the other one assumes atoms rearrange through collisions, as exemplified by the free volume model. To assess the validity of these two viewpoints, we computed with molecular dynamics simulations the transport properties of the Lennard-Jones fluid, and tested how well the Arrhenius equation and the free volume model describe the temperature dependence of the viscosity and of the diffusion coefficient at fixed pressure. Although both models reproduce the simulation results in a large range of pressure and temperature covering the liquid and supercritical states of the Lennard-Jones fluid, we found that the parameters of the free volume model can be estimated directly from local structural parameters, also obtained in the simulations. This consistency of the results gives more credibility to the free volume description of transport properties in liquids.

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