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Effect of heavy impurities on thermal conductivity of glass-forming liquids

The unique low-temperature characteristics exhibited by disordered materials have garnered significant research attention over an extended period. These materials' specific heat and thermal conductivity properties are termed as *anomalous* to emphasize their intriguing deviations from those observed in crystalline materials. Consequently, they have attracted substantial investigative efforts, both in experimental and theoretical domains. Our study involves an investigation into the impact of heavy impurities on the thermal conductivity of glass-forming liquids. To achieve this, we employ a combination of non-equilibrium molecular dynamics simulations and numerical techniques. Within our model for glass formers, heavy impurities are introduced by a random selection of particles, with their mass adjusted accordingly. In the extreme scenario, quenched disorder is introduced by randomly pinning a fraction of the particles. With increased quenched disorder via increasing the fraction of pinned particles, the energy current in the system set due to the application of thermal gradient in non-equilibrium simulation decreases, and as a result the thermal conductivity decreases rapidly. Our findings demonstrate a swift transformation in the localization characteristics of low-frequency vibrational modes of the underlying solid, resulting in a marked reduction in thermal conductivity as the mass of impurities or the fraction of pinned particles increases. Further, it is shown that it is possible to transform the low-frequency extended modes to acquire quasi-localized character by the introduction of quenched disorder, which in turn contribute to the reduction of thermal conductivity.

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