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Vibrations and thermal conductivity in inorganic and polymeric glasses. SERGEI SHENOGIN, ARUN BODAPATI, PAWEL KEBLINSKI, Rensselaer Polytechnic Institute — The mechanism of thermal transport in amorphous materials was studied by means of vibrational mode analysis and classical nonequilibrium molecular dynamics (MD) simulations. We studied four different model systems of (a) Lennard-Jones glass, (b) bead-spring model of an amorphous polymer, (c) amorphous silicon with Stillinger-Weber potential; and (d) all-atom model of glassy polystyrene with PCFF-type force field. For all structures we evaluated thermal conductivity from the harmonic theory of disordered solids [P.B.Allen, and J.L.Feldman, Phys.Rev.B 48, 12581 (1993)] and from direct MD simulations. We found that for all models but polystyrene, the harmonic theory accurately predicts thermal conductivity. By contrast, in the case of polystyrene, only $\sim 1/2$ of thermal conductivity can be explained within the harmonic approximation. Consequently, a major part of the transport has to be attributed to anharmonic coupling between vibrational modes. The reasons for the failure of harmonic theory of disordered solids to model amorphous glassy polymers will be discussed.

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