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Thermal Transport in Graphene from Large-scale Molecular Dynamics Simulations LUIZ FELIPE PEREIRA, DAVIDE DONADIO, Max Planck Institute for Polymer Research — Carbon-based materials display exceptional thermal properties. The thermal conductivity of carbon allotropes can range five orders of magnitude. In the bulk, amorphous carbon is a very poor heat conductor, with $\kappa \approx 0.01$ W/m/K, whereas diamond has the highest thermal conductivity among elemental solids, $\kappa \approx 2000$ W/m/K at room temperature. Even broader ranges can be achieved by considering carbon nanostructures. Thermal conductivities as large as 5000 W/m/K have been measured for suspended graphene and carbon nanotubes. In spite of intense investigations, there is much controversy over the actual value of the thermal conductivity of graphene, both experimentally and theoretically. Here, we present results from equilibrium and non-equilibrium molecular dynamics simulations aimed at understanding the mechanism of heat transport in graphene. In particular, we investigate the influence of finite-size and uniaxial strain on the thermal conductivity of graphene, performing large scale molecular dynamics simulations of micrometer-size models containing up to 10^6 atoms.

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