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Thermal transport in low-dimensional systems: the case of Graphene and single layer Boron Nitride LUIZ FELIPE PEREIRA, DAVIDE DONADIO, Max Planck Institute for Polymer Research — Low-dimensional systems present unusual transport properties in comparison to bulk materials. In contrast with the three-dimensional case, in one- and two-dimensions heat transport models predict a divergence of the thermal conductivity with system size. In reality, in a low-dimensional system the mean-free-path of heat carriers (phonons) becomes comparable to the micrometer size of experimental samples. Recent developments in nanostructure fabrication allow a direct comparison between theory and experiments for such low-dimensional systems. We perform extensive molecular dynamics simulations of heat transport in graphene and single layer BN, in order to clarify the behavior of the thermal conductivity in realistic low-dimensional systems. In particular, we address the influence of system size on the simulation results. Equilibrium molecular dynamics predicts a convergence of the thermal conductivity with system size, even for systems with less than one hundred nanometers and thousands of atoms. Meanwhile, large scale non-equilibrium molecular dynamics shows a divergence of the thermal conductivity with system size up to the micrometer scale. We analyse the discrepancy between methods in terms of perturbations in phonon populations induced by the non-equilibrium regime.

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