Abstract Submitted
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Computational study of the thermal conductivity of defective carbon nanostructures[1] ZACHARIAS FTHENAKIS, DAVID TOMANEK, Michigan State University — We use molecular dynamics simulations to study the role of defects on the thermal conductivity in low-dimensional graphitic nanostructures such as schwarzites (3D), graphene (2D), carbon nanotubes and graphene nanoribbons (1D). Since the simulations are very demanding due to the very long phonon mean free path, we describe forces acting on carbon atoms by a parameterized valence force field. Our calculations make use of the non-equilibrium molecular dynamics technique, which incorporates the constant-temperature Nose-Hoover thermostat and non-equilibrium driving forces, which mimic the effect of the heat flow. We study different types of defects, including vacancies and isotope impurities, and show that their importance changes with changing dimension of the system.

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