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Optimal matching of thermal vibrations into carbon nanotubes: theory and simulations[1] K.G.S.H. GUNAWARDANA, Department of Physics and Astronomy University of Oklahoma, KIERAN MULLEN, Department of Physics and Astronomy, University Of Oklahoma, A.A. MOUSSA, Department of Physics and Astroomy University of Oklahoma — Carbon nanotubes (CNTs) and graphene sheets (GS) are promising candidates to improve the thermal conductivity of nano- composites and to use as a thermal interface materials. The main obstacle to these applications is the extremely high thermal boundary (Kapitza) resistance. It is possible to lower the Kapitza resistance by inserting a secondary atomic chain linking CNT or GS to the external medium. We have previously shown a theoretical approach optimizing this interface atomic chain in the continuum limit. To probe the limitations of the continuum model, an atomistic simulation was carried out. It was observed that the low frequency contribution to the thermal transport can be improved according to the continuum limit optimization. Further we have developed a theoretical tool based on R-Matrix theory to analyze the interfacial thermal transport taking phonon dispersion into account.

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