THERMAL CONDUCTIVITY REDUCTION DUE TO ISOTOPE SUBSTITUTION IN SINGLE-WALLED CARBON NANOTUBES AND GRAPHENE NANORIBBONS

UPAMANYU RAY[1]*, GANESH BALASUBRAMANIAN[2]

[1] Department of Mechanical Engineering,
103 Nuclear Engineering,
Iowa State University, Ames, IA 50011, USA
E-mail: uray@iastate.edu

[2] Department of Mechanical Engineering,
2092 Black Engineering,
Iowa State University, Ames, IA 50011, USA
Tel.: +1 -515-294-9226
Email: bganesh@iastate.edu

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Introduction

Using non-equilibrium molecular dynamics simulations, we study the decrease in thermal conductivity (k) in isotopically impure carbon nanotubes (*CNTs)* and graphene nanoribbons. It is observed that the decrease in k for the doped *CNT*s, developed from the zone-folding approach of graphene sheets, is more than that of the doped graphene nanoribbons since the edge scattering effects due to development of dangling bonds in graphene increases the participation of phonon modes there. We analyze the vibrational density of states (*DOS*) both along and perpendicular to the direction of heat transfer. We find that the high energy modes of vibration shift to lower wave numbers and the highest peaks of the vibrational modes become shorter reflecting the strong influence of mass disorder that impedes formation of delocalized modes in impure materials. At wave numbers less than $1500 cm^{-1}$, the out-of-plane flexural acoustic modes in graphene nanoribbons and the delocalized longitudinal modes in *CNT*s play a more prominent role in the heat transfer process. The presence of isotopic dopants perturbs the *DOS* as well as the phonon dispersion curves thereby decreasing the overall phonon group velocity and reducing k. In summary, our atomistic simulations predict the decrease in thermal conductivity of isotope substituted 1D and 2D carbon nanomaterials. The relative decrease in thermal conductivity for a constant percentage of isotope substitution in CNTs and GNRs of equivalent lengths is similar for the whole length scale leaving the ballistic-diffusive regime. The induced mass disorder shifts the vibrational spectra to lower wave numbers. This is observed for both the acoustic flexural out-of-plane modes in GNR and the low frequency delocalized transverse modes in CNTs as well as the short-ranged longitudinal modes in CNT and in-plane vibrations in GNR thus influencing thermal transport. Contribution of isotope substitution to the thermal conductivity is consistent over a range of material lengths for both the nanostructures.

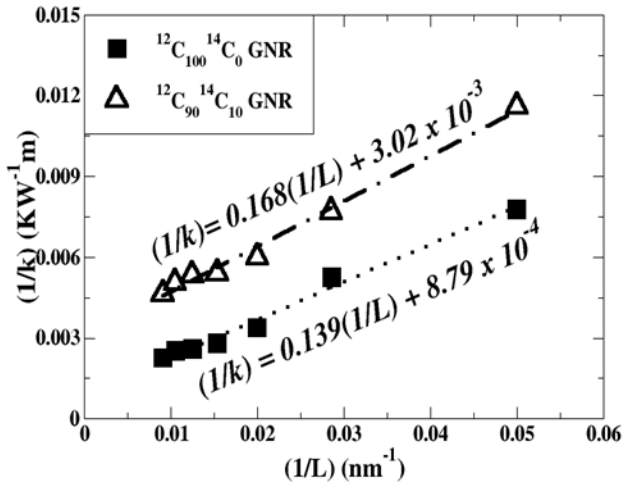
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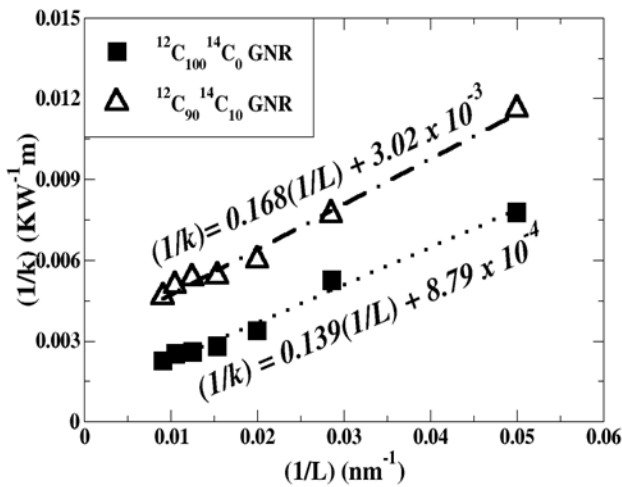
1. Figures:

Figure 1(a)

Figure 1(b)

Figure 1: The variation of 1/k with 1/L for both pure and 10% isotope substituted (a) CNTs and (b) GNRs of lengths L = 20 nm, 35 nm, 50 nm, 65 nm, 80 nm, 95 nm & 110 nm are presented. The fitting curves shown as dashed lines represent the linear inter-relationship between k and L for both pure and isotope substituted nanomaterials.

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