

Phonon Transport in Large Scale Carbon-Based Disordered Materials: Implementation of an Efficient Order N and Real Space Kubo Methodology

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In recent years, the understanding of phonon transport in carbon-based materials such as carbon nanotubes (CNTs) and graphene-based materials has become particularly important for both fundamental studies of coherent transport but also in view of novel applications. Conventional Green function approach cannot be used to study large system since it requires matrix inversions. An efficient computational approach is demanded in order to tackle large scale (and realistic) simulations of material of interest. In this poster, using the Kubo formalism[1] we demonstrate that a time-dependent phonon wavepacket formalism can be connected to the calculation of the thermal conductance, which has exactly the same form as the real space Kubo approach studying electronic transport[2]. After validating this numerical approach by comparing the obtained phonon mean free paths (MFP) in disordered CNTs (with isotope impurities) with previously computed ones by means of Green functions-based method [3], we apply the new algorithm to large width GNRs, and focus on the impact of edge disorder profiles. Scaling properties of phonon MFP and temperature-dependent thermal conductance are calculated as a function of edge disorder strength and for ribbon lateral sizes accessible to today's state-of-the-art lithography. A strong impact of smooth edge disorder on the thermal conductance was found, pinpointing towards good thermoelectrical properties of large width nanoribbons[4]. The broad generality of our method could offer a novel frame to explore other types of complex materials, including Boron-nitride-based materials or silicon-based materials (nanowires, superlattices, etc.).[5]

References

- [1]P. B. Allen and J. L. Feldman, Phys. Rev. B **48**, 12581 (1993).
- [2]F. Triozon et al., Phys. Rev. B **69**, 121410(R) (2004);
A. Lherbier et al., Phys. Rev. Lett. **100**, 036803 (2008).
- [3]I. Savic, N. Mingo, D. A. Stewart, Phys. Rev. Lett **101**, 165502 (2008).
- [4]H. Sevinçli and G. Cuniberti, Phys. Rev. B **81**, 113401 (2010).
- [5]W. Li, H. Sevinçli, G. Cuniberti and S. Roche, *submitted*

Figures

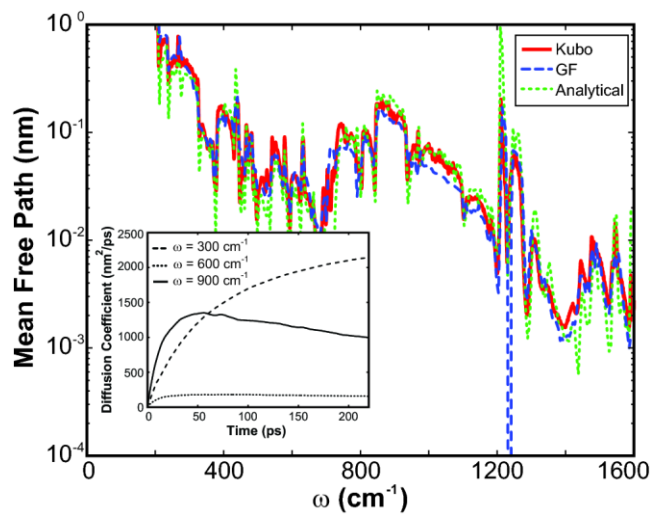


FIG.1. Main frame: frequency dependent MFP in CNT (7,0) with isotopic disorder with the GF method[3], Kubo method and the analytical formula. Inset: time dependent diffusion coefficients for three chosen frequencies.

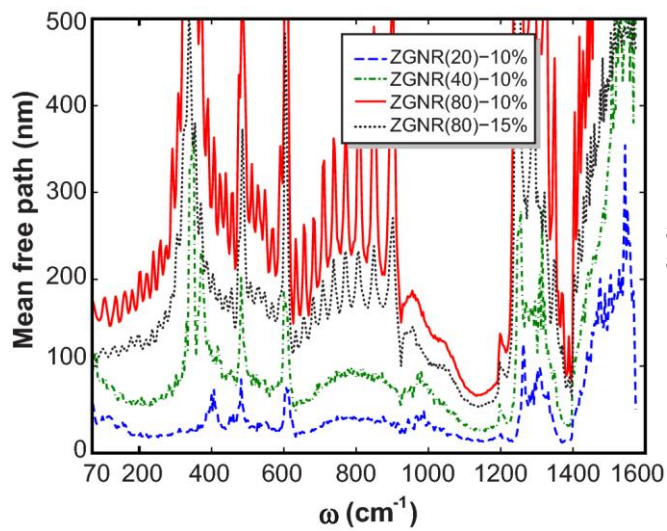


FIG.2. Elastic MFP for ZGNR of widths $N_z = 20, 40$ and 80 with disorder density of 10% , and also for 80 and 15% disorder for comparison.