Phonon transport studies in ultra-narrow graphene nanoribbons: Understanding features of heat flow in 1D

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Abstract

We investigate phonon transport in low-dimensional, disordered graphene nanoribbons (GNRs) in order to provide generic insight into features of phonon transport in low-dimensional materials. We employ lattice dynamics for the phonon spectrum and the Non-Equilibrium-Green's Function method for the calculation of phonon transport. We focus on how different parts of the phonon spectrum are influenced by geometrical confinement and line-edge-roughness, and how that influences heat transport. We show that, depending on the channel geometry, with the introduction of line-edge-roughness disorder, phonons in the different energy regions of the spectrum can flow either ballistically, diffusively, or become localized. *'Effective transport gaps'* in phonon transmission are observed, which severely reduce heat transport. In addition, we discuss the trends of the thermal conductivity as a function of the channel's length and width in the form of characteristic exponents (L^{α} and W^{β}) in the presence of line-edge roughness. In the case of the length-dependence we show how transport crosses from the ballistic to the diffusive regime within a few hundred nanometers, whereas in the case of width-dependence, we show that the dependence predicted by the Casimir model is still surprisingly valid even for channels with widths as low as 2nm. Finally, we explore the possibility of periodic width-modulation to reduce the thermal conductivity below the Casimir limit. Our results could be particularly useful for advanced thermoelectric applications which dictate drastic reductions in a material's thermal conductivity.

Biosketch: **Neophytos Neophytou** received his PhD in Electrical and Computer Engineering from Purdue University, West Lafayette, IN, USA in 2008. He worked as a Post-Doctoral Researcher at the Institute of Microelectronics at the Technical University of Vienna in Austria until 2013. He is currently an Associate Professor at the University of Warwick in the UK. His area of specialization is theory, computational modeling and simulation of transport in nanoelectronic materials and devices including nanowires, ultra-thin body devices, carbon nanotubes, and graphene nanoribbons. His current research interests include thermoelectric transport in nanostructured devices for energy conversion and generation applications.