Phonon transport effects in disordered graphene nanoribbons

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Abstract. In this work we investigate phonon transport in low-dimensional, disordered armchair 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 (Fig. 1a-b) 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 [1]. In the ballistic case, phonons throughout the entire phonon energy spectrum contribute to thermal transport. We show that with the introduction of line-edge-roughness, the phonon transmission is reduced, but quantitatively and qualitatively in different ways in different parts of the energy spectrum, i.e. phonons in specific energy regions can flow either ballistically, diffusively, or become localized depending on the channel geometry. Four distinct behaviors within the phonon spectrum in the presence of disorder are identified: i) the low-energy, low-wavevector acoustic branches are affected the least by edge disorder; ii) energy regions that consist of a dense population of relatively 'flat' phonon modes (including the optical branches) are also not significantly affected; iii) 'quasi-acoustic' folded bands that lie within the intermediate region of the spectrum are strongly affected by disorder; iv) the strongest reduction in phonon transmission is observed in energy regions that are composed of a small density of phonon modes, in which case roughness can introduce *effective transport gaps* (Fig. 1c) and band-mismatch, and drive transport into the localization regime. 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 [1]. 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 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, as also discussed earlier for different materials [2].

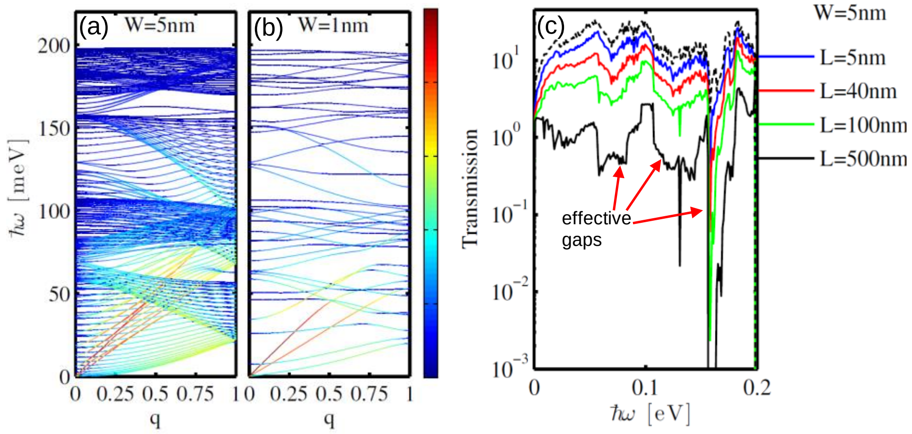

Fig. 1. Phonon dispersions for (a) W=5nm, (b) W=1nm wide GNRs. The colormap shows the contribution of each phonon state to the total thermal conductance (red: largest contribution, blue: smallest contribution). (c) The transmission function versus energy for rough edge GNRs of width W=5nm. The ballistic transmission (pristine GNRs, non-roughened ribbons) is depicted by the black-dashed line. Results for nanoribbons with lengths L=5nm (blue line), L=40nm (red line), L=100nm (green line), and L=500nm (black-solid line) are shown.

References

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