Thermal Transport in Suspended and Supported Graphene Nanostructures

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Thermal conductivity of graphene and graphene-based nanostructures [1], such as graphene nanoribbons (GNRs) [2], CVD-grown polycrystalline graphene (PCG) [3], and nano-patterned single-layer graphene (SLG) is of great interest due to their potential applications as logic devices, high-frequency amplifiers, and heat spreaders in future nanoelectronic circuits [4]. Device applications of graphene typically rely on samples supported on SiO_2 and cut into ribbons [5]. For switching applications, GNR-FETs have to be made from very narrow ribbons in order to lithographically tune the band-gap and achieve the required on-off ratios. High-frequency applications also lead to strong dissipation in GNR-FET [6], which further motivates the present interest in the thermal properties of narrow, suspended and supported ribbons.

Line edge roughness along the sides of narrow graphene ribbons has been shown to reduce the lattice thermal conductivity relative to its value in large flakes [7]. Initially, it was found that the ballistic thermal conductivity of graphene is isotropic; however, it was subsequently discovered that, when graphene is cut into nanoribbons, directional anisotropy of thermal conductivity appears [2]. Despite tremendous experimental and theoretical progress, a study treating both substrate and edge roughness effects on thermal transport, as well as their mutual interplay and the anisotropy of the lattice thermal conductivity tensor, has been lacking.

We explore lattice thermal transport in supported graphene nanoribbons (GNRs). We demonstrate the sensitivity of the lattice thermal conductivity in GRNs to the edge properties, based on solving the phonon Boltzmann transport equation (pBTE) under the relaxation time approximation. We derive a solution to the pBTE in the cross-ribbon direction with partially diffuse edges in the presence of competing scattering from the substrate, umklapp phonon-phonon, and isotope scattering processes, as depicted schematically in Figure 1. We compute the lattice thermal conductivity tensor, with excellent agreement with experiment (Figure 3) and show that is has two very distinct components: one along the ribbon, and another one in the cross-ribbon direction, as shown in Figure 2 (b-c). The parallel/cross-ribbon anisotropy increases in narrower ribbons and with increased line edge roughness, shown in Figure 4 (a-c).

In supported nanoribbons, we identify three ranges based on the width W of the GNR and the competition between edge roughness and substrate scattering: narrow ribbons (W<100 nm), where line edge roughness scattering dominates and anisotropy is very high, medium ribbons (100 nm<W<1μm) where substrate and roughness scattering compete and the two edges are effectively decoupled, and wide ribbons (W>1um) where substrate scattering dominates and thermal transport becomes nearly isotropic, shown in Figure 4 (d). Based on our model, we conclude that thermal conductivity of narrow GNRs can be effectively controlled by controlling their width and edge properties. Coupled with good electronic transport properties, this opens up the possibility of using GNRs for high-efficiency thermoelectric conversion. High degree of anisotropy in narrow ribbons also opens up the possibility of using GNRs as heat guides to move heat in a directed way by patterning the graphene ribbons into heat conduits.

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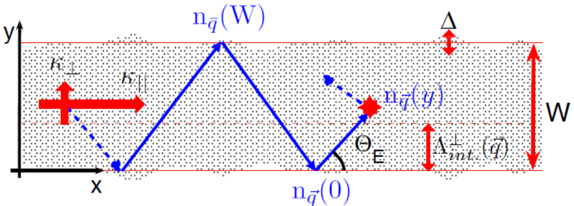

Figure 1: Schematic representation of the graphene nanoribbon, showing ribbon width W, line edge roughness Δ, and a phonon path through the ribbon [9].

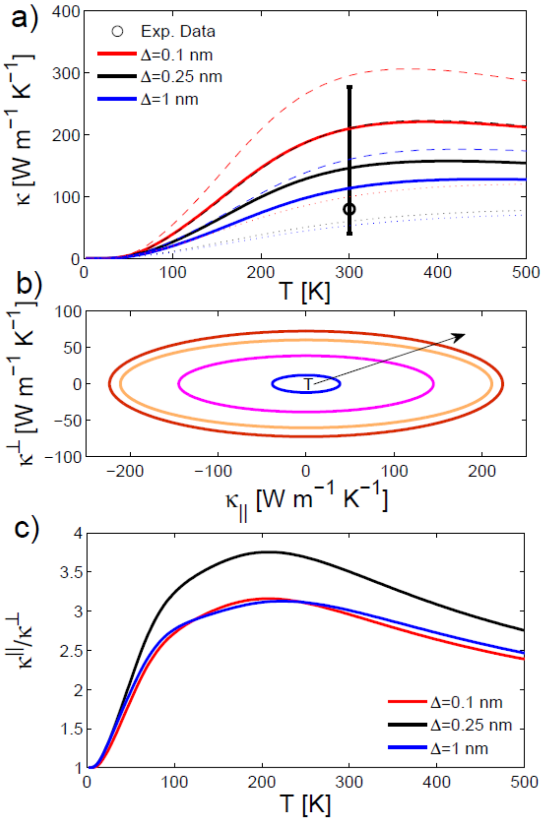

Figure 2: Effective lattice thermal conductivity of a 15 nm wide graphene nanoribbon supported on a SiO_2 substrate (a). Experimental data is from Ref. [5]. Parallel and perpendicular components of the tensor (b) show strong anisotropy at all temperatures (c). From Ref. [9].

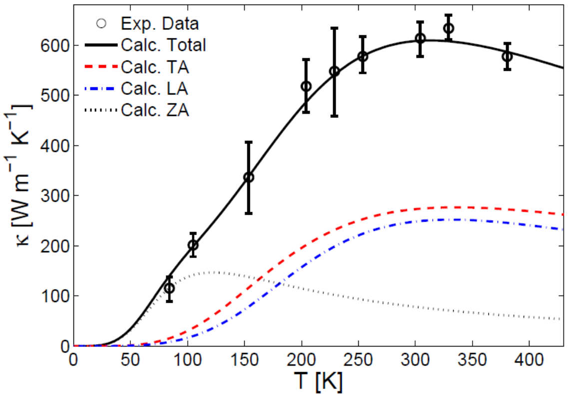

Figure 3: Comparison of lattice thermal conductivity of a wide (W=2 μm) graphene ribbon supported on SiO_2 with experimentally measured data from Ref. [8], showing excellent agreement throughout the temperature range.

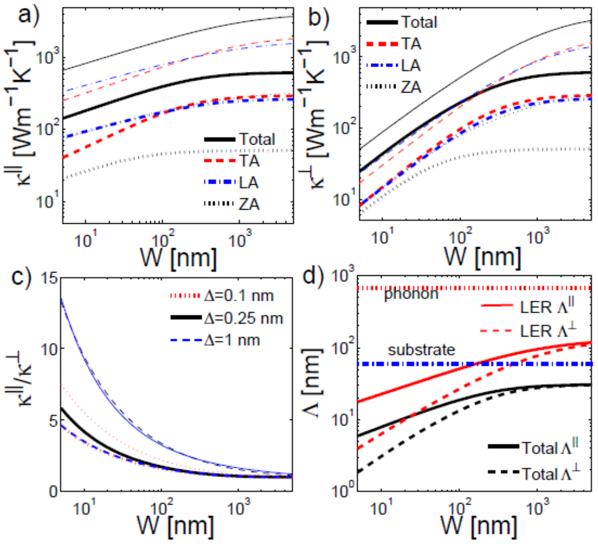

Figure 4: Dependance of room-temperature parallel (a) and perpendicular (b) components of the lattice thermal conductivity of supported graphene nanoribbons on the ribbon width W. The ratio of parallel to perpendicular components of the thermal conductivity tensor are shown in panel (c). Strong dependence of the parallel and perpendicular components of the LER and total phonon mean-free-paths on width W is shown in (d). Figure adapted from Ref. [9].