The role of dimensionality on phonon-limited charge transport: from CNTs to graphene

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Graphene and carbon nanotubes (CNTs) are two-dimensional (2D) and one-dimensional (1D) allotropes of pure sp^2 carbon. Their intrinsic electronic and transport properties are, therefore, intimately related. In particular, the transport properties of CNTs are expected to approach those of graphene when increasing tube diameter. However, this 1D to 2D transition, which gives insights into the role of dimensionality, has never been carefully studied.

In order to investigate this transition, an atomistic computational model for the phonon-limited carrier mobility in carbon materials has been developed. The carrier mobility is obtained from an exact solution of Boltzmann transport equation. A tight-binding model with the latest parameters extracted from first principle calculations is used for the electronic band structure. A force-constant model is used for the phonon band structure, and has been refined in order to reproduce the admixture of optical components into the acoustic phonon modes at non-zero wave-vectors. This admixture has significant impact on the carrier mobility.

This model has been validated against DFT calculations and experimental data. At high carrier density, the agreement with the DFT calculations of Ref. [1] (Fig. 1) and the experimental data of Ref. [2] (Fig. 2) is very satisfactory. At low carrier density, the agreement with experiment [3] (Fig. 3) is also very good, when the additional scattering by surface optical phonons in the substrate is taken into account [4].

The same model and parameters were used to study the transition from 1D to 2D in CNTs with diameter up to 16 nm. The mobility in CNTs converges to the mobility in graphene when increasing tube diameter (Fig. 4), but with very different (and possibly non monotonic) behaviors depending on the nature of the CNTs. The convergence is much faster at high carrier density (Fig. 5) and high temperature (Fig. 6). A simple explanation starts with the electronic band structure of CNTs – which can be viewed as a sampling of the 2D band structure of graphene by a bundle of lines parallel to the tube direction. In general, the mobility in CNTs approaches that of graphene when the number of bands in the transport energy window (a few kT around the Fermi energy) is large enough to smooth out the effect of 1D confinement on the band structure and on the electron-phonon interactions. The absence of linearly dispersive bands in semiconducting nanotubes and the selection rules for intervalley scattering are mostly responsible for the differences between CNT chiralities. Details will be given at the conference.

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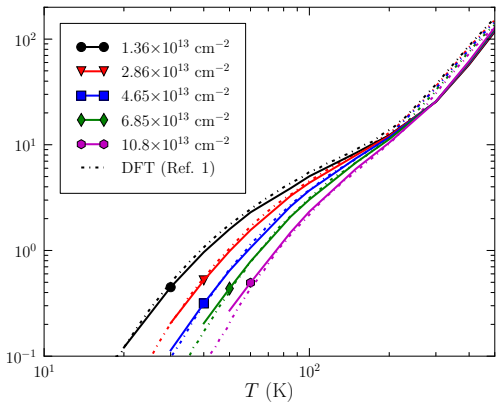

Fig. 1. Resistivity of graphene at high carrier (hole) density compared with recent DFT calculations [1].

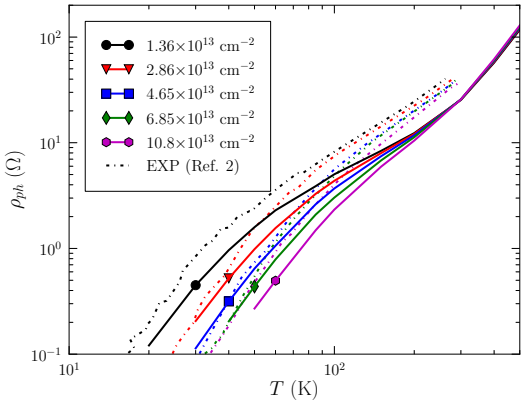

Fig. 2. Resistivity of graphene at high carrier (hole) density compared with experiment [2]. Note that our calculations only include the intrinsic electron-ponon scattering, and therefore underestimate the experimental mobility.

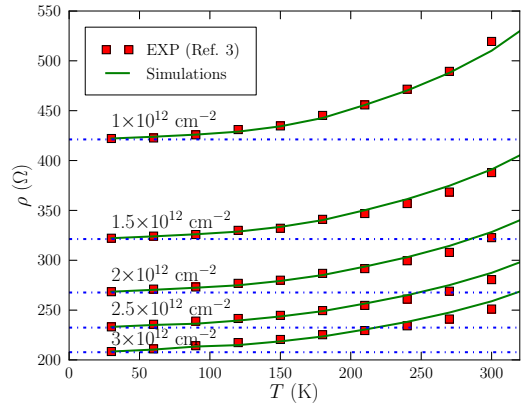

Fig. 3. Resistivity of graphene at low carrier (hole) density compared with experiment [3]. Scattering by surface optical phonons in the substrate is also included here.

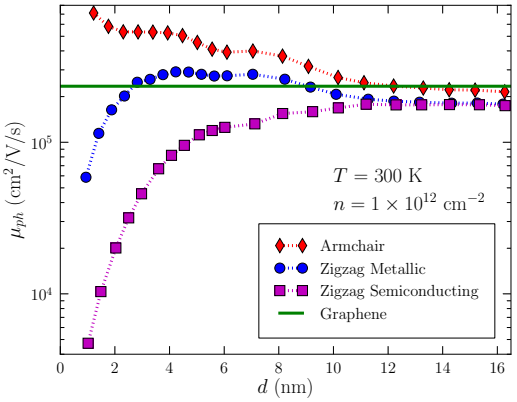

Fig. 4. Evolution of the mobility with the diameter of the CNTs.

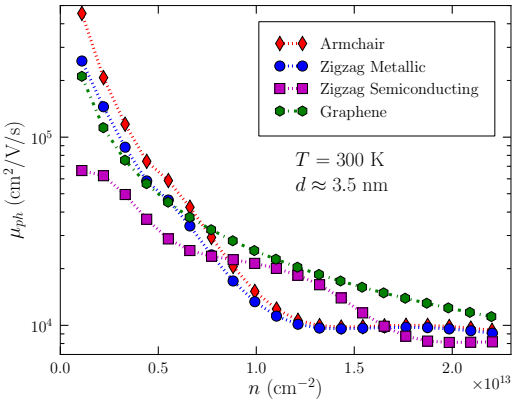

Fig. 5. Evolution of the mobility with the carrier (hole) density.

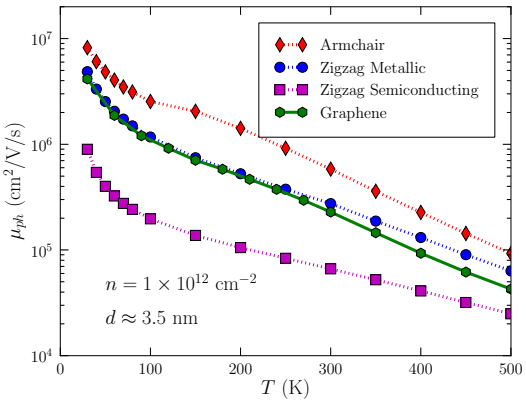

Fig. 6. Evolution of the mobility with temperature.