Electron Transport and Hot Phonons in Carbon Nanotubes

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Single-wall carbon nanotubes (SWNTs) can carry the highest current density of any material before they break. This makes them the best candidates as interconnects in integrated circuits. The current vs. voltage (IV) curve of metallic SWNTs has been measured by several groups. For voltages > 0.2 V, it is observed a sudden increase of the resistivity which is due to the scattering with optical phonons. The understanding of this phenomenon is a crucial step towards finding methods to boost SWNTs performances. In a recent paper [1] we have shown that, at high bias, the electron transport in metallic SWNTs induces an anomalously-high optical-phonon occupation (hot phonons) which, in turn, induces the measured resistivity increase. The fundamental quantity determining this phenomenon is the electron-phonon coupling (EPC).

In the first part of the seminar I will discuss our ab-initio calculations (based on density functional theory) of the EPC of SWNTs. I will show that SWNTs EPC can be obtained via a simple folding model from the EPC of graphite. The values obtained are used to explain a wide range of experimental facts: i) the large EPC value induces two Kohn anomalies in the phonon dispersion of graphite, which can be measured by inelastic X-ray scattering [2]; ii) the linewidth of the G peak in Raman spectra of graphite is almost entirely determined by the EPC [3]; iii) the differences in the Raman spectra of metallic and semiconducting SWNTs (the splitting and linewidths of the G+ and G- peaks) are determined by the EPC [3]. In the second part of the talk I will use the ab-initio EPCs to compute the electron scattering lengths in metallic SWNTs during transport. The comparison with experimental IV curves shows the existence of hot phonons with an effective temperature of several thousands K [1]. I will discuss a model for the quantitative description of phonon heating. The essential ingredient is the coupled Boltzmann transport equations for both phonons an electrons to determine in a consistent way the IV curve and the phonon occupation. A remarkable agreement with measured IV curves is found [4].

[1] Lazzeri et.al. Phys.Rev.Lett. 95, 236802 (2005);
[2] Piscanec et.al. Phys.Rev.Lett. 93, 185503 (2004);
[3] Lazzeri et al. Phys. Rev. B 73, 155426 (2006).
[4] Lazzeri et.al. Phys.Rev.B 73, 165419 (2006).