Raman bands in small diameter carbon nanotubes

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We carried out first principles calculations to obtain the phonon dispersion of single walled carbon nanotubes with small diameter. The calculations on the density functional level became possible by making use the helical symmetry of the tubes. It is very important that the Raman-spectrum of a carbon nanotube is dominated not only by Gamma-point phonons. Similarly to graphene, zone boundary phonons can be observed as well, when double resonance conditions are fulfilled. The two most important double resonant Raman bands are the disorder induced D band and its 'overtone', the 2D band (also known as G' band). After briefly introducing our results for Gamma-point phonons I will concentrate on double resonance processes.

Recently an interesting band in the region of the D band was observed in bilayer graphene when the two layers were rotated with respect to each other. We have shown that similar effect may be observed in double walled carbon nanotubes with different chiralities. The effect of disorder in such cases can be replaced by interaction between the two layers. However for double walled tubes two extra constraints exist as compared to bilayer graphene.

† In memory of my PhD student Ádám Rusznyák who died tragically in May 22 2013.