Optical Properties of Single and Double Wall Carbon Nanotubes

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Many striking properties of single wall (SWCN) and double wall (DWCN) carbon nanotubes are consequences of their symmetry [1]. We combined the density functional and the tight binding methods with the modified group projector technique [2], to develop numerical algorithm completely implementing symmetry in nanotube band structure calculations. The resulting code POLSym [3], enables us to perform very precise calculations of the electron and phonon (within the force constants approach) bands of quasi 1D periodic systems. Its efficiency is determined by the amount of the symmetry of the considered system.

Extremely high symmetry of SWCNs, generating whole compound from a single atom, to a large extent determines most of SWCNs properties. Therefore, SWCNs are exceptionally convenient for our approach, and we have been able to calculate electronic [4] and phonon [5] bands for several hundreds of chiral and achiral SWCNs.

On the contrary, the symmetry of DWCNs is greatly reduced with respect to the constituent layers. Nevertheless, it turns out that just this symmetry breaking is DWCNs important characteristic, being decisive with many respects. Analyzing the breaking, we have selected particularly interesting DWCNs and performed the numerical calculations for the few tents of the commensurate ones among them [5].

Here we list some of the results related to the light scattering in SWCNs and DWCNs. This includes optical activity, absorption and infra red (IR) and Raman scattering.

At first, the optical activity has been analyzed [1]. Due to the high isogonal group principle axis, the optical activity tensor is isotropic in the perpendicular to the tube plane. In addition, only in the achiral tubes this tensor vanishes, meaning that all the chiral tubes are active. As for the DWCNs, many various possibilities may occur, depending on the resulting symmetry (i.e. symmetry breaking), which is partly determined also by the relative coaxial position if the walls. Let us mention that even the tubes with both walls achiral may be active.

Next, we studied dichroism (birefrigence) [6]. Related to the optical activity, this property involves electronic bands, their quantum numbers, and selection rules for the optically induced transitions. The very prediction is based on the rough model [7]. Nevertheless, for reliable quantitative results for this and other properties as optical absorption, plasmon excitations, dielectric permeability, loss spectra, etc., the detailed calculations must be performed. Besides the robust precise calculations taking care of all the orbitals and their non-orthogonality, we have also applied a variety of different simplifications. The comparison of all these results gives insight to the relevance of different physical factors: orbital hybridization, collective phenomena, tube deformations and defects.

The results prepared and analyzed for many tubes are combined to get some insight to the real samples, containing different tube bundles, ropes etc.
As for the DWCNs, the Van der Waals interaction between the walls of DWCN still has not been successfully estimated by the density functional approach. Therefore, to calculate their electronic bands, we use more rough methods, but the exact symmetry is used to suite the form and the amplitude of the relevant potentials.

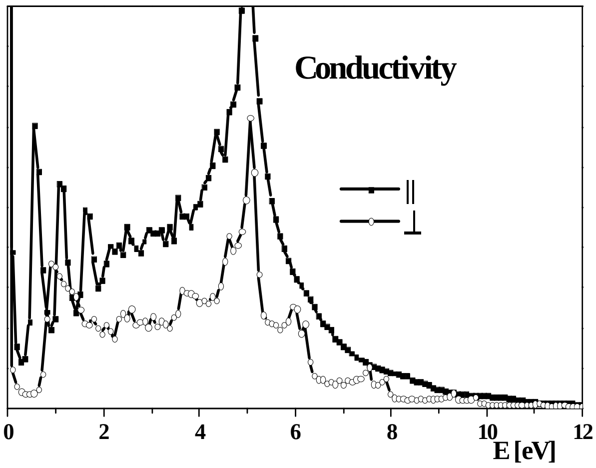

Figure 1 Parallel and perpendicular absorption averaged over the bundle of 29 SWCNs with diameters close to that of (10,10).

The calculations for IR spectra are naturally based on the phonon bands, while the Raman properties calculations combine both electron and phonon domain. For SWCNs the dependence of frequencies of all the Raman and IR active modes on the tube diameter and chirality is established. Analogous results are found for DWCNs. The lowest $k=0$ (nonacoustic) frequencies correspond to the relative coaxial motions of the walls; being only 5-20 cm^{-1} they give experimentally verifiable evidence on the extremely low friction of the walls.

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