11th International Conference on Advanced Materials
Rio de Janeiro Brazil
September 20 - 25
ICAM2009

Natural Torsion in Small Diameter Carbon Nanotubes

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Abstract – This work investigates the possibility that small diameter chiral carbon nanotubes have a natural torsion originating from the symmetry breaking due to chirality effects. This natural torsion is calculated using an extended tight-binding model and is found to decrease as the inverse cube of the diameter. The dependence of the natural torsion on the chiral angle is found to be di®erent for metallic and semiconducting nanotubes, especially for near-armchair nanotubes, for which the behavior of semiconducting nanotubes deviates from the simple sin(6θ) behavior observed for metallic nanotubes.

Several theoretical and experimental studies indicate that the electronic and optical properties of carbon nanotubes are extremely sensitive to structural deformations such as axial, radial or torsional strains.[1-4] However, these reports assume that in its natural state, carbon nanotubes are free from such geometrical deformations. In the case of radial and axial strains, this assumption can always be asserted since these deformations maintain the full symmetry of the nanotube and thus the nanotube structure can be renormalized to the new parameters without losing its basic properties. However, in the case of a torsional strain, the pure translational symmetry of the nanotube is broken and thus, the usual representation of the nanotube unit cell needs to be revised. In this work we calculated the natural torsion of small diameter single wall carbon nanotubes using an extended tight-binding (ETB) approach [5] considering a DFT calculation-based parameterization [6]. Although the torsion breaks the pure translation symmetry of the nanotube, the screw–rotational symmetry is preserved, enabling for a symmetry-based calculation of the electronic band structure. The torsional deformation affects the interatomic distances, changing the calculated band structure. The natural torsion is found by minimizing the total energy with respect to the torsional deformation. This procedure was performed to calculate the natural torsion in all carbon nanotubes with diameters (d_t) ranging from 0.5 to 1.75 nm and a d_t^{-3} dependence was found for the value of the natural torsion. Also, the dependence of the natural torsion on the chiral angle was found to be different for metallic and semiconducting nanotubes. Also, this natural torsion was found to increase the minigap found in metallic nanotubes by up to 50%, this gap opening was found to depend on the square of the chiral angle(θ).

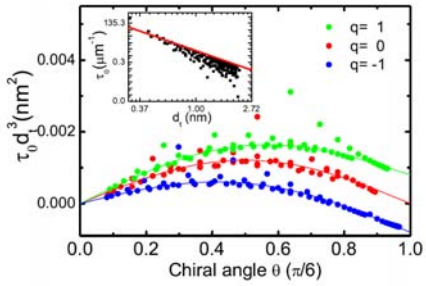

Figure 1: Dependence of the natural torsion (τ_0) on the chiral angle (θ) . The inset shows the diameter (d_t) dependence τ_0 in log scale. The solid line represents a d_t^{-3} dependence.

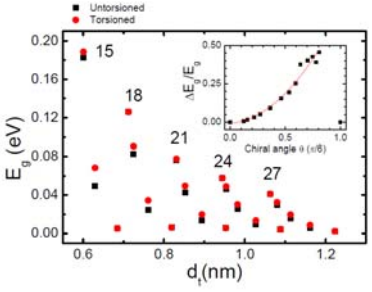

Figure 2: Dependence of the minigap in untorsioned (square box) and torsioned (circle) metallic nanotubes on the nanotube diameter (d_t). The inset shows the chiral angle dependence of the relative change in the minigap

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