The Importance of Defects in Carbon Nanotubes: How to Identify them using Different Techniques

Mauricio Terrones

Advanced Materials Department, IPICyT, Camino a la Presa San José 2055
78216 San Luis Potosí, SLP, México

It is clear that defects are always present within carbon nanotubes (single- and multi-walled). The amount of defects depends on the production method, which involves the process temperatures. For example, arc discharge and laser ablation methods involve extremely high temperatures close to 2500 – 3500 °C, and these processes result in the generation of highly crystalline nanotubes. However, chemical vapor deposition (CVD) techniques, usually involve lower temperatures ranging from 650 – 1200 °C. Unfortunately, these tubes contain large number of defects and the walls appear to possess vacancies, carboxyl groups, and other elemental dopants. In practice, it is difficult to identify the type of defects contained in carbon nanotubes, and researchers have never systematically distinguished them. However, depending on the defective surface, the chemical activity, as well as the mechanical ad electronic properties of the tubes may be quite different.

In this talk, defects within carbon nanotubes will be categorized in 4 different groups: 1) *Structural defects*, related to imperfections that significantly distort the curvature of the hexagonal carbon honeycomb structure; these defects are usually caused by the presence of non-hexagonal rings (e.g. pentagons, heptagons, or octagons; 2) *Topological defects*, occurring on the nanotube surface, which do not result in large curvature distortions of the tubule. In particular, these defects could be 5-7 pairs embedded in the hexagonal network or Stone-Wales (SW-type) defects that could be created by rotating a carbon bond within 4 neighboring hexagons, thus resulting in the transformation of 2 pentagons and 2 heptagons; 3) *Doping-induced defects*, arising from substitutional non-carbon atoms embedded (or incorporated) into the tubular lattice, and 4) *Non-sp^2 carbon defects or edge-sites* caused the presence of highly reactive carbons such as dangling bonds, carbon chains, interstitials (free atoms trapped between SWNTs or between graphene sheets), edges (open nanotubes), add-atoms and vacancies.

From the theoretical standpoint, the structural stability and electronic properties of nanotubes containing hexagons, pentagons and heptagons will also be discussed in detail. These structures, now termed Haeckelites, are predicted to be metallic and exhibit enhanced electronic conductances when compared to standard pure carbon nanotubes. High resolution transmission electron microscopy (HRTEM) studies and theoretical calculations reveal that these type of structures are likely to be synthesized.

This presentation will review recent work related to different techniques used to identify defects using HRTEM, scanning tunneling microscopy (STM), scanning tunneling spectroscopy (STS), Raman spectroscopy (RS), atomic force microscopy (AFM), thermogravimetric analyses (TGA), electron and thermal transport measurements, etc. It is important to mention that most of the time the presence of defects and their identification has been overlooked by numerous scientists. However these play a key role in the nanotubes' physico-chemical properties. There are numerous challenges that will be discussed in this presentation: How do we identify defects efficiently? Could we distinguish among various defects? Would it be possible to establish a protocol able to quantify and control the amount of these defects? How many defects are necessary to fabricate robust polymer composites or nanotube junctions? Could we observe ferromagnetism in defective nanocarbons?, etc.