

Carbon nanotubes: From the structure to electronic properties

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Carbon nanotubes (CNTs) are usually thought of as graphitic sheets with a perfect hexagonal network and sp^2 -bonded carbon atoms that have been wrapped up into a seamless cylinders. Since their discovery in 1991 by Iijima the peculiar mechanical and electronic properties of these materials have attracted much attention. It has been theoretically predicted and then experimentally established that the CNTs exhibit semiconducting or metallic properties depending on their geometrical characteristics as diameter and helicity of the arrangement of hexagonal rings within a single layer. In the case of the semiconducting nanotubes the band gap is roughly proportional to the reciprocal of the tube diameter. Therefore precise knowledge of their atomic structure is required to understand the measured electric transport and optical activity properties.

On the other hand experimental observations have shown that the CNTs are not necessarily as perfect as they have been thought to be. The possible defects that can occur are topological (non-hexagonal rings), re-hybridization defects (sp^2 - sp^3 intermediate bonding) and incomplete bonding defects (vacancies, dangling bonds, dislocations). The presence of pentagon-heptagon pairs is the most interesting because it can change the helicity of the tube and alter its electronic structure. Moreover, the nanotubes having different helicities can be connected forming nanoscale metal/semiconductor or semiconductor/semiconductor junctions, composed only of a single element. No other material offers such a possibility.

One of the most convenient ways of investigating the atomic configuration of the CNTs has been thought direct imaging techniques using high-resolution electron microscopy, scanning electron or atomic force microscopy. Electron diffraction or selected area electron diffraction have also been used to study the atomic structure of the CNTs. Although these methods are valuable in giving information on specific regions of the sample material they do not yield quantitative details for the total sample volume it is desirable to obtain more global information about their structure. In the present work applications of the X-ray and neutron diffraction techniques together with the method of the pair distribution function were used to characterise the structure of the CNTs on the atomic scale. A third generation synchrotron source and pulsed neutrons were applied providing the structural data with extremely high resolution in real space approaching 0.1 Å, inaccessible using any other diffraction technique. Different types of the CNTs were studied and usefulness of these complementary approaches accompanied by the modelling techniques is presented.

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