o.m7.o3 **Structural characterization of carbon nanotubes.**
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Keywords: carbon based materials.

Most of the properties of a single-wall nanotube depend on its diameter and on the helicity of its atomic structure. These two parameters, diameter and helicity, are related to the wrapping indices (n,m) that identify the nanotube. If the diameter of a nanotube can be measured accurately, the helicity is much more difficult to determine. In this talk, the few techniques giving access to both diameter and helicity will be reviewed.

In the case of isolated nanotubes, the most powerful structural techniques are scanning tunneling microscopy (STM) and selected-area electron diffraction. It will be shown that the analysis of the experimental data is greatly improved by comparison with computer-generated diffraction patterns or STM images. Illustrations from both theory and experiment will be presented.

o.m7.o4 **Crystal structure and properties of a sodium peroxide based graphite intercalation compound.**
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Keywords: graphite intercalation compound, sodium, oxygen.

It is easier to intercalate sodium into graphite, when a very small oxygen amount is added to the reagent metal (1 at. % approximately). By heating at 470°C for 1 or 2 days, in a stainless steel reactor and under a pure argon atmosphere, a pyrographite sample or a single crystal immersed in the previous oxidized metal, we synthesize a blue second stage graphite intercalation compound (1). This latter, which is poorly reactive in the ambient atmosphere, is a ternary graphite-sodium-oxygen phase, with a repeat distance of 1080 pm. Its chemical formula is $NaO_{0.44}C_{5.84}$.

The structural study of this compound exhibits clearly that the intercalated sheets are five-layered, according to the [Na-O-Na-O-Na] **c**-axis stacking. The distance between both oxygen layers is 152 pm. This value corresponds to the distance between both oxygen atoms of the peroxide O_2^{2-} anion. On the other hand, each sodium layer contains the same amount of alkali metal atoms. Thanks to these observations, it is possible to consider that the five-layered intercalated sheets are sodium peroxide slices, which have been cut perpendicular to their **c**-axis. Three successive sodium layers build a sheet constituted by two planes of octahedra : in each plane, these octahedra are connected by edges, and they are connected by faces, in the perpendicular direction. The peroxide anions occupy two adjacent octahedra, so that the oxygen-oxygen bonds are perpendicular to the common faces of the octahedra, that is to say parallel to the **c**-axis. All the double octahedra of each intercalated sheet are not occupied by the peroxide anions : two thirds of the double sites only are indeed occupied. The intercalation between the graphene layers of these sodium peroxide slices leads of course to several distorsions of these latter ; for instance, after intercalation of the peroxide slices, it appears that the octahedra are flattened along the **c**-axis.

Electrical resistivity measurements have been carried out for several samples : the basal plane conductivity exhibits a quasi-metallic behaviour, since the **c**-axis resistivity value presents a maximum around 245K. The resistivity anisotropy is particularly high (10^6 at the helium boiling point).

^{13}C NMR experiments corroborate the metallic character of this compound. On the other hand, XPS measurements show very clearly that the intercalated oxygen corresponds to O_2^{2-} peroxide anions and not to O^{2-} classical oxide anions. This result successfully confirms the previous structural model.

[1] M. El Gadi et al., J. Sol. St. Chem., 131, (1997), 282-289.