RESISTIVITY OF SAMPLES CONTAINING NANOTUBES

R. Heyd†,A. Charlier†,E. McRae‡,J.F. Marêché‡ and M.F. Charlier†

† Laboratoire de Physique du Solide, 1 Bld Arago, 57068 Metz, France

‡Laboratoire de Chimie du Solide, BP 239, 54506 Vandoeuvre, France

INTRODUCTION

A theoretical study of the electrical properties of compounds containing nanotubes is justified by the experimental results obtained during measurements of electrical resistivity. We submit a local deformation model for each type of studied tubules (i.e. zig-zag or armchair) within the framework of continuum elasticity theory. Deformation energy per atom of carbon and orbital overlap integrals are computed.

EXPERIMENTAL RESULTS

We measured the electrical resistivity ρ versus temperature between 295 and 4.2 K for a series of samples from carbonaceous rods prepared under different pure helium pressure P_{He} ranging from 20 to 750 torr and therefore containing various proportions of nanotubules. The van der Pauw technique was used with currents of the order of a few hundreds μA.

In all cases the resistivity rises as T decreases, with some correlations between the relative rise in resistivity and the helium pressure in the chamber used for the synthesis. The observations and results are in agreement with those indicated elsewhere [1,2]. The curves of normalized resistivities $\rho(T)/\rho(292)$ versus temperature T are shown in figure 1.

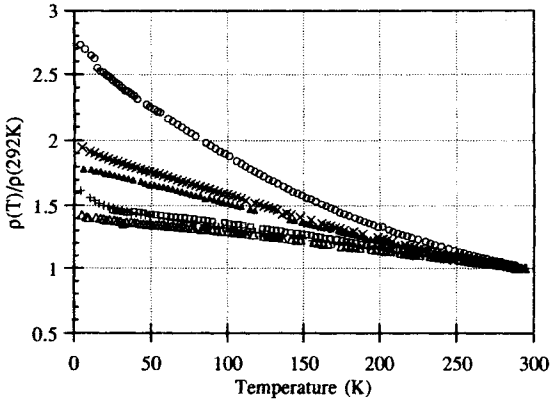

Figure 1 Relative resistivity vs temperature

As the temperature rises the conductivity is a stronger function of T for samples prepared under higher pressures, i.e. possessing more tubules. This suggests that tubules contribute to electrical properties in a specific way. In each case the experimental resistivity measurements obey a mathematical law represented by formula (1):

$$\rho(T) = C\exp(-AT)$$

where A and C are positive constants (see figure 1).

The temperature law presented in figure 1 is unusual. We submit a two level model, previously proposed for graphite resistivity measurements along c axis. The theoretical interpretation of oxydes' resistivity measurements near the Verwey transition was also performed ten years ago with success using this model[3]. The qualitative law given by formula (1) prompts us to examine electrical features of nanotubes.

NOMENCLATURE

We especially study two classes of nanotubes. According Hamada's et al. classification [4] we speak of zig-zag and armchair fibers.

We first choose an origin O and the two unit vectors $\vec{a_1}$ and $\vec{a_2}$ in the graphite plane. Next we roll the graphene sheet in such a way to superimpose the desired index point A(n_1,n_2) on the origin O: $\vec{OA}= n_1\vec{a_1}+n_2\vec{a_2}$. Where n_1 and n_2 are whole numbers.

For example Z(n,0) type tubules are called "zig-zag" fibers and have one Carbon-Carbon bond parallel to tubule axis at least. Thus A(2n,n) type is called "armchair fibers" and have one Carbon-Carbon bond perpendicular to tubule axis at least.

THEORETICAL APPROCH

Following the work done by Tomanek [5] we propose a local deformation potential model for each type of tubules studied, zig-zag or armchair, within the framework of continuum elasticity theory. We obtain a warping potential V(M) given by

$$V(M) = \frac{C}{R^2} z_M^2 \quad (2)$$

where C is a constant and R the tubule radius. The model used for zigzag fibers is a series of bended rods, with the following characteristics:

- thickness e=3.35Å
- height h=0.71Å
- periodicity h'=1.42Å

The evaluation of deformation energies per atom for different fibers in the limit of an infinite height gives results in good agreement with Tomanek's values[5] .This is shown by the following numerical results.

P	$R(Å)$	$e_P(eV/atom)$
5	1.96	4.546
7	2.74	2.319
10	3.91	1.136
20	7.82	0.284
30	11.73	0.126
40	15.66	0.071

P is the number of carbon atoms per ring, R is the corresponding radius and e_P the deformation energy per atom. We apply our local warping potential to overlap integrals computations. The results well agree with our theoretical values.

REFERENCES

1. S. Ijima, *Nature*, 354, 56, (1991)
2. T.W. Ebbesen, P.M. Ajayan, *Nature*, 358, 220, (1992)
3. I. Shiozaki, C.M. Hurd, S.P. Mc Alister, W.R. Mc Kinnon, P. Strobel, *J. Phys. C:Solid State Phys.*, 14, 4641, (1981)
4. N. Hamada, S. Sawada, A. Oshiyama, *Phys. Rev. Letters*, B68, 1579, (1992)
5. D. Tomanek, W. Zhong, E. Krastev, *Phys. Rev.*, B48, 15461, (1993)