Molecular Polarizabilities of Model Carbon Nanotubes from Atomic Increments

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The interacting induced dipoles polarization model implemented in our program POLAR is used for the calculation of the dipole-dipole polarizability $\overline{\overline{\alpha}}$ (1). The method is tested with single-wall carbon nanotube (SWNT) models as a function of nanotube radius and elliptical deformation (2-4). The results for the polarizability follow the same trend as reference calculations performed with our version of program PAPID. For the zigzag tubes, the polarizability is found to follow a remarkably simple law, *i.e.*, varies as the inverse of the radius. A dramatic effect is also found with elliptical deformation. It is found that the polarizability and related properties can be modified continuously and reversibly by the external radial deformation. These results suggest an interesting technology in which mechanical deformation can control chemical properties of the carbon nanotubes. POLAR calculations differentiate more effectively than PAPID computations among SWNT models with increasing radial deformation. Different effective polarizabilities are calculated for the atoms at the highest and lowest curvature sites. POLAR calculations discriminate more efficiently than PAPID computations between the effective polarizabilities of the highest and lowest curvature sites. This remarkable and significant tunable polarizability can have important implications for metal coverage of metals on nanotubes and selective adsorption and desorption of foreign atoms and molecules on nanotubes and can lead to a wide variety of technological applications, such as catalysts, hydrogen storage, magnetic tubes, *etc*.

Provisional conclusions follow.

1. The results of the present work indicate clearly that due to the differences between POLAR and PAPID results, it may become necessary to recalibrate POLAR. It appears that the results of good quality *ab initio* calculations might be suitable as primary standards.

2. It has been shown that the polarizability of a zigzag SWNT model can be modified reversibly and variably by the radial deformation. POLAR calculations differentiate more effectively than PAPID computations among SWNT models with increasing radial deformation.

3. Different effective polarizabilities are calculated for the atoms at the sharp site and flat site. POLAR calculations discriminate more efficiently than PAPID computations between the effective polarizabilities of the sharp site and the flat site.

4. The tunable polarizability reported in this paper can have important implications for metal coverage of metals on nanotubes and selective adsorption/ desorption of foreign atoms on the carbon nanotubes.

1. F. Torrens, J. Sánchez-Marín and I. Nebot-Gil, J. Mol. Struct. (Theochem), **463**, 27 (1999).
2. F. Torrens, J. Nanosci. Nanotech., in press.
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4. F. Torrens, Microelectron. Eng., submitted for publication.

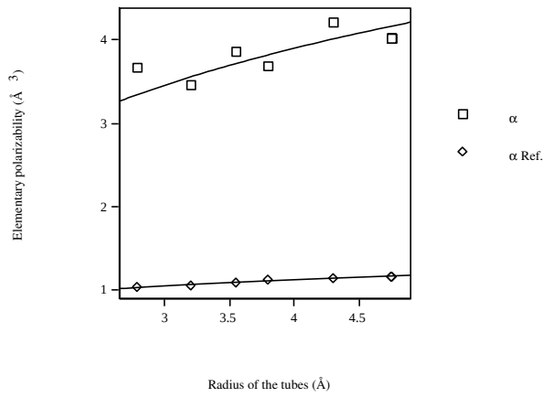

Figure 1. Elementary polarizability per atom of the zigzag $(n,0)$ $(7 \le n \le 12)$ SWNT models *vs*. the radius of the tubes.

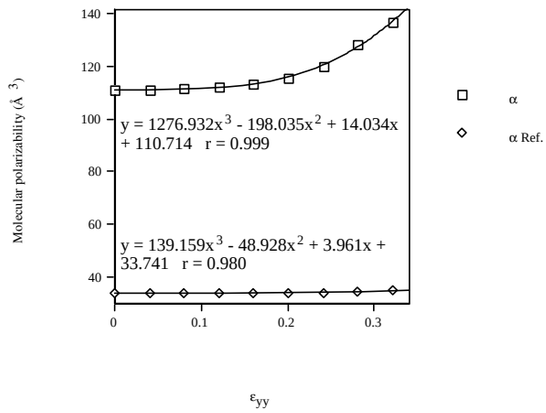

Figure 2. Molecular polarizability of the zigzag $(8,0)$ SWNT model *vs*. the elliptic radial deformation, ε_{yy}.

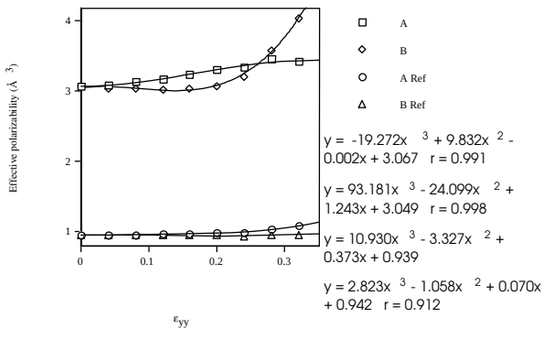

Figure 3. Effective polarizability of atoms near the end of the major axis *a (sharp site)* and minor axis *b (flat site)* for a $(8,0)$ SWNT model vs. the elliptic radial deformation, ε_{yy}. The upper curve corresponds to atoms on the high curvature region near the end of the major axis *a (sharp site)*. The lower curve corresponds to atoms on the low curvature region near the end of the minor axis *b (flat site)*.