MOLECULAR MODELING OF THE ELASTIC MODULI OF POLYETHYLENE –SWCNT COMPOSITES

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The aim of this work is to investigate the reinforcement effects of carbon nanotubes (CNT) in polymeric matrices for different physical properties (room and middle temperature mechanical properties, thermal properties and other functional ones). Because of their small physical size with high aspect ratio, high modulus and strength, good thermal and electrical conductivity, CNT are promising fillers in polymer composites at very low loading [1]. The prediction of mechanical properties of model samples of such composites is a useful counterpart to the much more expensive experimental techniques; the type of matrix to be used, the optimal crosslink degree and the degree of functionalization of the CNT are examples of chemical variables which can be suitably probed by Molecular Modeling.

In this preliminary stage of the study we want to investigate the dependence of a suitable property such as elastic constant on a chemical variable (such as the number of chains chemically bonded to the CNT for unity of length of the CNT, the degree of crosslink, the polymeric matrix). From the calculated dependence it is possible to predict which is the value of the chemical variable in order to get the best of the property, thus translating a calculation result in a hint to the experimentalist.

Because of the dimension of the system we have decided to use a “static” method to calculate the elastic constant matrices. The procedure involved several energy minimizations starting from different minima with different density (to simulate the effect of temperature). Different strains were applied on the starting minima and then the systems were allowed to relax completely. The resulted deformations were registered and strain tensors were computed. The obtained results will be compared with those calculated by Molecular Dynamics simulations.

With these ideas in mind, a model composite built up with 1 single walled carbon nanotube (SWCNT) (5,5) 48 angstrom long, embedded in a polymer matrix consisting of 34 chains of poliethylene (PE) 80 monomers long, was set up in order to be subjected to minimizations.
The system was prepared by putting the PE molecules around the SWCNT in a very low density system with the aid of the commercial program CERIUS^2 [2] [Fig.1a]; then periodic boundary conditions (PBC) are applied and the whole system is minimized with respect to both conformation and cell parameters by means of a home-made program [Fig.1b]. The force field (FF) employed is the Siepmann portable FF [3,4,5] where hydrocarbons are modeled following the united atom approach; also the Dreiding FF [6] available in CERIUS^2 reasonable choice as a first approach.

References:

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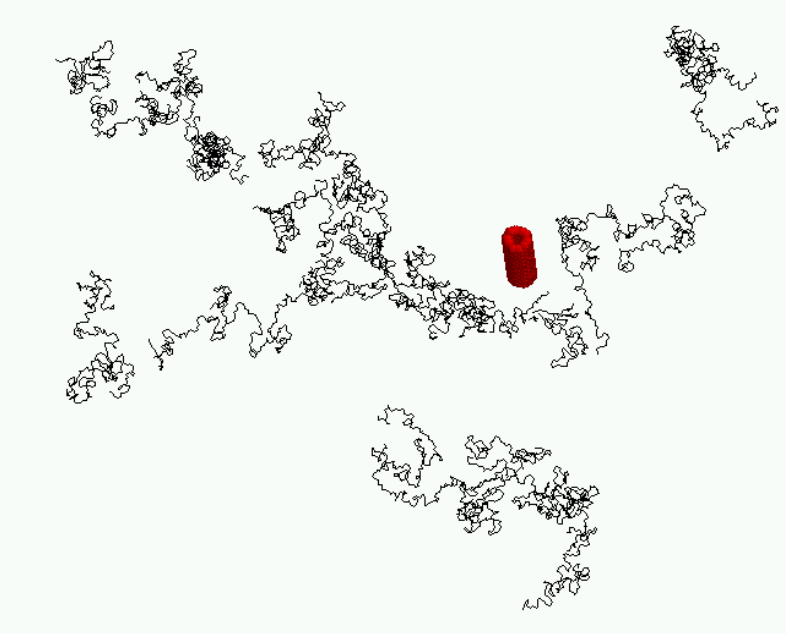

Figure 1a. Initial configuration of the PE-SWCNT composite built with the help of the CERIUS^2 software. The whole system is in vacuum and the PE chains are in random coil conformation.

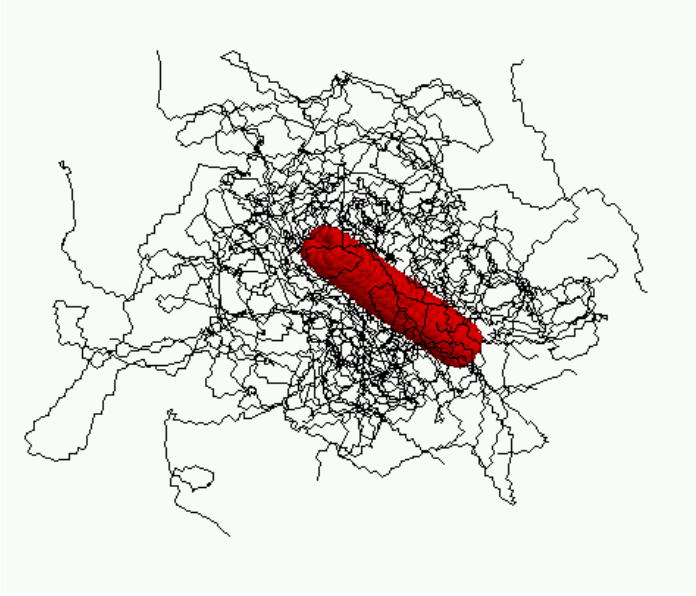

Figure 1b. The PE-SWCNT composite after application of PBC and minimization with respect to both conformations and cell parameters.