HOMOGENISATION MODELS OF CARBON NANOCOMPOSITES MECHANICAL PROPERTIES

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Introduction

It is well known that single walled (SWCN) or multi walled carbon nanotubes (MWCN) offer a significant amount of stiffness (1-4 TPa) or strength comparing with those obtained for classical graphite or carbon fibres. However, those nanomaterials cannot form structures used for engineering purposes. On the other hand, nanocomposites made of SWCN or MWCN can loose a lot of their magnificent mechanical properties when will be joined with the matrix. Of course, the same situation is observed for classical carbon/graphite microcomposites.

The general aim of the present paper is following:

- to present the theoretical homogenisation models for the evaluation of the Young modulus values for nanocomposites reinforced with SWCN and MWCN,
- to propose method of numerical modelling nanocomposites reinforced by SWCN and a polymer matrix,
- to compare the obtained results with classical microcomposites in order to demonstrate advantages and disadvantages of both composite materials.

Modelling of nanocomposites mechanical properties

Two theoretical models have been presented and discussed in details – see also [1]. The first one is based on the physical description by taking into account interatomic interaction and nonotubes geometry. This approach employs the form of the physical potential proposed by the Tersoff-Brenner. The elementary cell definition, here nanotube, with surrounding resin layer is treated as the homogeneous body - the material continuum. Next, the similar model to phenomenological engineering approach has been presented that is created by the junction of the law of mixture with the Cox mechanical model. This model describes the stress distribution along stretched short fibres surrounded by the resin matrix. The similarity between the composite materials reinforced by short fibres and nanotubes has been considered and pointed out. The evaluation of the Young modulus requires the basic information about the materials parameters of the nanotubes and resins. This method can be easily adopted in all engineering computations and possible applications.

The numerical model corresponds directly to the 3-D form of a single carbon nanotube (i.e. a graphene sheet rolled up to a cylinder) surrounded by a polymer resin layer. The interaction between two neighbourhood carbon atoms in the nanotube and between carbon atoms and the resin are expressed with the use of the Tersoff-Brenner potential and van der Waals forces. Numerically the interaction is modelled by a 1-D spring FE having a stiffness derived from the above mentioned relations. It is assumed that the single nanotube surrounded by the resin forms an elementary cell. That subcell is a starting point for the derivation of averaged mechanical properties using standard homogenisation rules – see e.g. [2].

Results and Concluding Remarks

In order to compare the interatomic interaction model with phenomenological model the value of Young modulus has been calculated for two different volume fraction of nanostructures: 10% and 20% - see Fig.1. The experimental investigations proved that the values of modulus are close to the modules, which is obtained from the interatomic interaction model.

The considered carbon nanocomposites have lower Young modulus than that for classical fibre microcomposites. In our opinion, the factors leading to such rather bad properties are following the low volume fraction of the reinforcement in composites, random distribution of the nanotubes and the length of reinforcement which deformation results in many unfavourable effects.

In present phase of evolution composites reinforced by nanotubes do not allow to get better mechanical properties than microcomposites. However, there is a great possibility of using nanotubes in industrial applications due to higher strength and Young modulus than analogous properties for micro-fibres.

Numerical homogenisation models are complicated due to necessity of taking into account specific nanotube geometry (see [1]), and not only the nanotube diameter. Therefore, the plot demonstrates only one pointed obtained from numerical analysis. However, it should be emphasised that carbon nanotubes have two general average dimensions: the diameter and the length and both of them that can affect significantly the nanocomposite mechanical properties. In our opinion, the length should be also taken into consideration, especially for short nanotubes, and it shows explicitly the advantages of numerical modelling.

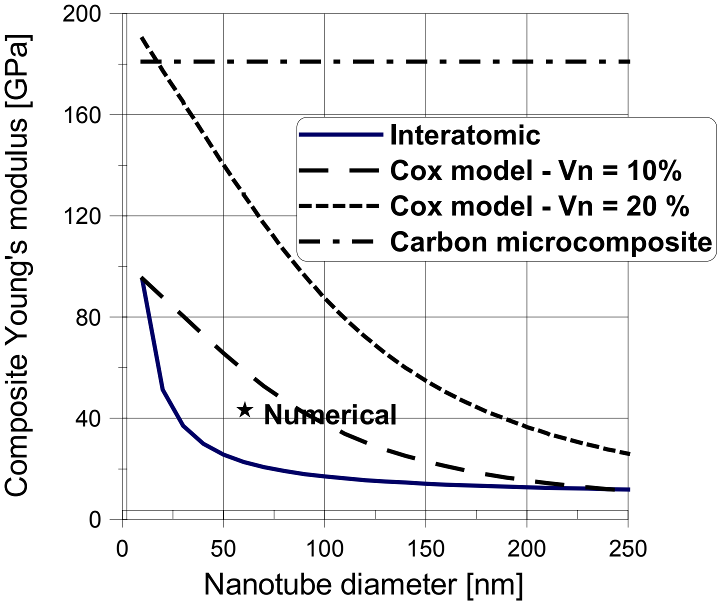

Fig.1 A comparison of mechanical properties for carbon micro- and nano- composites

In present phase of evolution composites reinforced by nanotubes do not allow to get better mechanical properties than microcomposites. However, there is a great possibility of using nanotubes in industrial applications due to higher strength and Young modulus than analogous properties for micro-fibres. Theoretical considerations demonstrate only modest improvement in mechanical properties for nanocomposites. To improve it is necessary to solve various technological problems dealing with: alignment of nanotubes, dispersion of nanotubes in the matrix, functionalization of the nanotubes to enhance matrix bond/load transfer, efficient use of the different types of nanotube reinforcements (SWCN vs. MWCN vs. nanoropes). Now, a number of methods have been used to achieve highly oriented CN – see e.g. [3]. All these methods are limited to microscale and are not suitable for commercial manufacturing process.

Validity of the assumptions relating the applicability of continuum based theories vs. physical models (understood in the sense of both solid state physics and quantum mechanics) is still an open problem. However, the results presented in the paper demonstrate that physical models gives much better description for low values of nanotubes diameters, whereas for high values two approaches leads to the almost same results.

References

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