CHARACTERIZING LOAD TRANSFER EFFICIENCY IN CARBON NANOTUBES NANOCOMPOSITES USING MULTISCALE SIMULATION

Ting-Chu Lu, Jia-Lin Tsai*
Department of Mechanical Engineering, National Chiao Tung University, Hsinchu, Taiwan
* Corresponding author(jialin@mail.nctu.edu.tw)

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1. Introduction

The load transfer efficiency from the matrix to the carbon nanotubes (CNTs) plays an important role in the mechanical response of the CNTs nanocomposites since it may affect the effectiveness of the nano-reinforcements. For the multi-walled carbon nanotubes (MWCNTs), not only the outer graphene layers but also the inner layers may be responsible for sustaining the load. Thus, the loading capacity within the inner layers may influence the whole performance of the nanocomposites. By applying load on the outer wall, Shen et al. [1] studied the load transfer between the adjacent walls of double-walled carbon nanotubes (DWCNTs). It was found that the loading on the outer wall can not be effectively transferred into the inner wall. However, when chemical bonding between the walls is established, the load transferred to the inner layer can be enhanced dramatically. How to introduce the interatomistic characteristics of DWCNTs in conventional composite model is an interesting task since the length scale in continuum mechanics and atomistic modeling is distinct. In this study, the load transfer efficiency from a surrounding matrix to the CNTs was examined using multi-scale simulations. Both single-walled carbon nanotubes (SWCNTs) and DWCNTs were taken into account in the investigation. The interatomistic behaviors between the adjacent graphite layers in DWCNTs were characterized by molecular dynamics (MD) simulation, from which a cylindrical DWCNTs continuum model was established. Subsequently, a representative volume element (RVE) containing the hollow cylindrical continuum (denoting the CNTs) and matrix was proposed and employed in the finite element analysis for characterizing the axial stress distribution as well as the load transfer efficiency of the CNTs within nanocomposites.

2. Molecular Dynamics Simulation

2.1 Interatomistic potentials

In MD simulation, the interatomistic behaviors between atoms were described using the potential functions which normally consist of bonded and non-bonded interactions. For the CNTs, AMBER force field [2, 3] was utilized in the simulation of bonded interactions, while, the non-bonded property was characterized using the Lennard-Jones potential [4]. It is noted that for the DWCNTs, in addition to van der Waals (vdW) force, the artificial build-up covalent bonds were considered as the interatomistic properties between the adjacent graphite layers. In order to evaluate the atomistic intensity of the adjacent graphite layers, the outer graphite layer was extended relative to the inner layer in MD simulation as shown in Fig.1. During the simulation, both the extension of the outer layer and the reaction of the inner layer were recorded. In this study, (3, 3) and (8, 8) DWCNTs with the lengths of 80, 162, 295 and 492Å were employed in the MD simulations which were conducted using a DL-POLY package [5].

2.2 Equivalent continuum solid of DWCNTs

Based on the extension versus reaction curves of DWCNTs obtained from MD simulation, a two-layer hollow cylindrical continuum in which the interaction of the neighboring layers was modeled using spring element was proposed. It is noted that the corresponding spring constants between the layers were determined so that the extension versus reaction curve derived from the continuum model would match with that obtained from the MD simulation. Basically, the spring constants

associated with the two interfacial properties (vdW interaction, covalent bonding) were determined, respectively. In addition to the interfacial properties, the atomistic configurations of DWCNTs with the diameter of the outer and inner layers being D_1 and D_2 were converted equivalently into its continuum counterpart as shown in Fig.2. It is noted that "h" indicates the interlayer spacing of the graphite walls which is normally equal to 0.34nm [6]. The geometric parameter R_{1o}, R_{1i}, and R_{2i} representing the inner and outer radius of each layer in the continuum solid can be expressed in terms of the atomistic configuration as $R_{1o}=(D_1+h)/2$, $R_{1i}=(D_2+h)/2$, and $R_{2i}=(D_2-h)/2$. In the continuum solid, it was assumed that the thickness of each layer is equal to "h" such that no gaps exit between the adjacent layers. This two-layer hollow cylindrical continuum model proposed to represent the discrete atomistic structure of the DWCNTs was then embedded in the matrix to form a continuum model of nanocomposites.

3. Continuum Finite Element Analysis Model

A cylindrical representative volume element (RVE) containing the hollow cylindrical continuum shell (denoting the CNTs) and matrix phases were employed in the FEM continuum analysis. Because of the cylindrical attribute of the RVE, a half-quarter symmetric 3-D finite element analysis (FEA) model was employed in the evaluation of the load transfer efficiency in the CNTs nanocomposites. Fig.3 demonstrates the continuum FEA model for the DWCNTs nanocomposites. By applying a loading σ_o, the corresponding stress distribution on the layer 1(outer layer) and layer 2 (inner layer) can be evaluated directly from FEA analysis. It is noted that in Fig.3, the DWCNTs is perfectly bonded to the matrix and the interface between the graphite layers is modeled using the spring element as described earlier. It is noted that there were four different lengths of DWCNTs adopted in the FEM model and the length effect in the load transfer efficiency was discussed in the next section. Moreover, the influence of interfacial adhesion between the neighboring graphite layers was also investigated in the study. The peculiarity of the FEM model is that the inherent atomistic interactions existing between the graphite layers in discrete DWCNTs structure was successfully implanted in the continuum nanocomposites by means of the spring element.

4. Results and Discussion

Fig.4 shows the axial stress distribution in layer 1 and layer 2 for the DWCNTs with length of 492Å. It can be seen that the stress in both layers increases from the CNT ends, while the increasing rate for the layer 1 is greater than that in layer 2. This tendency indicated that when the loading is moved from the matrix to the outer layer, most of the loading is still carried by the outer layer and only little loading is transferred to the inner layer. It can be found that the stress in outer layer eventually attained the saturated value while the inner layer is still in the low stress level. Apparently, through vdW atomistic interaction, the stress cannot be effectively transferred from the outer layer to the inner layer. In an attempt to improve the load transfer of DWCNTs, the artificial build-up covalent bonds were established between the graphene layers and the corresponding stress distribution is shown in Fig.5. Basically the stress distribution of outer layer is not affected by the covalent bonding, however, the stress in the inner layer increase significantly in the presence of the covalent bonds. This phenomenon demonstrates that the DWCNTs with covalent bonds can effectively enhance load transfer efficiency from the matrix to the outer layer and further into the inner layer. To effectively quantify the load transfer efficiency from the surrounding matrix to the DWCNTs, the concept of effective length is introduced as [7]

$$L_{eff} = \frac{\int_0^L (\sigma_{f1} + \sigma_{f2})dy}{2\sigma_f^s} \qquad (1)$$

where σ_{f1} , σ_{f2} indicate the axial stress in layer 1, and layer 2, respectively, and σ_f^s is the corresponding saturated stress of SWCNTs associated with the same length of DWCNTs. In the design of nanocomposites, the main concept is to facilitate the load applied on the materials being efficiently transferred into the reinforcement and carried by the reinforcement. Indeed, the effective length can be regarded as an index to evaluate the effectiveness of the reinforcement embedded in the

matrix. When the effective length is increasing, it indicates that the load carrying efficiency of the reinforcement is increasing, and the overall mechanical properties of the nanocomposites can be enhanced accordingly. When the effective length concept was implemented on SWCNTs, the effective length was calculated as

$$L_{eff} = \frac{\int_0^L \sigma_f dy}{\sigma_f^s} \quad (2)$$

where σ_f is the axial stress in the SWCNTs, and σ_f^s is the corresponding saturated stress. Fig.6 illustrates the load transfer efficiency of SWCNTs and DWCNTs and DWCNTs with covalent bond. It is shown that the covalent bond can effectively improve the load transfer efficiency of DWCNTs. However as compared to the SWCNTs, the improvement is still less. In addition, no matter in SWCNTs or DWCNTs, the increase of CNTs length basically can enhance the load transfer efficiency in CNTs nanocomposites.

5. Conclusion

The atomistic interaction of adjacent graphite layers in DWCNTs was characterized using MD simulation, based on which a spring element was introduced as the interface in the continuum DWCNTs model. Afterwards, the continuum DWCNTs was embedded in the matrix to form a continuum nanocomposites from which the load transfer efficiency were determined. It was found that the load transfer efficiency increases with the increment of CNTs length. In addition, the DWCNTs with covalent bonds exhibit superior load transfer efficiency than those with only vdW interactions. In addition, the SWCNTs still possess the best load transfer efficiency as compared with DWCNTs even though there are covalent bonds in the DWCNTs. Therefore, to achieve better mechanical properties, SWCNTs instead of DWCNTs are suggested as reinforcements.

References

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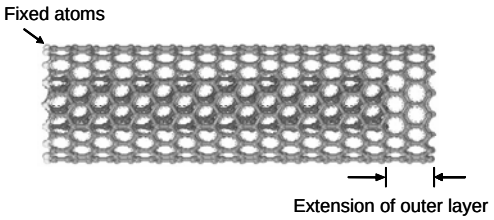

Fig.1. Extension of the outer layer in DWCNTs

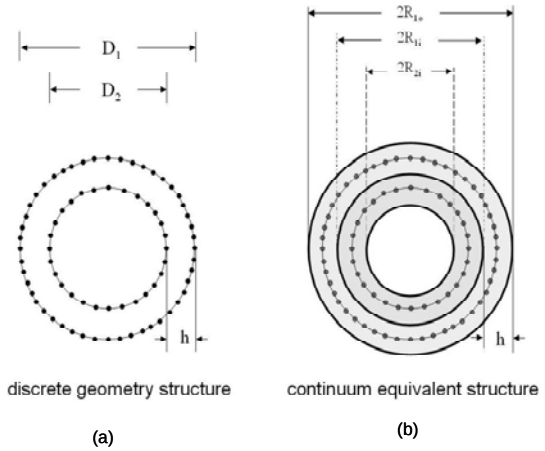

Fig.2. Conversion of DWCNTs discrete molecular structure into an equivalent continuum solid ((a) discrete molecular structures, (b) equivalent continuum solid).

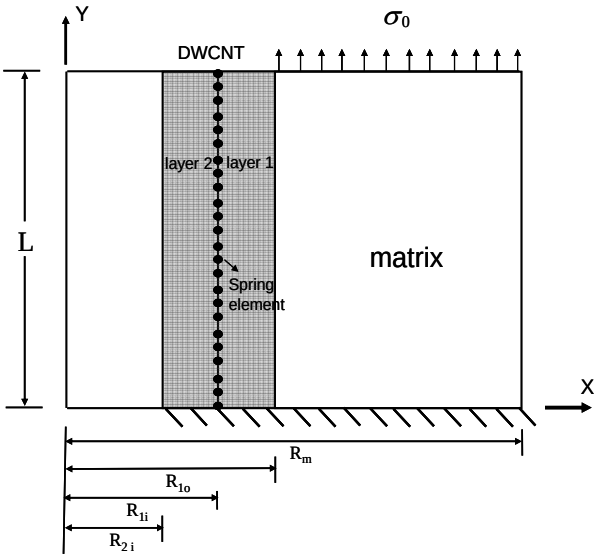

Fig. 3. Continuum FEM model for DWCNTs nanocomposites.

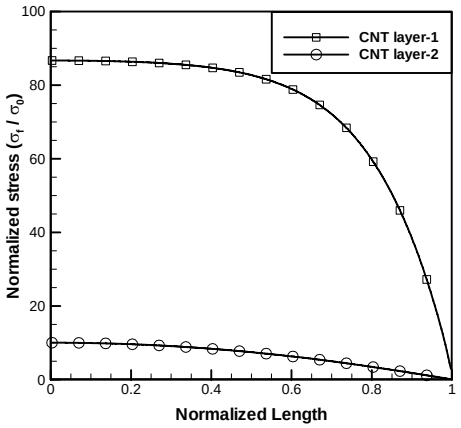

Fig. 4. Stress distribution in the DWCNTs

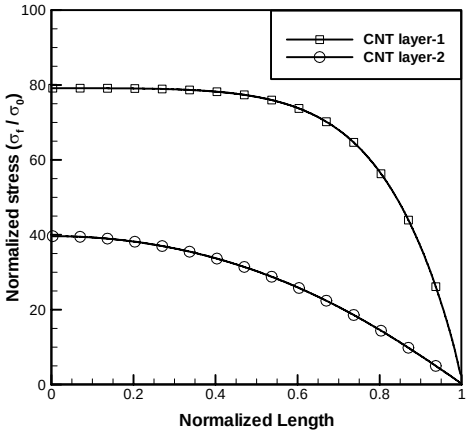

Fig. 5. Stress distribution in the DWCNTs with covalent bonds

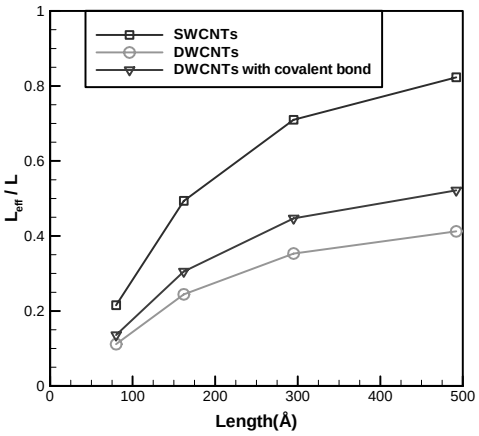

Fig. 6. Load transfer efficiency of SWCNTs and DWCNTs.