Research on the mechanical properties of the CNT composites

Luodan Su, Qingsheng Yang*

Department of Engineering Mechanics, Beijing University of Technology, Beijing 100124, China
*Corresponding author: qsyang@bjut.edu.cn

Abstract Carbon nanotube (CNT) can be used as a good reinforcement embedded into polymer matrix. However, properties of composites reinforced by CNT can't be improved efficiently, because of the damage of interface between CNT and polymer in CNT composites. In this paper, the cohesive zone model (CZM) was employed to express the damage and fracture of interface between CNT and the epoxy matrix. The key parameters of the bilinear CZM were deduced based on the existing theory work. The whole deformation and fracture process of the interface has been revealed through the FE simulation results. The performance of the interface decides the mechanical property of the CNT composites and the stress-strain curve of composites has been plotted. It is with great importance to study the mechanical property of the interface to improve the performance of CNT composites.

Keywords Carbon nanotude, Composite, Interface, Damage, Crack Growth

1. Introduction

Since the discovery of carbon nanotube (CNT) by Iijima [1], CNT has wide application potential because of their wonderful physical and mechanical property, it has been thought as a promising candidate as the ideal reinforcing fibers for advanced composite with high strength and low density. However, mechanical property of composites reinforced by CNT can't be improved efficiently, owing to the deep affect of interface between CNT and polymer in CNT composites. The damage and fracture of the interface leads to stress redistribution in CNT composite, and decides the effective mechanical property of the composite. The mechanical property of the interface is the key factor of the CNT reinforced composite [2].

The Cohesive zone Model (CZM) describes material separation with a traction-separation law (T-S law) and links the micro-structural failure mechanism to the effective properties of the composite [3,4]. Because of the nano-scale interface in CNT composite, the van der Waals force plays an important role in the property of the interface [5,6]. The Cohesive zone Model(CZM) can reflect the characteristic and working principles of the van der Waals force phenomenologically, by two important parameters, the cohesive strength Tc and the energy release rate Gc , as shown in Fig.1[7]. The effective separation and damage parameter from view point of stiffness reduction are employed. The different T-S law has been developed with continuous study of the cohesive model, and the CZM has been widely used in interface decohesion and crack growth.

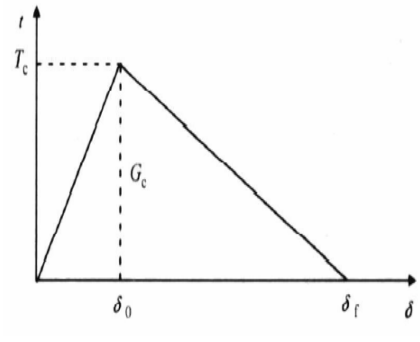

Figure 1. Bilinear cohesive law

Nowadays, many researchers have realized the significance of the van der Waals force in the interface between the CNT and the matrix, and study mechanical property of the interface of CNT composite with various method, such as the experimental method and the Melecular Dynamics (MD) method [8]. There are still many technical limitations in experimental method, and the calculation cost of the MD method is too huge. The Finite Element Method (FEM) combined with the CZM is the effective and economy method to study mechanical property of the interface of CNT composite, and the CZM was utilitied in this paper to predict local damage initiation and fracture propagation.

2. CZM Model of Interface

The key problem of the CZM is the definition of the two important parameters, the cohesive strength Tc and the energy release rate Gc. There is few experimental data providing the interface parameters accurately and directly for the CZM. Gou[9] has calculated the shear strength by the MD simulation of the CNT's pull out from the matrix. The result 75MPa was adopted to be the shear strength .Tan[6] has deduced the normal strength 470MPa and the energy release rate 0.107Jm^{-2}, from the Lennard-Jones potential from the van der Waals interactions, the results was adopted as the normal cohesive strength and the energy release rate Gc. The interface between the CNT and the matrix was modeled by the 2 dimension, 4 node cohesive element COH2D4 to reproduce the damage of interface between the CNT and polymer. The Young's modules of the CNT and the epoxy matrix are respectively 1 TPa and 4GPa.

The FEM model of the CNT composite was established by the generally used software ABAQUS. It is with three phases: the CNT fiber phase, the cohesive interface phase employing the CZM and the epoxy matrix phase. The unit cell was extracted to represent the effective properties of CNT composite based on the homogenization theory, as is shown in Fig. 2.

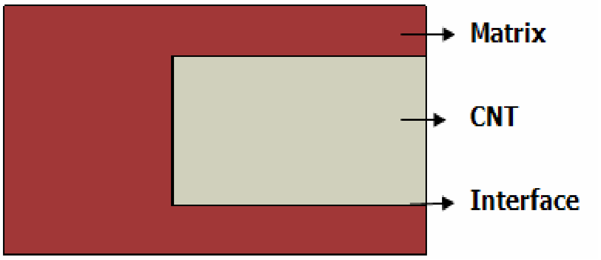

Figure 2. Unit cell of CNT composite

Since composite structures are usually designed for the loading in the reinforcement orientation, the displacement load was exerted at one side of the unit cell, and the other side was fixed, the boundary conditions of the unit cell was demonstrated in Fig. 3.

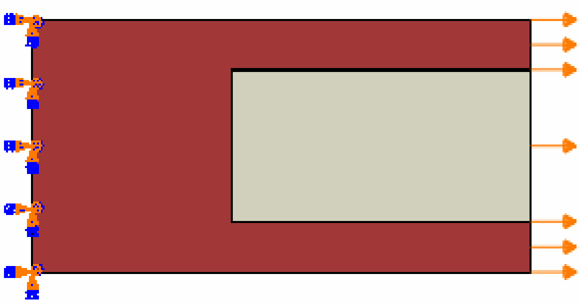

Figure 3. Boundary conditions of unit cell

3. Results and discussion

One of the advantages of the FE simulation is that the whole deformation and damage process can be observed clearly in the simulation. From the FE results, three obvious stages of mechanical properties of the interface were found: the linear elastic stage, the damage initiation stage and the crack propagation stage, as is shown in Figs. 4-6. The unit of the labels of the stress distribution nephogram is GPa.

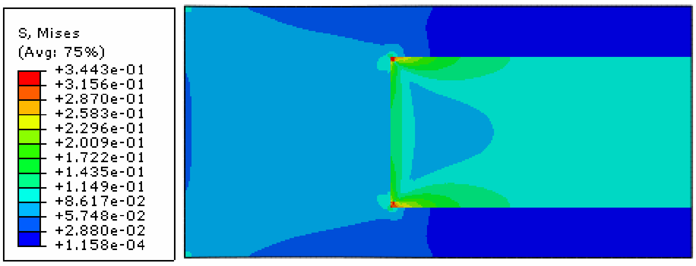

Figure 4. Stress distribution at linear elastic stage

In the linear elastic stage, the epoxy matrix and the CNT were bonded by the interface. The high cohesive strength ensures the effective transfer of the stress between CNT and the matrix. CNT takes more load than the matrix, the properties of CNT composites have been improved by the strong interface. The stress in the matrix where near by the CNT end is larger than the other positions in the matrix, and the stress in the CNT where near by the interface is larger than the other positions in CNT. In addition, the stress concentration appears at the corner of the CNT end.

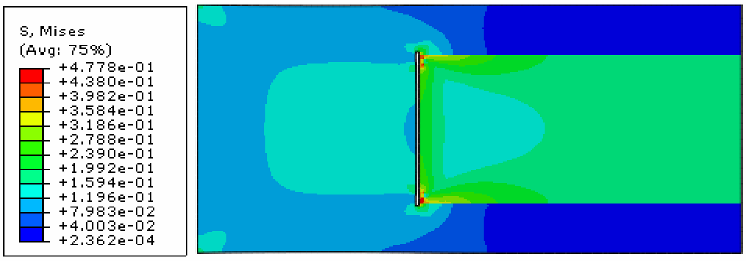

Figure 5. Stress distribution at damage initiation stage

As the displacement increasing, the damage initiation stage comes up, the damage initiated at the corner of the interface due to stress concentration. The damage of the interface leads to the stiffness reduction and stress redistribution in the composite, although the composite still has the capacity to bear the load. Then the microcracks at the corner grows, the crack extends to the end side of the interface.

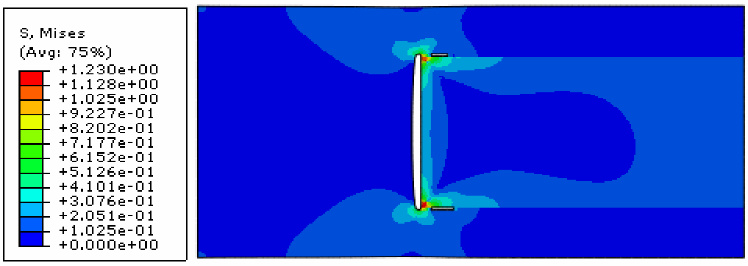

Figure 6. Stress distribution at crack propagation stage

At the crack propagation stage, the shear sliding comes up after the normal debond in the corner of the interface, as can be seen from the Fig.6, the normal crack hasn't connected to the shear crack, the shear crack initials at a position near the interface end . For the damage and the debond of the interface, the CNT composite has been failed to take the load. The interface plays an important role to the mechanical property of the composites. The maximum stress appears in the corner of the interface, the stress concentration effect should be considered to predict the damage initiation and the crack propagation.

4. The discussion of mechanical property of CNT composites

The crack progress and the fracture mechanism of the interface has been studied by the CZM model. The influence of the interface to the CNT composites can be reflected in the stress--strain curve of the whole unit cell, as is shown in Fig.7. Because of the effect of the interface, the relationship between stress and strain is nonlinear. At first, the composite displays linear characters, on account of the valid function of the interface before the stress gets to its strength value. The effective modules of the composites in the linear stage is 9.44GPa, CNT has the obvious reinforcing performance. Then accompanies with the crack propagation in the interface, the stress has an abrupt drop. The performance of the interface decides the mechanical property of the CNT composites.

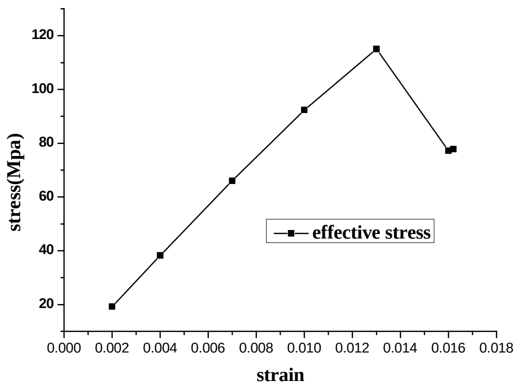

Figure 7. Stress-strain curve of CNT composites

5. Conclusion

1. The CZM of the interface between the matrix and CNT has been established to predict the mechanical property of interface, and it is proved that CZM is effective in the nanocomposites.
2. The whole deformation and damage process of the interface has been studied through the FE simulation results.
3. The stress--strain curve of composites has been plotted to research the mechanical properties of the composites. It is with great importance to study the mechanical property of the interface to improve the performance of CNT composites.

Acknowledge
This work is supported by the National Natural Science Foundation of China under the Project Number 11172012, and the Ph. D programs foundation of the Ministry of Education under the Project Number 20101103110005, which are gratefully acknowledged.

Reference

[1] Iijima S. Helical microtubules of graphite carbon . Nature, Vol 354(1991)56-61.
[2] Tserpes,K.I. , Papanikos, P. , Labeas,G. Multi-scale modeling of tensile behavior of carbon nanotube-reinforced composites. Theoretical and Applied Fracture Mechanics, 49(2008)51-60.
[3] N.Chandraa，H.Lia. Some issues in the application of cohesive zone mode For metal-ceramic interfaces. International Journal of Solids and Structures, 39(2002)2827-2855.
[4] D.Stevanovic. FEA of crack-particle interactions during delamination in inter layer toughened polymer composites. Engineering Fracture Mechanics,72(11)(2005)1738-1769.
[5] Jiang LY, HuangY, Jiang H, et al. A cohesive law for carbon nanotube/polymer interfaces based on the van der Waals force. J of Mech and Phys of Solids, 54(11) (2006)2436-52.
[6] H.Tan, L.Y.Jiang, Y.Huang, et al. The effct of van der Waals-based interface cohesive law on carbon nanotube-reinforced composite materials. Composites Science and Technology, 67(2007)2941-2946
[7] X. Guo, aA.Y.T. Leung ,A.Y. Chen. Investigation of non-local cracking in layered stainless steel with nanostructured interface. Scripta Materialia, Vol 63(2010)403-407.
[8] Li C Y, Chou T W. Modeling of elastic buckling of carbon nano-tubes by molecular Structural mechanics approach. Mechanics of Materials,36(2004)1047-1055
[9] Gou J H, Minaie B, Wang B, et al. Computational and experimental Study of interfacial Banding of single-walled nano-tube reinforced composites. Computational Materials Science, 31(2004)225-236