# The mechanical behaviors of polymer-carbon-nanotube composites suffering from compressing or tensile loading

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## Abstract:

Carbon nanotubes (CNTs) have attracted great interest in using CNTs as reinforcement in nano-composite due to its exceptional properties such as high stiffness and strength, light and high toughness characteristics as well as superior electrical and thermal properties. Thus, this paper studies the uniaxial stress-strain behaviors of the polymer-CNTs composites by using the molecular dynamic (MD) simulations. The composite consists of single-wall CNTs and crystalline polyethylene, and the direction along the length of the CNT is uniform as that of the polyethylene chains. In the MD simulation, the original simulation cell is approximated as $67\,\mathring{A} \times 46\,\mathring{A} \times 58\,\mathring{A}$ with the periodical boundary condition in all three directions applied. The interactions in the whole molecular system are described by the potential functions, including the Morse potential for all bonds, the harmonic cosine potential for all angles, the cosine potential for all dihedral angles and the short-range potential of the 12-6 potential for the VDW interaction among atoms. Additionally, the planar potential for all inversion angles in the CNT is also used. The total energy of the whole system $E_{\text{total}}$ is equal to the sum of the total energy of the polyethylene matrix $E_{\text{polyethylene}}$ and the total energy of the carbon nanotube $E_{\text{CNT}}$, which are expressed as

$$\begin{cases} E_{\text{total}} = E_{\text{polyethylene}} + E_{\text{CNT}}, \\ E_{\text{polyethylene}} = E_{\text{bond}} + E_{\text{angle}} + E_{\text{dihedral}} + E_{\text{short-ranged}}, \\ E_{\text{CNT}} = E_{\text{bond}} + E_{\text{angle}} + E_{\text{dihedral}} + E_{\text{inversion-angle}} + E_{\text{short-ranged}}. \end{cases} \tag{1}$$

The loading is applied by the displacement increment $0.5\,\mathring{A}$ along the length direction of the cell step by step. Under the different volume fraction of the CNT, the stress-strain curves of the composites suffering from compressing or tensile loading are calculated by the MD software DL-POLY. The obtained stress-strain curves are shown in Fig.2. It can be seen from Fig.2 that the obtained elastic modulus of pure polymer agree well with the experiment results (150~180GPa)

[1]. The modulus of the composite increases with the increase of the volume fraction of the CNT, and an increment 16.23% of the modulus by the volume fraction 10.72% is achieved.

## Reference:


[1] Peacock A J. Handbook of polyethylene: structures, properties, and applications. New York: Marcel Dekker, Inc.; 2000. p. 544


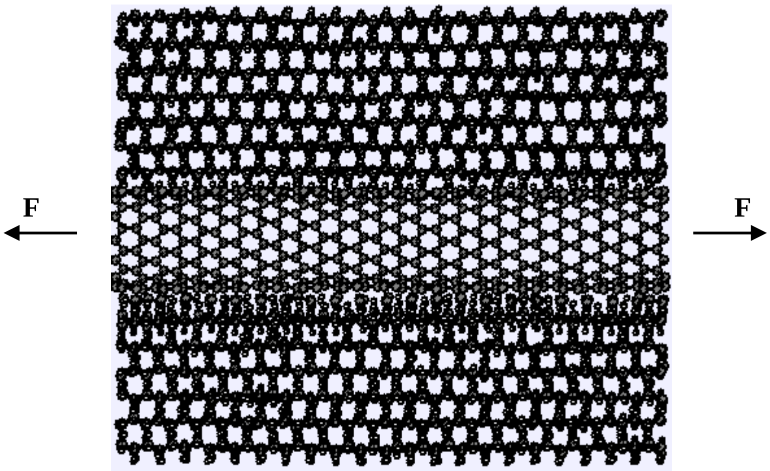


Fig.1 The simulation cell of the composite of polymer-CNT under

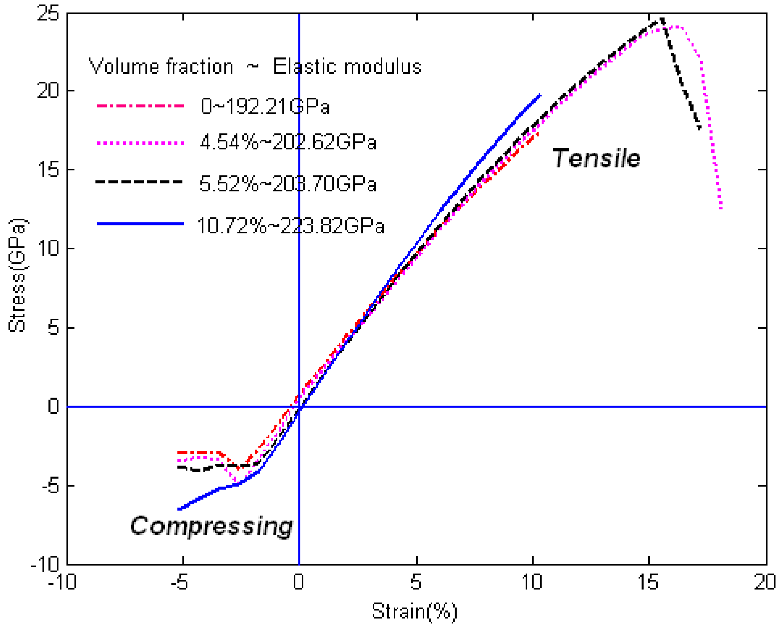


Fig.2 The stress-strain curves of composites with different volume fraction of CNT