Electronic Supplementary Material (ESI) for Nanoscale

Supplementary Information

Microstructural evolution of carbon nanotube fibers: deformation and strength mechanism

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In our CGMD modeling, the energy associated with the torsion of CNTs was neglected. In the following, we explain this simplification from the viewpoints of both physical deformation mechanism and validity of the modeling approach.

Physical deformation mechanism

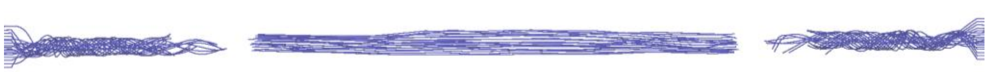
In actual CNT fibers, the lengths of CNTs range from several hundred micrometers to several millimeters, and the CNT diameter is only several nanometers. This results in the extremely high aspect ratio and high flexibility of CNTs. Thus, in the process of spinning a CNT fiber by twisting CNT films, for example, it is reasonable to assume that the intertube van der Waals forces play the dominate role in the deformation of CNTs. Furthermore, experimental observations show that the surface twist angles of CNT fibers are usually less than 30 degrees. Meanwhile, in the interior of a CNT fiber, the twist angles decrease as the distances between the CNTs and the fiber axis become smaller and overall CNTs in the fiber have not been twisted severely. Consequently, the torsion of CNTs would not have an effect as significant as stretching, bending and van der Waals interaction during CNT fiber fabrication and deformation, and could be neglected in the current modeling.

CGMD modeling with CNT torsion

To further illustrate the feasibility of neglecting CNT torsion in the current modeling, we have simulated the twisting of a CNT film with regular CNT distributions where the torsional energy of CNTs is taken into account. The energy associated with the torsion of a CNT is represented as $E_T = k_T[1-\cos(\beta)]$[1], where k_T is the torsional stiffness of the dihedral angle associated with four adjacent beads, and β is the dihedral angle. By fitting to the classical molecular dynamics modeling of CNT under torsion[2],

(a)

(b)



(c)

Figure S1. Morphology of a twisted CNT film when the CNT torsion is taken into account: (a) the whole twisted film, (b) the upper CNT layer and (c) the lower CNT layer.

the coefficient k_T is estimated as 3116.29 kcal/mol for the CNT (5,5) with interbeads equilibrium length of 5nm. Figure S1a shows the configuration of a twisted CNT film, and Figure S1b and S1c are the configurations of the upper and lower layer, respectively. It can be seen that this CNT film has not been twisted uniformly. While the segments under direct end loading (two red CNT segments and two side blue CNT segments) are twisted uniformly, the central blue CNT segment is hardly twisted at all. This finding in numerical simulation is incompatible with the experimental observation that CNT films are twisted uniformly. The main reason for such non-uniform twisting is that the CNTs modeled in Fig. S1 are relatively short, thus the intertube van der Waals interaction is not strong enough to overcome the torsional resistance of CNTs. This might also be the reason why the torsion of CNTs has not been considered in previous studies of CNT films[3-7], where the CNTs were somewhat twisted. Ref. [1] has considered CNT torsion in the study of CNT films. However, the effect of CNT torsion on the mechanical behavior of CNT films has not been discussed.

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