Thermo-mechanical properties of carbon nanothread and diamond nanothread reinforced-polymer composites

Chengkai Li[A], Haifei Zhan[A], and Yuantong Gu[A]

[A]School of Chemistry, Physics and Mechanical Engineering, Queensland University of Technology (QUT), Brisbane, QLD, 4001, Australia

The ultrathin sp^3 one-dimensional diamond nanothreads (NTHs), have attracted wide research attention since their first discovery in 2005 [1] and been regarded as a promising reinforcements in the composites [2]. In this work, we use molecular simulation (MD) to study the thermo-mechanical behaviors of three representative NTHs/polyethylene (PE) nanocomposites. The transition glass temperature is firstly assessed, and it is found that the transition glass temperature changes slightly with the nanothread reinforcements. Further investigation includes the relationship between temperature and interfacial behavior. Two different tensile deformation scenarios have been considered, including the tensile load being applied only to the polymer matrix, and the tensile load being applied to both the nanothreads and the polymer matrix. As expected, the polymer composites exhibit totally different tensile behaviors under these two loading scenarios. An in-depth analysis has also been conducted to assess interfacial properties between polymer matrix and the nanothreads. This work provides a comprehensive understanding about the influence from the reinforcements in the nanocomposites under mechanical loading.

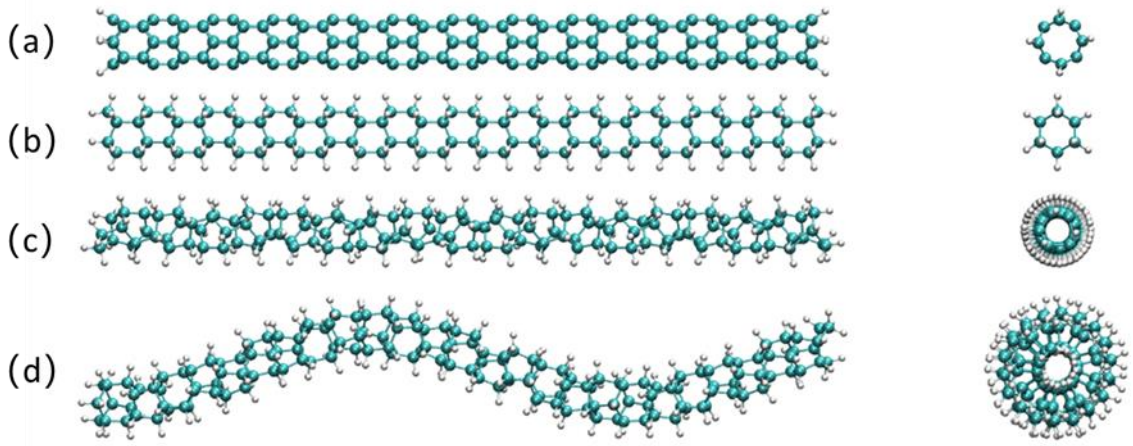

Fig.1 Side view and cross-section view of the atomic configurations of nanothreads as reinforcements (a) CNT (4 0) (b) NTH-1 (c) NTH-7 and (d) NTH-13.

References

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2. Zhan, H.F., Zhang, G., Tan, V.B.C., Cheng, Y., Bell, J.B., Zhang, Y.-W., Gu, Y.T. (2016), Diamond nanothread as a new reinforcement for nanocomposites, Adv. Funct. Mater., 26, 5279-5283.