Deformation mechanisms of diamond nanothread-based nanofiber

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Abstract

Carbon fibers have attracted intensive interests from both scientific and engineering communities due to their outstanding mechanical, chemical and physical properties. They have shown promising applications as multifunctional nano-textiles, structural composites, artificial muscles, and others. Our recent work has shown that the recently synthesized ultrathin diamond nanothread can be applied as a novel building block for nanofiber, which not only possesses excellent torsional deformation capability, but also has excellent interfacial load transfer efficiency. It does not show the flattening phenomenon as observed from the (10,10) carbon nanotube bundles, and has a high torsional elastic limit that is almost three times higher than the carbon nanotube bundle. Motivated by these findings, this work has focused on the deformation mechanisms of the individual diamond nanothread. Based on the large-scale molecular dynamics simulation and theoretical analysis, we firstly identified the deformation components, including bending, torsion, compression, and tension. Thereafter, the contribution of each deformation component is analyzed, from which the failure mechanism of the nanofiber is unveiled. This study has established a fundamental understanding of the deformation mechanisms of diamond nanothread-based nanofiber, which will greatly facilitate its engineering application.

Keywords: nanofiber, diamond nanothread, molecular dynamics simulations, interfacial, load transfer