MOLECULAR DYNAMICS STUDY OF STRESS-STRAIN BEHAVIOR AND EFFEECTIVE ELASTIC MODULI OF CARBON NANOTUBE REINFORCED EPON862

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Single-wall carbon nanotubes (CNTs) are the toughest fibres known, and structural materials that incorporate CNTs could have superior properties, which make them highly promising materials for reinforcing polymer composites. Epon 862 is a member of the epoxy family, in which its properties categorize itself as a thermosetting polymer. Thermosets are highly-cross linked polymer chains that form an irreversible network structure. As a result, this material is very strong due to their tight linkage; unfortunately, however, it is very brittle. The excellent mechanical properties of CNTs should be helpful in taking care of the inherent brittleness of Epon 862. There has been growing interest in using high-aspect-ratio CNTs to toughen Epon composites. This originates from the notion that CNTs are exceptionally stiff, strong, tough, and that by combining CNTs with brittle materials one can impart some of the attractive mechanical properties of the CNTs to the resulting composites.

Though some experiments of CNT reinforced polymer have been done, with the resulting composite nearly triple its resistance to fracturing, the reinforcement theory is still not clear so far. During the mixture and high temperature produce process, some of the CNTs must be destroyed and alignment of CNTs can not be exactly strait. Consequently, the theoretical prediction on the strength increase would be much more accurate than that from the experimental result.

In this paper, by using the molecular dynamics simulation, we study how the interface between CNTs and Epon862 interact to each other and thus explain how CNTs can be utilized as “fibers” to increase the mechanical properties of Epon862 composites reinforced with CNTs. Two different ways will be used to put CNTs inside Epon862 matrix: empty CNTs and CNTs with filled ENTs (with Epon862 molecule inside).

Keywords*:* carbon nanotube, Epon862, reinforcement, composites

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