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Evaluation of mechanical characteristics of nano modified epoxy based polymers using molecular dynamics

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ABSTRACT

Epoxy polymers are finding large scale application in construction industry for repair and retrofitting of deficient concrete structures, because of their great compatibility with construction materials and laminate composites. There is a scope to enhance the physico-chemical and mechanical properties of commercially available epoxy polymers through nanoscale modification. But, the improvement in the properties of the polymeric matrix mainly depends on the compatibility and extent of interaction of nanoparticles with the epoxy polymers. With the exponential growth in the field of nanotechnology and nanoscience, number of potential and compatible nanoparticles is available which can be judiciously explored to engineer the epoxy polymer to attain the desirable properties. In view of this, Molecular Dynamics (MD) studies have been carried out to investigate the interaction of filament type nano materials such as Carbon Nanotube (CNT) with different types of epoxy polymers. Various types of resins and hardeners available in market and usually adopted in industrial applications have been considered for the study. Steered Molecular Dynamics simulation has been carried out individually on CNT and epoxy resins. CNTs of different chiralities and diameters and epoxy resins are subjected to constant velocity pulling and their responses are observed. Then, the interaction of each of the epoxy polymer with CNT is investigated. In order to verify the results obtained from the affinity test using the interaction energy, pull out simulations have also been carried out. It has been found that pull out test results strongly supports the results obtained from the study using interaction energy in choosing the best and worst performing resins for nano engineering using CNT. From the study, the suitable resin and compatible epoxy is identified for CNT modification to ensure better performance of structures towards their repair and retrofitting. A new parameter has been proposed in the present study to uniquely quantify the extent of interaction of the polymer with CNT.

1. Introduction

The wide-spread use of nanotechnology paved the way for development of many experimental and computational techniques at molecular level for better understanding of nanomaterials and to find out the source for certain phenomena observed at the macro-level. Molecular mechanics is a computational technique that lies between Quantum mechanics and Mesoscale modeling and deals with the length scale of few angstroms to nanometers. The basic assumption of molecular mechanics is that the matter consists of a collection of atoms and from the interaction of atoms, the energy can be calculated. Molecular mechanics has found its success stories in determining the reaction rates, vibrational spectrum, thermodynamic and structural properties of the system [1–3].

Molecular Dynamics (MD) and Monte-Carlo (MC) simulations are the two major simulation types under molecular mechanics. MD is more widely used than MC owing to its ability to determine the dynamic properties of materials. The objective of a MD simulation is to compute the particle position as a function of time. It is assumed that the particles behave classically, thereby, obey Newton's second law of motion. For carrying out MD, the atomic system should be defined by specific forms of inter-particle interactions, proper initial and boundary conditions and thermo-dynamic constraints. The applications of MD is diverse; it is used in Chemo-informatics to discover and design new molecules; Proteomics to study the folding, misfolding and aggregation of proteins and structural change of a protein upon mutation of one or more amino acids; Biochemistry to study the drug delivery system; Material

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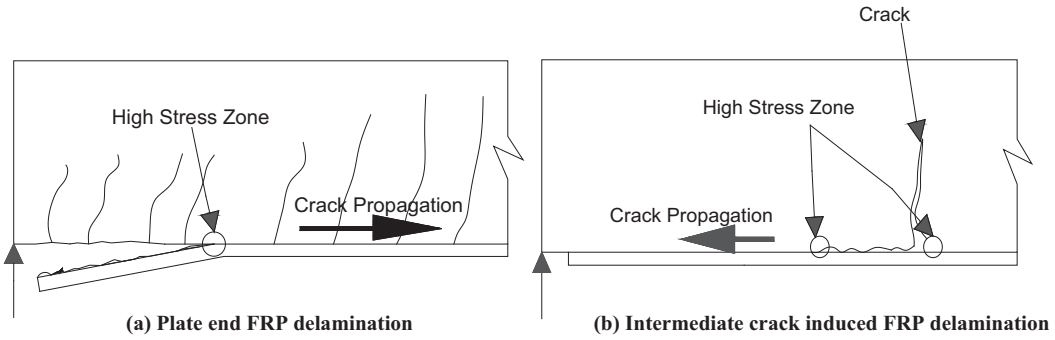

Fig. 1. Schematic diagram of FRP delamination.

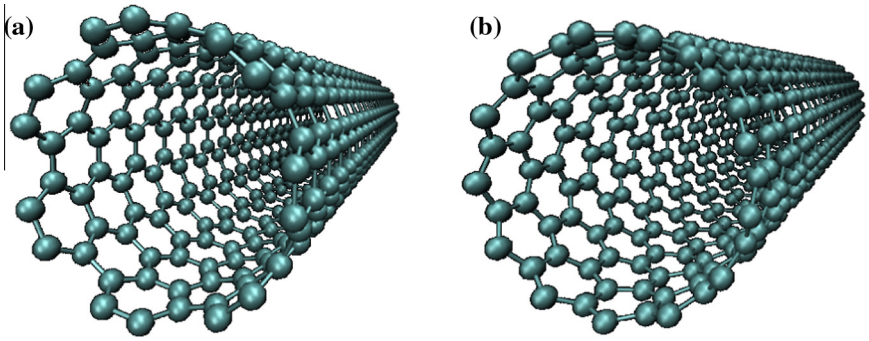

Fig. 2. Atomic structure of (a) 7,7 and (b) 13,0 nanotube.

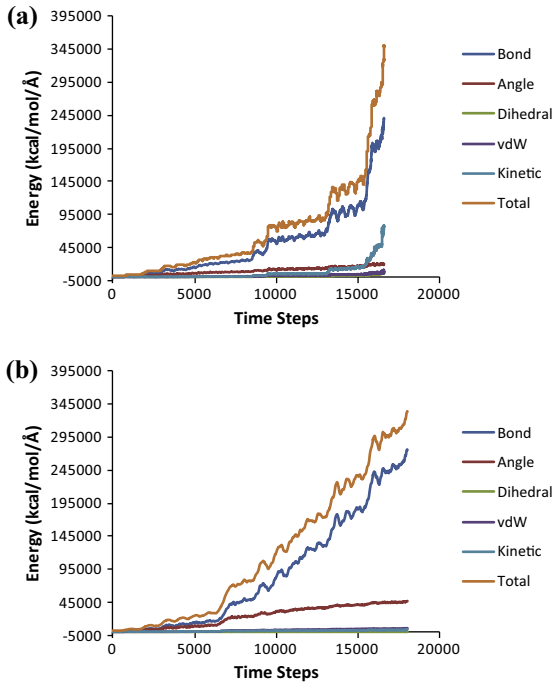

Fig. 3. Energy vs. time for (a) armchair and (b) zigzag.

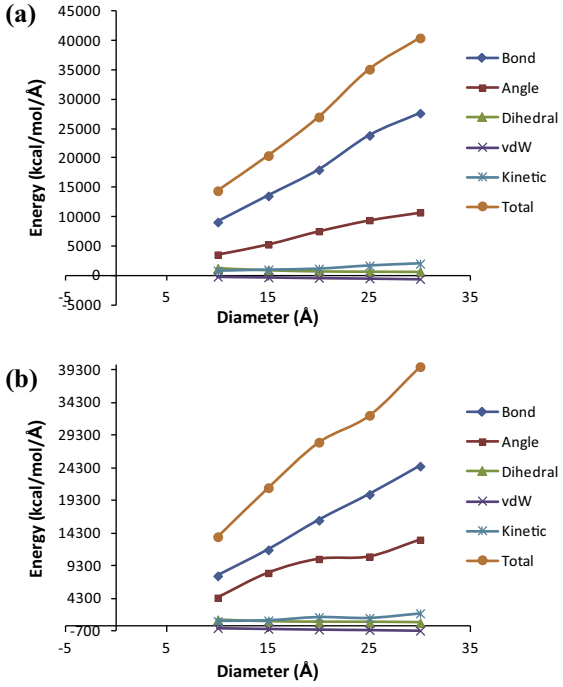

Fig. 4. Energy vs. diameter for (a) armchair and (b) zigzag.

Science to predict the rheological, thermal and mechanical properties of polymers. Recently, it is being used by the civil engineers to understand the structure and properties of various materials used for construction, repair and rehabilitation of structures and to study the behavior of these materials when some foreign materials like fibers and nanomaterials are added to it.

Epoxy polymers are widely used in construction industry. Epoxy polymers have been identified as the best binding agent for construction materials like wood, metal and concrete. This excellent property with its strain compatibility with construction materials has made them to find its application in repair and rehabilitation of structures and in developing laminate composites.