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Molecular dynamics study of toughening mechanisms in nano-composites as a function of structural arrangement of reinforcements

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ABSTRACT

Molecular dynamics (MD) simulations were carried out to investigate how structural arrangement of reinforcements affects the mechanical properties of a nano-composite under transverse loading. The cases studied are rectangular, hexagonal and random arrangements of reinforcements in a matrix. MD simulations of simple 2D LJ model nano-composites indicate hexagonally arranged reinforcements provide better toughness. In contrast, 3D simulations of CNT-aluminium composites suggest that rectangular arrangement is better. The present study also indicates that reinforcing a matrix with nano-fibers may not always increase its mechanical performance, particularly in transverse loading, as it does in the case of macro-composites. We discuss the likely sources of these differences as well as their implications.

1. Introduction

Nanocomposites are made up of two or more materials, and at least one of them has a dimension in the nanoscale. Since nanocomposites consist of distinctly dissimilar materials mixed at the nanometer scale, they open up opportunities for creating materials with highly enhanced and customizable mechanical properties compared to that of existing uniform materials [1,2].

Research in nanocomposite materials could be undertaken by experimental methods [3,4]. However, computational methods could greatly enhance our understanding of these materials, and pave the way for development and realization of these nanocomposites. Many numerical studies have been conducted to investigate the mechanical behavior of nanocomposites. However, most of these were conducted to find out the mechanical response and deformation mechanisms under longitudinal loading [5,6] and a few under transverse loading [7,8]. In the case of transverse loading one potential challenge is the structural arrangement of the reinforcements. The influence of such structural arrangements on the mechanical response has been considered, but only at the microscale. For example, finite element method was used to investigate the stresses in composites in the vicinity of the fibers in hexagonal, square and random arrangements [9], as well to compare the crack growth in hexagonal and rectangular arrangements [10,11]. Recently, the effect of hexagonal, random and rectangular arrays on the transverse tensile moduli of composites was also examined [12]. Other methods, such as discrete element methods, were also used for finding the damage initiation and progression of transversely loaded 2D composites [13]. However, there seems to be scant literature available on the effect of the various structural configurations at the nanoscale on the mechanical behavior and deformation mechanisms. Therefore, in the present study, focus is laid on the specific case of transverse loading of a nanocomposite.

The results of analysis of microscale composites cannot be extrapolated to the nano-scale composites, due to extremely high surface area to volume ratio in nanostructures compared to macrostructures [14]. Moreover, since nanocomposites cannot be considered as a continuum, Finite Element Analysis is inept to carry out the study. An alternative approach is molecular dynamics (MD). Molecular dynamics can take care of the discrete nature of atoms at the atomic scale [6,15] and can provide reliable analysis about the mechanical behavior of nanocomposites.

In molecular dynamics the forces between molecules are calculated based on a force field (potential), and thereafter the Newton's equation of motion is solved using numerical integration techniques [9]. The initial positions, velocities and a potential is prescribed. The positions, velocities, and forces of atomic particles are calculated at every subsequent time step [9,16]. MD has been extensively used for the analysis of mechanical response and deformation mechanisms of nanoscale materials [17] including carbon nanotube composites [18] and particulate nanocomposites [19]. In view of this, in the present work, MD is used to study the influence of structural arrangement on the composite strength and toughness. Three different arrangements are considered: hexagonal, rectangular, and random (Fig. 1). LAMMPS is used for the simulations and Visual Molecular Dynamics (VMD) [21] is used to

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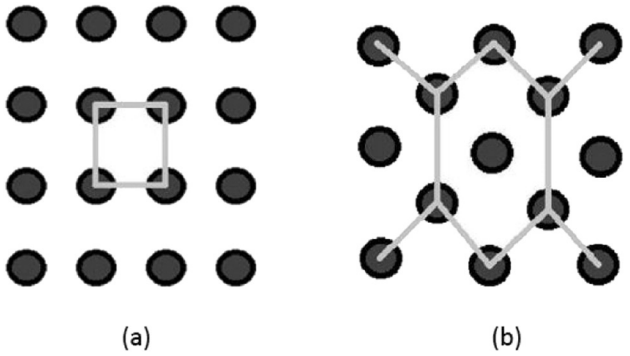

Fig. 1. Structural arrangements of reinforcements considered in this study: (a) rectangular, (b) hexagonal.

view the results. Two examples are considered in the present study to investigate this influence of structural arrangement:

(a) A generic 2D LJ model of a nano-composite with hard reinforcements interspersed in a relatively soft matrix.
(b) A 3D CNT-aluminium nanocomposite.

Following the introduction, details of the 2D model of a generic nano-composite are presented. 3D model of a CNT-aluminium nanocomposite is discussed next. Section 3 looks at the results and discusses probable causes and inferences. Important conclusions are given in the concluding section.

2. Computational model

The unidirectional nanocomposites considered in this work contain symmetrically placed reinforcements in one of the rectangular, hexagonal or random arrangements. In each composite, the reinforcements are sufficiently separated by matrix to prevent direct reinforcement-reinforcement interactions. A schematic illustration of the system under consideration is given in Fig. 2. The representative volume used for MD simulation is shown enclosed by the dashed boxes.

The nanocomposites are subjected to tensile loading and the stress-strain relationships are obtained. The effect of structural arrangement on the overall mechanical properties of the composite is investigated by examining these configurations at different time-steps.

Table 1
Lennard-Jones parameters used for the 2-D model.

Component	ϵ	σ	r_{cutoff}
Matrix	1	1	2.5
Reinforcement	1.3	1	4
Matrix-reinforcement interaction	1.14	1	3

2.1. 2D simulation: LJ model

The dimensions of simulation box are 80 lattice units in x and 84 lattice units in y direction. A small thickness of 0.5 lattice units in z direction is given to accommodate the thickness of atoms in z direction. Hex lattice with reduced density of 0.93 is used. Lenard-Jones (L-J) potential is used to simulate inter-atomic interaction. L-J potential is a pair potential described by the formula:

$$\phi = 4\varepsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right) \quad (1)$$

where, ε is the depth of potential well and σ is the distance from the atom (origin) where potential becomes zero, or inter-atomic force is minimum [22]. The value of sigma dictates the equilibrium distance, where as epsilon is responsible for the stiffness and strength.

The pair potential parameters (ε and σ) were desired to be such that the stress-strain curves of the matrix and reinforcement are analogous to stress-strain curves of concrete and cast iron to simulate realistic composite behavior. After some trial and error, the parameters were locked at values shown in Table 1. Interaction between matrix and

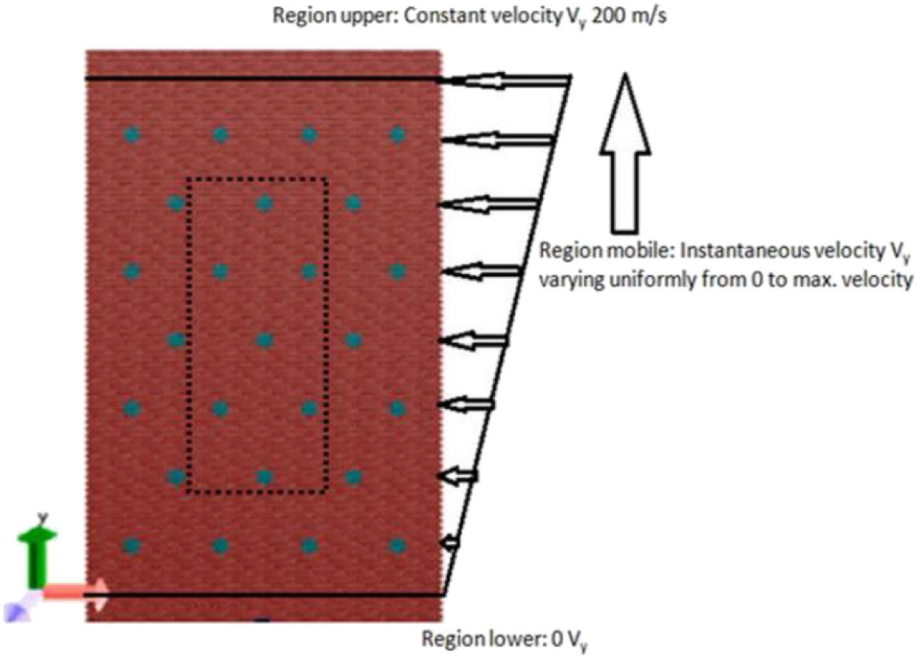

Fig. 2. Illustration of applied load on 2D nanocomposite models.