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Investigation of deformation mechanisms of staggered nanocomposites using molecular dynamics

S. Mathiazhagan *, S. Anup

Department of Aerospace Engineering, Indian Institute of Space Science and Technology, Thiruvananthapuram, Kerala, India

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ABSTRACT

Biological materials with nanostructure of regularly or stair-wise staggered arrangements of hard platelets reinforced in a soft protein matrix have superior mechanical properties. Applications of these nanostructures to ceramic matrix composites could enhance their toughness. Using molecular dynamics simulations, mechanical behaviour of the bio-inspired nanocomposites is studied. Regularly staggered model shows better flow behaviour compared to stair-wise staggered model due to the symmetrical crack propagation along the interface. Though higher stiffness and strength are obtained for stair-wise staggered models, rapid crack propagation reduces the toughness. Arresting this crack propagation could lead to superior mechanical properties in stair-wise staggered models.

1. Introduction

Platelet reinforced unidirectional nanocomposites, inspired from the nanostructure of biological materials such as nacre and bone [1], have potential applications in fabricating advanced synthetic composites [2]. We develop ceramic–ceramic nanocomposite models inspired from these biological composites. Though ceramic–matrix composite materials exhibit higher stiffness and strength, the low toughness of these materials restricts their use in commercial applications [3,4]. However, having one of the constituents in the nanometer regime could substantially improve their properties. In the present study, we analyze the mechanical behaviour of the regularly staggered (RSM) and stair-wise staggered (SSM) bio-inspired nanocomposites [5]. MD simulation, which has been extensively used in studying atomistic plastic deformation mechanisms [6,7], is used to investigate the deformation behaviour of nanocomposites.

Moreover, we use the concept of "model material" in MD simulations [8–10] to study the generic features of the materials' behaviour. We model both the matrix and platelets as brittle materials in order to obtain the generic failure mechanisms of ceramic–ceramic nanocomposite materials. Our MD study could provide clues to designing new ceramic–ceramic nanocomposites. Details of the computational methods used in the present study are explained in the next section. The results of our analysis and discussion with other results from literature are done in Section 3. The main conclusions are presented in Section 4.

2. Simulation methodology

We use two-dimensional hexagonal lattice to model the crystal structure of constituents and Lennard–Jones (LJ) potential to simulate the inter-atomic forces. LJ potential has been used to study the fundamental deformation mechanisms at atomic level and to obtain generic mechanical behaviour [11–14]. The LJ potential is given as $\phi(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$, where σ & ϵ are referred to as the LJ parameters. Dimensionless or reduced units are used in all the simulations, also known as LJ units. This units system also serves the purpose of generating a generic material. The platelets are modeled as hard and matrix as soft by keeping the value of ϵ as 1 and 0.1 respectively. However, value of σ is kept as unity for both cases to generate an ideal coherent interface.

The simulated geometry is shown in Fig. 1. The platelet thickness, platelet transverse and axial gaps as well as platelet overlap lengths are kept same in both the models. The models are subjected to uniaxial tension by applying a constant strain rate of 1E-6 (reduced units) under isothermal–isobaric conditions. In order to mimic the uniaxial tensile test, stresses normal to the loading

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* Corresponding author.
E-mail addresses: smathi.research@gmail.com (S. Mathiazhagan), anupiist@gmail.com (S. Anup).

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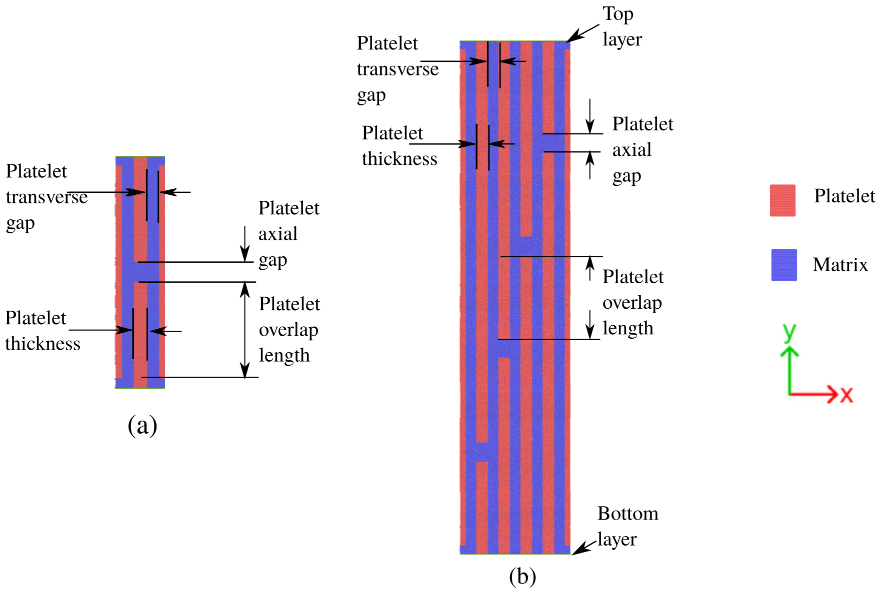
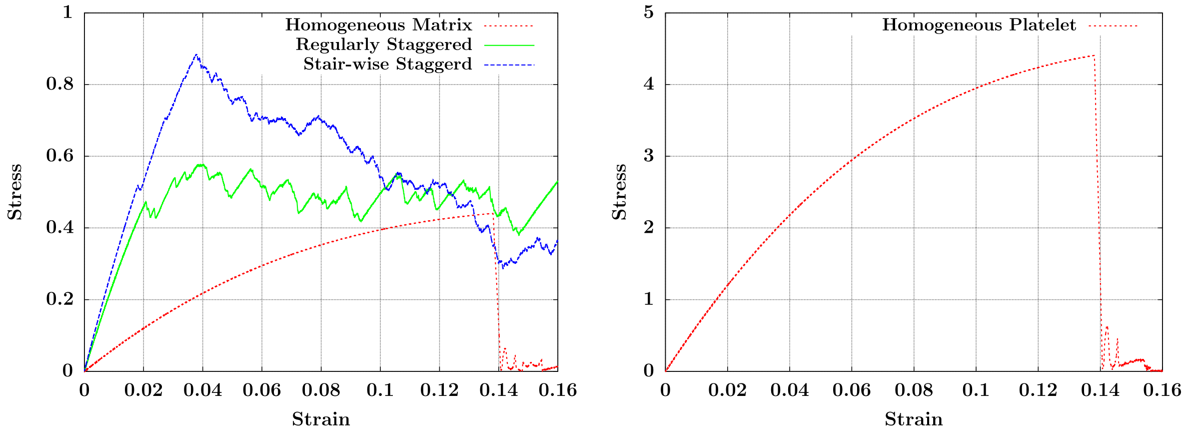


(a)

(b)

Fig. 1. Details of the simulated model. (a) Regularly staggered model (RSM), and (b) stair-wise staggered model (SSM). All the four characteristic dimensions such as platelet thickness, overlap length, axial and transverse gaps are kept same for both the models shown.



(a)

(b)

Fig. 2. (a) Stress–strain diagram for the homogeneous matrix, RSM, and SSM models. (b) Stress–strain diagram of homogeneous platelet. The hard platelet has stress–strain diagram similar to that of matrix and undergoes brittle failure, but the values of stiffness and strength are ten times that of the matrix.

directions are maintained zero. Moreover, a constant temperature of 0.0001 is maintained throughout the tensile test in all simulations. This low temperature is used to focus our attention on the influence of structural features rather than on the effect of temperature, which is used in MD simulations [15,16]. Further modeling and other details can be found in [9,10]. All simulations were carried out using parallel molecular dynamics code LAMMPS [17]. The open visualization tool (OVITO) is used to visualize MD data and generate snapshots [18].

3. Results and discussion

The stress strain diagrams obtained using MD simulations are shown in Fig. 2. In order to find the mechanical behaviour of constituent materials, homogeneous models of constituents materials are also studied. In Fig. 2, the stress–strain diagrams of homogeneous matrix and platelet are shown. The homogeneous matrix model shows continuous increase of stress with strain and undergoes brittle failure. The homogeneous hard platelet also has similar stress–strain behaviour, but the stiffness and strength are ten times that of matrix. As the homogeneous models are defect-free, the dislocations are not generated during tensile test and the models undergo rapid fracture at the maximum stress. Therefore, it has a smooth stress–strain curve.

The RSM and SSM models show mechanical behaviour very different from the above described homogeneous models. Though these nanocomposite models are made of the brittle constituents, the stress–strain diagrams show post-peak flow behaviour (where stress remains approximately a constant value) which is very similar to the ductile materials. The stress–strain diagrams of these composite materials also show ups and downs beyond the peak stress. In these models, the tips of the platelets act as a source for generation of dislocations (refer to Fig. 3). The interactions of the dislocations generated in the matrix phase as well as the intermittent pullout of platelets during tensile test cause the ups and downs in the stress–strain diagram (see the following discussion on analysis of deformation mechanisms and further details in [9]).

The RSM model shows uniform flow behaviour beyond the peak stress, i.e., ups and downs of stress about a constant value. Whereas, the SSM model shows continuous decreasing of stress with strain after reaching the maximum stress. The reason for this behaviour is analyzed as follows. Fig. 3 shows the deformation be-