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Influence of Platelet Aspect Ratio on the Mechanical Behavior of Bio-inspired Nanocomposites using Molecular Dynamics

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Abstract

Superior mechanical properties of hierarchical biocomposite materials such as nacre, bone and tendon are attributed to their basic building blocks. These basic building blocks, often having nanoscale features, play a major role in achieving combined stiffening, strengthening and toughening mechanisms. Bio-inspired composites based on these basic building blocks, such as the regularly staggered and stair-wise staggered arrangements of hard platelets reinforced in soft matrix, have huge potential for developing advanced materials. The study of applicability and transferability of the mechanical principles of biological materials to engineered materials will pave the way for these advanced materials. In order to probe the generic mechanical characteristics of the bio-inspired nanocomposites, the concept of model material in molecular dynamics (MD) simulation is used. In this paper, we investigate the effect of aspect ratio (AR) of platelets on the mechanical behavior of bio-inspired nanocomposites in uniaxial tension. The results of our MD simulations agree closely with the available theories of Young's modulus. Further, the results obtained for the strength of the regularly staggered model from our MD simulations agrees with the strength theory available in literature. However, the results of the stair-wise staggered model show significant difference. For the stair-wise staggered model, we have demonstrated the existence of two critical AR's, i.e., i) a smaller critical AR above which platelet fracture occurs, ii) another higher critical AR above which composite strength remains constant. Further, our MD study has shown that the pull-out mechanism occurs for platelet AR lower than the critical AR and platelet fractures for a higher AR. Pull-out mechanism acts as a major source of plasticity and energy absorbing mechanism of these nanocomposites. Further, we could find that i) the regularly staggered model is efficient in achieving a combination of high Young's modulus, flow strength and toughness, and ii) the stair-wise staggered model is efficient in achieving high Young's modulus and tensile strength.

Keywords:
Strengthening and mechanisms, Mechanical properties, Bio-inspired nanocomposites, Molecular dynamics, Design optimisation