Atomistic Simulations on the Mechanical Behavior of Bio-inspired Brittle Matrix Nanocomposites

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by

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ABSTRACT

There is a huge interest in the development of materials with superior mechanical properties, which have simultaneously high stiffness, strength, and toughness. Brittle matrix composites (BMC) are good candidates for such materials; they possess high stiffness and strength; however, their low toughness limits their industrial applications. In order to develop advanced materials with high toughness, the principles of structural biocomposite materials such as the staggered arrangements of reinforcements and the reinforcements in the form of nanometer-sized platelets are carried forward to the brittle matrix composites (BMC) in this thesis.

The mechanical behavior of bio-inspired brittle matrix nanocomposites is studied using atomistic simulations; moreover, the differences and similarities between the regularly staggered (RSM) and stair-wise staggered (SSM) arrangements of platelets are examined in detail. The effects of different strain rates on both the models are analyzed; different strain rate regimes and critical strain rates are found based on the different deformation mechanisms observed. The effect of aspect ratio (AR) of platelets is investigated and the existence of two critical ARs for SSM is found: a smaller critical AR which separates the platelet pullout and platelet fracture mechanisms, and a larger critical AR upto which the composite strength increases and remains constant thereafter. Further, the study of effect of platelet-matrix interface strength is done. The existence of critical interface strength is shown through our atomistic simulations; decohesions between platelet and matrix occur when the interface strength is below this critical value. Moreover, when the interface strength is weak i.e., below this critical value, SSM models show high toughness due to platelet sliding. However, in RSM models, strong interface strengths lead to high toughness. We also studied the length scale effect on these BMCs and the existence of critical length scale is found. The pull-out of platelet is the dominant mechanism and observed in all length scales studied. Whereas, a large amount of dislocation activities in matrix are observed when the length scale is above the critical length scale and geometric confinement on dislocation activities are found on smaller length scales. This thesis provides beneficial guidelines in designing tough bio-inspired brittle matrix nanocomposites.