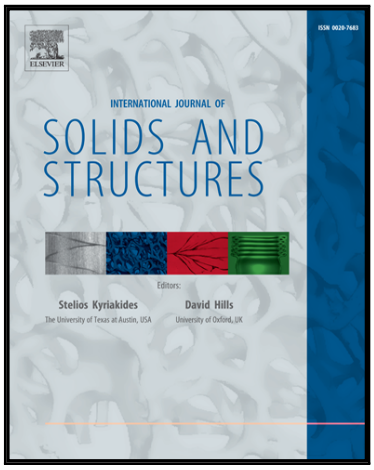

Computational Modeling of Interfacial Behaviors in Nanocomposite Materials

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Computational Modeling of Interfacial Behaviors in Nanocomposite Materials

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Abstract: Towards understanding the bulk material response in nanocomposites, an interfacial zone model was proposed to define a variety of material interface behaviors (e.g. brittle, ductile, rubber-like, elastic-perfectly plastic behavior etc.). It also has the capability to predict bulk material response though independently control of the interface properties (e.g. stiffness, strength, toughness). The mechanical response of granular nanocomposite (i.e. nacre) was investigated through modeling the "relatively soft" organic interface as an interfacial zone among "hard" mineral tablets and simulation results were compared with experimental measurements of stress-strain curves in tension and compression tests. Through modeling varies material interfaces, we found out that the bulk material response of granular nanocomposite was regulated by the interfacial behaviors. This interfacial zone model provides a possible numerical tool for qualitatively understanding of structure-property relationships through material interface design.

Keywords: Material interface modeling; organic interface; nacre; biological nanocomposite; polycrystalline structure

1. Introduction

Biological nanocomposites such as fish scale, bone and nacre are increasingly attracting attention from engineers and researchers due to their remarkable mechanical performances (Vernerey et al., 2014). In this kind of mineralized nanocomposites, the volume fraction of mineral generally is over 85vol% (Dastjerdi et al., 2013; Ritchie, 2011; Wang and Gupta, 2011). In some extreme cases, such as tooth enamel or shell of Strombus gigas, the volume fraction of mineral is up to 99vol% (Kamat et al., 2000; Yahyazadehfar and Arola, 2015). However, these biological nanocomposites exhibit outstanding strength and toughness with high contents of brittle minerals due to their ingenious design of microstructures. The universal microstructural feature of these

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