A generalized interfacial interaction model for prediction of mechanical behavior in bionanocomposite materials

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Towards understanding the bulk material responses in bionanocomposites, a generalized interfacial interaction model is proposed to characterize difference material interface properties, which has the capability to predict bulk material responses via independently control of the interface properties in bionanocomposites. It characterizes both attractive and repulsive interfacial interactions and can be applied to model various material interface behavior. To validate current interfacial interaction model, the mechanical response of extrafibrillar matrix of bone was investigated through modeling the organic interface with wet and dry interface conditions bounding the HA polycrystals. Comparison with experimental measurements of mineral strain-applied strain curves under simple tension and compression loading validated the effectiveness of the proposed model. The simulation results demonstrated that the proposed interfacial interaction model could successfully capture the different interfacial interaction properties and features by adjusting the model parameters. It was also found that the properties of organic interface in extrafibrillar matrix of bone play an important role on the mechanical response of bone. This model provides a possible numerical tool for qualitatively understanding of structure-property relation through material interface design.