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# Mechanical properties and scaling laws of interpenetrating phase nanocomposites via multi-scale simulations

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**Key Words:** *Interpenetrating phase nanocomposites, multi-scale simulations, scaling laws.*

Interpenetrating phase nanocomposites are a class of novel functional materials, in which the composed phases are each spatially continuous and interconnected in three dimensions. In this paper, we perform multi-scale simulations to investigate the dependence relation between the effective mechanical properties and the microstructures of interpenetrating phase composites. A phase field method is adopted to construct the random bicontinuous microstructure of the composite. Molecular dynamics simulations are then employed to calculate the interfacial properties. To make a scale transition from the atomistic to the continuum scale, we propose a interface layer model which is informed by molecular dynamics simulations. Using this multi-scale approach, the deformation and fracture mechanism of the composite are revealed. It is found that the tensile strength of interpenetrating phase nanocomposite is not sensitive to the interfacial failure. In addition, scaling laws for the effective Young's modulus, yield stress as functions of the characteristic sizes and the volume fraction of composed phases are suggested. The present study leads to better understanding of the mechanical behaviors and underlying physical mechanisms of nanocomposites, and provides design guidelines for enhanced-performance nanocomposites.

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