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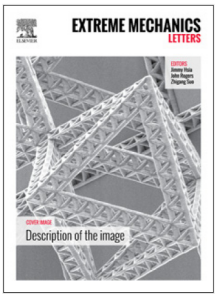

Theoretical framework and design of mechanochemically augmented polymer composites

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Theoretical framework and design of mechanochemically augmented polymer composites

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Abstract

Interfacial debonding is an important failure mode for polymer composites. A novel approach for managing this damage mechanism is to develop self-healing and self-reporting capabilities by augmenting the matrix/filler interfaces with mechanophores. Mechanophores are chemical groups that have useful reactions (e.g. fluorescence, cross-linking) in response to mechanical work. We refer to such a composite system as an Interfacial Mechanophore Augmented Composite (IMAC). Here we build the framework for understanding the governing physics and predicting the mechanochemical response of IMACs. By using an extensible link mechanophore model that assumes sparse mechanophore loading, we are able to utilize classical mechanics composite solutions for deformation fields in composites to predict mechanophore response as a function of macroscale stress, filler geometry, and component material properties. Using a 2D plane strain scenario of a fiber within an infinite matrix, we develop a comprehensive understanding of the progression of debonding and mechanophore activation. We find that the mechanophore activation length relative to the debond length is critical in determining the relative onset of debonding and activation. The change in the separation of the mechanophore attachment points between the not-activated and activated states therefore needs to be considered for mechanophore selection in addition to the required chemical functionality. Other factors such as matrix elasticity, particle elasticity, and particle size are found to have secondary effects on this relative progression. This modeling approach can readily be applied to diverse loading modes and material properties and can be ex-

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