Investigation on toughening behavior of thermoplastic modified epoxy

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Abstract

Epoxy resins are widely used as matrix phase materials in fiber-reinforced composites providing various industrial applications. On the other hand, highly crosslinked structure with interconnected networks by the strong covalent bonds called crosslinks entails brittle characteristics. This inherent drawback imposes many challenges on their engineering applications in the fields requiring high toughness. To circumvent such a limited usage of epoxy at higher conversion ratios, toughened epoxy by the incorporation of thermoplastic polymers has been extensively studied as a promising way to enhance the fracture toughness of epoxy. Unlike the toughened mixtures with rubbers, high performance thermoplastics can serve as a toughening agent without sacrificing other important properties of epoxy such as stiffness or in-service temperature. However, the understanding of detailed mechanism on toughening behavior at the molecular scale is stile limited.

The primary purpose of this study is to investigate toughening behavior of thermoplastic modified epoxy using molecular dynamics (MD) simulations. For establishing molecular models, PES is used as a toughening agent into the crosslinked epoxy system composed of TGAP and DDS. In this model, a simple bilayer structure consisting of PES layer and the crosslinked epoxy layer is modeled as a toughened epoxy system, since the size and shape effect of PES-rich phase is not considered in the present study. In order to provide a fundamental understanding on toughening mechanism, energy dissipations from the epoxy phase to the PES region during tensile loading simulations are rigorously examined using the bilayer structure. The degree of plastic deformation of each phase is monitored and compared with that of neat epoxy and PES system. Moreover, interfacial characteristics between epoxy and PES phase are intensively studied. Molecular morphology at the interface is discussed considering varying crosslinking conversions of epoxy. Traction separation responses are examined as well to reflect debonding phenomena at the interface.

Keywords: Toughened epoxy, Molecular dynamics simulation, Interface, Toughening mechanism

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