A molecular dynamics study on toughening of thermoplastic modified epoxy

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This work presents an investigation of toughening behavior for polyethersulfone (PES) modified triglycidyl-amino-phenol (TGAP) epoxy systems using molecular dynamics (MD) simulations. The 4,4'-diaminodiphenylmethane (DDS) is used as a curing agent to form cross-linked epoxy structures. Toughening mechanism of the modified mixtures (PES/TGAP/DDS) is studied in an atomistic scale. The molecular models consisting of PES and cross-linked epoxy are established. From the equilibrated models, the stress-strain curves are obtained and the tensile strength is predicted. The molecular morphology changes and the interfacial characteristics of PES/epoxy matrix with tensile strains are examined. Influences of cross-link conversion and PES content are further investigated. Findings of the study provide physical insights to understand the toughening mechanism is an atomistic perspective.

Keywords: Toughness, Cross-linking, Interface, Molecular dynamics.

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