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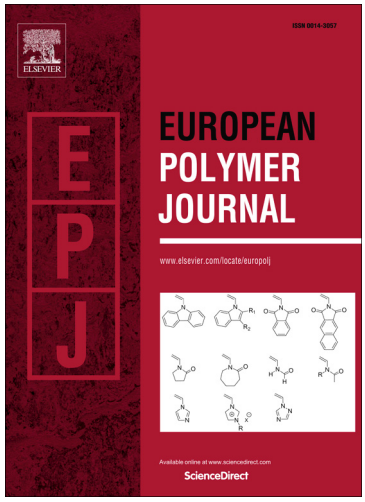

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Molecular Dynamics Simulation of Crosslinked Epoxy Resins: Curing and Mechanical Properties

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Abstract

We performed molecular dynamics (MD) simulation that includes multidisciplinary characteristics from synthesis to mechanical properties of epoxy resin. First, to reproduce the actual chemical reaction between matrix and curing agents, we conducted curing simulation wherein the activation energy and heat of formation are considered for the chemical reaction. Subsequently, we performed MD simulations using cross-linked structure obtained from curing simulation to derive density and Young's modulus. Results indicated that crosslinked structures involving both activation energy and heat of formation could reproduce experiment results that are evaluated using differential scanning calorimetry (DSC) measurements and mechanical tests. The simulated results imply that electrostatic interaction plays an important role in Young's modulus. The density of the hydrogen bond between the oxygen of the hydroxyl group and the hydrogen atom is a key factor for the difference in Young's modulus for each base resin. These findings confirm that MD simulation is a potential alternative to experiments for the appropriate material selection of epoxy resin.

Keywords: Curing characteristics, Thermosetting resin, Molecular dynamics, Mechanical properties

1. Introduction

Polymer matrix composites (PMCs) are key structural materials in transportation systems. Because of their lighter weight and grater stiffness, compared to conventional materials such as aluminium, half of the conventional metal in

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