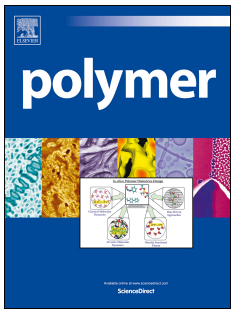

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A Study of Thermo-mechanical Properties of The Cross-linked Epoxy: An Atomistic Simulation

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Abstract

In this paper, crosslinking process and thermo-mechanical properties of epoxy materials containing diglycidyl ether bisphenol-A (DGEBA) as the epoxy resin and JEFFAMINE® D-230 polyoxypropylenediamine as the hardener have been studied using molecular dynamics simulation. An algorithm to create the crosslinked epoxy has been developed, and the crosslinking process is monitored. The simulation results disclose the effectiveness of the using annealing in the crosslinking process to achieve higher crosslinking densities within shorter reaction radiuses while producing more desirable conformation. The evolution of the complex network of cured epoxy is studied by radial distribution function (RDF). The important properties of the epoxy material such as glass transition temperature (T_g), the coefficient of thermal expansion (CTE), and elastic constants are calculated. Furthermore, the variation of the properties through the evolution process is considered, and the improvement of them is captured. The results obtained from our simulation are in good agreement with the experimental results, revealing the strength of molecular dynamics to predict the material properties.

Keywords: Atomistic simulation, Crosslinked Epoxy, Thermo-mechanical properties

1. Introduction

Epoxy is the product of the reaction between the epoxy resin and a curing agent. Epoxy resins are the class of polymers containing epoxide groups, and they may react with each other or with other curing agents to create an epoxy material with outstanding properties. The curing agents usually include co-reactant groups such as amines and phenols. The result of the reaction between epoxide groups and co-reactant groups in curing agents usually is a thermosetting polymer with superior thermos-mechanical properties. Due to their excellent properties, epoxies have a wide range of applications in various industries including but not limited to aircraft structures, FRP-concrete bonding, electrical components, and shipbuilding.

Since the introduction of molecular dynamics (MD) by Alder and Wainwright [1] in the late 50's and later by Rahman[2], there are numerous research works focusing on the application and improvement of MD, mostly in the field of science. MD is computationally demanding, and it was not until recently that modern computers made it possible for researchers to use its privileges in the

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