# Simulation and Analysis of Epoxy Polymer Networks: Advanced Crosslinking Approaches and Topological Modifications in LAMMPS

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**Abstract**

In this study, we focus on generating and analyzing the polymer network topology of epoxy resins, specifically DGEBA and DETDA molecules, using two crosslinking approaches within the LAMMPS simulation software. The first method utilizes the REACTER(1,2) approach to simulate the curing process, while the second approach employs a modified version of the bond/create(3,4) to ensure the topology of molecules is dynamically updated after bond formation. This modification enhances the precision and reliability of the simulated network structures. Both methodologies are evaluated to compare their effectiveness in capturing the network formation process, with an emphasis on their suitability for characterizing microstructure-property relationships and mechanical behavior. The results provide insights into the advantages and limitations of each approach for simulating crosslinked polymer systems, with potential implications for the design of highperformance bio-sourced epoxy materials.

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