Molecular Dynamics Simulations of Epoxy Resin Systems

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Introduction

Epoxy resins are a class of thermoset polymers that have a wide range of applications in everyday lives, including adhesives, coatings, encapsulants, casting materials, etc. To fulfill different criteria in these applications, one can let the epoxy resins cross-link with amine hardeners, producing cured resin system. The number of cross-linked molecules can influence the physical properties of the system significantly. In this project, we investigate how cross-linking affects physical properties by using Molecular Dynamics (MD) simulation.

The MD simulation consists of computer algorithms which is based on classical equations of motion. The forces and position of atoms are calculated over a very short timestep of 1 femtosecond. By equilibrating the system for a long time period, in the range of 100 nanoseconds, the physical properties can be properly studied. Moreover, we can perform measurements that are difficult to conduct in real experiments as they are expensive in human-hours and in material costs.

Preparation of the System

1. Build Molecules in VMD
2. Optimize Structure in NWChem
3. Pack Molecules into a Box
4. Crosslinking Monomers
5. Minimize the Energy of the System
6. Conduct Testing
7. Glass Transition Temperature

Underlying Mechanism to LAMMPS Simulation

LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) is the software which we used to run molecular dynamics simulations. All movement of atoms within LAMMPS stems from solutions to equations that describe forces on each atom. There are four distinct types of interactions: bonds, angles, dihedrals, and non-bonded interactions. Each atom has a specific type, which is based on its element as well as the atoms that surround it. Additionally, each bond, angle and dihedral is given a parameter based on the types of atoms which surround the central atom.

The CHARMM (Chemical at HARvard Macromolecular Mechanics) General Force Field was used to describe the forces on each atom given the atom-type and specified parameters.

\[ V_{\text{CHARMM}} = \sum V_{\text{bond}}(r) + \sum V_{\text{angle}}(\theta) + \sum V_{\text{dihedral}}(\phi) + \sum V_{\text{non-bonded}}(r) \]

Crosslinking Reaction

Propane, 2,2-bis(2,3-epoxypropoxy) phenyl (BADGE) and Isophoronediamine (IPDA) react to form an epoxy resin. The reaction is exothermic and releases heat, which can be monitored using a calorimeter.

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Conclusions and Future Steps

Successes:
- Construct epoxy resin systems and optimize structure.
- Cross-link systems and measure glass transition temperature.
- Preliminary results are close to experimental values.

Struggles:
- Implementation of measurement of systems in LAMMPS.
- Type matching each atom within our system.

Future Steps:
- Measure the thermal expansion coefficient and isothermal compressibility.
- Measure the glass transition temperature of DGEBA-IPDA system and compare with experimentally obtained values.

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References