Atomistic Molecular Dynamics Simulations of Cross-linked Epoxy using LAMMPS

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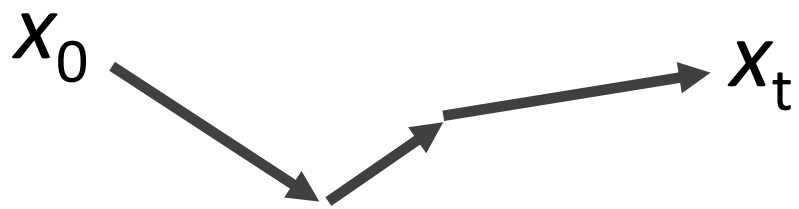
1. Specific Volume-Cooling Rate Analysis

Khare, K. S.; Phelan, F. R., Jr.; "Quantitative Comparison of Atomistic Simulations with Experiment for a Cross-Linked Epoxy: A Specific Volume – Cooling-Rate Analysis", *Macromolecules*, 51, 564 (**2018**).

2. Translational Dynamics

$$R^2(t) = < (x_t - x_0)^2 >$$



Khare, K. S.; Phelan, F. R., Jr.; "Integration of Atomistic Simulation with Experiment Using Time−Temperature Superposition for a Cross-Linked Epoxy Network", *ChemRxiv*, DOI: 10.26434/chemrxiv.8326172 (**2019**). [Preprint]