Thermomechanics in Cross-linked Epoxy: Quantitative Comparison between Atomistic Simulation and Experiment

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Direct quantitative comparisons between atomistic simulations and experiment are non-trivial due the inability to access experimental length and timescales using molecular dynamics (MD). Particularly for viscoelastic materials like cross-linked epoxy networks, thermomechanical properties show rate dependence in addition to temperature dependence, which makes such comparison even more challenging. Here, we show that theoretically informed simulation and analysis protocols together with material specific time-temperature superposition principle (TTSP) data that can be extracted from both experiment and simulation allow us to bridge the disparate time-scales, and thus, enable direct quantitative comparisons. Specifically, we study (1) the cooling rate dependence of specific volume with temperature, and (2) the temperature and time trend of translational and rotational dynamics using atomistically detailed molecular dynamics simulation. Upon relating these trends with relevant experimental data in the literature, we find that the specific volume trend in experiments can be predicted within 0.5 % using simulations. Further, we find that master curves of the dynamical properties obtained via simulations can be constructed independently of experiments, and that the temporal features of these master curves from simulations show excellent agreement with the creep compliance master curve obtained via experiment.