Thermodynamic and Dynamic Properties of a Resin Mixture with Embedded Sio_2 from Molecular Simulations

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We have studied a mixture of the epoxy resin consisting of diglycidyl ether of bisphenol-A (DGEBA) and the curing agent poly(oxypropylene) diamine (POPDA-X, where X is the number of repeated units, 2 or 3 in this study), with in-situ growth of SiO_2 clusters. Due to its mechanical properties such as high tensile strength, good adhesion and high corrosive resistance, epoxy has been considered as good material for high-voltage insulation. Initial experimental work on DGEBA resin functionalized with SiO_2 nanoparticles has shown improved thermal stability and mechanical strength of the hybrid material [1,2]. Using Classical Molecular Simulations and the OPLS-AA forcefield [3], we have created a model for the 4:1:1 DGEBA/POPDA-2/POPDA-3 mixtures, with 0%, 58% and 87% crosslinking degree. The model is verified against experimental XRD data, and we estimate the glass-transition temperature for the various mixtures.

With the newly developed model, we can study mechanical as well as thermodynamic properties of the various cross-linked models. The results are found to be in good agreement with experimental results. With use of classical simulations, we show how the thermal and mechanical properties of the resin changes as a function of temperature and cross-linking degree. We further predict properties of the material with addition of different oxide nanoparticles, and use this to guide the experimental efforts.

References

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