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Molecular Simulation of Highly Crosslinked Epoxy Resin and POSS-Epoxy Nanocomposites PO-HAN LIN, RAJESH KHARE, Department of Chemical Engineering, Texas Tech University — Generation of atomistic model structures of crosslinked epoxy at realistic density is a challenging task. In this work, we present an efficient approach for generating such model structures of highly crosslinked matrices. The approach utilizes simulated annealing optimization technique for carrying out one-step polymerization of the reaction mixture in the simulation box. The structures so generated are relaxed using a combination of molecular mechanics and molecular dynamics (MD) simulations. The developed technique is computationally efficient and has been used for creating atomistic model structures of both crosslinked epoxy and a nanocomposite formed by the incorporation of the polyhedral oligomeric silsesquioxane (POSS) molecules in the crosslinked epoxy matrix. MD simulations are used to determine the volume-temperature behavior of these structures. The density and the glass transition temperature of the simulated structures are compared with the literature experimental data. Furthermore, the molecular packing behavior of the POSS-epoxy nanocomposite is compared with the molecular packing in the crosslinked epoxy matrix.

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