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Computational Modeling of Aging Effects of Epoxy Polymers. THOMAS CLANCY, SARAH-JANE FRANKLAND, National Institute of Aerospace, THOMAS GATES, NASA-LaRC — Due to the increased usage of non-metallic materials in aircraft, there is interest in the effects of aging on the performance of these materials. In order to gain insight into the molecular mechanisms of failure or reduced performance of these materials, computational modeling has been performed. Crosslinked epoxy systems were studied at the atomistic level. Atomistic models of crosslinked epoxy polymers were built by performing molecular dynamics simulations of unreacted epoxy and crosslinker molecules, followed by the formation of chemical crosslinks. Further molecular dynamics simulations were employed to equilibrate the models. These atomistic crosslinked epoxy models were also built with a range of moisture content. In addition, the crosslinking density was varied. The mechanical properties of these atomistic models were calculated in order to assess the effect of hygrothermal aging on the epoxy models.

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