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Mechanical and Thermal Properties of Cross-Linked Phenolic Resins Using Molecular Dynamics JOHN LAWSON, JOSHUA MONK, JUSTIN HASKINS, CHARLES BAUSCHLICHER, NASA Ames Research Center — To gain insight into the design of materials, it is valuable to understand how the chemical make-up at the nano-scale can influence the thermal and mechanical bulk properties. An atomistic computational study allows us to manipulate the structural make-up of individual phenolic chains as well as generate various cross-linked (or cured) systems. In this study, molecular dynamics simulations of bulk phenolic systems were performed with the software LAMMPS. An all-atom force field was chosen to investigate how the strength and thermal conductivity of the phenolic material varies as a function of the degree of cross-linking and chemical make-up of the phenolic chains. Small-scale mechanical tests were performed to compute various moduli for the phenolic systems above and below the glass transition at varied degrees of cross-linking. The thermal conductivity was obtained using the Green-Kubo approach for the virgin phenolic system as well as the strained systems.

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