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Computational Modeling of Polymers and the Influence of Molecular Level Structural Features on Mechanical Properties THOMAS CLANCY, SARAH-JANE FRANKLAND, National Institute of Aerospace — The role of molecular structure on the mechanical properties of polymer based materials is investigated through atomistic based molecular dynamics simulations. Models of crosslinked polymers were built with a range of moisture content in order to study the effect of environmental exposure on mechanical properties. Another key structural parameter, the degree of crosslinking, was also varied. The molecular structural features associated with these parameters are studied for their influence on the mechanical properties. The relative motion of crosslink points and the influence of penetrants such as water are investigated under deformation conditions. The mobility of penetrants within the polymer matrix is studied under equilibrium and deformation conditions in order to assess the role of these structural features on the mechanical properties as well as to assess the influence of deformation on diffusion rates.

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