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The effect of nanoconfinement on network topology and thermo-mechanical properties of glassy polymers dynamically reacted using MD simulation KATHERINE SEBECK, JOHN KIEFFER, University of Michigan - Ann Arbor — The interaction of polymers with an ordered surface affects the thermo-mechanical properties of polymer matrix composite and nanoconfined polymeric materials. Atomistic simulations of glassy polymers such as epoxides offer unique insights to the network topology of such structures. A series of epoxide network structures using a bifunctional epoxide and polyfunctional aliphatic amines have been generated using a dynamic polymerization simulation technique. This allows for natural evolution of the network topology in both bulk and confined structures. The nature of structural organization at the surface of confined structures will be analyzed as a function of distance from the interface using various metrics including spatial distribution functions. These structural characteristics are then correlated with dynamical properties such as Tg and modulus, comparing nanoconfined networks to bulk systems.

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