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An explicit 3D chain and node mesoscale network model for silica-filled polydimethylsiloxane DAVID HANSON, Los Alamos National Laboratory — We present a numerical mesoscale model that describes the stress/strain properties of a mesoscale volume element of silica-filled polydimethylsiloxane (PDMS) under tensile or compressive strain. An explicit 3D network, composed of randomly dispersed nodes (filler particles), multiply connected by a large number of chains (PDMS polymers), is strained by an affine transformation. The resulting macroscopic stress is computed by summing the chain tensile forces over free surfaces of the volume element. The non-entropic forces used in the model are computed from atomistic simulations of individual chains for two cases: chains undergoing extension from a natured initial state, or a chain interacting with a hydroxylated silica surface. The forces are computed from changes in the internal energy as a function of the end position of the chain. The distribution of chain lengths of the interparticle connecting segments and free ends are assumed to be Gaussian. The model is validated by comparison of the predicted stress/strain behavior to experimental data.

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