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Transport properties of mechanically deformed polymer networks[1] HASSAN MASOUD, ALEXANDER ALEXEEV, Georgia Institute of Technology — We develop a hybrid computational method to probe how the permeation and hindered diffusion change when an isotropic polymer network is deformed by an externally applied force. We use a bond-bending lattice spring model to capture the micromechanics of random networks of interconnected elastic filaments coupled with the dissipative particle dynamics to explicitly model the viscous fluid and diffusive solutes. Our simulations reveal that the network transport properties are defined by the network porosity and by the degree of network anisotropy due to network mechanical deformations. We also show that the internal network structure does not affect the permeation and diffusion of stressed and unstressed networks. Furthermore, our results indicate that permeability of mechanically deformed networks can be predicted based on the alignment of network filaments that is characterized by a second order orientation tensor. Our findings have implications for designing drug delivery agents, tissue engineering, and understanding the function of certain biological systems.

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