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Rubber elasticity from a micromechanical model of polymer chains

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Abstract

A traditional approach in continuum theories of rubber elasticity is to derive the strain energy function from statistical mechanics of long-chain molecules. In particular, the freely jointed chain model leads to the well-known inverse Langevin function, which governs the limiting chain extensibility in rubber networks. In this contribution, we propose an alternative approach based on a semi-flexible microstructure that deforms elastically. The microstructure consists of rigid bars representing the Kuhn segments of an ideal polymer chain, combined with elastic springs. These springs account for long-range interactions and topological constraints on the freedom of motion of the chain. By enforcing equilibrium, we derive an analytical response function for the polymer chain. This function not only captures finite chain extensibility but also reproduces the nonlinear decrease in tangent shear modulus at moderate strains, a feature commonly observed in rubbers. The macroscopic strain energy of the continuum is obtained through network averaging and involves four constitutive parameters with clear physical interpretation. The effectiveness of the model is demonstrated by fitting to various sets of experimental data from biaxial tension tests. Applications to inhomogeneous deformations, such as membrane inflation, further confirm the predictive capability of the model.

Keywords:

Hyperelasticity Micro-mechanics Polymer network Finite deformation