Micromechanical modelling of rubbery networks: discrete and continuum approaches

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Abstract

Micromechanics-based constitutive models for rubbery networks, such as elastomers and hydrogels, are usually formulated within the framework of rubber elasticity theory. Starting from a description of the behaviour of a single chain derived from statistical mechanics considerations, the behaviour of the network is obtained by averaging the response of individual chains arranged in a simplified unit cell, dictating the partitioning of stretches among the chains. Representative examples include the three-chain model, eight-chain model, and the full-network (microsphere) model. However, these models fall short in describing the role of the (possibly evolving) network structure on the mechanical behaviour. In recent years, computational discrete network (DN) models have emerged as a promising approach to investigate structure-property relationships in rubbery networks. In this approach, chains are represented as entropic springs connected at junction points representing the crosslinks. By explicitly representing the random network structure, the effect of network heterogeneities and defects can readily be described. In this work, we used discrete network models to investigate the role of network topology on the elastic response. The effect of chain pre-stretch on the mechanical properties is emphasised. We further use DN simulations to assess the accuracy of stretch partitioning assumptions used in analytical models. Damage by chain scission is described by coupling the DN model with a Kinetic Monte Carlo algorithm. Simulation results highlight the impact of heterogeneous force distribution on the failure response. Implications for the formulation of advanced constitutive models are discussed.