Micromechanical modelling of rubbery networks

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Abstract

The mechanical properties of soft materials such as elastomers and hydrogels fundamentally depend on the structure of the underlying polymer network and the intrinsic response of the polymer chains. Structural features of interest include the polymer chain length, the density and functionality of the crosslink points, and network inhomogeneities and defects. Understanding structure-property relationships thus requires a modelling approach that addresses the microscale of the polymer network. Conventional constitutive models based on rubber elasticity theory usually fall short in this respect, as they cannot capture the effect of network topology on the chain stretch distribution. On the other hand, molecular simulations remain computationally prohibitive at the network length and time scales, calling for new, complementary modelling strategies.

In this talk, I will present our recent efforts in the development of micromechanical models for rubbery networks, with the objective of linking the behaviour of single polymer chains to the macroscopic behaviour. Discrete Network (DN) models will be introduced as a conceptually simple and cost effective computational approach to investigate the role of network topology on the deformation and failure behaviour, while being firmly grounded in statistical mechanics. DN models can also be used as a guide for the development of advanced continuum constitutive theories. In the second part of the talk, I will present our new model for the force-extension response of a single polymer chain, which accounts for both entropic and energetic effects. The model captures the chain response across all force regimes, while also providing an estimate of the bond stretch, which is critical to predict chain scission. This presentation is primarily based on the works of two PhD students, Lucas Mangas Araujo and Jie Zhu.

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