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A Mesoscale Discrete Network Model for Rubbers

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Abstract

Understanding, predicting, and optimising the mechanical behaviour of elastomers necessitates models that effectively address how their molecular networks form, reorganise, and deform under load. The state-of-the-art approaches either look at a very small scale by performing molecular dynamics simulations or are based on empirically designed or micromechanically motivated constitutive models. On the one hand, all-atom models can accurately describe the mechanics of such polymers and the effect of cross-linking at the nanoscale, while on the other hand, constitutive models often make idealised assumptions to describe the polymeric networks, failing to fully account for, e.g., the chain-level heterogeneity. This limitation hinders our ability to connect the processes of synthesis, gelation, and network evolution to the macroscopic behaviour of rubbers such as ethylene propylene diene monomer (EPDM). In this work, we introduce a discrete element method (DEM)-based coarse-grained network model framework designed to bridge these scales by explicitly representing polymer chains, crosslinks, and emergent topology within a computationally manageable mesoscale simulation. Implemented in the open-source MUSEN platform, this model computationally models the EPDM compounding process using a coarse-grained chain-of-beads structural representation. Each repeating monomer unit of EPDM rubber is treated as a discrete particle connected by non-linear springs, allowing for direct tracking of entropic elasticity, bond formation, chain mobility, and the heterogeneous force pathways that develop during network formation. A functional model regulating diffusion, polymer bonding, and interaction mechanisms governs the kinetics within

a periodic representative volume element. Ongoing work includes coupling this simulation framework with planned experimental studies on peroxide-cured EPDM to quantitatively validate network formation and deformation mechanisms. This integrated modelling-experimental approach aims to establish a DEM-based network model as a predictive tool for understanding and designing elastomers.

Keywords:

Discrete element Method(DEM) Rubbers Polymer networks