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A cross-scale continuum model for the mechanics of cross-linked elastomer composites reinforced with nanofibers

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Introduction

The parameterized modeling method of constitutive equations guided by molecular dynamics simulation has been widely employed to achieve a bottom-up mechanical property optimization of elastomers. However, previous works highlighted the lack of damage mechanics model related to the interfacial debonding between nanofibers and elastomers. The present study was designed to construct a multiscale continuum model for the mechanics of cross-linked elastomer composites reinforced with nanofibers, which may have practical application value for the structural design and performance optimization of nanofiber-filled hyperelastic composites.

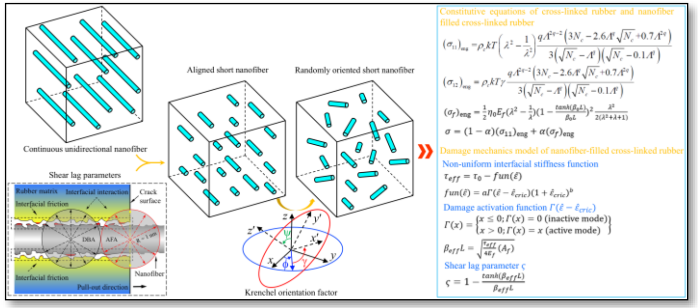

Fig. 1 Schematic diagram of the development of nanofiber-filled elastomer composite model.

In this work, the coarse-grained and all-atomic molecular dynamics simulations were used to investigate the physical parameters of cross-linked elastomer networks and the cohesive and damage mechanics models of nanofiber-filled cross-linked elastomer, respectively. As representative nanofibers and elastomers, carbon nanotubes and natural rubber were adopted.

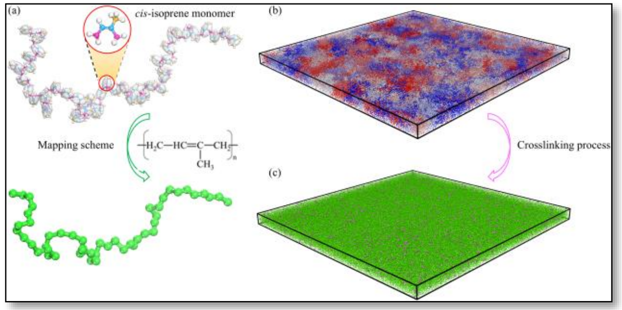

Fig. 2 Coarse-grained molecular models of rubber networks: (a) mapping scheme for rubber chains; (b) uncross-linked rubber model (Molecular chains are distinguished by different colors); (c) cross-linked rubber model (Green and pink represent rubber and sulfur atoms, respectively).

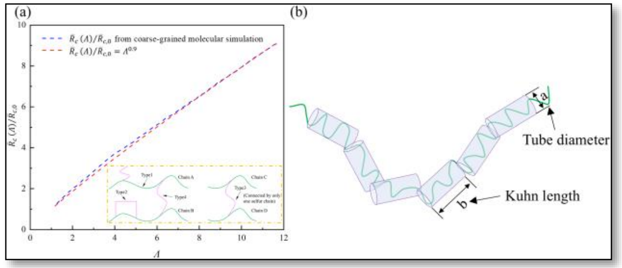

Fig. 3 (a) Macroscopic and microscopic transition factor in cross-linked rubber networks, with the inset showing four main types of chain segments in cross-linked rubber networks ; (b) Schematic diagram of the primitive path.

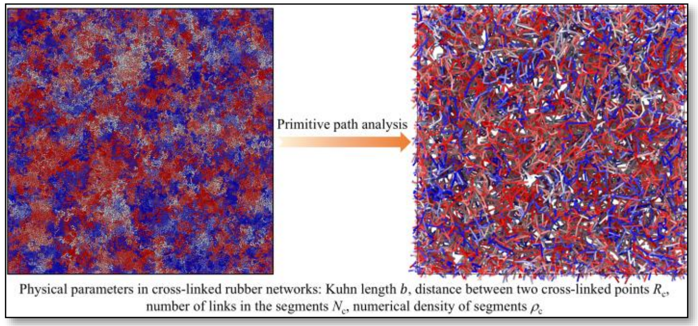

Fig. 4 Snapshot of the primitive path analysis of rubber networks.

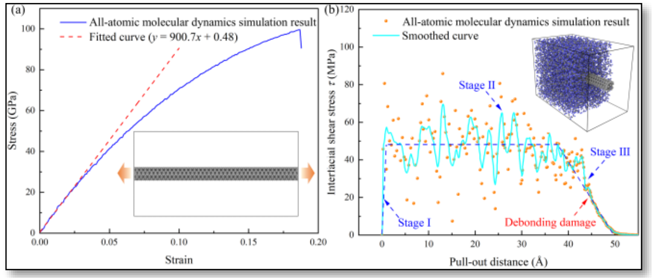

Fig. 5 (a) Stress-strain curve of carbon nanotube nanofiber during uniaxial tension; (b) load-displacement curve based on the cohesive model.

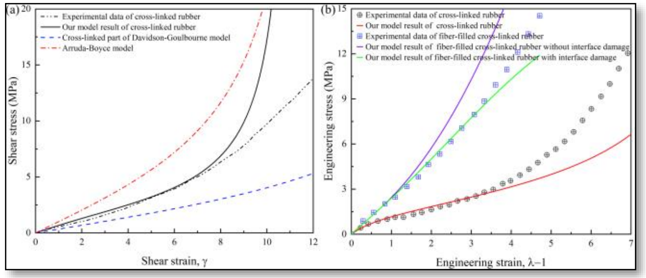

Fig. 6 (a) Comparison of prediction and experimental results[1] of cross-linked rubber under simple shear; (b) comparison of prediction and experimental results[2] of cross-linked rubber and carbon nanotube nanofiber-filled cross-linked rubber composites under uniaxial tension.

Conclusions

By introducing the macroscopic and microscopic transition factor, shear lag theory, Krenchel orientation parameter, and non-uniform interfacial stiffness function, the constitutive equations of cross-linked natural rubber and nanofiber-filled cross-linked natural rubber composites considering interfacial debonding damage were constructed. The physical parameters of the proposed constitutive equations were obtained through coarse-grained and all-atomic molecular dynamics simulations, achieving a cross-scale analysis of elastomers from micro to macro levels.