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Simulation of Microheterogeneous Networks and Extraction of Segment Orientation Behavior from D-NMR Spectra BERNARDO AGUILERA-MERCADO, CLAUDE COHEN, FERNANDO ESCOBEDO, School of Chemical and Biomolecular Engineering, Cornell University — The degree of heterogeneity in the microstructure of end-linked elastomer networks has been shown to have a very strong impact on the network mechanical and elastic properties such as: ultimate strain, modulus, and toughness. Networks with crosslinks and chains inhomogeneously distributed are expected to exhibit heterogeneous segment orientation responses. The global segment orientation of systems with frozen inhomogeneities, and a significant amount of highly stretched chains at the unperturbed state, cannot be captured by measurements of the deuterium NMR spectra splits solely. Spectrum frequency splits quantify the segment orientation due to local excluded volume interactions only and do not account for the contributions arising from large end-to-end chain deformations. Long wings of the spectrum reflect the presence of strongly aligned segments ignored when one considers only the split. A new methodology based on the Maximum-Entropy method is proposed to find the probability density of an order parameter that describes the network segment orientation from which the global orientation behavior can be completely characterized. The methodology is validated with both molecular simulation and experimental data.

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