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A Multi-scale Mechanics Model for Disordered Biopolymer Gels Incorporating Intrinsic Incompressibility

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ABSTRACT

Disordered biopolymer gels, such as gelatin, agar, carrageenan, and polysaccharide gels, exhibit a complex microstructure composed of amorphous regions and junction zones, the latter stabilized by physical bonds such as hydrogen bonding and ionmediated adhesion. The amorphous regions consist of polymer chains in a random conformation, which can be described using coil models such as freely jointed chains. In contrast, the junction zones serve as physical cross-links, where polymer chains associate to form structured connections, often behaving like rigid rods. This interplay between flexible and rigid components is important to the macroscopic mechanical response of biopolymer gels, making their modeling both challenging and essential for understanding their behavior in various applications. To predict the stress-stretch relationship of biopolymer gels, numerous theoretical models have been developed. Among them, the eight-chain network model combined with a coil-rod microstructure has successfully captured essential features such as unzipping/zipping of molecular chains during loading/unloading, presence of a permanent set upon unloading, and energy dissipation under cyclic loading. Despite its success, a major limitation of this model is its failure to enforce the incompressibility constraint, leading to unphysical predictions where volume changes occur even when there is no zipping/unzipping. In reality, biopolymer gels are largely incompressible due to the retention of solvent molecules, and any observed volume change should be more reasonably attributed to the unzipping/zipping of polymer chains rather than an inherent expansion or contraction of the network. The present work addresses this limitation by introducing a new formulation that explicitly incorporates the incompressibility constraint, ensuring that any volume change is strictly a consequence of zipping/unzipping within the coil-rod structures. By doing so, it eliminates the counterintuitive volume variations present in previous formulations and provides a more physically accurate description of biopolymer gel mechanics. This improved framework has significant implications for understanding and predicting the mechanical behavior of soft biological materials, hydrogels, and polymer networks used in biomedical and industrial applications. By capturing the interplay between molecular conformations and macroscopic mechanical properties, this approach enhances the predictive capability of constitutive models, offering valuable insights for designing materials with tailored mechanical responses.