

# STATISTICAL MECHANICS ANALYSIS OF COIL-ROD-COIL STRUCTURE IN BIOPOLYMER GELS

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## ABSTRACT

Due to the unique properties of biopolymer gels, they are extensively used in the food industry and biomedical applications such as drug delivery. Unlike the rubber-like materials, the constituting chains in biopolymer gels interlock together through physical rather than covalent cross-linking. Biopolymer gels are characterized by two principal regions: the disordered zone containing coiled chains, and the ordered zone manifesting in the form of ion-mediated aggregation of macromolecules and/or helical structures. Thus, the associated coherent network is formed by combining these two regions such that the ordered structures serve as junction zones between the disordered chains. On the macroscopic scale, there are abundant studies on the prediction of biopolymer gels properties by using phenomenological models. However, to gain deeper insight into the fundamental nature of such polymers and their underlying mechanical properties, it is preferable to apply statistical mechanics on the atomic scale. In this regard, the entire polymer network can be envisaged as a collection of coil-rod-coil structures representative of the building blocks of the network. In addition, previous studies revealed that biopolymer gels under cyclic mechanical loadings possessed healing properties. This feature can be explained by the reversible zipping and unzipping of the physical junction zones, which is the dominant mechanism in biopolymer gels compared with bond scission of the chains in rubber-like materials. The coil-rod-coil structure can model this phenomenon as the ordered rod part and disordered coiled parts are interchangeable.

The present work aims to extend the existing formulations of coil-rod-coil structures to predict their pertinent rheological properties. First, the coil-rod-coil structure is modelled by a sizeable rigid rod located between two freely jointed chains. Then the relationship between the force and end-to-end distance of the coil-rod-coil structure is developed from statistical mechanics. Finally, the formulation is extended to incorporate the zipping mechanism with the aid of kinetic reaction theory and the results are compared with those in the previous studies. The rigorous formulation presented in this work paves the way for constructing biopolymer network models with more complex chain interactions in future studies.