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Relationship between model bacterial peptidoglycan network structures and AFM force-distance curves AIDAN BROWN, ROBERT WICKHAM, University of Guelph, AHMED TOUHAMI, University of Texas at Brownsville, JOHN DUTCHER, University of Guelph — Recent atomic force microscopy (AFM) measurements have involved pulling on Gram-negative bacterial sacculi with the AFM tip as a means of distinguishing between different proposed structures of the peptidoglycan network. The goal of the present study is to provide the theoretical connection between a given network structure and its response to the pulling force. We model the glycan strands as hinged rods, and the peptide cross-links as wormlike chains. Using Monte Carlo simulation to equilibrate the three-dimensional network, subject to a fixed AFM tip-to-substrate distance, we can compute the force exerted by the network on the AFM tip. The effects of adhesion of the sacculi to the substrate and enzymatic action on the network are included. We have modeled both the layered and the scaffold model for the peptidoglycan network structure. We have compared our theoretical force-distance curves for each network structure with experimental curves to determine which structure provides the best agreement with experiment.

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