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ORIGINS OF MECHANICAL ANISOTROPY IN ICOSAEDRAL VIRAL CAPSIDS.

Content

Icosahedral viral capsids are nanoscale protein containers that protect and deliver the viral genome. Despite their high degree of geometric symmetry, experimental evidence has revealed that their mechanical response is not uniform in all directions. This phenomenon—mechanical anisotropy—is not yet fully understood, and its biological relevance remains underexplored. Current knowledge is limited by experimental constraints and the challenge of isolating geometric versus atomic contributions to mechanical behavior. This study aims to investigate the structural origins of mechanical anisotropy in icosahedral viral capsids through numerical simulation. We hypothesize that the observed anisotropy arises primarily from surface geometry and quaternary structural organization, rather than from atomic-scale interactions. Our objective is to characterize how the directionality of mechanical response varies with capsid architecture and indentation site. We will perform in silico nanoindentation simulations on eight viral capsids—CCMV, HK97-like bacteriophage HII, Bacteriophage T7, Hepatitis B virus, Minute Virus Mice, AAV2, Simian Virus 40 and Escherichia phage HK97. Structural data will be retrieved from VIPERdb or the Protein Data Bank and preprocessed to ensure complete quaternary assembly. Capsids will be discretized into high-quality hexahedral meshes using an octree-based algorithm, preserving essential topological features. Finite element simulations will apply static loads at specific symmetry axes (2-fold, 3-fold, 5-fold) to probe directional stiffness. Understanding the mechanical anisotropy of viral capsids can shed light on their biological roles, including stability, uncoating, and host interaction. This research provides a computational framework to disentangle structural and mechanical determinants of anisotropy, offering insights into viral evolution and design principles for biomimetic nanomaterials.

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