CONTINUUM MECHANICS OF MOLECULAR ASSEMBLIES DERIVED FROM MOLECULAR DYNAMICS SIMULATION

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Mechanical properties of macromolecular assemblies have typically been derived from experiments, either from measurements of the thermal fluctuations of individual filaments (e.g., actin filaments, microtubulues), or from macroscopic rheological measures. From these, properties of an effective continuum material are often derived such as bending stiffness (K_B) or Young's modulus (E). To date, the use of simulation to investigate mechanical properties has been limited due to lack of knowledge of the particular structure or computational constraints. Here we demonstrate several complimentary approaches to the determination of K_B and E from atomistic simulation. We investigate filaments formed from a self-assembling peptide ac-$[RARADADA]_2$-am that forms a double layer β-sheet filament whose structure was determined through a combination of simulation and comparison to images obtained by atomic force microscopy. Three independent simulation methods - thermal motion analysis, normal mode analysis, and steered molecular dynamics - were used to determine the continuum mechanical properties of the filament. We found that while side chain interactions determine the energetics of self-assembly, the backbone hydrogen bond network that forms the filament's `elastic core' dominates the structural stiffness. Values for bending stiffness (0.5-2.0 Nm^2) suggest an effective Young's modulus in the range of several GPa, comparable to the range of values obtained from experimental measurements on actin filaments [1] and microtubules [2]. Results demonstrate the feasibility of using computational methods to derive mechanical properties of macromolecular assemblies, and to probe the fundamental interatomic interactions that influence elasticity.

References

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