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Simulation of Microtubules: Mechanical properties MARK STEVENS, Sandia National Labs — In order to understand microtubule assembly and the necessary monomeric properties to design artificial polymers that possess features similar to those of microtubules, we have developed a coarse-grained model of a monomer that self-assembles into tubules. In this model the monomer has a wedge shape which promotes tubule formation. There are attractive binding sites on the vertical and lateral sides of the monomer. We previously performed molecular dynamics simulations to calculate the set of structures that form upon self-assembly as we vary the lateral and vertical interaction strengths. In this talk, we will present the results of mechanical studies of the coarse-grained tubule system. The persistence length and various elastic moduli have been calculated. Microtubules have some of the largest persistence lengths of polymers. We have found that the persistence length is indeed very long for this coarse-grained model system. We calculate elastic moduli for varying the interaction strengths of the lateral and vertical interactions. We gain insight into the values that occur in microtubules, with respect to mechanical stability and stiffness.

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