

Abstract Submitted
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Structural control in model microtubule self-assembly¹ SHENGFENG CHENG, MARK STEVENS, Sandia National Laboratories — Being able to control the structure formed in self-assembly is the goal of many nanoscience studies. Here we explore various ways to control the structure of self-assembled tubules. We have previously developed a model wedge-shaped monomer that can self-assemble into tubule structures. We now add chirality and a lock-and-key mechanism to the model to enhance structural control of the self-assembly. Previously, we found that helical tubes are frequently formed despite the fact that chiral symmetry is not present in the monomer. We now identify the physical origin of helicity as the large overlap in the energy distributions between nonhelical and helical tubes. The helical tubes typically undergo a twist deformation that lowers the energy substantially. We find that a modification of the location of binding sites on the bottom and top surfaces of the wedge into a lock-and-key configuration leads to a better control of the helicity and twist deformation of the assembled tubes. Better control occurs when the interaction strength between the vertical binding sites is stronger than that between the lateral ones. We can also control the pitch of the helicity by adjusting the location of binding sites on the lateral surfaces of the monomer. Our results shed new light on the structure of in vitro microtubules formed with various numbers of protofilaments of tubulins, which also exhibit twisted structures when the number is different from 13.

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