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A mechanochemical model of microtubule growth dynamics

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Summary

Microtubules experience growing and shrinking alternatively. This dynamic property is intrinsic for microtubules and is essential for them to function. Revealing the mechanism for microtubules to maintain a stable growth phase is important and fascinating. It has been recognized that the hydrolysis of the nucleotides bound on the tubulins and the associated configuration changes of the tubulins highly influence the growth and shrinkage process of microtubules. In consideration of the hydrolysis effect, a "GTP cap" model has been widely supposed to answer for the stabilizing mechanism of microtubule growth. Meanwhile, experiments shown that there exists an open sheet structure curving outward at the end of a microtubule and the growth process experiences a "sheet-to-tube" curvature transition. This growth mode may also help stabilize the microtubule growth, and is referred to as a "conformational cap" model. The microtubule growth process and the stabilizing mechanism involve complicated mechanical-chemical couplings. However, early works are mostly experimental, and analytical consideration lacks. Detailed insights are needed for the spatiotemporal energy distribution and variation which governs the microtubule behaviors, and the linkages between mechanics and biochemistry should be taken into account. Here, we present a novel model to describe the dynamic attributes of microtubules at a resolution of one monomer. Firstly, the structures for a sheet-ended microtubule are characterized, which involve complex twisting and bending of each protofilament, and exhibit colorful forms. Secondly, the "sheet-to-tube" process is simulated, and the energy evolution is analyzed. The results verify that the sheet structure can work as a stabilizing mechanism for microtubule growth, and the length of this conformational cap should be no less than 2 dimers. Thirdly, it is shown that such conformational cap can be uncoupled with the GTP cap, meaning that mechanical factors could be pivotal in biochemical systems. Fourthly, based on the obtained results, we put forward a growth style for microtubule as Tetris: the stochastic tubulin assembly is regulated by energy, and is harmonized with the zipping of the seam, thus keeping a practically constant sheet length. Simulation for such a growth mode is done. In addition, the model is used to simulate the microtubule macroscopic static properties that are characterized by a radial indentation.