«Microtubule stochastic dynamics modeling and the application of optical methods for their research»

Abstract

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Microtubule (MT) is a complex biological heteropolymer that performs such functions as the formation of the cytoskeleton of the cell, the formation of the mitotic spindle during mitosis and it also enables intracellular transport. The study of its unique dynamic properties is carried out both experimentally (including the usage of optical methods) and theoretically, using the construction of numerical models. This paper presents the results of constructing a mechanical-molecular model of a microtubule based on the Brownian dynamics method taking into account all possible degrees of freedom of particles in the system. It was shown that, within the framework of the model, the law of motion of each structural element of a microtubule (monomer) is a system of six Langevin equations. The obtained equations were converted into an iterative algorithm, after which a computer program was written that carries it out. The constructed model was calibrated on simple systems (such as monomer and tetramer in several different modes). It was shown that the selected modeling algorithm as a whole correctly reproduces the basic properties inherent in the studied systems. During the simulation, the value of the equilibrium establishment time for the free tetramer was obtained and it was found that the equilibrium conformation angles in the model are slightly different from those in the parameterization. It was revealed that the lateral bonds formed by four monomers in each protofilament (PF) are insufficient to compensate for the bending of the studied PF in the radial plane. In addition, it was found that the bend of the protofilament in the tangential (to the MT body) plane practically does not change in the presence of lateral bonds. Thus, it was shown that the constructed model can be successfully used to simulate the behavior of an entire MT and interpret the results of various experiments.