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A nonlinear model of the dynamics of radial dislocations in microtubules

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ABSTRACT

We have established a new dynamical model of microtubules based on their intrinsic dipolar character. The model assumes a single angular degree of freedom per dimer describing the conformational displacements of constituent dimers in radial direction. A corresponding nonlinear dynamical equation of motion is solved both analytically, using the simplest equation method, and numerically. It is shown by both approaches that kink solitons could be elicited and sustained to propagate along the microtubule. We suggest that this model could explain some dynamical functional properties of microtubules, including the triggering of the onset of their depolymerization.

1. Introduction

Microtubules (MTs) form an important part of the cellular skeleton and represent a network for intracellular transport of motor proteins. They also play a crucial role during cell division, forming a dynamic structure that spatially separates duplicated chromosomes.

Microtubules represent hollow cylinders formed by protofilaments (PFs) aligned in directions that are parallel to their axes [1–5]. There are in vivo usually 13 longitudinally ordered PFs covering the cylindrical walls of MTs. The lengths of MTs span dimensions from the order of micrometers to the order of millimetre. The approximate values of the outer and the inner radii of MT cylinder are 25 nm and 15 nm, respectively [6–8].

PF represents a series of proteins known as tubulin heterodimers. Each dimer is effectively an electric dipole whose length is $l = 8$ nm, as shown in Fig. 1. Its electric dipole moment and charge displacement are: $p = 337\text{Debye} = 1.13 \times 10^{-27}$ Cm and $d \approx 4$ nm, respectively [6,9–11].

Microtubules are very dynamic polymers whose polymerization and disassembly are determined by whether their dimers are in a straight position within PFs or in radially displaced positions pointing out of cylindrical surface. These circumstances are the basis for our attempt to describe MT dynamics relying on the nonlinear model expressed by this single degree of radial displacement of tubulin dimer within PF.

The paper is organized as follows. In Section 2 we establish the nonlinear model of collective conformations of the dimers within PF. Section 3 deals with the analytical solution of equation of motion in terms of the simplest equation method. The numerical solutions of higher-order expansion of cosine function are presented in Section 4. The conclusions including the possible biological implications are presented in Section 5.

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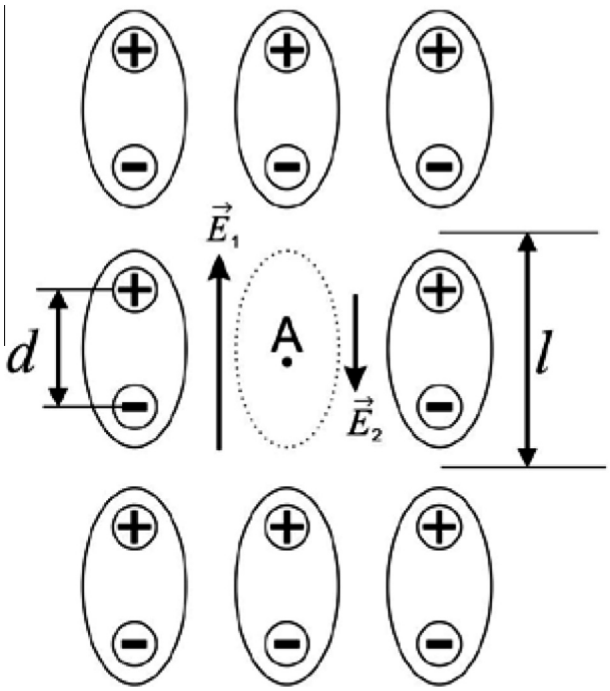

Fig. 1. A segment of three protofilaments (PF1, PF2 and PF3, from left to right) with the fields $\vec{E}_1$ and $\vec{E}_2$ in the point A, arising from the same protofilament PF2 and from the neighbouring PFs, respectively. The dipole moment $\vec{p}$ of the tubulin dimer has the displacement of the opposite charges depicted with d.

2. Dynamical model of microtubules

A simplified picture, relevant for the model established in this paper, is shown in Fig. 1. Let us consider the dimer in the middle, belonging to PF2. It feels electric fields of the neighbouring dimers. The field $\vec{E}_1$ comes from the dimers belonging to the same PF2, while $\vec{E}_2$ is the longitudinal component of the field which originates from the dimers belonging to the neighbouring PFs, i.e. PF1 and PF3. Details about the calculations of the above fields are published in Ref. [12]. It might be noticed that PF1 and PF3, in Fig. 1, should be respectively displaced up and down in order to match the real MT structure, i.e. its intrinsic helicity. These displacements lead to a component of $\vec{E}_{2p}$ in perpendicular direction to $\vec{E}_1$. However, the component $\vec{E}_{2p}$ is not taken into account in the present model as being irrelevant for the considered degree of freedom.

The tubulin dimers within PFs can perform conformational changes that may propagate along either individual PFs or small groups of PFs. The bending of PFs during disassembly of MT is the consequence of such cooperative conformations [13]. It was shown that the relative displacement of two neighbouring dimers can reach 32° prior disrupting PF. In addition, the angular displacements of the monomers within a single dimer can be up to 13° [14]. These facts motivated us to restrict our modeling to the angular conformations of dimers φ in radial directions from the line of the dipolar electric field $\vec{E} = \vec{E}_1 + \vec{E}_2$. Therefore, we assume that the whole dimer rotates and the corresponding angular displacement is φ. What the point is, around which this rotation occurs, is not known in this moment. It may be a dimers tip, its centre or any point in between. This is only important for the estimation of its moment of inertia, which is beyond the topic of this paper.

A dipolar potential energy of a single dimer is simply expressed as a scalar product

$$U(\varphi) = -\vec{p}\cdot\vec{E} = -qdE\cos\varphi, \tag{1}$$

where q represents the excess charge of the monomer within the dipole. It is assumed that the inequalities $p > 0$ and $E > 0$ hold.

In the nearest neighbour approximation, the expression for the Hamiltonian of one PF in a discrete version is

$$H = \sum_n \left[\frac{I}{2}\dot{\varphi}_n^2 + \frac{k}{2}(\varphi_{n+1} - \varphi_n)^2 - pE\cos\varphi_n\right], \tag{2}$$

which, after a series expansion of the cosine function, becomes

$$H = \sum_n \left[\frac{I}{2}\dot{\varphi}_n^2 + \frac{k}{2}(\varphi_{n+1} - \varphi_n)^2 - pE + pE\left(\frac{\varphi_n^2}{2} - \frac{\varphi_n^4}{24}\right)\right]. \tag{3}$$