MECHANO-ELECTRICAL OSCILLATIONS OF SUPRAMOLECULAR NETWORKS

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Abstract

Under physiological conditions, supramolecular biological structures undergo nanoscale mechanical vibrations. Since proteins, which form building units of these structures, are usually highly electrically polar, mechanical oscillations will be accompanied by oscillating electric field. However, molecular modeling methods are not yet able to perform all-atom mechanical simulation of larger structures, nor its electric field. A number of simplifications must be done in order to accomplish such a simulation. In this contribution we present a model of mechano-electrical oscillations of microtubule and microtubular network. We represented subunits of microtubule - the tubulin heterodimer - by two charged particles forming an elementary electric dipole. Mechanical oscillations for given vibration modes are then implemented as a spatial function modulating the distance between particles, and modulating thus the dipole moment of subunits as well. Field around oscillating microtubule was then calculated as a vector superposition of contribution from all subunits. This method gives realistic results in reasonable time and computational intensity.

1 Intoduction

As was predicted theoretically and confirmed experimentally, supramolecular biological structures undergo nanoscale mechanical vibrations under physiological conditions. Since proteins, which form building units of these structures, are usually highly electrically polar, mechanical oscillations will be accompanied by oscillating electric field. However, even cutting edge technology is not yet able to measure this electric field directly. It is then needed to employ computational methods, which give us deeper insight into the character of this field.

Nevertheless, molecular modeling methods are not yet able to perform all-atom mechanical simulation of larger structures, nor its electric field. A number of simplifications must be done in order to accomplish such a simulation. In this contribution we present a model of mechano-electrical oscillations of microtubule and microtubular network. Leaving aside biophysical role of mechano-electrical oscillations and technical aspects of its measurement, which is discussed elsewhere [1, 4], we aim mainly at the computational method developed for this purpose.

2 Microtubule

Microtubules, one of three filaments forming cytoskeleton, resemble hollow rods with inner and outer diameter 17 and 25 nm, respectively. They are mostly composed of 13 protofilaments. The subunits of protofilaments are tubulin heterodimers, which are polar structures, composed of $\alpha-$ and $\beta-$ tubulin. The tubulin heterodimers have the dipole moment of 337 Debye in direction of microtubule axis. Artistic representation of the single microtubule is depicted on the Fig. 1.

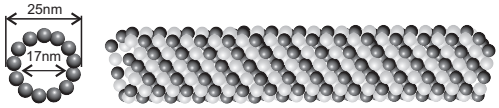

Figure 1: A single microtubule with 13 protofilaments.

3 Computational Method

Electrical properties of tubulin heterodimers are approximated by elementary electric dipole as depicted see on Fig. 2. Elementary electric dipole is described by following equations (1 - 3).

$$H_\varphi = -\frac{I\mathrm{d}l}{4\pi}k^2 \sin\left(\vartheta_p\right)\left(\frac{1}{\mathrm{j}kr} + \frac{1}{(\mathrm{j}kr)^2}\right) e^{-\mathrm{j}kr} \tag{1}$$

$$E_r = -\frac{I\mathrm{d}l}{2\pi}Zk^2 \cos(\vartheta_p)\left(\frac{1}{(\mathrm{j}kr)^2} + \frac{1}{(\mathrm{j}kr)^3}\right) e^{-\mathrm{j}kr} \tag{2}$$

$$E_\vartheta = -\frac{I\mathrm{d}l}{4\pi}Zk^2 \sin(\vartheta_p)\left(\frac{1}{\mathrm{j}kr} + \frac{1}{(\mathrm{j}kr)^2} + \frac{1}{(\mathrm{j}kr)^3}\right) e^{-\mathrm{j}kr} \tag{3}$$

where E is electric field intensity, H is magnetic field intensity, I is equivalent current, dl is length of the dipole, Z is wave impedance, k is propagation constant, ω is angular frequency, p is dipole moment, j is imaginary unit (j^2 = -1), $I\mathrm{d}\vec{l} = \mathrm{j}\omega\hat{p}$, and other symbols are according to Fig. 2a.

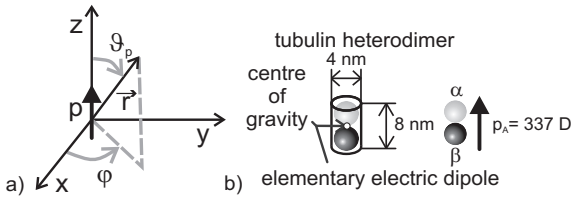

Figure 2: (a)A dipole in the Cartesian coordinate system. (b) An approximation of a heterodimer by an elementary electric dipole.

We put the elementary electric dipole in the center of gravity of each tubulin heterodimer of single microtubule and then we have simple model in Matlab (Fig. 3).

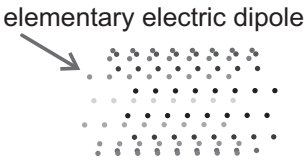

Figure 3: Model of microtubule in Matlab.

We calculated electric and magnetic field and Poynting vector around single microtubule as well as a simple microtubule net. The calculation is executed by adding all contributions from all elementary electric dipoles in one point of the field of evaluation. We repeated this calculation for all points of the field of evaluation.

We approximated microtubule vibrations by vibrations of each protofilament. Oscillations of tubulin heterodimers in one protofilament were aproximated as oscillations of the chain of the rigid two-type particles (α - and β tubulin). Movement of particles and corresponding oscillations of dipole moment is described by spatial modulation function

$$p_m = p_A \cdot \sin(mv) \tag{4}$$

where p_m is a modulated dipole moment, for p_A see Tab. 1, and mw is basically distance along the microtubule.

Modulation function is specific for each mode from mode zero to max mode. The mode zero represents oscillations of all dipoles in phase and the max mode represents oscillations of neighboring dipoles in antiphase. Higher modes resemble longitudinal wave.

Dipole moment - static:	$p_0 = 1.29\ 10^{-26}$ Cm (337 Debye) [5]
Dipole moment - oscillating:	$p_A = \frac{1}{80} p_0$ [2]
Relative permittivity:	$\varepsilon_r = 60$ [3]
Conductivity:	$\sigma = 1$ S/m [3]
Frequency:	f = 1 GHz
Theta:	$\vartheta = 0°$
Longitudinal shift of protofilaments:	4.92 nm (lattice A) [5]

Table 1: Material constants defining medium and geometry of a microtubule.

4 Selected Results

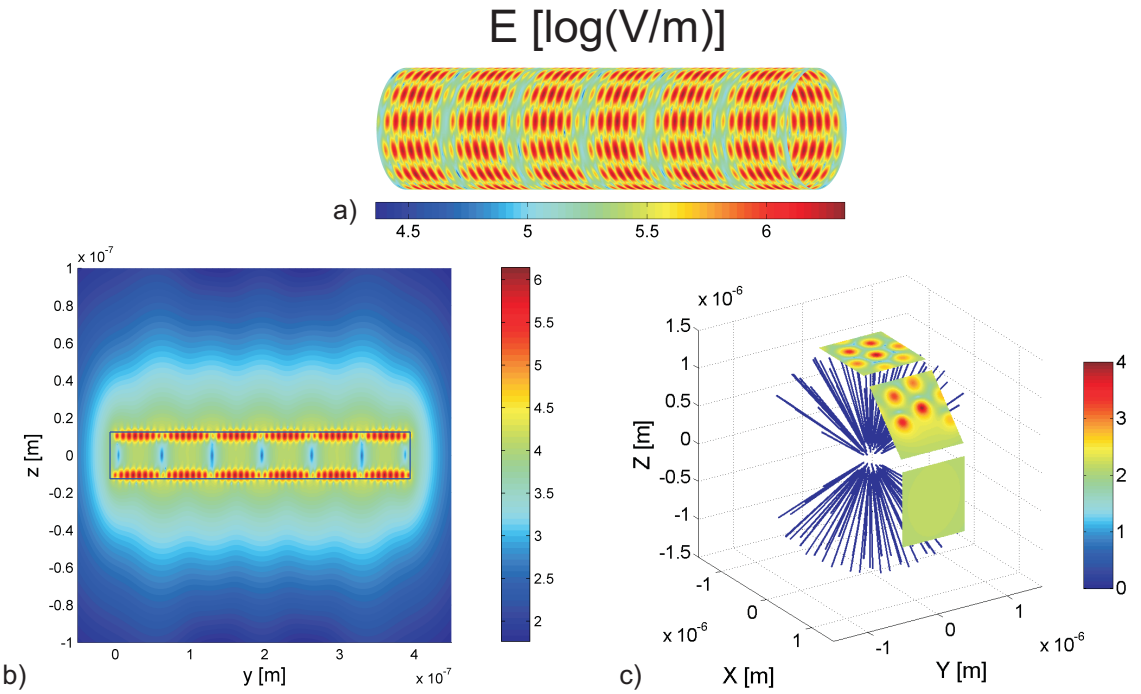

Figure 4: a) Instantaneous value of the intensity of electric field in logarithmic scale on the coaxial surface 1 nm above the microtubule wall, b) instantaneous value of the electric field in logarithmic scale in section through axis of the MT, c) instantaneous value of electric filed generated by microtubule net.

5 Discussion

The method presented omits quantum nature of processes which occur in the microtubule. That is the disadvantage of this method since microtubules are considered promising bio-structure for quantum computing. However, there is no need for such precision in other applications, such as bioelectromagnetics. Moreover, contemporary available computing power is not sufficient for such calculation, especially in the case of larger networks of supramolecules.

Ongoing development in this field leads to reduction of computational intensity taking the advantage of spatial symmetry of objects under examination. Together with increasing computing power, it will enable higher structural precision of the model, desirably all-atom model with quantum properties.

6 Conclusion

The method for calculation of mechano-electrical oscillations of supramolecular networks was presented, implemented, discussed, and typical results were shown. We may conclude that this method gives realistic results in reasonable time and computational intensity. Physical advisability of results presented will have to be confirmed experimentally, preferably by direct nanoscale measurement, if the technology is ripe enough to do so.

7 Acknowledgments

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