Mathematical Model for Study the Microtubules Using Shear Deformation Theories

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Abstract

In this paper, mathematical model for the study of microtubules, which are beam in shape inside of the cellular structure and where the shear modulus is very low, has discussed. Governing differential equations and boundary conditions obtained by using the principle of virtual work. The thick simply supported isotropic beams considered for the numerical studies. The parabolic shear deformation theory for flexure of thick microtubules, taking into account transverse shear deformation effects, is developed. The noteworthy feature of this theory is that the transverse shear stresses can be obtained directly from the use of constitutive relations with excellent accuracy. Results obtained and discussed critically with those of other theories and illustrated graphically for each case considered.

Keywords: Mathematical model, Microtubules, Bending, Parabolic shear deformation theory

1 Introduction

As the most rigid cytoskeletal filaments, microtubules bear compressive forces in living cells, balancing the tensile forces within the cytoskeleton to maintain the cell shape. The cytoskeleton is composed of three different types of filaments organized in networks: microfilaments (MF), intermediate filaments (IF) and microtubules
(MT). Each of them has specific physical properties and structures suitable for their role in the cell. These results show that the theory (parabolic shear deformation beam) provide a model united in one dimension, could explain rigidity flexural based on length, as well as its applications on several special issues microtubules and in many science, A.M. Abd-Alla, et al. [1-2]. These results demonstrate that the theory (parabolic beam shear deformation) model provide combined in one dimension could explain the bending stiffness based on the length as well as its use in several special issues in many biomechanics of microtubule science, Odde, D.J., et al., [3], Jordan, M.A., Wilson, L. [4], Mechab, I., et al. [5], Keten, S. et al. [6]. Moreover, the idea was to investigate Chretien, D., et al. [9] MTs membranes based vehicle model. Orthogonal with a rubber band shell pattern indicates that rely on bending stiffness due to the very low shear modulus. MTs unit circle, which have an impact on a significant reduction in the rigidity of emotion when the MTs called for short as the impact of the weakness disappears longer MTs. Recently, however, Timoshenko beam theory is not compatible with zero shear stress in the upper and lower surfaces of the structures. Microtubules configuration can be described by a pair of integers N-S, where N is the number of protofilaments and S the plexus starting number. 13-3 MT is the most common type of MTs collected in the vivo, as protofilaments in parallel with the longitudinal axis (i.e. deviation angle is zero)

In this work, analysis of bending of microtubules based on higher order theory indicates that the research work dealing with flexural analysis of microtubules using First-order beam theory is very scarce and is still in infancy. By comparison, the previous theories, third (higher) order theory, and its application to thick simply supported Microtubules is presented.

2 Formulation of the problem

Consider the bending of a beam with length $L$, moment of inertia $I$ and Young's modulus $E$, and subjected to distributed axial force $f(x)$ and transverse load $q$. The displacement field using Third-order beam, theory in this case given by

\[
U(x, z, t) = u_0(x, t) + z\phi(x, t) - c_1 z^3 \left( \phi + \frac{\partial w_0}{\partial x} \right),
\]

\[V(x, z, t) = 0,
\]

\[W(x, z, t) = w_0(x, t).
\] (1)

where $c_1 = 4/(3h^2)$, ($h$ being the height of the beam (MT)), $u_0$ is the axial displacement, $w_0$ he transverse displacement, and $\phi$ the rotation of a point on the centroidal axis $x$ of the beam.

Although one can use the general nonlinear strain-displacement relations, here we restrict the development to small strains and displacements. The nonzero strains of the refined beam theory are:
\[ \varepsilon_{xx} = \varepsilon_{xx}^{(0)} + z\varepsilon_{xx}^{(1)} + z^3\varepsilon_{xx}^{(3)}, \]
\[ \gamma_{xz} = \gamma_{xz}^{(0)} + z^2\gamma_{xz}^{(2)}, \quad (2) \]

where the linear strains associated with the displacement field are

\[ \varepsilon_{xx}^{(0)} = \frac{\partial u_0}{\partial x}, \quad \varepsilon_{xx}^{(1)} = \frac{\partial \phi}{\partial x}, \quad \varepsilon_{xx}^{(3)} = -c_1 \left( \frac{\partial \phi}{\partial x} + \frac{\partial^2 w_0}{\partial x^2} \right). \]
\[ \gamma_{xz}^{(0)} = \frac{\partial w_0}{\partial x} + \phi, \quad \gamma_{xz}^{(2)} = -c_2 \left( \frac{\partial w_0}{\partial x} + \phi \right). \quad (3) \]

and \( c_2 = 4/h^2 \). Note that \( \gamma_{xz} = 2\varepsilon_{xz}, \sigma_{xz} = G\gamma_{xz}, \) \( (4) \)

are quadratic functions of \( Z \). From the dynamic version of Hamilton's principle, we have, the principle of virtual work is

\[ 0 = \delta \int_{t_1}^{t_2} (K - (V + U)) dt, \Rightarrow 0 = \int_0^T \left( \delta U + \delta V - \delta K \right) dt, \quad (5) \]

where \( \delta U \) : virtual strain energy (volume integrate of \( \delta U_0 \)), \( \delta V \) : virtual work done by applied force, \( \delta K \) : virtual kinetic energy, and

\[ \delta U = \int_v \sigma_{ij} \delta \varepsilon_{ij} dv, \quad \delta V = -\int_{s_2} \dot{t}.\delta u ds, \quad \delta K = \int_v \frac{\rho}{2} \frac{\partial^2 u}{\partial t^2} dt dv. \quad (6) \]

Therefore, from the virtual strain energy of the parabolic shear deformation beam theory, we have

\[ \delta U = \int_0^L A \int_0^L \left[ \sigma_{xx} \left( \delta \varepsilon_{xx}^{(0)} + z\delta \varepsilon_{xx}^{(1)} + z^3\delta \varepsilon_{xx}^{(3)} \right) + \sigma_{xz} \left( \delta \gamma_{xz}^{(0)} + z^2\delta \gamma_{xz}^{(2)} \right) \right] dA dx, \]

\[ \delta K = \int_0^L A \int_0^L \rho \left[ \dot{u}_0 + z\dot{\phi} - c_1 z^3 \left( \dot{\phi} + \frac{\partial \dot{w}_0}{\partial x} \right) \right] \left[ \delta \dot{u}_0 + z\delta \dot{\phi} - c_1 z^3 \left( \delta \dot{\phi} + \frac{\partial \delta \dot{w}_0}{\partial x} \right) \right] + \dot{w}_0 \delta \dot{w}_0 \right] dA dx, \]

\[ \delta V = \int_0^L \left( q \delta w_0 \right) dx. \]

From Hamilton's principle, we obtaine
\[ 0 = \int_0^T \int_0^L \left[ \sigma_{xx} \left( \delta \varepsilon_{xx}^{(0)} + \varepsilon_{xx}^{(1)} + z^2 \varepsilon_{xx}^{(3)} \right) + \sigma_{xx} \left( \delta \gamma_{xx}^{(0)} + z^2 \gamma_{xx}^{(2)} \right) \right] dA dx dt \]

\[ - \int_0^T \int_0^L \rho \left[ \dot{u}_0 + z \dot{\phi} - c_1 z^3 \left( \dot{\phi} + \frac{\partial \dot{u}_0}{\partial x} \right) \right] \delta \dot{u}_0 + z \delta \dot{\phi} - c_1 z^3 \left( \delta \dot{\phi} + \frac{\partial \delta \dot{u}_0}{\partial x} \right) \right] + \dot{u}_0 \delta \dot{u}_0 \) dA dx dt \]

\[ - \int_0^T \int_0^L \left[ I_0 \dot{u}_0 \delta \dot{u}_0 + I_2 \dot{\phi} - c_1 I_4 \left( \dot{\phi} + \frac{\partial \dot{u}_0}{\partial x} \right) \right] \delta \dot{\phi} + q \delta \ddot{u}_0 \right\} dx dt \]

\[ - \int_0^T \int_0^L \left[ -\dot{c}_1 I_6 \left( \dot{\phi} + \frac{\partial \dot{u}_0}{\partial x} \right) \right] \delta \dot{\phi} + \frac{\partial \delta \dot{u}_0}{\partial x} + I_0 \delta \ddot{u}_0 \right\} dx dt \]

\[ - \int_0^T \int_0^L \left[ \dot{u}_0 \left( -c_1 z^3 \left( \delta \dot{\phi} + \frac{\partial \delta \dot{u}_0}{\partial x} \right) \right) + \delta \dot{u}_0 \left( -c_1 z^3 \left( \dot{\phi} + \frac{\partial \dot{u}_0}{\partial x} \right) \right) + z \left( \dot{u}_0 \delta \dot{\phi} + \delta \dot{u}_0 \dot{\phi} \right) \right\} dx dt, \]

where

\[
\begin{bmatrix}
N_{xx} \\
M_{xx} \\
P_{xx}
\end{bmatrix} = \int_{-h/2}^{h/2} \begin{bmatrix} 1 \\ z^2 \end{bmatrix} \sigma_{xx} dz,
\begin{bmatrix}
Q_x \\
R_x
\end{bmatrix} = \int_{-h/2}^{h/2} \begin{bmatrix} 1 \\ z^2 \end{bmatrix} \sigma_{xx} dz,
I_i = \int_{-h/2}^{h/2} \rho z' dz,
\]

Therefore

\[ 0 = \int_0^T \int_0^L \left[ N_{xx} \frac{\partial \ddot{u}_0}{\partial x} + M_{xx} \frac{\partial \dot{\phi}}{\partial x} + P_{xx} \left( -c_1 \left( \frac{\partial \phi}{\partial x} + \frac{\partial^2 w_0}{\partial x^2} \right) \right) \right] + \frac{Q_x}{x} \left( \frac{\partial w_0}{\partial x} + \phi \right) + R_x \left( -c_2 \left( \frac{\partial w_0}{\partial x} + \phi \right) \right) dx dt \]

\[ - \int_0^T \int_0^L \left[ I_0 \dot{u}_0 \delta \dot{u}_0 + I_2 \dot{\phi} - c_1 I_4 \left( \dot{\phi} + \frac{\partial \dot{u}_0}{\partial x} \right) \right] \delta \dot{\phi} + q \delta \ddot{u}_0 \right\} dx dt \]
Now integration-by parts in the last relation, we get

\[
0 = \int_0^T \left\{ -\frac{\partial N_{xx}}{\partial x} + I_0 \frac{\partial^2 u_0}{\partial x^2} \right\} u_0 + \left\{ -\frac{\partial M_{xx}}{\partial x} - Q_x + K_2 \frac{\partial^2 \phi}{\partial t^2} - c_1 J_4 \frac{\partial^4 u_0}{\partial x \partial t^2} \right\} \frac{\partial \phi}{\partial x} \\
+ \left[ -c_1 \frac{\partial^2 P_{xx}}{\partial x^2} - \frac{\partial Q_x}{\partial x} - q + c_1 \left( J_4 \frac{\partial^3 u_0}{\partial x \partial t^2} - c_1 I_6 \frac{\partial^4 u_0}{\partial x^2 \partial t^2} \right) + I_0 \frac{\partial^2 u_0}{\partial t^2} \right] \frac{\partial u_0}{\partial x} \right\} dx dt \\
+ \int_0^T \left\{ N_{xx} \frac{\partial u_0}{\partial x} + M_{xx} \frac{\partial \phi}{\partial x} - c_1 P_{xx} \frac{\partial^2 u_0}{\partial x^2} + \left[ Q_x + c_1 \left( \frac{\partial P_{xx}}{\partial x} - J_4 \frac{\partial^2 \phi}{\partial t^2} + c_1 I_6 \frac{\partial^3 u_0}{\partial x \partial t^2} \right) \right] \frac{\partial u_0}{\partial x} \right\} dt.
\]

where all the terms involving \[^T \int_0^T \] vanish because the assumption that all variations and their derivatives are zero at \( t = 0 \) and \( t = T \), and the new variables introduced in arriving at the last expression are defined as follows:

\[
\bar{M}_{xx} = M_{xx} - c_1 P_{xx}, \quad \bar{Q}_x = Q_x - c_2 R_x, \quad c_1 = \frac{4}{3h^2}, \quad c_2 = \frac{4}{h^2}, \\
J_4 = I_1 - c_1 I_6, \quad K_2 = I_2 - 2c_1 I_4 + c_1^2 I_6.
\]

Note that \( I_i \), are zero for odd values of \( i \) (i.e., \( I_1 = I_3 = I_5 = 0 \)),

Thus, the Euler-Lagrange equations are

\[
\delta u_0 : \frac{\partial \bar{Q}_x}{\partial x} + c_1 \frac{\partial^2 P_{xx}}{\partial x^2} + q = I_0 \frac{\partial^2 w_0}{\partial t^2} + c_1 \left( J_4 \frac{\partial^3 \phi}{\partial x \partial t^2} - c_1 I_6 \frac{\partial^4 u_0}{\partial x^2 \partial t^2} \right),
\]

\[
\delta \phi : \frac{\partial M_{xx}}{\partial x} - \bar{Q} = K_2 \frac{\partial^2 \phi}{\partial t^2} - c_1 J_4 \frac{\partial^3 u_0}{\partial x \partial t^2}.
\]

The last line of Eq. (10) includes boundary terms, which indicate that the primary variables of the theory are (those with the variationally symbol)

\( u_0, w_0, \phi, \) and \( \frac{\partial u_0}{\partial x} \).
The corresponding secondary variables are the coefficients of 
\( \delta u_0, \delta w_0, \delta \phi, \) and \( \frac{\partial \delta w_0}{\partial x} \):

\[
N_{xx}, \bar{Q}_x + c_1 \left( \frac{\partial P_{xx}}{\partial x} - J_4 \frac{\partial^2 \phi}{\partial t^2} + c_1 I_6 \frac{\partial^3 w_0}{\partial x \partial t^2} \right), \bar{M}_{xx}, - c_1 P_{xx}.
\]

From above we get

\[
M_{xx} = EJ \frac{\partial \phi}{\partial x} - c_1 EJ \left( \frac{\partial \phi}{\partial x} + \frac{\partial^2 w_0}{\partial x^2} \right), \quad P_{xx} = EJ \frac{\partial \phi}{\partial x} - c_1 EK \left( \frac{\partial \phi}{\partial x} + \frac{\partial^2 w_0}{\partial x^2} \right).
\]

\[
Q_x = G\bar{A} \left( \frac{\partial w_0}{\partial x} + \phi \right), \quad R_x = G\bar{T} \left( \frac{\partial w_0}{\partial x} + \phi \right).
\]

Now, if we neglected effect of time, Eqs. (12,13) reduced to

\[
c_1 \left[ EJ \frac{\partial^3 \phi}{\partial x^3} - c_1 EK \left( \frac{\partial^3 \phi}{\partial x^3} + \frac{\partial^4 \phi}{\partial x^4} \right) \right] + G\bar{A} \left( \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial \phi}{\partial x} \right) + q = 0
\]

\[
E\bar{T} \frac{\partial^2 \phi}{\partial x^2} - c_1 E\bar{J} \left( \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^3 w_0}{\partial x^3} \right) + G\bar{A} \left( \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial \phi}{\partial x} \right) = 0,
\]

(14)

(15)

3. Solution the bending problem of Microtubules

This is because our goal is to study the oscillation frequency as the mechanical properties of the microtubules, we will look at a simple case: the free vibration isolated microtubules. Simply boundary conditions along the support microtubules L are:

\[
u_0 = 0 \quad \text{and} \quad M = 0 \quad \text{at} \quad x = 0, L.
\]

(16)

The following expansions of the generalized displacements \( w \) and \( \phi \) satisfy the boundary conditions in Eq. (16):

\[
w_0(x) = W_n \sin \left( \frac{n\pi x}{L} \right), \quad \phi(x) = \Phi_n \cos \left( \frac{n\pi x}{L} \right), \quad q(x) = q_0 \sin \left( \frac{n\pi x}{L} \right).
\]

(17)

Substitution of the expansions for \( w_0 \) and \( \phi \) from Eqs. (17) into Eqs. (14, 15) we obtain,
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\[ -G\bar{A}\left(\frac{n\pi}{L}\right) + c_1E\bar{J}\left(\frac{n\pi}{L}\right)^3 \right) \Phi_n - \left(\frac{n\pi}{L}\right)^2 + c_2KE\left(\frac{n\pi}{L}\right)^4 \right) W_n + q_0 = 0, \quad (18) \]

\[ -G\bar{A} - E(\bar{I} - c_i\bar{J})\left(\frac{n\pi}{L}\right)^2 \right) \Phi_n + \left(\frac{n\pi}{L}\right)^3 - G\bar{A}\left(\frac{n\pi}{L}\right) \right) W_n = 0, \quad (19) \]

\( \bar{I} = I - c_iJ, \quad \bar{J} = J - c_iK, \quad \bar{A} = A - c_i\bar{I} \quad \bar{A} = A - c_iJ. \)

\[ a_1 = -G\bar{A}\left(\frac{n\pi}{L}\right) + c_1E\bar{J}\left(\frac{n\pi}{L}\right)^3, \quad b_1 = G\bar{A}\left(\frac{n\pi}{L}\right)^2 + c_2KE\left(\frac{n\pi}{L}\right)^4, \]

\[ a_2 = -G\bar{A} - E(\bar{I} - c_i\bar{J})\left(\frac{n\pi}{L}\right)^2, \quad b_2 = \left(\frac{n\pi}{L}\right)^3 - G\bar{A}\left(\frac{n\pi}{L}\right). \]

The solution of above equations

\[ \Phi_n = \frac{q_0\left(GA + \left(\frac{n\pi}{L}\right)^2\right)}{\left(\frac{n\pi}{L}\right)E(c_1KE\bar{J} + \bar{J})c_1\left(\frac{n\pi}{L}\right)^4 + \left(2GA^2 + E\bar{K} - 1\right)GA\left(\frac{n\pi}{L}\right)^2}, \quad (20) \]

\[ W_n = -\frac{q_0\left(GA + E\bar{J}\right)}{\left(\frac{n\pi}{L}\right)^2E(c_1KE\bar{J} + \bar{J})c_1\left(\frac{n\pi}{L}\right)^4 + \left(2GA^2 + E\bar{K} - 1\right)GA\left(\frac{n\pi}{L}\right)^2}. \quad (21) \]

When \( c_1 = 0 \) in Eq. (1), it corresponds to the displacement field of the Timoshenko beam theory. Thus, the equations of motion of the Timoshenko beam theory can be obtained directly from Eqs. (12, 13) by setting \( c_1 = c_2 = 0 \).

### 4 Numerical results and discussion

It used most methods experimental determination of bending microtubules model of classical beam, static torsion, Dogterom and Yuri [7], Kikumoto et al. [8], Jansson and Dogterom [10]. In the future, we will study the free vibration isolated microtubules using higher order shear deformation theory. PSDT and effectiveness can be studied with more accurate comparison with the 2D model.
Considering the support simply microtubules circle half the average diameter \( r = 12.8 \text{nm} \), Young's modulus \( E = 1 \text{GPa} \), Poisson's ratio \( v = 0.3 \), density and mass per unit volume \( \rho = 1.47 \text{g/cm}^3 \) and the proportion of the shear modulus \( \beta = G/E \) of between 0.000001 and 0.001. According to the literature, and it will be considered circular cross section of MTs and is equivalent to a circular annular shape, with a thickness \( h = 2.7 \text{nm} \) equivalent. First, we identify the critical length of the isolated MTs, and then the relative error in the yard of thickness in the model of Euler-Bernoulli beam model (PSDT) is less than 10\%. This is shown in Fig.1-4 critical length, depending on the value \( \beta \). Assuming that the multilateral trading system and the length of the cells tend to be shorter \( 40 \mu m \), it can be assumed that the critical length of the above \( 40 \mu m \) does not constitute a material interest. As it is shown in the Fig.1-4 that if the critical length is about \( 11 \mu m \), if \( \beta = 0.0001 \) or \( 36 \mu m \) if \( \beta = 0.00001 \).

Fig. 1. Dispersion curves for displacement \( W \), versus \( x \) at \( \beta = 0.001 \) in first-order beam, theory and the computations are carried out for field \( E = 10,20,30 \). Fig. 2. Dispersion curves for normal stress \( \sigma_{xx} \), versus \( x \) at \( \beta = 0.001 \) in first-order beam, theory and the computations are carried out for field \( E = 10,20,30 \). Fig. 3. Dispersion curves for displacement \( W \), versus \( x \) at \( \beta = 0.001 \) in third-order beam, theory, the computations are carried out for field \( E = 10,20,30 \). Fig. 4. Dispersion curves for normal stress \( \sigma_{xx} \), versus \( x \) at \( \beta = 0.001 \) in third-order beam, theory, the computations are carried out for field \( E = 10,20,30 \).

5 Conclusion

The consistent theoretical formulation of the theory with general solution technique of governing differential equations of microtubules is studied. The general solutions for beam with varying load are obtained in case of thick simply supported microtubules. The displacements and stresses obtained by present theory are in excellent agreement with those of other equivalent refined and higher order theories. The present theory yields the realistic of axial displacement and stresses through the thickness of microtubules. Thus, the validity of the present theory is established. Hence, the parabolic shear deformable beam model can be used as a simple and relevant model for 1D beam-like mechanics of microtubules. This conclusion could have some interesting consequences to mechanical behavior of cells.

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References


Fig. 1. Dispersion curves for displacement $W$, versus $x$ at $\beta = 0.001$ in first-order beam, theory

Fig. 2. Dispersion curves for normal stress versus $x$ at $\beta = 0.001$ in first-order beam, theory

Fig. 3. Dispersion curves for displacement $W$, versus $x$ at $\beta = 0.001$ in higher-order beam, theory

Fig. 4. Dispersion curves for normal stress versus $x$ at $\beta = 0.0001$ in higher-order beam, theory