# Analyzing Thermal Influences on Protein Microtubules in Eukaryotic Cells through Nonlocal Elasticity Modeling

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**Abstract:**

In this research, the dynamic behavior, along with the thermal impacts using isolated protein microtubules, is investigated. Microtubules are one of the bio-beam structures, which is a significant part of the cytoskeleton in eukaryotic posses and cells. A significant role in the dynamic characteristics is to model the microtubules consistent with a beam element. The equation of motion is constructed along with the parametric investigations to scrutinize the impacts of shear deformation, thermal effect, and coefficient of length scale. The obtained form of the results is compared with the classical systems along with the literature results designating the system provided in this study as more precise than other systems in better agreement using the experimental data.

**Keywords:** Biomechanics; Protein Microtubules; Heat Stress Mitigation; Comparative Modeling; Nonlocal Elasticity, Cytoskeleton .

## 1. Introduction

The study of protein microtubules and their dynamic responses to thermal effects holds considerable potential for advancements in cattle health, particularly in relation to cellular stability and essential biological functions critical for animal health and reproduction. The findings from this research suggest several key applications:

Enhancement of Disease Resistance: Gaining insights into the thermal sensitivity of microtubules at the cellular level may facilitate the development of vaccines or therapeutic strategies aimed at enhancing cellular stability during disease states, particularly for conditions that disrupt cell division or intracellular transport—processes vital to immune response in cattle.

Improvement in Fertility: Microtubules play a pivotal role in mitosis, a process central to reproductive biology. Understanding their response to thermal stress could inform approaches to support embryo development and reproductive health in cattle, potentially benefiting in vitro fertilization practices and other breeding technologies aimed at improving reproductive outcomes.

Heat Stress Mitigation: Given that heat stress negatively impacts cattle productivity, knowledge of how cellular structures, such as microtubules, respond to temperature variations could aid in developing management strategies to preserve cellular health, thereby sustaining productivity even under high-temperature conditions.

Advances in Antimicrobial Development: Understanding the thermal sensitivity of microtubules could also support the development of antimicrobials that selectively target cellular mechanisms in pathogens without harming the host cells, thereby enhancing animal health and reducing the spread of disease in livestock populations.

These applications illustrate how cellular-level research into microtubule dynamics and thermal responses can translate into practical solutions for cattle health, reproductive efficiency, and resilience. This contributes to broader advancements in veterinary science and livestock management. Microtubules (MTs), integral components of the cytoskeleton in eukaryotic cells, play pivotal roles in a myriad of biological processes. These tubular structures are crucial in facilitating cell division and motility, as well as the movement of motor proteins. They also contribute significantly to intracellular transport mechanisms and are instrumental in the formation of cilia and flagella, which are essential for cellular mobility and function. The multifaceted functions of microtubules underscore their importance in the intricate network of cellular activities. [1-5]. Comprising α-tubulin and β-tubulin, as illustrated in Figure 1, microtubules distinguish themselves with remarkable flexibility and stiffness, surpassing other filamentous structures by an order of magnitude. Their composite and anisotropic structural nature endows them with unique mechanical properties. Characteristically, microtubules adopt a hollow cylindrical architecture, predominantly composed of 13 parallel protofilaments in vivo, although this count can fluctuate between 9 and 16 in vitro settings, as documented in studies [6-10]. Typically, microtubules exhibit external and internal diameters of approximately 25 nm and 15 nm, respectively, and vary in length from 10 nm to 100 µm, as established in recent research [11].

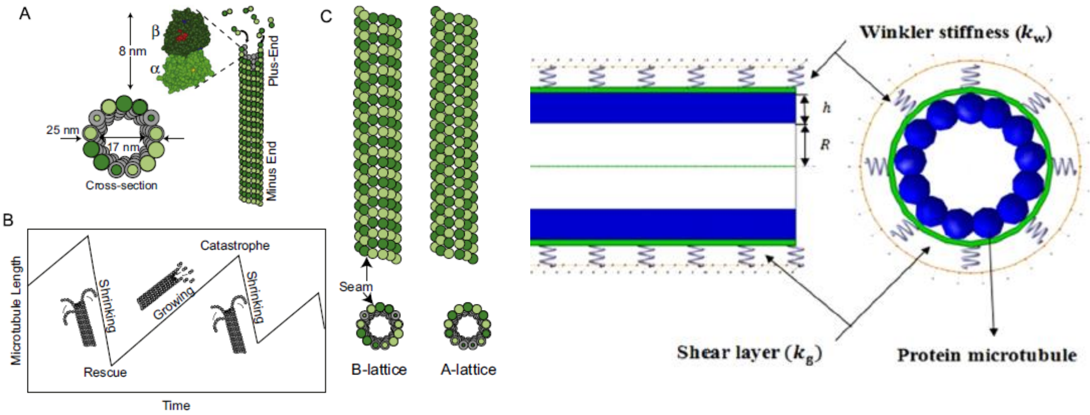


Fig. 1. Geometry of a microtubule with the cytoplasm environment affects Pasternak

Figure 1 offers an incisive portrayal of microtubule dynamics and structural configuration, elucidating their pivotal role in cellular architecture and function.

Panel A delineates the polymer filament formation of microtubules, constituted by tubulin heterodimers comprising alpha (light green) and beta (dark green) subunits. These subunits coalesce, facilitating the polymer growth, with each subsequent dimer attachment contributing to the elongation of microtubules. The plus-end is characterized by its dynamic nature, capable of rapid elongation or contraction, while the minus-end remains relatively static. The depicted microtubules have defined outer and inner diameters, approximately 25 nm and 17 nm, respectively. Panel B describes the dynamic instability of microtubules, a process modulated by the addition and subtraction of dimers, which are subject to stochastic transitions known as catastrophes and rescues—transitions from elongation to contraction and vice versa. Enhancing microtubule stability involves curtailing catastrophes and bolstering rescue frequency. Panel C contrasts the seamless continuity of the A-lattice, where alpha subunits consistently interface with beta subunits, against the B-lattice, which features a seam resulting from the staggered alignment of these subunits. This structural dichotomy is integral to the versatility of microtubule function within the cell [12]. This figure encapsulates the intricate interplay between MT stability and flexibility, a testament to the robust yet adaptive nature of cellular structures.

The insights garnered here have profound implications for the understanding of cytoskeletal dynamics in eukaryotic cells [12]. The mechanical behavior of microtubules in response to environmental conditions, particularly within viscoelastic or elastic media and varying temperature regimes, presents a complex landscape for scientific inquiry. Numerous studies have examined the temperature-dependent rigidity of microtubules, revealing a decrease in flexural rigidity of taxol-free microtubules with an increase in temperature [13]. Specifically, a reduction in flexural rigidity at one end of the microtubules was observed when the temperature was raised from 20 °C to 35 °C. Data pertaining to the flexural rigidity of microtubules, with lengths spanning 8-12 mm, were collected within this temperature range, indicating that temperature fluctuations significantly influence mechanical attributes such as natural vibrational frequencies and critical buckling force of microtubules. Despite these findings, simulation-based studies examining the temperature-dependent mechanical behavior of Microtubules remain scarce. The few experiments that have been conducted with these parameters offer limited insight due to the narrow scope of tested values. Consequently, there is a clear imperative to delve into the buckling and vibrational characteristics of Microtubules through computational mechanical models that incorporate temperature variables, providing a more comprehensive understanding of their mechanical performance under varying thermal conditions [14]. Contemporary simulations of microtubules have increasingly incorporated environmental temperature effects to scrutinize their mechanical performance. Through the integration of a constitutive relationship derived from atomistic continuum principles, a sophisticated computational mesh-free framework has been constructed to encapsulate the influence of temperature fluctuations. This innovative approach in the realm of mesh-free mechanical simulation not only accommodates temperature effects on the rigidity of Microtubules but also aligns with empirical data from experimental endeavors [15-16]. Leveraging this temperature-inclusive mechanical simulation, the performance of Microtubules, specifically their vibrational frequencies and critical buckling forces, is thoroughly analyzed to refine the atomistic-continuum mesh-free model. While a spectrum of studies [17-19] has illuminated various aspects of MT vibrational behavior, the specific responses to temperature variations remain less explored. This gap highlights the novelty and necessity of research focused on the temperature-dependent behavior of Microtubules, aiming to provide a more granular understanding of their mechanical properties under diverse thermal conditions.

In the present article, we delve into the intricate vibrational behaviors of microtubules, fundamental constituents of the cytoskeleton within living cells. The study puts forth a novel representation of Microtubules as beam-like structures through the Application of nonlocal Timoshenko beam theory. This advanced theoretical framework allows for an in-depth analysis of the propagation of transverse waves in Microtubules, considering the dual influences of temperature variations and the small-scale parameters inherent to the nonlocal Timoshenko beam model. The model proposed herein stands as a significant contribution to the field, poised to captivate the attention of a vast array of biophysicists focused on the mechanics of filamentous structures. It promises to extend beyond the traditional engineering community, inviting interdisciplinary exploration and potentially catalyzing new lines of inquiry in the study of cellular mechanics. The analysis of elastic microtubule (MT) systems through the lens of nonlocal continuum mechanics is a pivotal step in understanding the complex interplay between cellular structures and their mechanical environment. Within this framework, nonlocal elasticity theory is employed, which posits that the stress at a reference point x is a function not merely of the strain at x, but also of the strain at every other point in the body. This theoretical approach is deeply rooted in the atomic theory and experimental observations of lattice dynamics, particularly the dispersion of phonons.

## 2. Analysis of elastic microtubules systems in nonlocal continuum mechanics

In this paradigm, when the effects of strain are considered only at point x, neglecting its influence at other points, the classical local elasticity theory is recovered. However, by accounting for the influence of nonlocal strain, a more comprehensive understanding of material behavior can be achieved. Employing the Timoshenko beam theory, a sophisticated model for analyzing transverse waves within an elastic beam that also considers thermal effects is developed. The expressions derived from this model, referenced in literature [20-25], serve to deepen our understanding of the mechanical behaviors of Microtubules under various thermal and stress conditions. Fig.1. Schematic configuration of a microbeam subjected to an axial force and concentrated load $\ell$ is called material length scale parameter. Consider a microbeam with length $L$ and thickness $h$ subjected to an axial force $N_x$ and concentrated load $q_0$ shown in Fig.1. Based on Reddy beam theory, the displacement field is assumed as:

$$u_1 = u(x,t) + z\phi(x,t) - c_1 z^3\left(\phi + \frac{\partial w}{\partial x}\right), \qquad u_2 = 0, \qquad u_3 = w(x,t) \tag{1}$$

The non-zero strains of the refined beam theory are.

$$\begin{aligned}
\varepsilon_{xx} &= \frac{\partial u_1}{\partial x} = \frac{\partial u}{\partial x} + z\frac{\partial \phi}{\partial x} - c_1 z^3\left(\frac{\partial \phi}{\partial x} + \frac{\partial^2 w}{\partial x^2}\right)\\
2\varepsilon_{xz} &= (1 - c_2 z^2)\left(\phi + \frac{\partial w}{\partial x}\right)\\
\chi_{xy} &= \frac{1}{4}\left[\frac{\partial \phi}{\partial x} - c_2 z^2\left(\frac{\partial \phi}{\partial x} + \frac{\partial^2 w}{\partial x^2}\right) - \frac{\partial^2 w}{\partial x^2}\right]\\
\chi_{yz} &= -\frac{c_2}{2} z\left(\phi + \frac{\partial w}{\partial x}\right)
\end{aligned} \tag{2}$$

where $c_2 = 4/h^2$. The displacement field of the refined beam theory accommodates a quadratic variation of the transverse shear strain that vanishes on the top and bottom faces, $z = \pm h/2$, of a beam. Thus, there is no need to use shear correction factors in the Reddy beam theory. Where: $c_1 = \frac{4}{3h^2}$, $c_2 = \frac{4}{h^2}$,

To develop governing equations of motion and boundary conditions of the micro-Reddy beam, one should start from Hamilton's principle, which can be expressed by:

$$\int_0^T \delta K - \delta U + \delta W = 0 \tag{3}$$

According to the modified couple stress theory [26], the strain energy U of an isotropic linear elastic material can be considered as:

$$\delta U = \int_0^L \int_A \left(\sigma_{ij}\delta\varepsilon_{ij} + m_{ij}\delta\chi_{ij}\right) dA\,dx \tag{4}$$

$$\begin{aligned}
&\varepsilon_{ij} = \frac{1}{2}(\nabla u + (\nabla u)^T) = \frac{1}{2}(u_{i,j} + u_{j,i}) \\
&\sigma_{ij} = \lambda \operatorname{tr}(\varepsilon_{ij})\delta_{ij} + 2\mu\varepsilon_{ij} \\
&m_{ij} = 2\ell^2\mu\chi_{ij} \\
&\chi_{ij} = \frac{1}{2}(\nabla\theta + (\nabla\theta)^T) = \frac{1}{2}(\theta_{ij} + \theta_{ji}) \\
&\theta = \frac{1}{2}\operatorname{curl}(u)
\end{aligned} \tag{5}$$

where $\sigma_{ij}$ are the components of the Cauchy stress tensor, $m_{ij}$ are the components of the deviatoric part of the couple stress tensor, $\delta_{ij}$ is the Kronecker delta, $\lambda$ and $\mu$ are the Lamé constants in classical elasticity, $\ell$ is a material length scale parameter measuring the effect of couple stress and $\varepsilon_{ij}$ and $\chi_{ij}$ are, respectively, the components of the infinitesimal strain tensor and the symmetric curvature tensor, with $u_i$ being the displacement components and $\theta_i$ being the components of the rotation vector defined as

$$\theta_i = \frac{1}{2}\varepsilon_{ijk}u_{k,j}.$$

Also, the strain energy $U$ in a deformed isotropic linear elastic material. Clearly, Eqs. (5) reduce to those in classical elasticity when $\ell = 0$ (i.e., when the microstructure effect is neglected). For materials with non-negligible microstructure effects, the length scale parameter $\ell$ can be determined from torsion tests of slim cylinders of different diameters or bending tests of thin beams of different thicknesses. The variation of kinetic energy $\mathrm{K}$ is given by:

$$\delta K = \int_0^L \int_A \left(\frac{\partial u_1}{\partial t}\frac{\partial \delta u_1}{\partial t} + \frac{\partial u_3}{\partial t}\frac{\partial \delta u_3}{\partial t}\right) dA dx \tag{6}$$

Using displacement field again in Eq. 6 and integration by part the variation of kinetic energy $\delta\mathrm{K}$ is obtained as:

$$\begin{aligned}
\delta K \quad &= \int_0^L - \left(m_0\frac{\partial^2 u}{\partial t^2}\right)\delta u + \left(-m_0\frac{\partial^2 w}{\partial t^2} + c_1\widehat{m}_4\frac{\partial^3 \phi}{\partial t^2\,\partial x} + c_1{}^2 m_6\frac{\partial^4 w}{\partial t^2\,\partial x^2}\right)\delta w \\
&+ \left((-\widehat{m}_2 + c_1\widehat{m}_4)\frac{\partial^2 \phi}{\partial t^2} + c_1\widehat{m}_4\frac{\partial^3 w}{\partial t^2\,\partial x}\right)\delta\phi dx
\end{aligned} \tag{7}$$

Where the constants are defined as follows:

$$(m_0, m_2, m_4, m_6) = \int \rho(1, z^2, z^2, z^4) dA$$
$$\hat{m}_2 = m_2 - c_1 m_4 \text{ and } \hat{m}_4 = m_4 - c_1 m_6$$

The first variation of work done by the external force is denoted by $\delta W$ as follows:

$$\delta W = \int_0^L \left[ -(\bar{N}_x + N_T) \frac{\partial^2 w}{\partial x^2} + q \right] \delta w dx \qquad (8)$$

Where $q$ is applied shear forces. $\bar{N}_x$ and $\bar{N}_T$ Buckling load and axial force are applied due to the influence of temperature change. $\bar{N}_x$ is the applied buckling load, and w is the deflection of the beam. $N_T$ is defined as [27]:

$$N_T = A_{11} \alpha \Delta T \qquad \text{where} \qquad A_{11} = \int_{-h/2}^{h/2} (2\mu + \lambda) dz$$

The equation of motion in terms of displacement is as follows:

$$e_1 \frac{\partial^2 \phi}{\partial t^2} + e_2 \frac{\partial^3 w}{\partial t^2 \partial x} + e_3 \left( \phi + \frac{\partial w}{\partial x} \right) + e_4 \frac{\partial^2 \phi}{\partial x^2} + e_5 \frac{\partial^3 w}{\partial x^3} = 0$$
$$d_1 \frac{\partial^2 w}{\partial t^2} + d_2 \frac{\partial^3 \phi}{\partial t^2 \partial x} + d_3 \frac{\partial^4 w}{\partial t^2 \partial x^2} + d_4 \left( \frac{\partial \phi}{\partial x} + \frac{\partial^2 w}{\partial x^2} \right) + d_5 \frac{\partial^3 \phi}{\partial x^3} + d_6 \frac{\partial^4 w}{\partial x^4} - (\bar{N}_x + N_T) \frac{\partial^2 w}{\partial x} = 0 \quad (9)$$

The boundary conditions are also obtained:

$$d_2 \frac{\partial^2 \phi}{\partial t^2} + d_3 \frac{\partial^3 w}{\partial t^2 \partial x} + d_5 \frac{\partial^2 \phi}{\partial x^2} + d_6 \frac{\partial^3 w}{\partial x^3} + d_4 \left( \phi + \frac{\partial w}{\partial x} \right) + (\bar{N}_x + N_T) \frac{\partial w}{\partial x} = q$$
$$\text{or w at } x = 0 \text{ and } x = L$$
$$e_4 \frac{\partial \phi}{\partial x} + e_5 \frac{\partial^2 w}{\partial x^2} = M \text{ or } \phi = \bar{\phi} \qquad \text{at } x = 0 \text{ and } x = L \qquad (10)$$
$$d_5 \frac{\partial \phi}{\partial x} + d_6 \frac{\partial^2 w}{\partial x^2} = M_c \quad \text{or} \quad \frac{dw}{dx} = \frac{d\bar{w}}{dx} \qquad \text{at } x = 0 \text{ and } x = L$$

Where

$$e_1 = -\widehat{m}_2 + c_1\widehat{m}_4\,, \quad e_2 = c_1\widehat{m}_4 = -d_2\,, \quad e_3 = \mu\left(-\tilde{A} - \ell^2 c_2^2 I\right) = -d_4$$
$$e_4 = \left[(2\mu+\lambda)\left(\hat{I} - c_1\hat{j}\right) + \frac{1}{4}\mu\ell^2\tilde{A}\right], \quad e_5 = \left[(2\mu+\lambda)(-c_1\hat{j}) + \frac{1}{4}\mu\ell^2\left(-A + c_2{}^2 j\right)\right]$$
$$d_3 = c_1{}^2 m_6, \quad d_1 = -m_0\,, \quad d_5 = \left[(2\mu+\lambda)(c_1\hat{j}) + \frac{1}{4}\mu\ell^2(\bar{A} + c_2\bar{I})\right]$$
$$d_6 = -\left[(2\mu+\lambda)(c_1{}^2 K) + \frac{1}{4}\mu\ell^2\left(A + 2c_2 I + c_2{}^2 j\right)\right]$$
$$\bar{A} = A - c_2 I, \quad \tilde{A} = \bar{A} - c_2\bar{I}, \quad \hat{j} = j - c_1 K, \quad \bar{I} = I - c_2 j, \quad \hat{I} = I - c_1 j$$

## 3. Analytical solution

To illustrate the new model, buckling, and free vibration problems of a simply supported beam with the following property: $\rho = 1470\,\frac{\mathrm{kg}}{\mathrm{m}^3}$, $v = 0.3$, $E = 2\mathrm{GPa}$, $\alpha = 54 \times \frac{10^{-6}}{^\circ\mathrm{C}}$, $\ell = 17.6 \times 10^{-6}\mu\mathrm{m}$, are solved by the following expansions of the generalized displacements $w$ and $\phi$ that satisfy the boundary conditions in Eqs. (10)

$$w(x,t) = \sum_{n=1}^{\infty} W_n \sin\left(\frac{n\pi x}{L}\right) e^{i\omega_n t} \text{ and } \phi(x,t) = \sum_{n=1}^{\infty} \phi_n \cos\left(\frac{n\pi x}{L}\right) e^{i\omega_n t}$$
(11)

For buckling, we consider q and all-time derivatives to zero, and for free vibration, we also consider $\bar{N}_x$ and q to zero.

## 4. Results and Discussions

This study employed numerical simulations to analyze the critical buckling force and vibration frequencies of microtubules, with a particular focus on the impact of temperature variations. Initially, simulations were conducted to determine the critical buckling force of microtubules, aiming to align with the experimental values noted in the research by Kikumoto et al. [28, 29-30], which examined microtubules ranging from 6 µm to 20 µm in length. The congruence between the experimental findings and our simulation data serves as a testament to the effectiveness and precision of our developed model, as illustrated in Fig. 2. This figure clearly demonstrates that the critical compressive force values from our simulations closely track the experimental data.

Moreover, the study involved simulations to benchmark against traditional finite element analysis, exploring the free vibration behavior of microtubules. We extended our simulations to assess the critical buckling force of microtubules at temperatures between 10 °C and 45 °C, incorporating various boundary condition scenarios. The findings, depicted in Fig. 2, reveal a consistent decrease in the predicted buckling force with an increase in environmental temperature, a trend that held across different boundary conditions. These results underscore that temperature adversely affects both the critical buckling force and the structural rigidity of microtubules. Our simulations clearly demonstrate that higher temperatures compromise the strength of microtubules, affirming the temperature's significant influence on their mechanical integrity.

In this investigation, we delved into the influence of temperature on the vibration frequencies of microtubules. The study features detailed graphs representing the vibration frequencies across a broad spectrum of temperatures. Specifically, Fig. 3 showcases the natural vibration frequency in relation to the vibration mode number under environmental temperatures ranging from 10 °C to 45 °C. The analysis encompassed the first 14 vibration modes, considering various boundary conditions to gauge the temperature's effect on microtubule vibrational behavior. A notable observation from the study is the inverse relationship between vibration frequency and temperature; as the latter rises, the former declines. An in-depth examination of the first vibration frequencies for microtubules with lengths between 5 mm and 45 mm was conducted, with the findings illustrated in Fig. 4. Irrespective of the boundary conditions applied, the research consistently observed a detrimental effect of temperature on the natural vibration frequencies of microtubules. Additionally, the study considered vibration frequency versus microtubule length under different typical boundary scenarios. The conclusions drawn suggest that microtubules experience a reduction in rigidity when exposed to higher temperatures, explaining the observed decrease in vibration frequency with an increase in environmental temperature. The study conclusively demonstrates that elevated temperatures lead to a marked reduction in microtubule stiffness, subsequently causing a significant decrease in vibration frequencies.

In summary, This work encompasses a series of results that elucidate the impact of temperature on the mechanical properties of microtubules. Juxtaposes the critical buckling force with the length of microtubules, where the congruence between simulated and experimental data underscores the model's accuracy. Examines the natural vibration frequencies across different vibrational modes, showcasing a decrease in frequency with rising temperatures. Delineates the critical compressive force as a function of microtubule length under varying temperatures, indicating a temperature-induced reduction in structural integrity. Collectively, these figures provide a quantitative visualization of the temperature's detrimental effects on microtubule rigidity and vibration characteristics, which are essential for cellular mechanics. Our investigation reveals several key findings. Notably, temperature impacts, the reduction in rotary inertia in vibrational frequencies, transverse shear deformation, and the influence of small length-to-diameter ratios all contribute to the observed effects. Moreover, it is evident that employing the Readdy beam nonlocal theory, especially in scenarios with small length-to-diameter ratios and high vibration factors, yields better predictive frequencies compared to the Timoshenko beam nonlocal theory and Euler-Bernoulli beam system, which neglects the effects of rotary inertia and shear transverse deformation. This parametric investigation underscores the significance of considering these factors, especially for stubby, short beams, and higher vibration systems. The applications of this research in the vibrational analysis of protein microtubules using nonlocal elasticity theory are pivotal in biotechnology and nanotechnology [31-35]. The insights provided are instrumental in advancing nano-electromechanical systems (NEMS) and micro-electromechanical systems (MEMS) [36-41]. This is particularly relevant in developing more effective drug delivery mechanisms and precision biomedical devices, as well as in deepening our understanding of cellular mechanics. Additionally, the study significantly contributes to materials science, especially in enhancing the mechanical properties of nanoscale materials and structures [42-46]. These advancements are crucial for cutting-edge applications across various sectors, including electronics, robotics, and aerospace.

## 5. Conclusion

In this investigation, we explored the influence of temperature on the buckling and vibrational properties of microtubules. Our findings are consistent with previously reported experimental data, enhancing our understanding of microtubules' mechanical behavior in response to temperature variations. We observed that an increase in temperature adversely affects the rigidity of microtubule structures, leading to a reduction in the forces required for buckling. This trend was noted regardless of the boundary conditions applied to the microtubules. Furthermore, a detailed analysis of natural vibration frequencies helped to clarify the extent of temperature's impact. Higher environmental temperatures were associated with lower vibration frequencies, indicating a temperature-dependent change in mechanical behavior. The research establishes that temperature exerts a considerable effect on the mechanics of microtubules, with both the critical buckling force and natural vibration frequencies diminishing as temperatures rise. The outcomes of this study, which span a broad spectrum of microtubule lengths and temperature conditions, offer significant insights and contribute valuable references for the mechanical analysis of microtubules relevant to cellular functions.

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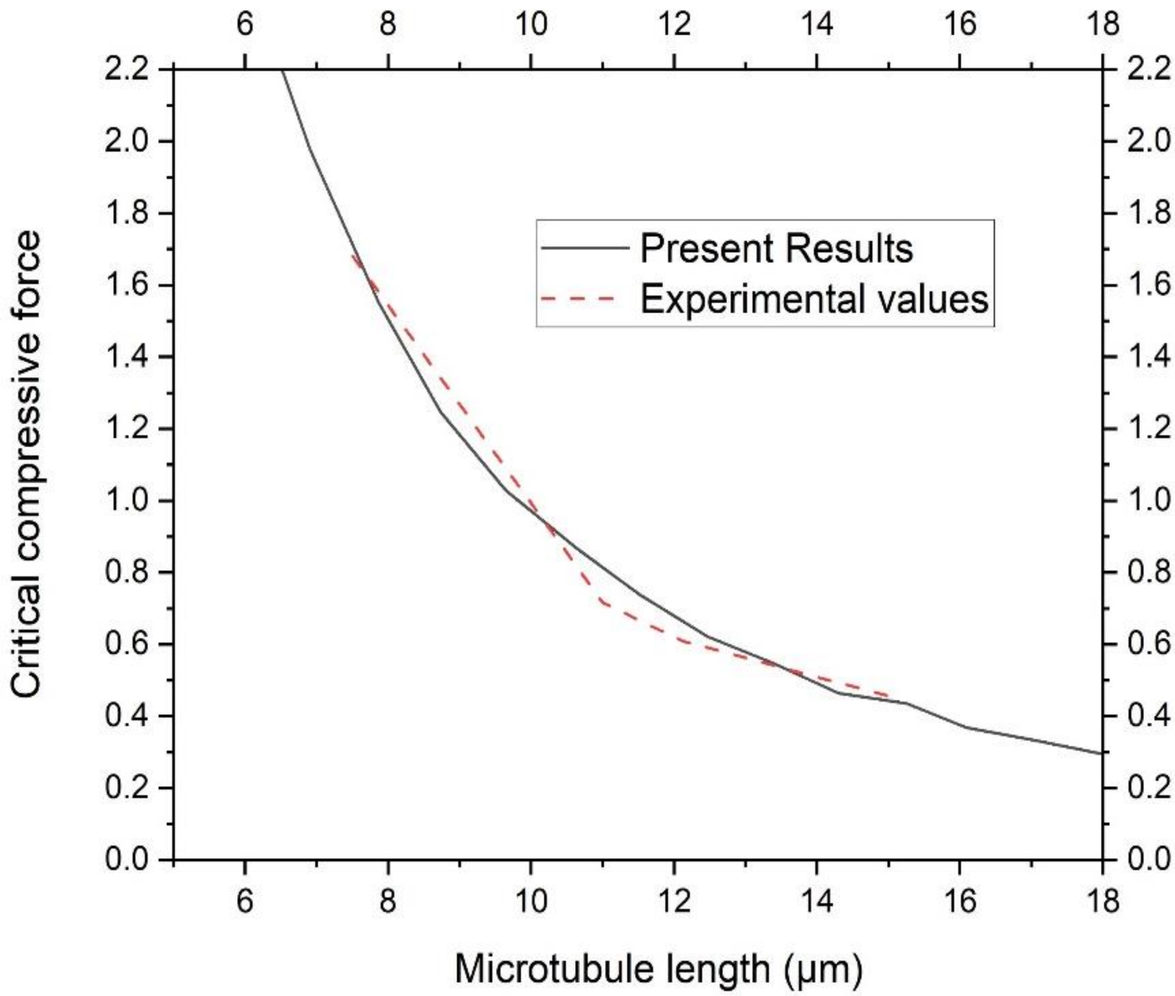


Figure 2 illustrates the relationship between critical buckling force and microtubule length. The continuous line represents the results obtained from our current study, while the dotted line reflects the outcomes derived from empirical testing [35,36].

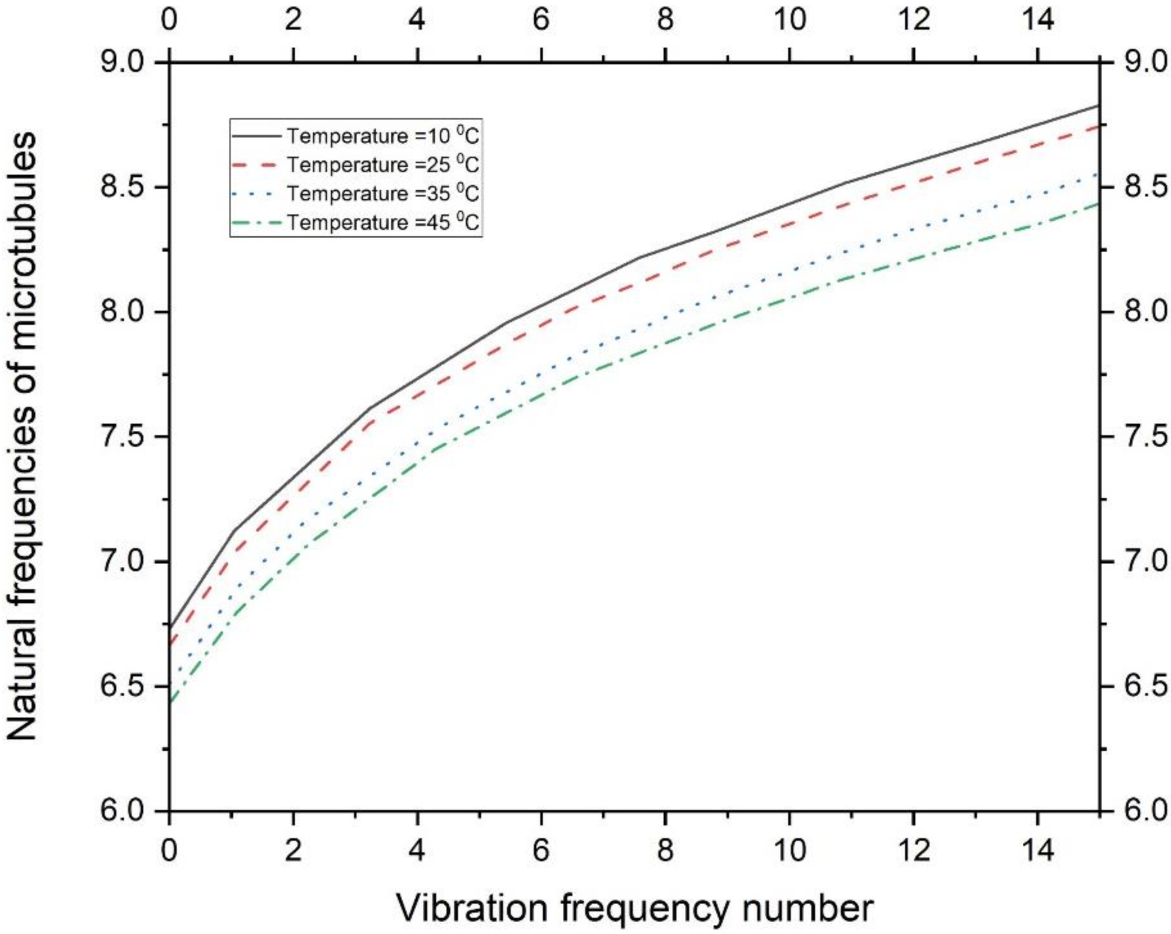


Figure 3 presents the relationship between natural vibration frequencies and vibration mode numbers, with a corresponding environmental temperature range from 10 °C to 45 °C, focusing on the first 14 vibration modes.

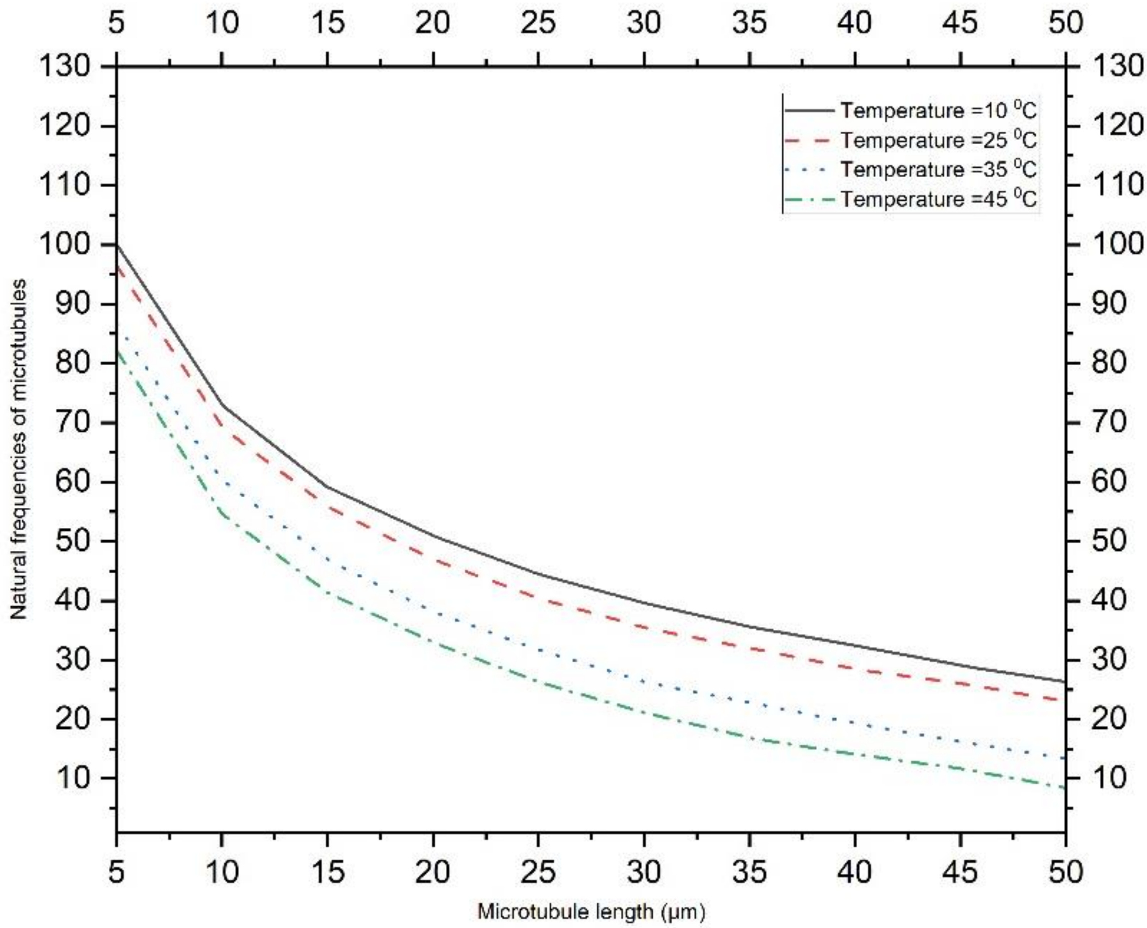


Figure 4 displays the correlation between critical compressive force and microtubule length as the environmental temperature ranges from 10 °C to 45 °C. It depicts microtubules with lengths extending from 5 mm to 45 mm.

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