Thermal Vibration of Zinc Oxide Nanowires by using Nonlocal Finite Element Method

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Abstract

Zinc oxide nanowires (ZnO NWs) can be used in some NEMS applications due to their remarkable chemical, physical, mechanical and thermal resistance properties. In terms of the suitability of such NEMS organizations, a correct mechanical model and design of ZnO NWs should also be established under different effects. In this study, thermal vibration analyses of elastic beam models of ZnO NWs are examined based on Eringen's nonlocal elasticity theory. The resulting equation of motion is solved with a finite element formulation developed for the atomic size-effect and thermal environment. The vibration frequencies of ZnO NWs with different boundary conditions are calculated under nonlocal parameter and temperature change values and numerical results were discussed.

Keywords: Finite element method, nonlocal elasticity, thermal environment, vibration, Zinc Oxide nanowire.

1. Introduction

It is seen that people use products with stronger physical, chemical, thermal, mechanical, optical, etc. properties. This is possible with the science of nanotechnology that is today’s pioneer technology. Nanotechnology is a science that aims to investigate the properties of materials with dimensions from 1 nm to 100 nm and to integrate these materials into classical applications of science and engineering disciplines. It can be stated that nanotechnology, which started its adventure with gave a conference by R. Feynman [1] in 1959, gained a serious importance with the discovery of the carbon nanotube material [2,3]. Additionally, properties of wide range of nanomaterials such as boron nitride nanotube [4], graphene [5] and metallic or molecular nanowires [6-8] are fundamental topics of this discipline. It can be expressed that such nanomaterials show their effect in different applications such as sensor, switch, actuator, bridge, transistor.

The structural-electronic applications containing nanomaterials are generally collected under the name of nanoelectromechanical systems (NEMS). To perform the accurate mechanical analyses of NEMS is essential for NEMS applications to work properly in terms of engineering. To perform mechanical analysis via experimental methods requires high operation costs, professional expert approaches and long processes. Also, it is a well-known fact that the results
obtained by experimental methods do not present results in accordance with the classical elasticity theory. These difficulties have been overcome by adapting the mathematical approaches developed in different periods to the classical elasticity theory. The new elasticity theories, namely, higher-order continuum theories, generally include parameters related to the atomic dimensions of nanomaterials. It can be said that nonlocal elasticity theory [9-10], couple stress elasticity theory [11,12], strain gradient elasticity theory [13,14], surface energy elasticity theory [15,16] and doublet mechanics elasticity theory [17] exemplify for higher-order continuum theories.

The nonlocal elasticity theory states that the stress and strain of other regions adjacent to that region must also be taken into consideration in order to calculate the stress and strain in a certain region of the atomic structure. Thus, the uncertainty in the strain energy that goes to infinity due to atomic factors is resolved. In the 1960s, the studies of Eringen et al. enabled the establishment of the nonlocal elasticity theory and the determination of its main principles. It can be stated that approximately 45 years later, analyses of continuous mechanical models of nanoscaled structures started to be handled with the nonlocal elasticity theory [18-20]. Following these, vibration, buckling and bending analyses of nonlocal Euler–Bernoulli nano beams are given [21-23]. Lu et al. studied the nonlocal vibration phase velocities of single and multi-walled carbon nanotubes by using Euler-Bernoulli and Timoshenko beam theories [24]. Numanoğlu examined axial and flexural vibration analyses of different nanowires and nanotubes [25]. Axial and torsional vibration analyses of nonlocal nanorods are also available in the literature [26-32]. Jalaei and Civalek studied the nonlocal elasticity dynamic instability of functionally graded porous beam under magnetic effects resting on viscoelastic foundation by employing Navier’s technique and Bolotins’s approach [33]. Apart from these, vibration and bending of some nanomaterials are tackled based on the classical theory [34-36]. Civalek presented the finite element formulations of plates and shells [37]. On the other hand, it can be stated that studies on the use of finite element formulation in mechanical analysis of nanostructures with nonlocal elasticity have taken place in the literature [27,28,38-52]. Additionally, the free vibration behavior of a functionally graded beam is researched for Euler-Bernoulli, Timoshenko, Shear and Rayleigh beam theories [53]. Moreover, mechanical analyses of different continuous structures have been performed via novel numerical approaches such as discrete singular convolution and differential quadrature [54-60].

In this article, vibration analyses of nanobeams modeled by using zinc oxide nanowires (ZnO NWs), which has an important area in the applications of nanotechnology science, are carried out with the nonlocal elasticity theory. The temperature effect is considered in the vibration analysis. A nonlocal finite element formulation (NL-FEM) is presented for the solution of equation of motion. Then, the vibration frequencies of simply supported ZnO NWs are calculated via analytical method and NL-FEM and compared. Also, thermal vibration frequency results are presented by using NL-FEM for beam models with boundary condition that is not possible to be solve analytically. In the solution of nonlocal free vibration, the accuracy of the proposed formulation is discussed. Finally, the most general results are summarized.

2. Nonlocal Finite Element Analysis for Thermal Vibration of Nanobeams

The equation of motion of nonlocal thermal vibration of nano scaled beams according to Euler-Bernoulli beam theory can be presented as follows:
\[
\begin{align*}
&
\left[ EI - (e_o a)^2 \right] \frac{\partial^4 w}{\partial x^4} + EA \alpha \Delta T \left( \frac{\partial^2 w}{\partial x^2} \right)^2 - f + \rho A \frac{\partial^2 w}{\partial t^2} - (e_o a)^2 \rho A \frac{\partial^4 w}{\partial x^2 \partial t^2} \\
&+ (e_o a)^2 \frac{\partial^2 f}{\partial x^2} = 0
\end{align*}
\]

(1)

where \( EI \) is bending rigidity, \( e_o a \) is nonlocal parameter and \( EA \) is axial rigidity. \( \alpha \) defines the thermal expansion coefficient. \( \Delta T \) is temperature change and \( w \) is transverse displacement. On the other hand, \( \rho A \) explains volume of unit length and \( f \) is transverse distributed force.

The solution of Eq. (1) will be performed in this current study by using finite element. The fundamental of this solution based on weighted residual method [49]. According to this, average weighted residue is written as

\[
I = \int_0^l \left( \left[ EI - (e_o a)^2 \right] \frac{\partial^4 w}{\partial x^4} + EA \alpha \Delta T \left( \frac{\partial^2 w}{\partial x^2} \right)^2 - f + \rho A \frac{\partial^2 w}{\partial t^2} - (e_o a)^2 \rho A \frac{\partial^4 w}{\partial x^2 \partial t^2} \\
+ (e_o a)^2 \frac{\partial^2 f}{\partial x^2} \right) dx = 0
\]

(2)

here, \( h \) is weighting function and \( l \) is length of finite element. The transverse motion of bending finite element is described as

\[
w = \phi w
\]

(3)

where \( \phi \) is shape function of beam finite element and \( w \) is displacement vector. Additionally, the first derivation of displacement of bending finite element can be written as

\[
\frac{\partial w}{\partial x} = D^k w = Bw
\]

(4)

where \( D^k \phi = B \) and \( D^k \) is defined as kinematic operator.

The partial integrations of all terms seen in Eq. (2) can be written as

\[
I_1 = \int_0^l EI h \frac{\partial^4 w}{\partial x^4} dx = EI h \frac{\partial^4 w}{\partial x^4} \bigg|_0^l - EI \frac{\partial h \frac{\partial^3 w}{\partial x^3}}{\partial x^3} \bigg|_0^l + \int_0^l EI \frac{\partial^2 h}{\partial x^2} \frac{\partial^2 w}{\partial x^2} dx,
\]

\[
I_2 = \int_0^l (e_o a)^2 \frac{\partial^4 w}{\partial x^4} dx = (e_o a)^2 \frac{\partial^3 w}{\partial x^3} \bigg|_0^l - (e_o a)^2 \frac{\partial h}{\partial x} \frac{\partial^2 w}{\partial x^2} \bigg|_0^l + \int_0^l (e_o a)^2 \frac{\partial^2 h}{\partial x^2} \frac{\partial^2 w}{\partial x^2} dx,
\]

\[
I_3 = \int_0^l EA \alpha \Delta T \frac{\partial^2 w}{\partial x^2} dx = EA \alpha \Delta T \frac{\partial w}{\partial x} \bigg|_0^l - \int_0^l EA \alpha \Delta T \frac{\partial h}{\partial x} \frac{\partial w}{\partial x} dx,
\]

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If above equations are substituted into Eq. (2) and weighted residual is evanished, the weak formulation is attained as follows

$$
I_4 = \int_0^l hf \, dx,
I_5 = \int_0^l \rho Ah \frac{\partial^2 w}{\partial t^2} \, dx,
I_6 = \int_0^l (e_a)^2 \rho Ah \frac{\partial^4 w}{\partial x^4 \partial t^2} \, dx + \int_0^l (e_a)^2 \rho A h \frac{\partial^3 w}{\partial x \partial t^3} \, dx
$$

$$
I_7 = \int_0^l (e_a)^2 h \frac{\partial^2 f}{\partial x^2} \, dx = (e_a)^2 h \frac{\partial f}{\partial x} \Bigg|_b - \int_0^l (e_a)^2 \frac{\partial h}{\partial x} \frac{\partial f}{\partial x} \, dx,
$$

(5)

To rearrange Eq. (6), following expressions can be used:

$$
h = \phi^T, \quad \frac{\partial h}{\partial x} = (\phi^T)' = B^T, \quad \frac{\partial^2 w}{\partial x^2} = B'w, \quad \frac{\partial^2 w}{\partial t^2} = \phi \ddot{w}
$$

(7)

Substituting of Eq. (7) into Eq. (6) yields following equation

$$
\int_0^l EI h \frac{\partial^2 w}{\partial x^2} \, dx - \int_0^l (e_a)^2 EA \alpha \Delta T \frac{\partial^2 h}{\partial x^2} \frac{\partial^2 w}{\partial x^2} \, dx - \int_0^l EA \alpha \Delta T \frac{\partial h}{\partial x} \frac{\partial w}{\partial x} \, dx - \int_0^l \rho A h \frac{\partial^3 w}{\partial x^3 \partial t^2} \, dx + \int_0^l (e_a)^2 \rho A \frac{\partial h}{\partial x} \frac{\partial f}{\partial x} \, dx = 0
$$

(6)

$$
\int_0^l \left(EI \begin{bmatrix} B^T & B' 
\end{bmatrix}
\right) w \, dx - \int_0^l (e_a)^2 EA \alpha \Delta T \begin{bmatrix} B^T & B' 
\end{bmatrix} w \, dx - \int_0^l EA \alpha \Delta T \begin{bmatrix} B^T & B' 
\end{bmatrix} w \, dx - \int_0^l \phi^T f \, dx + \int_0^l \rho A \phi \phi \, dx + \int_0^l (e_a)^2 \rho A \begin{bmatrix} B^T & B' 
\end{bmatrix} \phi \, dx - \int_0^l (e_a)^2 B^T f \, dx = 0
$$

(8)

this equation can be written as follows in the matrix form:

$$
\begin{bmatrix}
K - K_{T,c} - K_{T,cl} & \mathbf{w} + (M_c + M_{cl}) \ddot{w} = \mathbf{f}_c + \mathbf{f}_{cl}
\end{bmatrix}
$$

(9)

In here,

$$
K = \int_0^l \left(EI \begin{bmatrix} B^T & B' 
\end{bmatrix}
\right) \, dx = \int_0^l EI \begin{bmatrix}
\phi_1'' \\
\phi_2'' \\
\phi_3'' \\
\phi_4''
\end{bmatrix} \, dx = \begin{bmatrix}
12 & 6l & -12 & 6l \\
6l & 4l^2 & -6l & 2l^2 \\
-12 & -6l & 12 & -6l \\
6l & 2l^2 & -6l & 4l^2
\end{bmatrix}
$$

(10)
\[ K_{T,e} = \int_{0}^{l} E A \alpha \Delta T \left( B^T B \right) dx = \int_{0}^{l} E A \alpha \Delta T \begin{bmatrix} \phi_1' \\ \phi_2' \\ \phi_3' \\ \phi_4' \end{bmatrix} \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \end{bmatrix} dx \\
= \frac{E A \alpha \Delta T}{30l} \begin{bmatrix} 36 & 3l & -36 & 3l \\ 3l & 4l^2 & -3l & -l^2 \\ -36 & -3l & 36 & -3l \\ 3l & -l^2 & -3l & 4l^2 \end{bmatrix} \] (11)

\[ K_{T,ml} = \int_{0}^{l} (e_0 \alpha)^2 E A \alpha \Delta T \left( B^T B \right) dx = \int_{0}^{l} (e_0 \alpha)^2 E A \alpha \Delta T \begin{bmatrix} \phi_1'' \\ \phi_2'' \\ \phi_3'' \\ \phi_4'' \end{bmatrix} \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \end{bmatrix} dx \\
= \frac{(e_0 \alpha)^2 E A \alpha \Delta T}{l^3} \begin{bmatrix} 12 & 6l & -12 & 6l \\ 6l & 4l^2 & -6l & 2l^2 \\ -12 & -6l & 12 & -6l \\ 6l & 2l^2 & -6l & 4l^2 \end{bmatrix} \] (12)

\[ M_e = \int_{0}^{l} \rho A \left( \phi' \phi \right) dx = \int_{0}^{l} \rho A \begin{bmatrix} \phi_1' \\ \phi_2' \\ \phi_3' \\ \phi_4' \end{bmatrix} \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \end{bmatrix} dx = \frac{\rho A l}{420} \begin{bmatrix} 156l & 22l^2 & 54l & -13l^2 \\ 22l^2 & 4l^3 & 13l^3 & -3l^3 \\ 54l & 13l^2 & 156l & -22l^2 \\ -13l & -3l^3 & -22l^2 & 4l^3 \end{bmatrix} \] (13)

\[ M_{ml} = \int_{0}^{l} (e_0 \alpha)^2 \rho A \left( B^T B \right) dx = \int_{0}^{l} (e_0 \alpha)^2 \rho A \begin{bmatrix} \phi_1'' \\ \phi_2'' \\ \phi_3'' \\ \phi_4'' \end{bmatrix} \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \end{bmatrix} dx \\
= \frac{(e_0 \alpha)^2 \rho A}{30l} \begin{bmatrix} 36 & 3l & -36 & 3l \\ 3l & 4l^2 & -3l & -l^2 \\ -36 & -3l & 36 & -3l \\ 3l & -l^2 & -3l & 4l^2 \end{bmatrix} \] (14)

\[ f_e = \int_{0}^{l} f \phi^T \phi dx = \int_{0}^{l} f \begin{bmatrix} \phi_1' \\ \phi_2' \\ \phi_3' \\ \phi_4' \end{bmatrix} dx = \begin{bmatrix} 6 \\ l \\ 6 \\ -l \end{bmatrix} \] (15)
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\[ f_{nl} = \int_0^l (e_o a)^2 f^T B^T dx = \int_0^l (e_o a)^2 f' B^T dx = (e_o a)^2 f' \begin{pmatrix} \phi'_1 \\ \phi'_2 \\ \phi' \end{pmatrix} \begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix} \]  

(16)

where \( K \) is bending stiffness matrix. \( K_{T,c} \) and \( K_{T,nl} \) state the local and nonlocal negative stiffness matrices originating from temperature change, respectively. On the other hand, \( M_c \) and \( M_{nl} \) are local and nonlocal mass matrices, respectively. \( f_c \) and \( f_{nl} \) express local and nonlocal external force vectors, respectively.

If the \( f = 0 \) is taken for free vibration and \( w(x,t) = W(x)\sin(\omega t - \alpha) \) expression is utilized into Eq. (9), the eigenvalue formulation of finite element analysis is obtained as follows:

\[ \det[\sum[K] - \omega^2 \sum[M]] = 0 \]  

(17)

where \( \sum[K] \) and \( \sum[M] \) are total stiffness and mass matrices. \( \omega \) is natural frequency of nanobeam.

Also, the frequency equation of simply supported beams can be solved analytically. According to this, the series expansion as follows, ensures geometric and mechanical boundary conditions of simply supported beams:

\[ w(x,t) = \sum_{n=1}^\infty W_n \left( \frac{n\pi x}{L} \right) \sin(\omega t - \alpha) \]  

(18)

where \( W_n \) is unknown series coefficient, \( n \) is mode number, \( L \) is length of nanobeam. \( \omega \) explains the natural frequency of nanobeam. \( \omega \) is natural frequency of nanobeam. Additionally, \( t \) is time and \( \alpha \) is phase angle. Using Eq. (18) into Eq. (1), the following expression can be obtained

\[ m_1 \left( \frac{n\pi}{L} \right)^4 + m_2 \left( \frac{n\pi}{L} \right)^2 + m_3 = 0 \]  

(19)

Where

\[ m_1 = EI - (e_o a)^2 EA \alpha \Delta T, \quad m_2 = -EA \alpha \Delta T - \omega^2 (e_o a)^2 \rho A, \quad m_3 = -\omega^2 \rho A \]  

(20)

Substituting of Eq. (20) into Eq. (19) yields the natural frequency equation of simply supported nano beams for nonlocal parameter and temperature change:

\[ \omega^2 = \frac{EI - (e_o a)^2 EA \alpha \Delta T \left( \frac{n\pi}{L} \right)^4 - EA \alpha \Delta T \left( \frac{n\pi}{L} \right)^2}{\rho A \left( \frac{e_o a}{L} \right)^2 \left( \frac{n\pi}{L} \right)^2 + 1} \]  

(21)
3. Numerical Examples

In this section, vibration frequencies are calculated for thermal vibration analysis of ZnO NWs. The numerical results are given for simply supported (S-S), cantilever (C-F), propped cantilever (C-S) and clamped supported (C-C) boundary conditions. In order to include the nano scale effect in the analysis, nonlocal elasticity theory is considered. Mechanical properties are taken as follows in the thermal vibration analysis: modulus of elasticity $E = 58$ GPa [61], unit volume mass $\rho = 5600$ kg/m$^3$ [62] and thermal expansion coefficient $\alpha = 2.9 \times 10^{-6}$ K$^{-1}$ [63]. Additionally, the geometric features are chosen as follows: beam length $L = 20$ nm and circular cross-section diameter $d = 2$ nm. On the other hand, 20 finite elements are used for nonlocal finite element analyses.

In Table 1, the first three mode vibration frequencies of simply supported beams modeled with ZnO NWs are calculated and compared with analytical and finite elements for different nondimensional nonlocal parameter values. In addition, the frequencies of the beams not under temperature change were compared with frequencies of the beams under temperature change. First of all, nonlocal expression is a parameter that reduces classical vibration frequencies. By the increase of this value reveals, the frequencies of nanoscaled beams more decrease. Also, temperature change decreases the frequencies of ZnO NWs. In the case that the nonlocal parameter is higher, the temperature factor is more influential. On the other hand, it is seen that the values obtained by the finite element method are very close to the analytically calculated frequencies. In general, while the increase in the mode number raises the difference between calculated values by using the analytical method and NL-FEM, the increase of nonlocal parameter decreases this difference.

In Table 2, the first three mode frequencies of ZnO NWs are tabulated for three different boundary conditions and temperature change. Analytical vibration analysis for boundary conditions except S-S is not possible in case of nonlocal elasticity. Also, when it is considered that the temperature parameter is included in the analysis, an alternative to the analytical method has to be used and therefore the analyses are given only with the finite element formulation. When the stiffness states between the boundary conditions are compared, it can be said that the results obtained are reasonable. The frequencies of the clamped supported beams are the highest, while the frequencies of the cantilever beams are the lowest. Additionally, the boundary condition in which the nonlocal parameter has the highest effect is C-C.

Table 1. Comparison of the first three modes flexural frequencies (GHz) of simply supported Zinc Oxide nanowires.

<table>
<thead>
<tr>
<th>Nonlocal parameter</th>
<th>Mode Number</th>
<th>$\Delta T = 0$ K</th>
<th>$\Delta T = 300$ K</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Analytical</td>
<td>NL-FEM</td>
</tr>
<tr>
<td>$e_0a/L = 0$</td>
<td>1</td>
<td>6.3190</td>
<td>6.3190</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>25.2761</td>
<td>25.2763</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>56.8712</td>
<td>56.8731</td>
</tr>
<tr>
<td>$e_0a/L = 0.15$</td>
<td>1</td>
<td>5.7161</td>
<td>5.7161</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>18.3941</td>
<td>18.3942</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>32.8423</td>
<td>32.8434</td>
</tr>
<tr>
<td>$e_0a/L = 0.35$</td>
<td>1</td>
<td>4.2516</td>
<td>4.2516</td>
</tr>
</tbody>
</table>

Table 2. The first three modes flexural frequencies (GHz) of Zinc Oxide nanowires with different boundary conditions under temperature change.
4. Conclusions

In this study, a vibration analysis is performed for elastic beam models of ZnO NWs based on the nonlocal elasticity theory. It is also thought that the beams are under the influence of temperature change. Finite element formulation is used to solve the equation of motion. With this formulation, frequencies of different vibration modes of ZnO NW beams with different boundary conditions are calculated under nondimensional nonlocal parameter and temperature change values and the results are discussed.

In general, it is understood that the atomic scale effect and ambient temperature are definitely factors to be taken into account in the dynamic analysis of continuous models of nanoscale structures. In addition, it is concluded that the use of finite element formulation based on the size effect is an important way for the cases where dynamic analysis cannot be performed by analytical methods. It is thought that these results will guide the proper and optimum structural designs of NEMS using ZnO NWs.

References


