NUMERICAL STUDY OF SIZE-DEPENDENT INSTABILITY OF NEMS CONSIDERING MOLECULAR FORCE AND ELASTIC SUPPORT CONDITIONS

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ABSTRACT
Nano-electromechanical systems (NEMS) sensors are recently used as powerful medical detectors for detection of disease. In this research paper, the modified couple stress non-classic continuum theory is applied to examine the size effect on the pull-in instability of beam-type NEMS sensor at submicron separations considering the van der Waals attraction. The proposed model takes the non-classic support conditions into account using rotational springs at supported end of the simply supported nano-beam. In order to solve the nonlinear constitutive equation of the nano-beams, finite difference numerical solution employed. The results reveal significant influence of the size dependency, elastic support conditions and van der Waals attraction on the pull-in characteristics of beam-type NEMS.

Keywords: nano-electromechanical systems (NEMS) sensor, modified couple stress theory, elastic boundary conditions, size effects, van der waals force.

INTRODUCTION
Beam-type micro/nano-electromechanical systems (MEMS/NEMS) are widely used in many applications (Ke and Espinosa, 2006; Zhang et al., 2004). Consider a beam-type actuator constructed from two conductive electrodes where one is fixed and the other is movable. Applying voltage difference between these two causes the movable electrode to deflect towards the fixed one (ground electrode), because of the electrostatic forces. At a critical voltage, which is known as the pull-in voltage, the movable electrode becomes unstable and pulls-in onto the ground electrode. The pull-in behavior of MEMS has been studied for over two decades without considering nano-scale effects (Osterberg, 1995; Batra et al., 2007). With decrease in dimensions to nano-scale, many essential phenomena appear which are not important at macro scales. In this paper, three effects of these sub-micron phenomena are considered for simulation of pull-in instability of micro/nano-actuator.

The first phenomenon that becomes important at submicron distances is the presence of dispersion forces. These attractions can significantly influence the NEMS performance when the initial gap between the components of actuator is typically below several ten nanometers (Israelachvili, 1992; Koochi et al., 2011a; Soroush et al., 2012) Batra et al. (2008) studied the pull-in behavior of micro-plates considering van der Waals attraction. Spengen et al. (2002) studied the stiction in MEMS due to van der Waals force. Dequesnes et al. (2002) calculated the effect of van der Waals attraction on the instability voltage of carbon-nanotube-based NEMS switches.

The second issue that must be considered in modeling ultra-small structures at nano-scale is the characterization of real boundary conditions (B.C.). The B.C. of real nano-structures is not always homogeneous and may be flexible by rotation (Muthukumaran et al., 1999). The static and dynamic responses of structures vary under different boundary conditions. Rinaldi et al. (2008) characterized the non-classical support conditions of micro-cantilevers through electromechanical test. Yunqiang et al. (2008) studied the B.C. effect on the static and dynamic responses of micro-plates. According to limitations of manufacturing techniques in nano-scale productions, not all B.C. may be acceptable such as clamped or simply supported condition. Therefore, the boundary support conditions need to be theoretically quantified and experimentally validated (Gino et al., 2007).

Finally, the third effect that appears at small scales (specially for nano-dimensions and even for some micro-dimensions) is the size dependency of material characteristics. The classical continuum mechanics is not able to explain the size-dependent behavior of materials and structures at sub-micron distances. To overcome this problem, non-classical continuum theories such as non-local (Eringen and Edelen, 1972) and couple stress (Ejike, 1969; Kishidaand Sasaki, 1990) are developed considering the size effects. Compared to other non-classical continuum theories such as strain gradient theory, the modified couple stress theory has two advantages: the couple stress tensor is symmetric and only one internal length scale parameter is involved. These features make the modified theory easier to use by theoreticians and practical for experimental measurements (Gaoand Park, 2006). Some experimental results demonstrate that the size dependency is an inherent property of conductive metals when the characteristic size of the structure is comparable to the internal material length (Stolken and Evans, 1998; Lam et al., 2003). Recently, new modified couple stress theory has been proposed by Yang et al. (2002). In this theory,
two classical material constants in the couple stress theory are reduced to only one internal material length scale parameter. This theory has been applied to investigate Euler micro-beams by many researchers (Asghari et al., 2010; Ma et al., 2008; Abdi et al., 2011).

The Euler beam model is applied as a time-saving continuum approach to obtain the constitutive governing equations (Abadyan et al., 2010; Soroush et al., 2010; Koochi et al., 2011b; 2011c). The rotational artificial spring are used at the supported end to model the B.C. of simply supported nano-beams. In order to solve the constitutive equation of nano-structures, finite difference solution is employed. The obtained results are compared with other results reported in the literature.

Figure-1. Schematic representation of simply supported nano-beams.

MODIFIED COUPLE STRESS THEORY

Based on the modified couple stress theory, the strain energy density is written as (Stolken and Evans, 1998):

\[ u = \sigma \varepsilon + m : \chi, \]

where the stress tensor \( \sigma \), strain tensor \( \varepsilon \), deviator part of the couple stress tensor \( m \) and symmetric curvature tensor \( \chi \) are defined by the following:

\[ \sigma = \lambda tr(\varepsilon)I + 2\mu\varepsilon, \quad 2(a) \]

\[ \varepsilon = \frac{1}{2}((\nabla u) + (\nabla u)^T), \quad 2(b) \]

\[ m = 2l^2 \mu \chi, \quad 2(c) \]

\[ \chi = \frac{1}{2}((\nabla \theta) + (\nabla \theta)^T), \quad 2(d) \]

\[ \theta = \frac{1}{2} \text{curl}(u), \quad 2(e) \]

where \( \lambda, \mu, l \) and \( \theta \) are Lame constant, shear modulus, material length scale parameter and rotation vector, respectively (Gao and Park, 2006). According to the basic hypotheses of Euler-Bernoulli beams in one dimension, the displacement field is assumed as:

\[ u = -z \frac{\partial w(X)}{\partial X}, \quad v = 0, \quad w = w(X). \]

Consider ing small deformation and substituting relation (3) in equation (2), one obtains

\[ \chi_{xy} = \frac{1}{2} \frac{\partial^2 w(X)}{\partial X^2}, \quad 4(a) \]

\[ \chi_{xx} = \chi_{yy} = \chi_{zz} = \chi_{yz} = \chi_{zx} = 0 \]

\[ m_{xy} = -\mu l^2 \frac{\partial^2 w}{\partial X^2}, \quad 4(b) \]

\[ m_{xx} = m_{yy} = m_{zz} = m_{yz} = m_{zx} = 0 \]

\[ \varepsilon_{xx} = -z \frac{\partial^2 w(X)}{\partial X^2}, \quad 4(c) \]

\[ \varepsilon_{yy} = \varepsilon_{zz} = \varepsilon_{yz} = \varepsilon_{xy} = \varepsilon_{zx} = 0, \quad 4(d) \]

\[ \sigma_{xx} = -E \frac{\partial^2 w}{\partial X^2}, \quad 4(e) \]

\[ \sigma_{yy} = \sigma_{zz} = \sigma_{yz} = \sigma_{zx} = \sigma_{xy} = 0. \]

where \( E \) is the Young's modulus.

GOVERNING EQUATION

Figure-1 shows simply supported beam-type MEMS/NEMS actuator. The actuators are modeled by a beam of length \( L \) with a uniform rectangular cross section of width \( B \) and thickness \( H \) which is suspended over a conductive substrate. The artificial angular spring with spring stiffness of \( K_{1\theta} \) is used to model the real B.C. in SS simply supported nano-beams. For DS case, two springs with rotational stiffnesses of \( K_{1\theta} \) and \( K_{2\theta} \) are applied at the supported ends. Note that considering axial tractions along the beam (such as stretching, residual and thermal stress, etc.) will be considered in further works.

In order to develop the governing equation of the beams, we apply the minimum energy principle which implies equilibrium when the free energy reaches the minimum value. Substituting equation (4) into equation (1), integrating and adding the spring’s energy, the total elastic energy (U) of the system can be written as equation 5(a) (Gao and Park, 2006). Furthermore, the work (V) done by external forces is obtained by integrating the external forces distribution, \( q(X) \), along the beam length (equation 5(b)).

\[ U = \frac{1}{2} \int_0^L (EI + \mu l^2) \left( \frac{\partial^2 w}{\partial X^2} \right)^2 dX + \frac{1}{2} K_{1\theta} \left( \frac{\partial^2 w(0)}{\partial X^2} \right)^2 \quad 5(a) \]

\[ V = \int_0^L q(X) w(X) dX. \quad 5(b) \]

In above relations, \( I \) is the second moment of cross-sectional area and \( A \) is the cross-sectional area of the beam. By applying Hamilton principle i.e., \( \delta (V-U) = 0 \), the equilibrium of the beam is derived from equation (5) as:
\[(EI + \mu AI^2) \frac{d^4w}{dx^4} = q(X) \quad (6)\]

with the following B.C.:

\[w(0) = \frac{d^3w}{dx^3} (L) = \frac{d^3w}{dx^3} (L) = 0 \quad 7(a)\]

\[\left( EI + \mu AI^2 \right) \frac{d^3w(0)}{dx^3} = K_{vw} \frac{dw(0)}{dx} \quad 7(b)\]

In equation (6), \(q(X)\) equals to the summation of electrostatic (\(f_{\text{elec}}\)) and van der Waals (\(f_{\text{van}}\)) forces per unit length of the beam (Yang \textit{et al.}, 2002). The electrostatic force enhanced by the first order fringing correction can be presented as the following equation (Soroush \textit{et al.}, 2010):

\[f_{\text{elec}} = \frac{\varepsilon_0 B V^2 (g - w)}{2(g - w)} \left[ 1 + 0.65 \frac{g - w}{B} \right], \quad (9)\]

where \(\varepsilon_0 = 8.854 \times 10^{-12} \text{ C}^2 \text{N}^{-1} \text{m}^{-2}\) is the permittivity of vacuum, \(V\) is the applied voltage and \(g\) is the initial gap between the movable and the ground electrode. Considering ideal cases, the van der Waals force per unit length of the beam is (Koochi \textit{et al.}, 2011b):

\[f_{\text{van}} = \frac{A B}{6\pi(g - w)^{1.5}}, \quad (10)\]

where \(A\) is the Hamaker constant. In realistic cases, the dispersion interaction between two surfaces highly depends on dielectric properties of the surfaces and also on the geometric parameters.

One can use equations (9-10) and the substitutions \(\hat{w} = w/g\) and \(x = X/L\) to transform equation (6) into the following dimensionless boundary value problem:

\[\frac{d^4\hat{w}}{dx^4} = \frac{\alpha}{(1 - \hat{w}(x))^{3/2}(1 + \delta)} + \frac{\beta}{(1 - \hat{w}(x))^{3/2}(1 + \delta)} + \frac{\gamma \beta}{(1 - \hat{w}(x))^{3/2}(1 + \delta)} + \frac{\gamma \beta}{(1 - \hat{w}(x))(1 + \delta)}, \quad 11(a)\]

\[\hat{w}(0) = K \hat{w}(0) , \quad \hat{w}(0) = \hat{w}(1) = \hat{w}''(1) = 0 \quad 11(b)\]

In above equations, the non-dimensional parameters, \(\alpha, \beta, \gamma, \delta\) and \(K\) are:

\[\alpha = \frac{\overline{A} B L^4}{6\pi g^2 EI} \quad 12(a)\]

\[\beta = \frac{\varepsilon_0 B V^2 L^4}{2g^3 EI} \quad 12(b)\]

\[\gamma = 0.65 \frac{g}{B} \quad 12(c)\]

\[\delta = \frac{\mu AI^2}{EI} \quad 12(d)\]

\[K = \frac{K_{vw} L}{EI + \mu AI^2} \quad \text{(for SS case)} \quad 12(e)\]

It should be noted that special cases, i.e., clamped beams, can be easily modeled by setting \(K = \infty\). Therefore, one can use the following B.C. for special cases instead:

\[\hat{w}''(0) = \hat{w}''(1) = 0 \quad 13\]

Relations (11-13) present the governing equation of nano-beams.

**FINITE DIFFERENCE SOLUTION**

In order to numerically solve the governing equation of system, a procedure based on finite difference method (FDM) is developed in this study. Following the standard FDM procedure, the beam is discretized into \(n\) equal sections (elements) separated by \((n + 1)\) nodes. For each element, the governing equation (13) in the discretized form can be written as:

\[\hat{w}_{i+2} - 4\hat{w}_{i+1} + 6\hat{w}_i - 4\hat{w}_{i-1} + \hat{w}_{i-2} = F_i \quad 14\]

where \(h\) is the grid spacing, \(\hat{w}\) is the deflection of \(i\)th grid and:

\[F_i = \frac{\alpha}{(1 - \hat{w}_i)^3(1 + \delta)} + \frac{\beta}{(1 - \hat{w}_i)^2(1 + \delta)} + \frac{\gamma \beta}{(1 - \hat{w}_i)(1 + \delta)} \quad 15\]

Applying equation (15) to all of the elements and incorporating the boundary conditions (equation (11b)), a matrix form equation is obtained as:

\[\left[ A \right] \{ \hat{w} \} = \{ F \} \quad 16\]

where \(\{ \hat{w} \} = [\hat{w}_1, \hat{w}_2, ..., \hat{w}_n]^T \), \(\{ F \} = [F_1, F_2, ..., F_n]^T\) and \(A\) matrix can be defined as:
In this work MATLAB commercial software is employed to numerically solve equation (16) for the nodal deflections.

RESULTS AND DISCUSSIONS

To compare with the literature, the pull-in voltage of typical cantilever micro-actuators ($\alpha = \delta = 0, K = \infty$) have been calculated. The geometry and the constitutive material of the beams are identified in Table-1. The comparison between FDM results and those of the literature is presented in Table-2.

Table-1. Geometrical parameters and material properties of the nano-beam of Table-3.

<table>
<thead>
<tr>
<th>Case</th>
<th>Material properties</th>
<th>Geometrical dimensions</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$E$ (GPa)</td>
<td>$\nu$</td>
</tr>
<tr>
<td>Narrow beam</td>
<td>77</td>
<td>0.33</td>
</tr>
<tr>
<td>Wide beam</td>
<td>77</td>
<td>0.33</td>
</tr>
</tbody>
</table>

Table-2. Pull-in voltage comparison for cantilever beam of Table-2. Molecular force is neglected.

<table>
<thead>
<tr>
<th>Case</th>
<th>Pull-in voltage ($V$)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(Osterberg, 1995)</td>
</tr>
<tr>
<td>Narrow beam</td>
<td>1.23</td>
</tr>
<tr>
<td>Wide beam</td>
<td>2.27</td>
</tr>
</tbody>
</table>

Figure-2 depicts variation of $\beta_{PI}$ of SS beam vs. spring stiffness ($K$) and van der Waals force ($\alpha$) without considering the size effect. As seen, enhancing the spring stiffness leads to increase in pull-in voltage of SS actuator. On the other hand, van der Waals force decreases the pull-in voltage of the structure. For arbitrary $K$, increase in $\alpha$ leads to decrease in $\beta_{PI}$. Finally, when $\alpha$ reaches its critical value, $\alpha_c$, no $\beta_{PI}$ can be obtained. This means that for a sufficiently large value of molecular attraction the beam attaches to the ground plane even without applying voltage difference.

Figure-3 depicts variation of $\beta_{PI}$ vs. $K$ and $\alpha$ for $\delta = 0.5$. By comparing Figures 2 and 3 it is found that for arbitrary spring stiffness and intermolecular force, the size effect ($\delta\neq0$) produces higher values of $\beta_{PI}$. This effect can not be modeled via classical continuum theory.

Figure-2. Effect of van der Waals force ($\alpha$) and spring coefficient ($K$) on the pull-in voltage ($\beta_{PI}$) of SS nano-beam for $\delta = 0$ and $\gamma = 1$. 
Figure-3. Effect of van der Waals force ($\alpha$) and spring coefficient ($K$) on the pull-in voltage ($\beta_{PI}$) of SS nano-beam for $\delta = 0.5$ and $\gamma = 1$.

CONCLUSIONS

In this article, modified couple stress theory has been applied to investigate the effect of van der Waals force, elastic B.C. and size dependency on the pull-in behavior of MEMS/NEMS. The following points are concluded:

- Size effect can highly increase the pull-in voltage of thin MEMS/NEMS where the beam thickness is comparable to its material length scale. In comparison with the pull-in voltage, the pull-in deflection is less sensitive to variation of size effect parameter.
- The van der Waals force decreases the pull-in voltage and deflection of MEMS/NEMS at submicron scales. This emphasizes the importance of molecular forces consideration in design and analysis of MEMS/NEMS.
- Results show that the instability of MEMS/NEMS strongly depends on the rotational spring coefficients.

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REFERENCES


