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A NEW EFFICIENT APPROACH FOR MODELING AND SIMULATION OF NANO-SWITCHES UNDER THE COMBINED EFFECTS OF INTERMOLECULAR SURFACE FORCES AND ELECTROSTATIC ACTUATION

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This paper applies the homotopy perturbation method to the simulation of the static response of nano-switches to electrostatic actuation and intermolecular surface forces. The model accounts for the electric force nonlinearity of the excitation and for the fringing field effect. Using a mode approximation in the Galerkin projection method, the nonlinear boundary value differential equation describing the statical behavior of nano-switch is reduced to a nonlinear algebraic equation which is solved using the homotopy perturbation method. The number of included terms in the perturbation expansion for achieving a reasonable response has been investigated. Three cases have been specifically studied. These cases correspond to when the effective external force is the electrostatic force, the combined electrostatic and Casimir force and the combined electrostatic and van der Waals force. In all three cases the pull-in characteristics has been investigated thoroughly. Results have been compared with numerical results and also analytical results available in the literature. It was found that HPM modifies the overestimation of N/MEMS instability limits reported in the literature and can be used as an effective and accurate design tool in the analysis of N/MEMS.

Keywords: Nano-switches; Casimir force; van der Waals force; homotopy perturbation method; pull-in instability.

1. Introduction

Nanoelectromechanical systems (NEMS) which are a smaller version of micro-electromechanical systems (MEMS), are sensors, actuators, devices and systems

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with critical dimensions of the order of nanometers.[1] N/MEMS devices finds variety of applications such as micropumps,[2] micromirrors,[3] microphones,[4,5] microresonators,[6] random access memory,[7] nanotweezers for miniaturized robotics,[8] super-sensitive sensors[9,10] and devices for high-frequency operation and fast switching in communication networks.[1]

Technology of N/MEMS has experienced a lot of progress in testing and fabricating new devices recently. Their low manufacturing cost, batch production, light weight, small size, durability, low energy consumption and compatibility with integrated circuits, makes them even more attractive.[11,12]

Typical MEMS devices employ a parallel beam capacitor with variable capacity in which one beam is actuated electrically and as a result, this flexible microbeam deflects towards the rigid substrate, which is followed by capacitive changes.[13] Similar mechanisms are used in NEMS devices. For example one can indicate at carbon-nanotube based cantilever switches which are fundamental building blocks for the design of NEMS applications, such as nanotweezers and some other nanoscale actuators.[1]

The input voltage has an upper limit beyond which the restoring force of the micro/nano structure can no longer resist the electrostatic force, and consequently the structure spontaneously collapses. This behavior is known as pull-in instability, and the upper limit of input voltage is called pull-in voltage.

Determination of the static deflection and the pull-in voltage are critical in the design process of microsystems, to determine the sensitivity, instability and the dynamics of devices.[14] Several studies have investigated the static pull-in behavior of microbeams. Ijntema and Tilmans[15] have considered the static and dynamic responses of a microbeam under the actuation of the electrostatic force. Tilmans and Legtenberg[6] have studied microbeams using the Rayleigh–Ritz method, to generate an analytical expression for the pull-in voltage. Choi and Lovell[16] have calculated the static deflection of a microbeam using a shooting method. Their model accounts for both the electrostatic force and the midplane stretching. Abdel-Rahman *et al.*[14] have utilized a nonlinear model of a microbeam including the electrostatic force, mid-plane stretching and applied axial load. They used a shooting method to solve the static problem.

Comparing to MEMS switches, the operation of NEMS switches is different because of the importance of the intermolecular surface forces such as van der Waals and Casimir forces which can be neglected at micrometer scale. Even in the absence of electrostatic actuation, when the gap between cantilever tube and the rigid substrate is very small the pull-in phenomenon can occur because of the intermolecular forces.[17–20]

The intermolecular surface forces are especially significant when the nanobeams are working in vacuum without the effect of capillary forces and the separations between movable components are in the sub-micrometer range.[21] For separations much less than the plasma wavelength (for a metal) or much less than the absorption wavelength (for a dielectric) of the material constituting the surfaces (typically below 20 nm), the retardation, which is a result of the finite propagation speed of the electromagnetic field, is not significant.[22] In this case, the intermolecular force between two surfaces is simplified as the van der Waals attraction.[23] The Casimir force arises from the polarization of adjacent material bodies, separated by distances of less than a few microns.[24]

Van der Waals force and Casimir force can both be connected with the existence of zero-point vacuum oscillations of the electromagnetic field.[25–27] The microscopic approach to the modeling of both van der Waals and Casimir forces can be formulated in a unified way using Quantum Field Theory.[22,25,27] It is found that the Casimir force is generally effective at larger separation distances between the bodies than the van der Waals force. Whereas the Casimir force between semi-infinite parallel plates is inversely proportional to the fourth power of the gap, van der Waals force is inversely proportional to the third power of the gap. The dependence of these forces on the dielectric properties of the plates and the filling medium is studied in detail in Ref. 25. It is important to note that van der Waals and Casimir forces cannot in general be considered to simultaneously act in MEMS, since they describe the same physical phenomenon at two different length scales.

Effect of van der Waals force on the pull in instability of electrostatically actuated rectangular microplates has been studied by Batra *et al.*[28] Lin and Zhao[29] adopted a one degree of freedom mass spring model to study the influence of Casimir force on the nonlinear behavior of nanoscale electrostatic actuators. Dequesnes *et al.*[1] studied the pull-in voltage characteristics of several nanotube electromechanical switches, such as double-wall carbon nanotubes suspended over a graphitic ground electrode. They proposed parametrized continuum models for coupled electrostatic and van der Waals energy domains. They compared the accuracy of the continuum models with atomistic simulations. Their numerical simulations based on continuum models closely match the experimental data reported for carbon-nanotube-based nanotweezers.

Ding *et al.*[21] presented an analysis of Casimir effect with surface roughness, conductivity and temperature corrected on the deformation of a membrane strip structure. They provided a way of designing a membrane strip with high resistance to collapse. Ramezani *et al.*[19,30] investigated the two point boundary value problem of the deflection of nano-cantilever subjected to Casimir and electrostatic forces using analytical and numerical methods to obtain the instability point of the nanobeam. They computed the pull-in parameters of the beam under combined effects of electrostatic and Casimir forces. In their analytical approach, the nonlinear differential equation of the model was transformed into the integral form by using the Green's function of the cantilever beam. Then, closed-form solutions were obtained by assuming an appropriate shape function for the beam deflection to evaluate the integrals. They[20] used the same method to investigate the influence of van der Waals force on the pull-in voltage and deflection of nanomechanical switches using a distributed parameter model. The fringing field effect was also taken into account in their model.

Although the Static deflection and Pull-in instability of nanocantilevers has been investigated by many researchers, most of the methods used for this purpose are numerically cumbersome. Analytical approaches are usually more appealing than numerical one because of conveniences for parametric studies and accounting for the physics of the problem. Also analytical solutions give a reference frame for verification and validation of the numerical approaches.

The current paper uses the homotopy Perturbation method to investigate static deflection and pull-in parameters of nanocantilevers due to the combined effects of electrostatic and intermolecular forces. He[31] features a survey of some recent development in asymptotic techniques, which are valid not only for weakly nonlinear equations, but also for strongly ones. He[32] introduced the HPM as a relatively new method that is still evolving. This new perturbation technique, namely homotopy perturbation method does not depend upon the assumption of small parameters.[33] He[33] illustrated the well-known duffing equation as an example and found that even with using a first order approximation, the maximal relative error of the period is less than 7% even when the parameter ε approaches infinity. His new method takes full advantages of the traditional perturbation methods and homotopy techniques.[34] Blendez *et al.*[35] solved the nonlinear differential equations which govern the nonlinear oscillation of a simple pendulum and showed that even only one iteration leads to the relative error of less than 2% for the approximated period even for amplitudes as high as 130°. Blendez *et al.*[36] found improved approximate solutions to conservative truly nonlinear oscillators using He's homotopy perturbation method. They found that for the second order approximation the relative error in the analytical approximate frequency is approximately 0.03% for any parameter values involved.

As it is seen in the literature of the HPM, this method overcomes the limitations of classical perturbation methods and at the same time provides an accurate prediction of the behavior of the nonlinear systems. So here, it has been used for the first time to analyze the nonlinear boundary value problem of nanocantilever's static behavior under the effects of electrostatically actuation and intermolecular forces.

2. Problem Formulation

A common approach to nanoscale simulation is to use molecular dynamics (MD). However, MD simulations require the computation of all atoms of the system. The time step in MD simulations is typically of the order of 0.1 fs for a stable integration scheme. MD simulations involving more than a million atoms are very expensive and the dynamics of the system can only be probed for a few picoseconds. Therefore, MD simulations may not be easily used in an integrated design process or for design optimization.[1] Dequesnes *et al.*[1] proposed parametrized continuum models for the coupled electrostatic and van der Waals energy domains and compared the accuracy of the continuum models with atomistic simulations. Their numerical simulations based on continuum models closely match the experimental data reported for carbon-nanotube based nanotweezers. So in this paper a continuum model is implemented to model the static behavior of cantilever type nano-switches.

Following a continuum model Ramezani *et al.*[23] presented the following nonlinear boundary value model for static deflection of cantilever type nano-switch shown in Fig. 1 under the combined effects of electrostatic actuation and intermolecular forces.

$$EI\frac{\partial^4 \hat{w}}{\partial \hat{x}^4} + \rho bh\frac{\partial^2 \hat{w}}{\partial \hat{t}^2} = \frac{(1-n)\mathrm{A}b}{6\pi(d-\hat{w})^3} + \frac{n\pi^2\hbar cb}{240(d-\hat{w})^4} + \frac{1}{2}\varepsilon b\left(1+0.65\frac{d-\hat{w}}{b}\right)\frac{V^2}{(d-\hat{w})^2} \tag{1}$$

where E is the effective young modulus of the nanobeam, I is the second area moment of the inertia, $\hat{w}$ is the beam deflection, $\hat{x}$ is the coordinate along the length, ρ is density, b is the width of the beam, h is the beam thickness, $\hat{t}$ is time, A is the Hamaker constant, $\hbar = 1.055 \times 10^{-34}$ J.s is Planck's constant divided by 2π, c is the speed of light, d is the initial gap between the solid and flexible electrode and ε is the vacuum permittivity. The first term in the right hand side of equation (1) describes the van der Waals force, the second term represents the Casimir force, and the third and fourth terms describes the electrostatic force and its fringing field

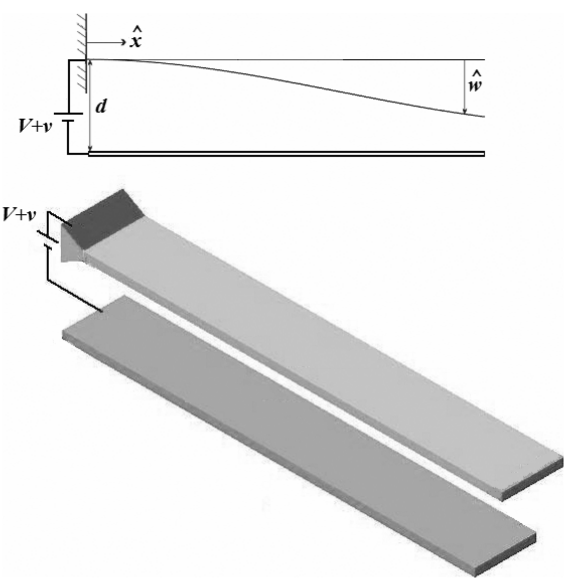

Fig. 1. Cantilever type nano-switch.

effect respectively. The index n is 0 when the effective intermolecular force is van der Waals force and is unity when the effective intermolecular force is Casimir force. Since this paper investigates the static deflection of the nano-switches, the inertia term, i.e. the second derivative of $\hat{w}$ with respect to $\hat{t}$ is neglected. Guo and Zhao[37] studied the stability of the torsional actuators considering van der Waals effects. In their model, when dealing with the static equilibrium problem, the resultant of the electrostatic and the van der Waals torques counterbalance with the elastic restoring torque. Here a similar situation occurs. In the absence of inertia term, when intermolecular surface forces are taken into consideration, the resultant of these forces with the electrostatic actuation force, reaches a balance with the elastic restoring force of the beam. So, by neglecting inertia terms, equation (1) can be nondimensionalized in the form of equation (2).

$$\frac{d^4 w_s}{dx^4} = \frac{(1-n)\alpha_3}{(1-w_s)^3} + \frac{n\alpha_4}{(1-w_s)^4} + \frac{\alpha_2 V^2}{(1-w_s)^2} + f\frac{\alpha_2 V^2}{1-w_s} \tag{2}$$

where

$$x = \frac{\hat{x}}{L} \tag{3}$$

$$w = \frac{\hat{w}}{d} \tag{4}$$

$$\alpha_2 = \frac{6\varepsilon L^4}{Eh^3 d^3} \tag{5}$$

$$\alpha_3 = \frac{\mathrm{A}bL^4}{6\pi d^4 EI} \tag{6}$$

$$\alpha_4 = \frac{\pi^2 \hbar c b L^4}{240 d^5 EI} \tag{7}$$

$$f = 0.65\frac{d}{b} \tag{8}$$

In these equations L represents the beam length.

The associated boundary conditions for solving equation (2) are

$$w(0) = 0 \tag{9}$$

$$\left.\frac{\partial w}{\partial x}\right|_{x=0} = 0 \tag{10}$$

$$\left.\frac{\partial^2 w}{\partial x^2}\right|_{x=1} = 0 \tag{11}$$

$$\left.\frac{\partial^3 w}{\partial x^3}\right|_{x=1} = 0 \tag{12}$$

Now using the first mode shape of the nanocantilever, the deflection of the nanoswitch is assumed to be as equation (13).

$$w_s(x) = a\phi(x) \tag{13}$$

where $\phi(x)$ is the first mode shape of the nanocantilever and a is some unknown coefficient. For cantilever beams $\phi(x)$ can be stated as follows.

$$\phi(x) = \cosh\beta x - \cos\beta x - \frac{(\cosh\beta + \cos\beta)}{(\sinh\beta + \sin\beta)}(\sinh\beta x - \sin\beta x) \tag{14}$$

For the first mode of the cantilever beam $\beta = 1.87510$. Following the Galerkin's decomposition method, by substituting equation (13) into equation (2) and integrating the residual over the nanoswitch nondimensionalized domain by weight $\phi(x)$, one may arrive at equation (15).

$$Ka - \int_0^1 \left[\frac{(1-n)\alpha_3}{(1-a\phi(x))^3} + \frac{n\alpha_4}{(1-a\phi(x))^4} + \frac{\alpha_2 V^2}{(1-a\phi(x))^2} + f\frac{\alpha_2 V^2}{(1-a\phi(x))}\right]\phi(x)dx = 0 \tag{15}$$

In this equation, K is defined as

$$K = \int_0^1 \phi(x)\frac{d^4\phi(x)}{dx^4}dx \tag{16}$$

The equation (15) can be decomposed to linear and nonlinear parts.

$$L(a) + N(a) = 0 \tag{17}$$

where

$$L(a) = Ka \tag{18}$$

$$N(a) = -\int_0^1 \left[\frac{(1-n)\alpha_3}{(1-a\phi(x))^3} + \frac{n\alpha_4}{(1-a\phi(x))^4} + \frac{\alpha_2 V^2}{(1-a\phi(x))^2} + f\frac{\alpha_2 V^2}{(1-a\phi(x))}\right]\phi(x)dx \tag{19}$$

Now the homotopy form is constructed as follows.

$$H(a,P) = (1-P)[L(a) - L(a')] + P[L(a) + N(a)] = 0 \tag{20}$$

or in a more simplified manner

$$L(a) - L(a') + P[N(a) + L(a')] = 0 \qquad P \in [0,1] \tag{21}$$

Here P is an imbedding parameter which serves as perturbation parameter and a' is the initial guess. It is obvious that as P increases from 0 to 1, the solution of equation (21) varies from the solution of the linear equation to the exact solution of equation (15). To apply the perturbation technique, one can assume that the solution of Eq. (21) can be expressed as a series in P as

$$a = a_0 + Pa_1 + P^2 a_2 + \cdots \tag{22}$$

It would be desirable to expand the nonlinear part of the equation (21) in Taylor series as equation (23).

$$\begin{aligned} N(a) = N(a_0) &+ (Pa_1 + P^2 a_2 \cdots + P^4 a_4) \left.\frac{dN}{da}\right|_{a=a_0} \\ &+ (Pa_1 + P^2 a_2 \cdots + P^4 a_4)^2 \frac{1}{2!} \left.\frac{d^2 N}{da^2}\right|_{a=a_0} \\ &+ (Pa_1 + P^2 a_2 \cdots + P^4 a_4)^3 \frac{1}{3!} \left.\frac{d^3 N}{da^3}\right|_{a=a_0} \\ &+ (Pa_1 + P^2 a_2 \cdots + P^4 a_4)^4 \frac{1}{4!} \left.\frac{d^4 N}{da^4}\right|_{a=a_0} + \cdots \end{aligned} \tag{23}$$

Substituting equations (22) and (23) into equation (21) and equating the coefficients of like powers of P, one obtains the following system of algebraic equations which can be solved consecutively.

$$\begin{aligned} P^0 &: L(a_0) - L(a') = 0 \\ P^1 &: L(a_1) + N(a_0) + L(a') = 0 \\ P^2 &: L(a_2) + a_1 N'(a_0) = 0 \\ &\vdots \end{aligned} \tag{24}$$

With solving these equations, coefficients a_i can be found as

$$\begin{aligned} a_0 &= a' \\ a_1 &= -a' + \frac{1}{K} \int_0^1 \left[\frac{(1-n)\alpha_3}{(1-a_0\phi(x))^3} + \frac{n\alpha_4}{(1-a\phi(x))^4} + \frac{\alpha_2 V^2}{(1-a_0\phi(x))^2} \right. \\ &\quad \left. + f \frac{\alpha_2 V^2}{(1-a_0\phi(x))} \right] \phi(x) dx \\ a_2 &= \frac{a_1}{K} \int_0^1 \left[\frac{3(1-n)\alpha_3}{(1-a_0\phi(x))^4} + \frac{4n\alpha_4}{(1-a\phi(x))^5} + \frac{2\alpha_2 V^2}{(1-a_0\phi(x))^3} \right. \\ &\quad \left. + f \frac{2\alpha_2 V^2}{(1-a_0\phi(x))^2} \right] \phi(x) dx \\ &\vdots \end{aligned} \tag{25}$$

Now letting the perturbation parameter P equals unity, a is obtained as equation (26).

$$a = a_0 + a_1 + a_2 + \cdots \tag{26}$$

And the static deflection of the nanobeam can be obtained from $w_s(x) = a\phi(x)$.

3. Results and Discussion

For obtaining acceptable results, the number of included terms in the perturbation expansion of a has to be investigated. For this purpose Table 1 has been prepared. This Table 1 shows that in the worst condition (i.e. when the applied voltage is around pull-in voltage) including more than seven terms in the perturbation expansion of a would not make a considerable change in the obtained response.

In Figs. 2 and 3, the deflection of nanobeam has been calculated using different orders in the perturbation approximation. It is observed that a six order approximation is acceptable for a highly precise response.

Figure 4 compares the results of HPM, numerical approach and previously reported analytical approaches[20] for the maximum deflection of the nanobeam in the absence of electric actuation when the effective intermolecular force is van der Waals force. As it can be seen, our analytical approach can gives better insight to the behavior of the system.

In Fig. 5, Similar comparison, has been made, when the effective intermolecular force is the Casimir force. This figure is another evident of the effectiveness

Table 1. Maximum deflection of nanobeam when $n = 1$, $\alpha_4 = 0.2$ and $d/b = 1$.

Number of included terms in the perturbation expansion of a	$\alpha_2 V^2 = 0$	$\alpha_2 V^2 = 0.225$	$\alpha_2 V^2 = 0.475$	$\alpha_2 V^2 = 0.725$	$\alpha_2 V^2 = 0.825$
2	0.0253	0.0820	0.1551	0.2532	0.3459
3	0.0270	0.0829	0.1573	0.2599	0.3699
4	0.0272	0.0830	0.1578	0.2621	0.3833
5	0.0272	0.0831	0.1579	0.2630	0.3929
6	0.0272	0.0831	0.1579	0.2634	0.4007
7	0.0272	0.0831	0.1579	0.2636	0.4073

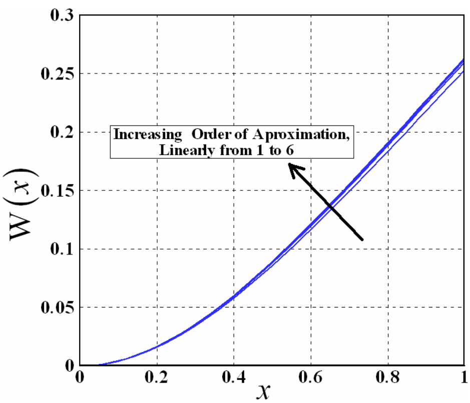

Fig. 2. Nanobeam deflection at $\alpha_2 V^2 = 0.725$ when $n = 1$, $\alpha_4 = 0.2$ and $d/b = 1$ using different orders of approximation for a.

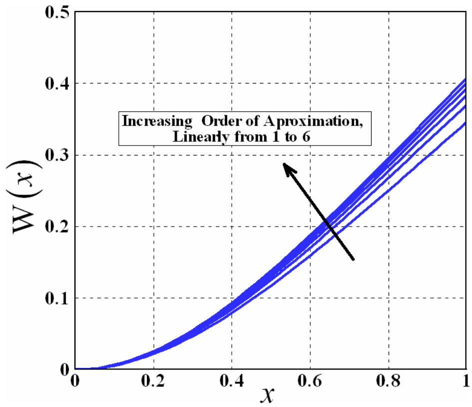

Fig. 3. Nanobeam deflection near pull-in voltage when $n = 1$, $\alpha_4 = 0.2$ and $d/b = 1$ using different orders of approximation for a.

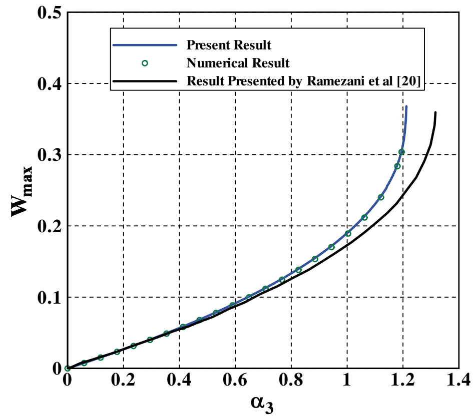

Fig. 4. Maximum deflection of the nanobeam in the absence of electric actuation when the effective intermolecular force is van der Waals force.

and accuracy of the HPM in dealing with strongly nonlinear boundary value problems.

Figures 4 and 5 also show that even when there is no electric actuation with increasing the values of α_3 and α_4 which can be accomplished by increasing the length of nanobeam, pull-in can still occur due to intermolecular forces. The maximum beam length around which the pull-in occur due to intermolecular forces is called freestanding length. Figures 4 and 5 serve as a tool for computing the freestanding length of nanobeams.

Maximum deflection of the nanobeam under the effect of electric actuation, including fringing field effect in the absence of intermolecular forces has been investigated in Fig. 6. Again it is clear that HPM gives better prediction of the systems behavior especially around the pull-in instability of the nanoswitch.

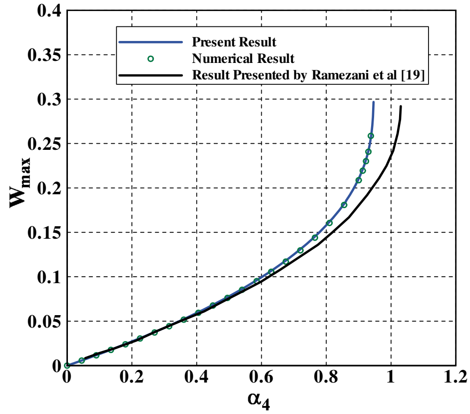

Fig. 5. Maximum deflection of the nanobeam in the absence of electric actuation when the effective intermolecular force is Casimir force.

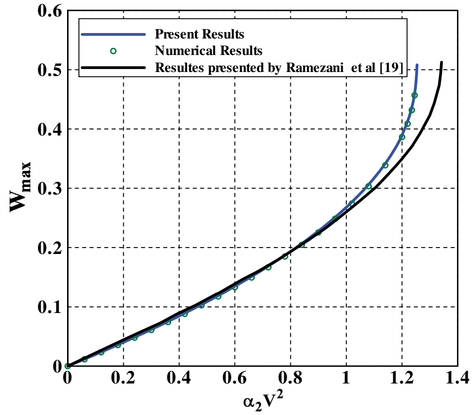

Fig. 6. Maximum deflection of the nanobeam under the effect of electric actuation and considering fringing field effect, in the absence of intermolecular forces when $d/b = 0.8$.

Figure 7 shows the effect of the parameter d/b, which is a measure of the fringing field effect on the pull-in and voltage deflection characteristics of the nano-switch. It is observed that with increasing the value of d/b, the value of the pull-in voltage decreases. This matter can be seen more clearly in Fig. 8.

Figure 9 shows the voltage deflection characteristics of a nano-switch under the combined effect of van der Waals force and electrostatic actuation for two different values for d/b and α_3.

In order to gain a more comprehensive understanding of the effect of van der Waals force, in Fig. 10 voltage-deflection curves of the nano-switch has been plotted for various values of α_3. With comparison of different curves in Fig. 10, one may conclude that in the analysis of NEMS, α_3 play an undeniable role. Figure 10 also shows

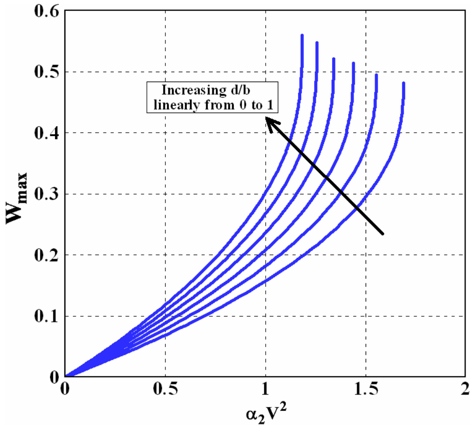

Fig. 7. Maximum deflection of the nanobeam under the effect of electric actuation, for various values of d/b.

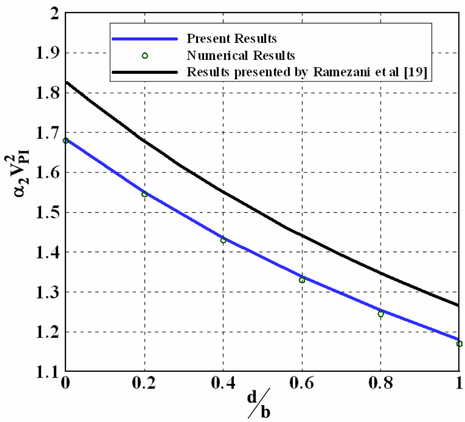

Fig. 8. Effect of fringing field on the pull-in characteristics of the nano-switch.

that with increasing the parameter α_3, the value of the pull-in voltage decreases. This has been shown in Fig. 11. Further more Fig. 11 greatly clarifies the importance of the fringing fields in the analysis of NEMS which neglecting its effect can make considerable errors for pull-in characteristics of the nano-switch.

The same discussions can be made when the effective intermolecular force is the Casimir force. Figure 12 shows the voltage deflection characteristics of a nano-switch under the combined effect of Casimir force and electrostatic actuation for two different values for d/b and α_4.

In Fig. 13 voltage-deflection curves of the nano-switch has been plotted for various values of α_4. This figure shows the important role of parameter α_4 in the analysis of NEMS.

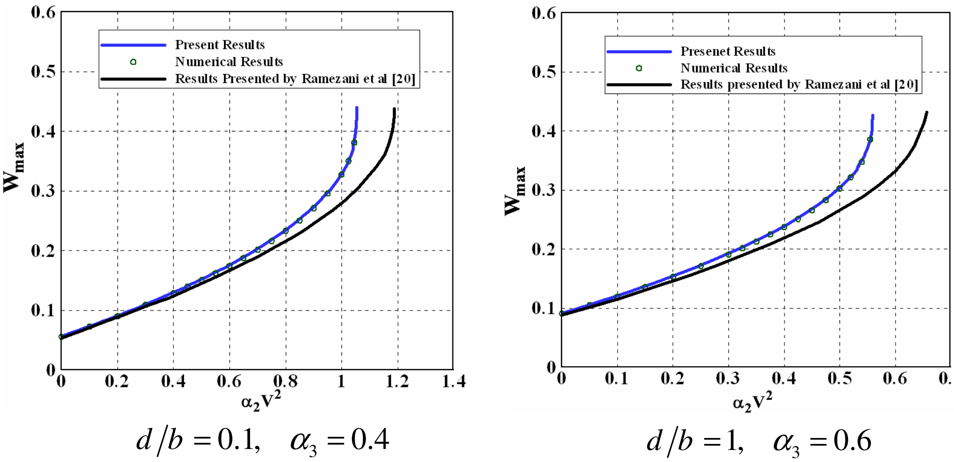

Fig. 9. Voltage deflection characteristics of a nano-switch under the combined effects of van der Waals force and electrostatic actuation.

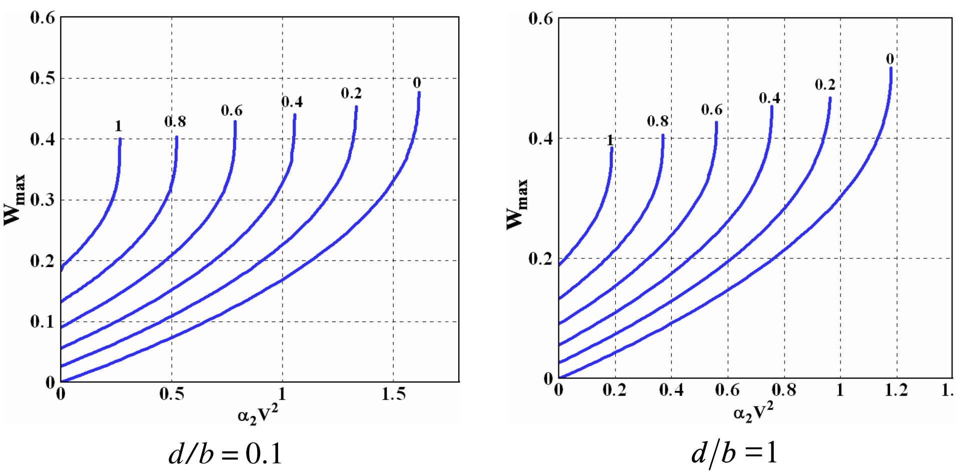

Fig. 10. Voltage-deflection curves of the nano-switch for various values of α_3.

One can use Fig. 13 to plot the value of the parameter $\alpha_2 V^2$ at the pull-in state at different values of α_4. The results have been shown in Fig. 14. Tong *et al.*[38] investigated the stability of nanodevices in the presence of Casimir and electrostatic forces. They calculated the pull-in parameters of the system and showed that for plates separated within the range of nanometer in distance, the Casimir effect can influence the stability of the device significantly. Figure 14 proves the same matter for nanobeams. Figure 14 also implies that when the effective intermolecular force is the Casimir force, fringing field effect cannot be ignored in the analysis of NEMS.

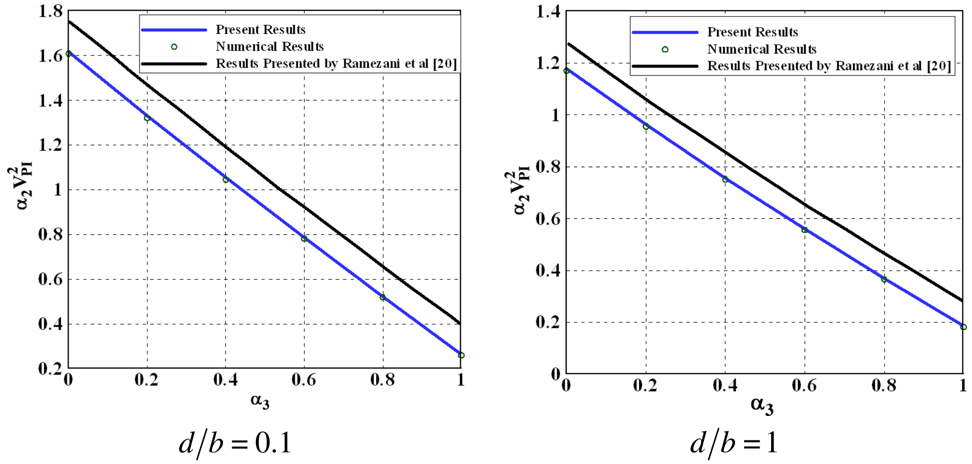

Fig. 11. Effect of the parameter α_3 on the value of $\alpha_2 V^2$ at pull-in.

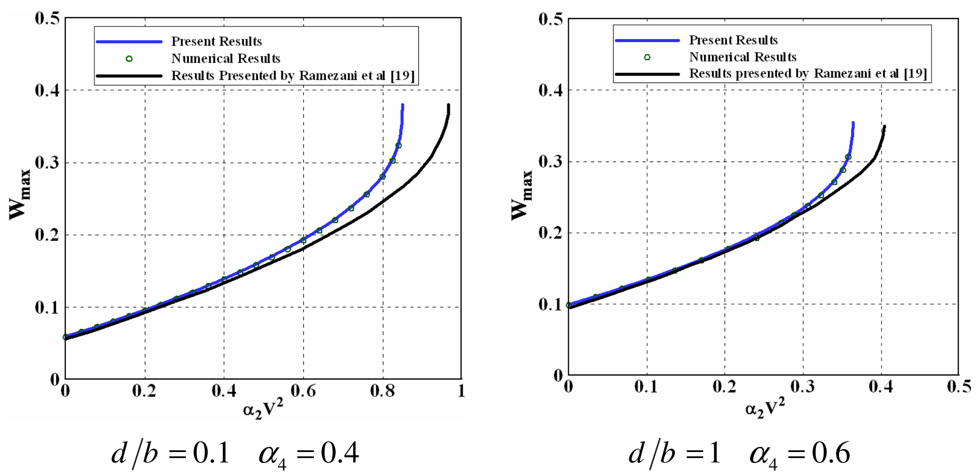

Fig. 12. Voltage-deflection characteristics of a nano-switch under the combined effects of Casimir force and electrostatic actuation.

From different figures in this paper one may easily conclude that HPM is an effective tool for analyzing N/MEMS devices. This method overcomes shortcomings of the previously reported Green function method,[19,20,23,30] which when dealing with distributed parameter models, usually overestimates instability of N/MEMS.

4. Conclusion

The current paper makes use of the HPM to analyze static deflection and pull-in characteristics of nano-switches under the effect of electrostatic and intermolecular

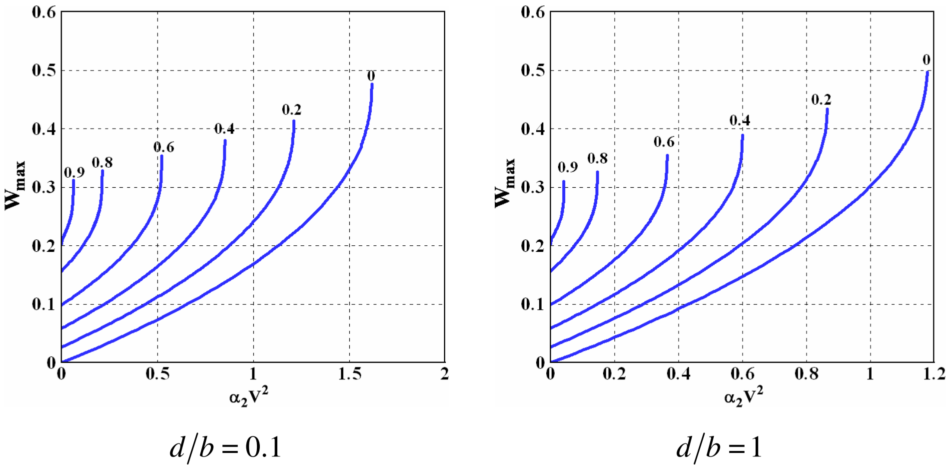

Fig. 13. Voltage-deflection curves of the nano-switch for various values of α_4.

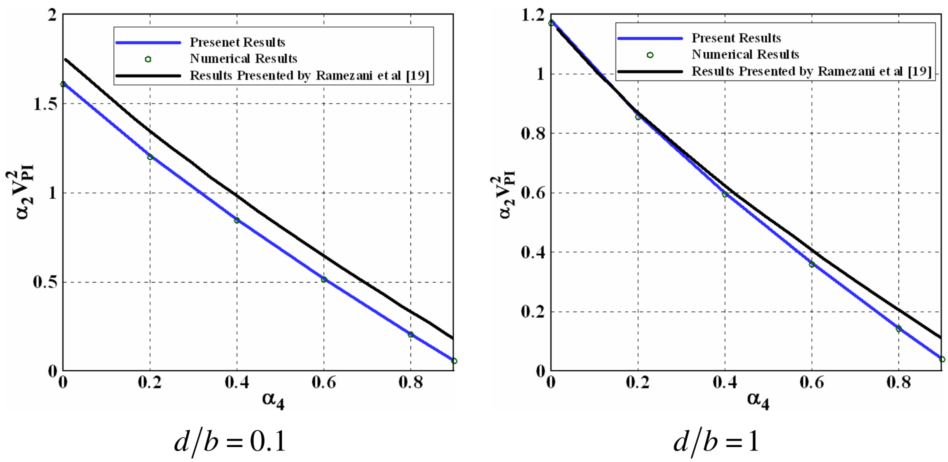

Fig. 14. Effect of the parameter α_4 on the value of $\alpha_2 V^2$ at pull-in.

surface forces. Using a Galerkin projection method, the nonlinear boundary value differential equation was reduced to a nonlinear algebraic equation which was solved by applying HPM. Three cases have been specifically investigated. These cases correspond to when the effective external force is the electrostatic force, the combined electrostatic and Casimir force and the combined electrostatic and van der Waals force. In all cases the pull-in characteristics has been investigated thoroughly. In most cases the results has been compared with numerical results and also with previously reported analytical results available in the literature. It was found that HPM modifies the overestimation of N/MEMS instability limits reported in the literature and can be used as an effective and accurate design tool in design optimization.

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