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Effect of Geometry in Frequency Response Modeling of Nanomechanical Resonators

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Abstract. The trend towards nanomechanical resonator sensors with increasing sensitivity raises the need to address challenges encountered in the modeling of their mechanical behavior. Selecting the best approach in mechanical response modeling amongst the various potential computational solid mechanics methods is subject to controversy. A guideline for the selection of the appropriate approach for a specific set of geometry and mechanical properties is needed. In this study, geometrical limitations in frequency response modeling of flexural nanomechanical resonators are investigated. Deviation of Euler and Timoshenko beam theories from numerical techniques including finite element modeling and Surface Cauchy-Born technique are studied. The results provide a limit beyond which surface energy contribution dominates the mechanical behavior. Using the Surface Cauchy-Born technique as the reference, a maximum error on the order of 50 % is reported for high-aspect ratio resonators.

Keywords: Nanomechanical Resonator, Finite Element Modeling, Frequency, Geometry

PACS: 02.70.Dh, 81.07.Gf, 85.85.+j, 68.35.Md

INTRODUCTION

High-frequency operation of nanomechanical resonators led to a new generation of detectors ranging from nanomechanical mass sensors with a resolution of 1.7 yoctogram [1] to force sensors of 12 nano-N [2] resolution and new biosensors [3]. These applications have resulted in the specific tendency in one-dimensional nanomechanical resonators made of nanowires (NWs) in the direction of ever smaller and stiffer systems. Such nanoelectromechanical systems (NEMS) with nanomechanical resonators usually operate as transducers, where their mechanical behavior necessitates a sound modeling approach [4]. Recently, it has been shown that due to the dominance of the free surface in nanoscale structures, mechanical properties exhibit a pronounced size dependence [5]. A distinct surface energy contribution at the nanoscale due to the difference in atomic arrangement is the main reason for the size dependence in nanostructures [6]. Recently, Park *et al.* proposed a multiscale Surface Cauchy-Born (SCB) method to incorporate surface energy in nanomechanical modeling. This method is based on the quasicontinuum approach, where the constitutive response in each quadrature point is obtained from atomistic calculations. This method has been shown to capture size dependence in resonance frequency of metals [7] due to stiffening and dramatic softening in Si NWs [8]. As the mechanical behavior in nanomechanical resonators is a key to the operation of the most of NEMS applications, modeling of their mechanical properties becomes a critical task. To do so, limitations of both analytical techniques and numerical tools including surface contribution have to be determined. The choice of the most suitable modeling approach for one particular application is subject to controversy, where a guideline is required for a specific set of geometry and mechanical properties. In this study, frequency response deviations in analytical models and numerical tools including the finite element method (FEM) and SCB as a function of aspect ratio (length-to-thickness ratio (L/a)) are investigated.

FORMULATION

There are several methods for frequency response modeling from simple classical strength approaches to more complicated numerical tools. In Euler-Bernoulli theory the motion is purely translational in thickness direction (rotational effects are to be neglected) and these transverse deflections are assumed to be small. Solving equation of motion in the transverse direction, w , in position x derives resonance frequency for a beam with given modulus

of elasticity (E), moment of inertia (I), density (ρ) and cross-sectional area (A). This approach can be improved by including rotatory inertia and shear effects based on Timoshenko beam theory. Additional parameters such as Timoshenko shear coefficient (k' : depending on the shape of the cross section) and shear modulus (G) (Figure 1) are required [9].

FIGURE 1. A snapshot of Analytical (Euler and Timoshenko) and Numerical (classical FEM and SCB) methods for frequency response modeling.

In FEM, the elastic modulus and mass density are implemented in numerical integrations and by utilizing the strain displacement matrix, the stiffness (K) and mass (M) matrix can be calculated. These two matrices are implemented in the generalized eigenproblem to derive the resonance frequency [10]. As opposed to the ordinary continuum approach one can extract the constitutive response from the interatomic potential based on the Cauchy-Born hypothesis [6, 7]. In this approach, Interatomic potential, U , for the total number of bonds, nb , in a representative atomic volume in undeformed body, Γ_0 , is converted into the strain energy density, $\phi(C)$. In order to convert this expression into a suitable form for the FEM calculations, atomic bond length, r_m , is deformed with the right stretch tensor, C . For nanoscale materials with high surface area, the surface energy will become important and contribute significantly to the total energy. At this point, the total energy for a continuum system should be divided into bulk and surface portions. The strain energy density on the surface, $\gamma(C)$, can be expressed in the same fashion as those of the bulk portions, while each point on the surface has fewer atomic bonds in comparison to those within the bulk. This difference in atomic arrangement on the surface causes a 3×3 surface tensor with normal components. This allows surface relaxation due to the lack of fully coordinated atoms at the surface. In each surface layer of the body, Γ_0 , atoms are not fully coordinated. The potential energy can be written in discretized form based on the nodal displacement u_i as

$$\psi(u_i) = \sum_{e=1}^{Ne} \left\{ \int \phi(C) d\Omega + \int \gamma(C) d\Gamma \right\} \quad (1)$$

The stiffness matrix with surface energy can be extracted by minimizing the total potential energy. Finally, the SCB resonance frequency can be found by solving equation (10).

CASE STUDIES

All numerical examples were performed on single-crystalline copper nanowires with $\langle 100 \rangle$ longitudinal orientation with 100 transverse surfaces as illustrated in Figure (1). Euler, Timoshenko, FEM and SCB models were utilized under fixed-fixed boundary conditions. Three different parametric studies are conducted in this work, which consider NWs with square constant cross-sectional area (SCSA), rectangular constant cross-sectional area (RCSA) and constant surface area-to-volume ratio (CSAV) as summarized in Table 1. Modulus of elasticity, shear modulus, mass density and Timoshenko shear coefficient were taken as 120 GPa, 48 GPa, 8960 kg/m³ and 5/6, respectively [11]. In finite

element and SBC calculations, the Lennard-Jones interatomic potential with interatomic distance $r_0 = 2.598\text{\AA}$, cut-off distance $r_c = 3.5\text{\AA}$, and potential constants of $\varepsilon = 0.167\text{eV}$, $\sigma = 2.315\text{\AA}$ were utilized to define the constitutive law [11]. Nanowires in SCB models were initially out of equilibrium due to the presence of the surface stresses. The minimum energy configuration was obtained while accounting for the surface stresses. Finite element meshes contained between 5000 and 11000 nodes. The eigenvalue problem (equation (10)) was solved by utilizing the Krylov-Schur method.

TABLE 1. Summary of geometries considered (All dimensions are $L \times b \times a$ in (nm)).

RCSA	RCSA	CSAV
$20 \times 10 \times 10$	$20 \times 20 \times 10$	$30 \times 10 \times 10$
$50 \times 10 \times 10$	$50 \times 20 \times 10$	$50 \times 9.375 \times 9.375$
$60 \times 10 \times 10$	$60 \times 20 \times 10$	$70 \times 9.13 \times 9.13$
$80 \times 10 \times 10$	$80 \times 20 \times 10$	$100 \times 8.955 \times 8.955$
$100 \times 10 \times 10$	$100 \times 20 \times 10$	$150 \times 8.823 \times 8.823$
$120 \times 10 \times 10$	$120 \times 20 \times 10$	$200 \times 8.759 \times 8.759$
$150 \times 10 \times 10$	$150 \times 20 \times 10$	$300 \times 8.696 \times 8.696$
$200 \times 10 \times 10$	$200 \times 20 \times 10$	$400 \times 8.665 \times 8.665$
$250 \times 10 \times 10$	$250 \times 20 \times 10$	
$300 \times 10 \times 10$	$300 \times 20 \times 10$	
$400 \times 10 \times 10$	$400 \times 20 \times 10$	

RESULTS AND DISCUSSION

Since the surface Cauchy-Born method provides the most accurate model for the frequency response, it was considered as the reference technique, against which the results of all other techniques are compared. Frequency responses for Euler, Timoshenko and FEM methods are normalized with the SCB method as a function of length to thickness ratio (Fig.2).

FIGURE 2. Fundamental resonance frequency as a function of the aspect ratio in Euler, Timoshenko and SCB methods for (a) RCSA, (b) CSAV, (c) RCSA for an aspect ratio range of 2 to 40, and (d) RCSA for an aspect ratio range of 10-40.

Three different aspect ratio zones - each with their particular deviation (more than 15%) from unity - are identified:

- Zone 1: A low aspect ratio beam, for which analytical formulations result in considerably larger resonance frequencies than the reference value estimated by the SCB-method.
- Zone 2: A conventional beam shape with close analytical and numerical calculations.
- Zone 3: A slender nanowire with high aspect ratio (aspect ratio more than 15), where surface tension has a significant contribution.

The overestimation of frequency by analytical techniques, especially Euler-Bernoulli, in zone 1 is evident in Figs. 2.a, 2.b and 2.d. This is due to neglecting shear and rotational effects (deformation in X and Z directions). The Timoshenko method has less deviation as the only involved assumption is keeping plane sections perpendicular to the deformed centroidal axis [9]. However, the analytical formulations in general show unreliability in this zone, whereas the finite element calculation can be utilized safely as they capture deformations with interpolation in all directions [10]. To evaluate the significance of this simplification in analytical calculations in Y direction, different RCSA geometries were studied (Fig. 2.b). The results show a geometrical dependence with the same overall trend as compared to SCSA, where three different aspect ratio zones including block form, normal beam and slender nanowire can be identified. Surface tension contribution has same fashion (Fig.2.c) as compared to SCSA, the main difference between the RCSA and SCSA cases is the increase of the deviation with respect to the analytical calculations. The results show that increasing the width leads to more deviation in analytical calculations due to strengthening influence of neglected deformation in X and Z directions.

An underestimation in all three methods for aspect ratios higher than 15 (zone 3) can be seen, where surface contribution is dominant. Results show an effective increase in resonance frequency due to the surface stress, which is created by unbalanced atoms on the surface. The surface-to-volume ratio is a key feature of a variety of studies in nanoscale mechanical response, where the surface effect is dominant [12]. But recent studies [7, 8] on frequency analysis for NWs show that the length to thickness ratio has a more profound effect. Hence, in the third study of the present work, CSAV was considered (Fig.2.d). Similar deviations for low aspect ratios in the analytical models as well as importance of the surface contribution for high aspect ratios can be seen same when comparing to the SCSA and RCSA cases. This underestimation in high aspect ratio for CSAV case represents that length-to-thickness ratio is a much more important parameter to analyze frequency response modeling than the surface-to-volume ratio.

CONCLUSION

The main findings of this work can be summarized as follows:

- The importance of geometrical limitations in the prediction of frequency response of flexural nanomechanical resonators.
- The general inapplicability of classical analytical calculations (Euler and Timoshenko beam theories) in low-aspect-ratio (less than 8).
- The importance of the surface stress effect in NWs with high aspect ratio (more than 15).

Deviation in the analytical calculations is more than 5 times and numerical calculation has twice deviation due to the surface stress. It should however be emphasized that all calculations have been performed for fixed-fixed boundary conditions. Other geometrical parameters and boundary conditions can be considered for further studies.

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