Proceedings of the 25th Nordic Seminar on Computational Mechanics
K. Persson, J. Revstedt, G. Sandberg, M. Wallin (Eds.)

The influence of surface elasticity on the flexural rigidity of nanowires

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Summary. This talk describes a recently derive continuum model for estimating the flexural rigidity of nanowires. The model is linear elastic and includes contributions of surface stiffness as a result of lowered coordination. Predictions of the model are validated by comparison to benchmark molecular dynamics and statics simulations via two examples: resonant properties of top-down nanowires and buckling of nanowires. Overall, the present work demonstrates that continuum mechanics can be utilized to study the elastic and mechanical behavior and properties of ultrasmall nanowires if surface elastic contributions to the flexural rigidity are accounted for.

Key words: surface elasticity, nanowires, molecular dynamics simulations

Introduction

Over the past two decades, dramatic technological progress made in the field of nanotechnology has made it possible not only to visualize but also manipulate, assemble and organize matter with high precision on the atomic scale. This has opened the possibility of fabricating structural nanodevices by piecing basic nanosized building blocks together to form grander, more complex and more elaborate systems; the so-called bottom-up strategy. This has led to a gain in interest from many different branches and disciplines in the scientific community, which has paved the way for the discovery and recognition of many novel physical properties of nanostructures that differ significantly from those of macroscopic structures [1].

However, applications where the mechanical properties are of importance have been plagued with difficulties in predicting the mechanical response accurately. An examples of this is, for instance, nanoscale resonators where the flexural rigidity plays a central role [2]. The flexural rigidity of nanowires is highly affected by surface elastic contributions as a result of the high surface to volume ratio of nanostructures and the lowered coordination of surface atoms.

The purpose of this talk is to discuss a recently derived continuum model for estimating the flexural rigidity of nanowires. The model is linear elastic and includes the surface elastic contributions to the flexural rigidity through the second moment, which accounts for the fact that surfaces are subjected to the greatest amounts of strain in bending. Details of the model can be found in [3].

Continuum model

Based on the seminal work by Dingreville and coworkers [4], it is assumed that the surface energy density, Γ, can be expanded in terms of the surface strains, $\epsilon^s_{\alpha\beta}$,

$$\begin{aligned}\Gamma(\epsilon^s_{\alpha\beta}) &= \Gamma_0 + \frac{\partial\Gamma}{\partial\epsilon^s_{\alpha\beta}}\epsilon^s_{\alpha\beta} + \frac{1}{2}\frac{\partial^2\Gamma}{\partial\epsilon^s_{\alpha\beta}\epsilon^s_{\gamma\eta}}\epsilon^s_{\alpha\beta}\epsilon^s_{\gamma\eta} + \cdots = \\ &= \Gamma_0 + \Gamma^{(1)}_{\alpha\beta}\epsilon^s_{\alpha\beta} + \frac{1}{2}\Gamma^{(2)}_{\alpha\beta\gamma\eta}\epsilon^s_{\alpha\beta}\epsilon^s_{\gamma\eta} + \cdots \end{aligned} \quad (1)$$

where Γ_0, $\Gamma^{(1)}_{\alpha\beta}$, and $\Gamma^{(2)}_{\alpha\beta\gamma\eta}$ are the area specific surface energy density, the surface stress, and the surface elastic constants, respectively. Greek indices are 1 and 2 and repeated indices are summed. These surfaces are assumed to be flat and of infinitesimal thickness, which is an approximation as the influence of the surfaces has a finite range. Moreover, it is assumed that the potential energy of the bulk can be expanded in terms of the bulk strains

$$\begin{aligned}\Phi(\epsilon_{ij}) &= \Phi_0 + \tfrac{\partial \Phi}{\partial \epsilon_{ij}}\epsilon_{ij} + \tfrac{1}{2}\tfrac{\partial^2 \Phi}{\partial \epsilon_{ij}\partial \epsilon_{kl}}\epsilon_{ij}\epsilon_{kl} + \cdots = \\ &= \Phi_0 + \sigma_{ij}\epsilon_{ij} + \tfrac{1}{2}C_{ijkl}\epsilon_{ij}\epsilon_{kl} + \cdots \end{aligned} \tag{2}$$

where Φ_0, σ_{ij}, and C_{ijkl} are the volume specific energy density, the bulk stress tensor, and the bulk elastic constants, respectively. Roman indices range from 1 to 3 and repeated indices are summed. The surface and bulk contributions add up to the total strain energy

$$U(\epsilon_{ij}) = \int_{V_0}\int_0^{\epsilon_{ij}} \frac{\partial \Phi}{\partial e_{ij}} de_{ij} dV + \int_{A_0}\int_0^{\epsilon^s_{\alpha\beta}} \frac{\partial \Gamma}{\partial e^s_{\alpha\beta}} de^s_{\alpha\beta} dA \tag{3}$$

The surfaces are assumed to be rigidly attached to the bulk, which means that the surface strains can be obtained from the bulk strains simply through an appropriate projection operation. The flexural rigidity can the be found from by taking a weighted integral of the elastic properties over the cross section and bounding surface

$$\mu^{(2)} = \int_A E_b z^2 dA + \oint_S E_s z^2 dS \tag{4}$$

where Young's modulus of the bulk and the surfaces are denoted E_b and E_s, respectively. This way the composite character of the elastic properties across the nanowire cross section is accounted for, which gives an improved estimate of the flexural rigidity.

Atomistic simulations

To benchmark the continuum formulation we consider the special cases of slender $\langle 100\rangle/\{100\}$ and $\langle 100\rangle/\{110\}$ metallic face centered cubic (fcc) doubly clamped nanowires with square cross sections. Two different boundary value problems have been considered: the fundamental eigenfrequency of top-down nanowires subjected to transverse vibrations, and the critical compressive strain leading to buckling instability. We have obtained benchmark results for both boundary value problems using both classical molecular statics (MS) and molecular dynamics (MD) simulations. The interatomic interaction is modelled through an embedded atom method (EAM) potential fitted to properties for gold [5]. The relevant surface properties are evaluated using the free surface strain meshing technique suggested by Shenoy [6].

Resonant properties

The nanowires are called top-down as they can be considered to have been etched out from a bigger piece of matter while being rigidly constrained at both ends. Because of this, the interplanar distance along the wire axis corresponds to that of the ideal. The atomistic simulations are performed at liquid Helium temperature, e.g. 4.2 K, as described by [5] and the reader is referred to that paper for numerical details.

In Fig. 1 we have compared the fundamental eigenfrequency attained from atomistic simulations of $\langle 100\rangle/\{100\}$ top-down nanowires with the aspect ratio 12, with predictions of the newly derived continuum model and the those of macroscopic Bernoulli-Euler beam theory for different cross sectional widths. It can be seen that the atomistic results are in great agreement with those derived from the continuum model, while macroscopic continuum beam theory severely underestimates the fundamental eigenfrequency. This discrepancy is attributed to two separate

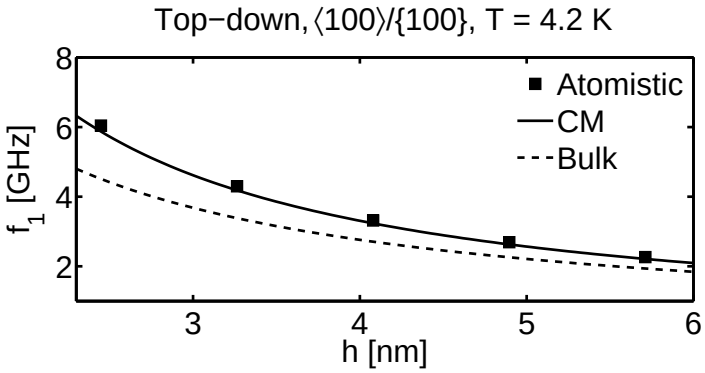

Figure 1. The fundamental eigenfrequency for $\langle 100\rangle/\{100\}$ top-down nanowires of different cross sectional dimensions. The aspect ratio of all nanowires is 12. The markers correspond to atomistic results, the solid and dashed lines are predictions from the newly derived continuum model and macroscopic beam theory, respectively.

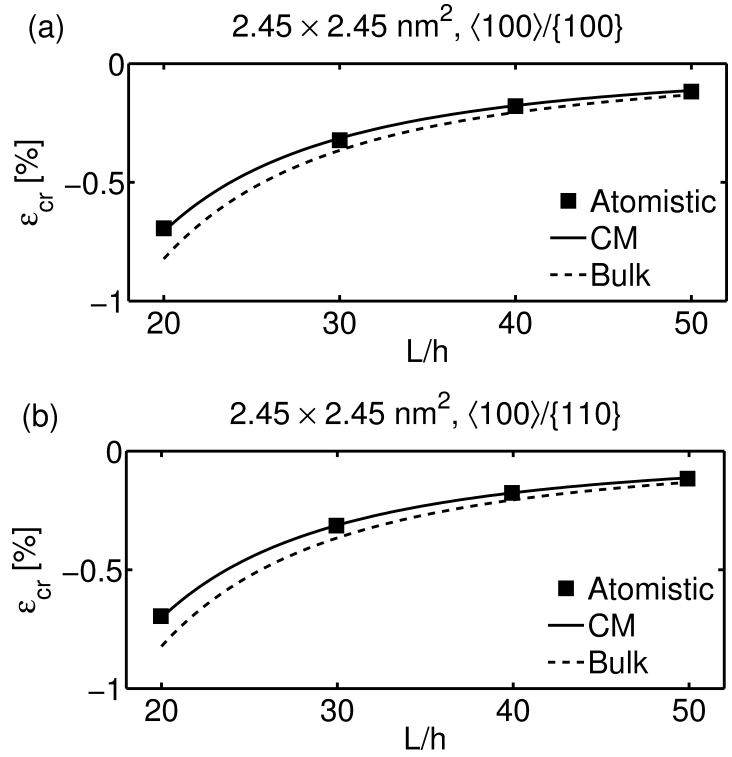

Figure 2. Critical buckling strain for (a) $\langle 100\rangle/\{100\}$ and (b) $\langle 100\rangle/\{110\}$ nanowires with $2.45 \times 2.45\text{nm}^2$ cross sections for different aspect ratios.

contributions. First, the lack of influence of surface elastic properties on the flexural rigidity. The second and most important mechanism is the lack of surface stress in the macroscopic beam picture. Both of these contributions are accounted for in the newly derived continuum model.

Buckling

The most important test of the new formulation is to evaluate how well buckling can be described by the present formulation. The reason why buckling is of greater interest than the eigenfrequency spectra of nanowires is due to the dependence of each boundary value problem

on the flexural rigidity. The atomistic results are taken from [7] where the numerical details are given.

In Figs. 2(a) and (b) we have compared the critical buckling strain for $\langle 100 \rangle / \{100\}$ and $\langle 100 \rangle / \{110\}$ nanowires with 2.45×2.45 nm^2 cross sections for different aspect ratios, respectively. It can be seen that the bulk predictions overestimate the atomistic results and the newly derived continuum model predicts critical strains that are in excellent agreement with the atomistic results. This is an effect that emanates solely from the heterogeneous description of the cross section when calculating the flexural rigidity.

Conclusions

In this presentation we have described a novel continuum formulation for dealing with the influence of surface effects influence on the mechanical properties of nanowires. The model has been compared with results from atomistic simulations and has been proven to show great accuracy. In addition to the benchmark tests in this abstract a plethora of comparisons have been documented in [3].

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