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Surface stress effects on the resonant properties of metal nanowires: The importance of finite deformation kinematics and the impact of the residual surface stress

Harold S. Park [a,*], Patrick A. Klein [b]

[a] Department of Mechanical Engineering, University of Colorado, Boulder, CO 80309, USA
[b] Franklin Templeton Investments, San Mateo, CA 94403, USA

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ABSTRACT

We utilize the recently developed surface Cauchy–Born model, which extends the standard Cauchy–Born theory to account for surface stresses due to undercoordinated surface atoms, to study the coupled influence of boundary conditions and surface stresses on the resonant properties of ⟨1 0 0⟩ gold nanowires with {1 0 0} surfaces. There are two major purposes to the present work. First, we quantify, for the first time, variations in the nanowire resonant frequencies due to surface stresses as compared to the corresponding bulk material which does not observe surface effects within a finite deformation framework depending on whether fixed/free or fixed/fixed boundary conditions are utilized. We find that while the resonant frequencies of fixed/fixed nanowires are elevated as compared to the corresponding bulk material, the resonant frequencies of fixed/free nanowires are reduced as a result of compressive strain caused by the surface stresses. Furthermore, we find that for a diverse range of nanowire geometries, the variation in resonant frequencies for both boundary conditions due to surface stresses is a geometric effect that is characterized by the nanowire aspect ratio. The present results are found to agree well with existing experimental data for both types of boundary conditions.

The second major goal of this work is to quantify, for the first time, how both the residual (strain-independent) and surface elastic (strain-dependent) parts of the surface stress impact the resonant frequencies of metal nanowires within the framework of nonlinear, finite deformation kinematics. We find that if finite deformation kinematics are considered, the strain-independent surface stress substantially alters the resonant frequencies of the nanowires; however, we also find that the strain-dependent surface stress has a significant effect, one that can be comparable to or even larger than the effect of the strain-independent surface stress depending on the boundary condition, in shifting the resonant frequencies of the nanowires as compared to the bulk material.

1. Introduction

Over the past decade, nanowires, both metallic and semiconducting, have drawn considerable interest from the scientific community (Xia et al., 2003; Lieber, 2003). The large interest in nanowires has largely been driven by their

* Corresponding author. Tel.: +1 303 492 7750; fax: +1 303 492 3498.
E-mail address: harold.park@colorado.edu (H.S. Park).

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remarkable physical properties, most of which emerge due to their small size and thus large surface area to volume (SAV) ratio. These properties range across the scientific disciplines, including unusual or enhanced optical (Canham, 1990; Barnes et al., 2003), electrical (Wiley et al., 2006; Rubio et al., 1996; Ohnishi et al., 1998), thermal (Li et al., 2003) and mechanical (Wong et al., 1997; Cuenot et al., 2004; Wu et al., 2005; Jing et al., 2006) properties.

Nanowires are also important as they will serve as the basic building blocks for future nanoelectromechanical systems (NEMS), which have been proposed for a multitude of cross-disciplinary applications, including chemical and biological sensing, force and pressure sensing, high frequency resonators, and many others (Cleland and Roukes, 1996; Huang et al., 2003; Craighead, 2000; Lavrik et al., 2004; Ekinci and Roukes, 2005; Ekinci, 2005). Because many of the proposed applications for nanowire-based NEMS, such as resonant mass sensing and high frequency oscillators (Craighead, 2000; Lavrik et al., 2004; Ekinci and Roukes, 2005) rely on the ability to control and tailor the nanowire resonant frequencies with a high degree of precision, it is critical to be able to predict and control variations in the nanowire resonant frequencies.

The potential of nanowires in future nanotechnologies has led to significant interest in experimental characterization of the size-dependent elastic properties of nanowires. The experimental techniques utilized have varied from time-resolved spectroscopy (Petrova et al., 2006) to AFM-induced bending (Wong et al., 1997; Wu et al., 2005; Heidelberg et al., 2006; Cuenot et al., 2004; Jing et al., 2006; Hoffmann et al., 2006; Chen et al., 2006; Namazu et al., 2000; Sundararajan et al., 2002) or resonance measurements (Verbridge et al., 2006, 2007; Cleland and Roukes, 1996; Husain et al., 2003; Nam et al., 2006; Dikin et al., 2003; Yang et al., 2001; Houston et al., 2002; Evoy et al., 2000). In general, resonance measurements to obtain the nanoscale elastic properties are predominant in the literature due to their relative simplicity as compared to bending and tensile experiments at the nanoscale due to the reduced amount of nanowire manipulation involved in resonance-based testing. The experimental results show significant scatter, with some predictions of enhanced elastic stiffness (Husain et al., 2003; Cuenot et al., 2004; Jing et al., 2006), some predicting reduced elastic stiffness (Petrova et al., 2006) with decreasing nanostructure size, and some predicting no change with respect to the bulk elastic stiffness (Wu et al., 2005; Heidelberg et al., 2006).

The difficulty in predicting the resonant properties of nanowires stems from the fact that they are characterized by a large SAV ratio; because of this, nanowires are subject to surface stresses (Cammarata, 1994; Haiss, 2001), which occur due to the fact that surface atoms have fewer bonding neighbors than do atoms that lie within the material bulk. Surface stresses have been predicted to cause many non-bulk phenomena in nanowires, including self-healing behavior and phase transformations (Diao et al., 2003; Park et al., 2005; Liang et al., 2005b), and non-bulk elastic properties (Zhou and Huang, 2004; Liang et al., 2005a; Dingreville et al., 2005; Cuenot et al., 2004; Jing et al., 2006; Shenoy, 2005).

The knowledge that surface effects are critical to understanding the mechanical behavior and properties of nanomaterials has motivated the development of enhanced continuum models, as standard continuum mechanics is length scale independent. Various analytic models have been developed to study the effects of surface stress on the resonant properties of nanobeams (Lu et al., 2005; Gurtin et al., 1976; Sader, 2001; McFarland et al., 2005), or more generally to capture the non-bulk mechanical properties of nanostructures (Gurtin and Murdoch, 1975; Miller and Shenoy, 2000; Shenoy, 2005; Sharma et al., 2003; Sun and Zhang, 2003; Dingreville et al., 2005; Wei et al., 2006; Wang et al., 2006; Tang et al., 2006; Lu et al., 2005; Gurtin et al., 1976; Sader, 2001; Huang et al., 2006; McFarland et al., 2005). Due to assumptions utilized to make the analyses tractable, the coupled effects of geometry, surface orientation and system size on the resonant properties of nanowires have not been quantified, nor have surface stress effects arising directly from atomistic principles been included in the analyses, which are generally in two-dimensions. The analyses also utilize overly simplistic pair-type atomic interactions to describe the surface physics, which tend to incorrectly predict a compressive surface stress for metals, whereas the surface stress for metals is almost always tensile. These errors indicate that quantitative analyses for real materials cannot be made using these approaches.

There are two major goals to the present work. The first is to quantify, for the first time, how surface stresses may be expected to alter the resonant frequencies for gold nanowires with a ⟨1 0 0⟩ axial orientation and {1 0 0} transverse surfaces considering both fixed/fixed and fixed/free boundary conditions as compared to the corresponding bulk material that does not observe nanoscale surface stress effects. These boundary conditions are ubiquitous in the study of NEMS, as most NEMS employ nanomaterials such as nanowires and nanotubes as the active beam element.

We obtain the resonant frequencies using the recently developed surface Cauchy–Born (SCB) model (Park et al., 2006; Park and Klein, 2007, 2008; Park, 2008a, b). The uniqueness of the SCB approach as compared to other analytical and theoretical (Gurtin and Murdoch, 1975; Miller and Shenoy, 2000; Shenoy, 2005; Sharma et al., 2003; Sun and Zhang, 2003; Dingreville et al., 2005; Wei et al., 2006; Wang et al., 2006; Tang et al., 2006; Lu et al., 2005; Gurtin et al., 1976; Sader, 2001; Huang et al., 2006; McFarland et al., 2005) surface elastic models is that it enables the solution of three-dimensional nanomechanical boundary value problems for displacements, stresses and strains in nanomaterials using standard nonlinear finite element (FE) techniques (Belytschko et al., 2002), with the nonlinear, finite deformation material constitutive response obtained directly from realistic interatomic potentials such as the embedded atom method (EAM) (Daw and Baskes, 1984). Furthermore, the usage of a standard FE formulation enables the consideration of arbitrary geometries and various materials once the SCB model has been developed.

Therefore, the resonant properties of the gold nanowires are determined by solving a standard FE eigenvalue problem for the resonant frequencies and associated mode shapes, with full accounting for surface stress effects through the FE stiffness matrix. The present analysis does not account for factors that are known to deleteriously impact the resonant properties of nanostructures, including clamping losses and thermoelastic damping (Ekinci et al., 2004; Cleland and