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Modification of the elastic properties of nanostructures with surface charges in applied electric fields

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ABSTRACT

The influences of applied electric fields and surface charges on elastic modulus of nanostructures such as nanowires and nanofilms are investigated within the framework of classic continuum mechanics. Under an applied electric field, the surfaces of structures are subjected to the electrostatic forces (negative pressure) along the direction of the electric field, and the resulting surface charges also change the surface mechanical properties due to the Hellman–Feynman (H–F) forces. Through incorporating the surface energy from the negative pressure and the H–F forces into surface free energy, the exact and analytical expressions of the effective elastic modulus of nanowires and nanofilms are addressed by considering the surface energy effects on the elastic modulus of nanostructures, which involves the contribution of the applied electric field and surface charges. The numerical results indicate that applied electric fields parallel to the axis of the nanowire and nanofilms enhance the transverse Young's modulus while reducing axial modulus of nanostructures. The effective modulus of nanowires and nanofilms with lateral surface charges depends on the surface charges density and the sign of the charges. In addition, the effect of electric field and surface charges on Young's moduli of nanowires and nanofilms has been found to be sensitive to structural geometric dimensions such as the thickness of the film and the diameter of the wire.

1. Introduction

With the reduction of the dimensions into nanoscale in microelectronic and micromechanical devices, nanostructures have attracted great interest in many scientific and technological fields. When one or more dimensions of a structural element are in the nano-level, the structures may arise completely different and exceptional physical properties including electronic, magnetic and optical properties (Wharam et al., 1988; Lee et al., 1995; Huang et al., 2001; Gudikson et al., 2002; Bauer et al., 2004; McGary et al., 2006), compared to those of corresponding macroscopic structures. Moreover, many researches have indicated that the nanostructures display novel mechanical behaviors that differ from the bulk ones, showing sizes effects such as the inverse H–P relationship of nanocrystalline materials and the size-dependent elastic properties of low-dimensional structures such as nanowires, nanotubes, nanobelts, nanofilms et al. (e.g., Chokshi et al., 1989; Konstantinidis and Aifantis, 1998; Li et al., 2003; Nilsson et al., 2004; Jing et al., 2006).

A great deal of research has been carried out both in theory and in experiment on the size effects of elastic properties for nanostructures. It is well-known that the surface plays much important role for nanostructures due to the increasing ratio of the surface area to the bulk, the mechanical property of the surface which differs from that of the bulk thus need to be taken into account for achieving the effective elastic properties of nanostructures. Theoretically, many attempts have been made to address the analytical expression of size-dependent elastic properties of nanostructure based on a framework of the continuum theory of mechanics, through incorporating the surface free energy into the total strain energy (e.g., Shenoy and Freund, 2002; Sharma et al., 2003, Sharma and Ganti, 2002, 2003, 2004; Wang et al., 2003; Zhang and Sharma, 2005; Duan et al., 2005; Dingreville et al., 2005; Lim et al., 2006; He and Lilley, 2008). Besides of the classical continuum theory, the first principle calculation (Miller and Shenoy, 2000; Yan et al., 2006; Zhang and Huang, 2006) is applied to investigate the elastic properties of nanostructures. On the other hand, researchers also utilized the atomistic or molecular simulations to analyze the size

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effects on elastic constants of nanostructures (Streitz et al., 1994a,b; Schioz et al., 1998; Miller and Shenoy, 2000; Sun and Zhang, 2003; Zhou and Huang, 2004; Diao et al., 2004; Shenoy, 2005; Park et al., 2006; Olsson et al., 2007; McDowell et al., 2008; Park and Klein, 2008). Experimentally, it has been proved in many measurements that the elastic properties of the structural elements at the nanoscale represent size-dependent notably (e.g., Wong et al., 1997; Cuenot et al., 2000, 2004; Wu et al., 2005; Jing et al., 2006; Chen et al., 2006; Nam et al., 2006). For experimental measurements on the mechanical properties of nanostructures, electromechanical and magnetomechanical approaches are often applied, e.g., Wang et al. (2001) and Dikin et al. (2003) determined the Young's modulus of nanotubes/nanowires based on the electromechanical resonances induced by *in-situ* transmission electron microscopy(TEM) and scanning electron microscope(SEM) respectively (Lefevre et al., 2005; Tabib-Azar et al., 2005; Hall et al., 2006).

The previous studies for the mechanical properties of nanostructures, however, are quite scarce to investigate the impact of applied fields, for example the electromagnetic fields, on the elastic properties of nanostructures (Zheng and Zhu, 2006; Desai and Haque, 2007). Not only on the aspects of the applications of nanoelectromechanical systems(NEMS) but also of the measurements of mechanical properties for nanostructures based on electromechanical and magnetomechanical drive, it can be arised for the multi-fields coupling problem between the electromagnetic and mechanical fields. Therefore, it is very important to study the influence of applied fields as well as surface charges on the mechanical properties of nanostructures for the veracity of the measured Young's modulus of nanostructures and the evaluation of mechanical properties of nanostructures in NEMS. The objective of this paper is to discuss the effects of electric fields and surface charges on the elastic properties of nanostructures such as nanowires and nanofilms.

Some of previous works have shown that there exists the relationship between the mechanical and electric properties for the elements of NEMS. For example, Purcell et al. (2002) used field emission to observe the vibration resonances of carbon nanotubes which can be tuned by the tension stemmed from the applied field; Sapmaz et al. (2003) analyzed the interaction theoretically between electrical and mechanical properties of suspended, doubly clamped carbon nanotubes subjected to charging effects, and showed that the tube is bended by the applied gate voltage to change the stress and thus influences the electrical and mechanical properties; Xu et al. (2005a,b) studied the mechanical resonance of a carbon nanotube in in-site transmission electron microscopy and found the coupling interaction between the field emission (FE) of a nanotube under a dc voltage applied longitudinally and its mechanical resonance stimulated transversely by an ac field; Kozinsky et al. (2006) addressed an electrostatic mechanism for nonlinearly tuning resonant frequencies of SiC beam for nanomechanical resonators and a theoretical model is developed to qualitatively explain the experimental results. Gao and Suo (2003) and Suo et al. (2004) presented a diffusion equation based on the free energy functional which accounts for the influence of surface charges on the surface stress, to simulate the pattern transfer process for the molecules dipoles on the metal surface. Nevertheless, these works haven't discussed the interplay between applied electromagnetic fields and elastic properties such as Young's modulus of nanostructures. Even though some of researchers investigated the coupling interaction between electrical and mechanical properties of carbon nanotubes (Keblinski et al., 2002; Gartstein et al., 2002; Verissimo-Alves et al., 2003; Hartman et al., 2004; Tang et al., 2006), these studies haven't presented the influence of applied electrical field on elastic modulus of nanostructures. The mechanical properties of nanostructures are one of the key factors for fabricating NEMS, it is quite important for nanostructures to carry out mechanical properties evaluation precisely to help design reliable NEMS.

In this paper, the Young's moduli of nanowires and nanofilms under applied electric fields are studied. Thanks to the presence of electrostatic charges on the surfaces of structures arising from the applied electric field, the surfaces suffer from the negative pressure and the surface energy can be modified notably. Meanwhile, Hellman–Feynman forces which result from the surface charges can also change the state of the surface stress and strain (Weigend et al., 2006). Therefore, with the aid of incorporating the surface energy stemmed from the surface electrostatic force into the surface free energy of nanostructures, the exact and analytical expressions of effective elastic modulus of nanowires and nanofilms are obtained by considering the surface energy effects on the elastic properties of nanostructures. According to the definition of Young's modulus, the modulus of nanowires and nanofilms in three orthogonal directions can be obtained, and a further quantitative discussion is made to illuminate the electric field effects and size effects of Young's modulus of nanowires and nanofilms under applied electric fields. The calculated results indicate that the transverse and axial Young's modulus are dependent significantly on the magnitude and direction of applied electric fields as well as the geometrical parameters of nanowires and nanofilms.

2. Theoretical model

2.1. Surface energy of nanostructures with surface charges in applied electric fields

When a structure is in an applied electric field **E**, the electrostatic forces arising from the electric charges induced on the surfaces of structure will be exerted on its surface. Generally, the electrostatic forces on the surfaces are weak so that it can be considered for a few atomic layers near the surface. Therefore, the surface stress generated by the electrostatic force can be introduced as the normal component of surface stress tensor which is always excluded in the absence of applied electric field. Have denoted the normal component of surface stress tensor as ${}_{n}^{E}\boldsymbol{\Gamma}^{s}$ and the corresponding strain normal to the surface as ${}_{n}\boldsymbol{\varepsilon}^{s}$, the increased surface energy $U^{s}{}_{E}$ arising from the applied electric field can be written as $\int_{A}{}_{n}^{E}\boldsymbol{\Gamma}^{s}\cdot{}_{n}\boldsymbol{\varepsilon}^{s}\mathrm{d}A$. It is noted that the bulk tensile stress and strain relevant to the electrostatic force can be expressed as ${}_{n}\boldsymbol{\sigma} = \mathbf{F}/A^{s} = \rho_{e}\mathbf{E}$ and ${}_{\mathrm{n}}\boldsymbol{\varepsilon}$, respectively. Here, A^{s} is the area of a surface of the structural element with electrostatic charges, the subscript n is the normal direction of the surfaces, $\rho_{\mathrm{e}} = \mu E$ is the charge density per area in the surfaces where μ is the permittivity of vacuum. According to the equivalency between the surface strain energy and the body strain energy stemmed from the electrostatic force, namely

$$U_{E}^{s} = \int_{A}{}_{n}^{E}\boldsymbol{\Gamma}^{s}\cdot{}_{n}\boldsymbol{\varepsilon}^{s}\,\mathrm{d}A = \int_{V}{}_{n}\boldsymbol{\sigma}\cdot{}_{n}\boldsymbol{\varepsilon}\,\mathrm{d}V, \tag{1}$$

one can obtain the surface stress ${}_{n}^{E}\boldsymbol{\Gamma}^{s}$ normal to the surface for structural elements in the electric field through the coordinate transformation between the bulk strain and the surface strain.

On the other hand, the change of surface stress and strain produced by the H–F forces on the charged surfaces must be taken into account in the total surface strain energy comparing with the one without surface charges for nanostructures. It has been demonstrated in the previous work (Weissmüller and Kramer, 2005) that the surface stretch and the tangent strain can be regarded as