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Surface effects in non-uniform nanobeams: Continuum vs. atomistic modeling

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ABSTRACT

Nanobeams are expected to be one of the key structural elements in nanotechnology. Contrary to macroscopic structures, surface effects can strongly influence the stress and deformation properties of nano-devices. In addition, at such small scales, material non-uniformity becomes significant and must be considered.

In this work, a continuum model for nanobeams, including both surface effects and material heterogeneity is developed. The model treats the surfaces as separate material layers with finite thickness. The continuum solution is compared with atomistic simulations, from which the effective bulk and surface properties are computed independently. A special case of self-deflection due to surface non-uniformities, which is important for design of nanosensors, is studied. A comparison between continuum and atomistic solutions reveals differences, which originate from local transition effects in the neighborhood of strong non-uniformities. This discrepancy is addressed by defining an effective length, found by correlating the beam deflections from both methods.

1. Introduction

In macroscopic and even microscopic structural elements, such as beams and plates, surface effects can be neglected and classical theories (Reddy, 1999) are sufficient. As the structural size decreases towards the nanoscale regime, the surface-to-bulk energy ratio increases and surface effects must be taken into account.

Surface effects can be characterized by two mechanical properties derived from surface energy: surface integrated residual stress and surface integrated modulus, denoted here by τ' and S'. Both τ' and S' are defined effectively by integration along the surface thickness that is assumed to be infinitesimal. These properties can be understood from either thermodynamic or atomistic considerations (Cammarata, 1994; Haiss, 2001; Müller and Saúl, 2004). For a given inter-atomic potential, τ' and S' can be calculated either analytically or numerically (Shenoy, 2005). It was found that the surface integrated residual stress can be either tensile ($\tau' > 0$) or compressive ($\tau' < 0$) and that the surface integrated modulus (S') can be either positive or negative. S' is associated with hardening or softening of nano-components, relative to their macroscopic counterparts, as observed for example in the experiments of Cuenot et al. (2004).

A continuum theory incorporating surface effects was originally developed by Gurtin and Murdoch (1975). Their work was followed by many theoretical studies on different structural elements, such as plates and beams (Lim and He, 2004; Sader, 2001, 2002; Lu et al., 2006; Huang, 2008; Bar On, 2010; Bar On and Altus, 2010). Miller and Shenoy (2000) used a continuum approach that included τ' and S', which were computed by atomistic simulation. Their study led to the definition of a critical thickness for nanobeams, above which surface integrated modulus effects can be neglected.

Another effect that characterizes the nanoscale is inherent material heterogeneity. Two types of heterogeneities are possible: surface and bulk. Heterogeneities may originate either from the basic structure of the material, such as grains in a polycrystal, or from various types of defects or contaminations. A complete theoretical model for nanobeams must address both surface and heterogeneity effects.

In this work, we study the displacements of a heterogeneous nanobeam under plane strain conditions, including geometric nonlinearity (rotations). The displacement governing equations (continuum) are formulated based on an equivalent single-layer approach normally used for composite materials (Reddy, 2003). The model is validated by comparison with atomistic simulations using a Lennard-Jones inter-atomic potential.

The study is focused on the case of self-deflections (no external loads) of nanobeams, caused directly from surface non-uniformities. These non-uniformities may originate from either directed design (actuation by local surface doping) or spontaneous effects (environmental), which can be used for the design of self-activated sensors (Lavrik et al., 2004; Bar On, 2010; Bar On and Altus, 2010).

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Symbols and signs

Atomistic parameters

a_0	lattice parameter
r_{cut}	interaction cutoff radius
σ	Lennard-Jones characteristic length
ε	Lennard-Jones characteristic energy

Continuum parameters

$E^{(k)}$	layer modulus
$t^{(k)}$	layer residual stress
$h^{(k)}$	layer thickness
$\sigma^{(k)}$	layer stress
$\varepsilon^{(k)}$	layer strain

Normalized structural parameters

d	axial stiffness
k	bending stiffness
f_s	surface residual force
m_s	surface residual moment
λ^2	total cross-sectional internal force

2. Governing equations for a heterogeneous nanobeam with surface effects

2.1. Descriptions and definitions

Consider a beam under plane strain conditions with thickness h, length L ($h/L \ll 1$) and width b in the out-of-plane direction. The classical approach for including surface effects is to treat the surface as a uniform layer with infinitesimal thickness and *integrated* effective properties: surface integrated residual stress τ' and surface integrated modulus S' (Gurtin and Murdoch, 1975). In case of nanobeams, with thickness on the order of 10–100 atomic layers, the surface thickness is small but not infinitesimal. Moreover, material non-uniformities must be considered as well.

We are interested in generalizing the classical approach by considering a heterogeneous nanobeam composed of three layers: a "bulk layer" (middle) and two finite thickness "surface layers" (upper and lower). The three layers are denoted by a superscript $k = 0,1,2$ for bulk, lower and upper surface, respectively (Fig. 1). Each layer is characterized by residual stress $t^{(k)}$ and modulus $E^{(k)}$, which are constant along the layer thickness $h^{(k)}$. These parameters are related to τ' and S' from the classical theories through:

$$\tau' = t^{(k)}h^{(k)}, \quad k = 1,2, \tag{2.1}$$

$$S' = (E^{(k)} - E^{(0)})h^{(k)}, \quad k = 1,2. \tag{2.2}$$

The layer longitudinal stress and strain are denoted by $\sigma^{(k)}$ and $\varepsilon^{(k)}$, respectively. The layer constitutive equation is:

$$\sigma^{(k)} = t^{(k)} + E^{(k)}\varepsilon^{(k)}. \tag{2.3}$$

All layer parameters $\left(h^{(k)},\ t^{(k)},\ E^{(k)},\ \sigma^{(k)} \text{ and } \varepsilon^{(k)}\right)$ are functions of the longitudinal coordinate x_1. The cross-sectional coordinates (x_2 and x_3) are measured relative to the local weighted center of gravity (centerline), which may vary along x_1.

2.2. Beam displacement equations of the continuum model

Following Reddy (2003), an equivalent single-layer model is used to describe the displacements along the beam. Consider the in-plane displacement field $\hat{\mathbf{v}}(x_1, x_2)$, which under Euler–Bernoulli assumptions can be expressed as

$$\hat{\mathbf{v}} = \hat{v}_i\mathbf{e}_i = \left(v_1(x_1) - \frac{\mathrm{d}v_2(x_1)}{\mathrm{d}x_1}x_2\right)\mathbf{e}_1 + v_2(x_1)\mathbf{e}_2;$$
$$v_i(x_1) = \hat{v}_i(x_1, x_2)|_{x_2=0}, \tag{2.4}$$

where v_1 and v_2 are, respectively, the "axial displacement" and "deflection" along the centerline of the beam ($x_2 = 0$). For compactness, Einstein's summation convention is adopted. The longitudinal nonlinear Von-Karman strain for moderate rotations (Reddy, 2003) is:

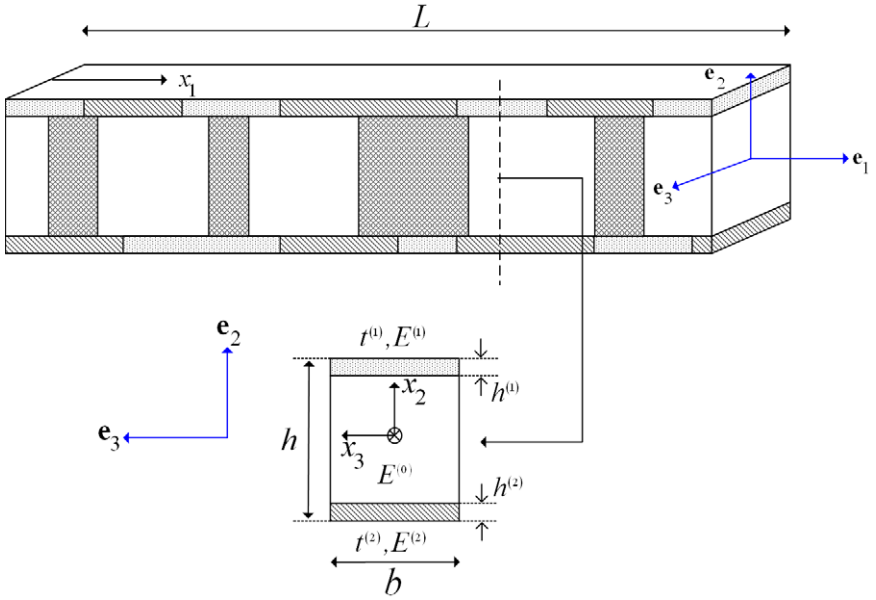

Fig. 1. Schematic diagram of a heterogeneous nanobeam and a selected cross-section.