EFFECTIVE ELASTIC CONSTANTS AND SURFACE CHARACTERISTICS OF FILMS WITH NANOMETRIC THICKNESS

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1. General

Nano-structures are necessarily delimited by such boundary defects as surfaces, edges, and corners which in turn effect disturbance in the atomic positions in their close vicinity. Atomic disruption alters the interatomic bond lengths and charge density distribution creating a so-called surface layer as the aftermath. Mindlin [3] proposed second strain gradient theory in which strain energy density function depends on the strain field and its first and second derivatives. This approach introduces surface characteristic lengths and modulus of cohesion as the surface parameters. Gurtin and Murdoch [4], however, treated elastic surfaces and their complementary bulk materials differently, giving rise to the notion of surface stress, surface strain, and surface elastic constants.

In this work, it is proposed to interrelate surface and second strain gradient theories. Consequently, based on the two new key equations for net surface stress and total elastic energy, surface elastic parameters of nano-film like surface energy, surface elastic constants, surface residual stress, and effective elastic constants are analytically derived in terms of Mindlin's additional parameters, Lamé constants, and film thickness. In continue, by employing ab initio calculations and available experimental values for surface stress and surface energy, the above-mentioned surface parameters are evaluated.

2. Deformation of a free-standing film of nanometric thickness

Consider an infinitely extended planar free-standing film of thickness, t defined as $-\infty < x_2,\ x_3 < \infty, |x_1| \leq t/2$ with boundary surfaces $x_1 = \pm t/2$, Fig. 1.

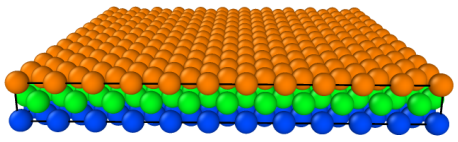

Figure 1. Atomistic modeling of infinitely extended film of three-atomic-layers.

The bulk and its complementary surfaces are treated as separate interacting entities. Second strain gradient theory governs the bulk which exerts some tractions to its two-dimensional bounding surfaces. Surface equilibrium condition, however, is based on the notion of surface stress and its surface gradient. Solving the coupled governing equations, the displacement field within the free-standing film due to the surface effect is obtained; subsequently, the residual surface stress tensor is derived in terms of Mindlin's parameters and film thickness. In continue, by considering the film under uniform biaxial tension and shear loading, the expressions for surface as well as effective elastic constants of the film are derived.

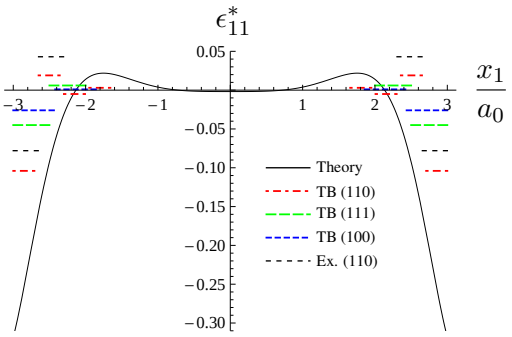

Figure 2. Surface relaxation delineated by strain component, ϵ_{11}^* versus normalized coordinate x_1/a_0 for Ag film of thickness $6a_0$, where a_0 is the lattice parameter. The available values of the average strain computed via tight-binding scheme [1] as well as the experimental data [2] are plotted for comparison.

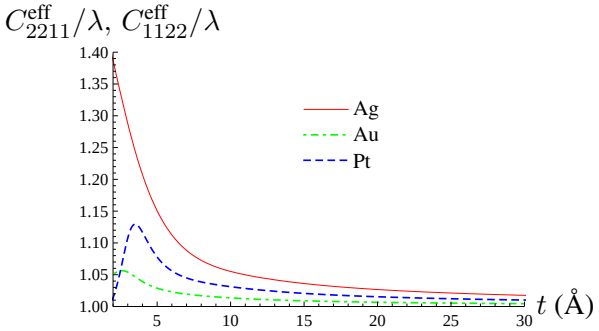

Figure 3. The normalized components of the effective elastic constants, $C_{2211}^{\text{eff}} = C_{2211}^{\text{eff}}$ with respect to Lamé constant, λ versus film thickness in units of Å for Ag, Au, and Pt.

3. Numerical results

Combining lattice dynamics and second strain gradient elasticity, Lamé constants and bulk internal lengths are related to the atomic force constants [5, 6]. Utilizing ab initio computations, atomic force constants and subsequently, the above-mentioned material constants are evaluated. Also, surface characteristic length and modulus of cohesion are calculated via the present formulations and pertinent available experimental values. Finally, for different film thicknesses, all surface characteristics are calculated. For example, Fig. 2 depicts the surface relaxation of Ag film and compares the results with the available experimental and computational data. Moreover, the variation of the effective elastic component, C_{2211}^{eff} with thickness for some metallic films is portrayed in Fig. 3, for illustration.

4. References

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