Frontiers in Applied Mechanics
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A NEW ELASTIC THEORY FOR NANOMATERIALS AND ITS APPLICATIONS

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Prof. Dr. Shaohua Chen is the group leader of "Micro-scale mechanics of Biomaterials and Solids" at Institute of Mechanics, Chinese Academy of Sciences. He received his Ph.D from Beijing Jiaotong University in 1999. Then, he joined Institute of Mechanics, Chinese Academy of Sciences to be a post-doctor, after that he stayed in the institute to engage in scientific research to date. He was ever a visiting scholar at Max Plank Institute for Metals Research in Germany for two years and the University of Hong Kong for five months.

Research Interests

His research interests include the mechanics of surface and interface, including surface/interface contact; mechanics of micro and nano materials, such as size effects in micro-nano-scales and self-assembly of nano-devices; biomimetics, including bio-inspired adhesion mechanism, such as geckos and ants, and rolling transport mechanism of oosperm; and mechanics of advanced composite materials, such as carbon nanotube (CNT) or carbon nano-scroll (CNS) reinforced composites. Establishing theoretical models is his main research technique, in addition to the numerical calculations.

A New Elastic Theory for Nanomaterials and Its Applications

Compared to large-scale bulk materials, nanomaterials exhibit a large surface-to-volume ratio. It is well known that the energy of each atom in the surface region deviates significantly from those in the interior of a nanomaterial, and this discrepancy has been identified as the main cause of size effects associated with the elastic moduli, resonant frequency, and thermal conductivity of nanoscale materials. Based on surface elastic theory, a large number of theoretical models have been successfully created to analyze size effects in nanomaterials. However, the involved surface elastic constants in those models can not be measured experimentally till now, which are much difficult to determine even using MD calculation. Recent investigations into surface-energy density of nanomaterials lead to a ripe chance for us to propose, within the framework of continuum mechanics, a new theory for nanomaterials based on surface-energy density. In contrast to previous theories, the linearly elastic constitutive relationship that is usually adopted to describe the surface layer of nanomaterials is not invoked and the surface elastic constants are no longer needed in the new theory. Instead, a surface-induced traction γ to characterize the surface effect in nanomaterials is derived, which is introduced into the boundary conditions and depends only on the bulk surface-energy density ϕ_0 and the surface-relaxation parameter λ_i, ($i=1,\ 2$)

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$$\boldsymbol{\gamma}_t = \nabla_s \phi = \frac{\nabla_s \phi_0}{J_s} - \frac{\phi_0 (\nabla_s J_s)}{J_s^2}, \quad \gamma_n \boldsymbol{n} = \frac{\phi_0 (\boldsymbol{n} \cdot \nabla_s) \boldsymbol{n}}{J_s}$$

where γ_n and $\boldsymbol{\gamma}_t$ are the normal and tangential components of the surface-induced traction $\boldsymbol{\gamma}$, respectively; J_s is a Jacobian determinant characterizing the deformation between the initial configuration and the relaxed or deformed one; ∇_s is a surface gradient operator with respect to position vectors $\boldsymbol{x}_s$ of a material point in the current configuration on curved surface S; $\boldsymbol{n}$ is the unit normal vector perpendicular to S.

The new theory is further used to characterize the elastic properties of several fcc metallic nanofilms under biaxial tension and nanowires under bending, the theoretical results agree very well with existing experimental and numerical results (Figs. 1 and 2). An interesting finding is that the whole property of nanomaterials may exhibit nonlinearly elastic due to the nonlinear boundary conditions on surface though the inside of nanomaterials is linearly elastic. Furthermore, it is found that the stiffening or softening behavior of a nanofilm results essentially from the competition between the residual surface strain induced by the surface relaxation and the excess surface strain caused by an external loading. The present theory should be much convenient for predicting the mechanical behavior of nanomaterials since the involved parameters are easy to ascertain.

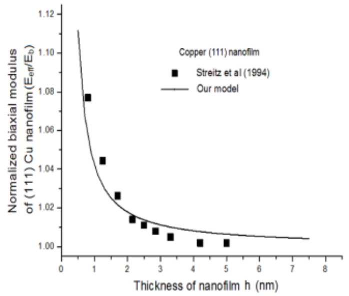

Fig. 1. Nanofilm under biaxial tension

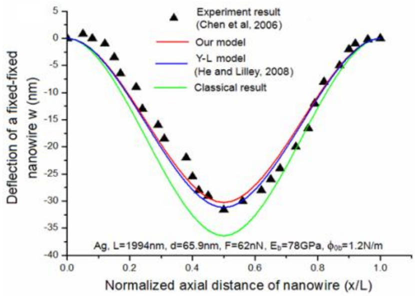

Fig. 2. Nanowire under bending

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