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Spherical Lame-Type Problem in Second Strain Gradient Theory

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ABSTRACT: Second strain gradient theory is employed to examine the spherical single/double-phase Lame-type problem. Due to the capability of strain gradient theory to capture the effects of the surface, size, and discrete nature of materials, the pertinent relaxed configuration is sought. The theory is written in the spherical coordinate system and the equilibrium equations, stress/strain components, constitutive relations, and tractions are derived. The relaxed configuration is obtained for both the diamond carbon and carbon-coated crystalline silicon shell. Afterwards, the external symmetric loading is applied to the relaxed configuration to analyze the mechanical response. The elastic material parameters are calculated via the quantum computations, lattice dynamics, and material continuum description. The analysis shows that the mechanical response in the augmented theory is significantly different from that in the classical elasticity. For example, in the single-phase problem with an inner and outer radius equal to two and ten lattice parameter, respectively, under a normalized external pressure of about 0.0001, the classic elasticity predicts an approximately constant normalized radial stress of about -0.0001 in the nanoshell. However, in the framework of strain gradient theory, the normalized radial stress is varying from about -0.001 and -0.0002 in the vicinity of the inner and outer boundaries, respectively, to about 0.0003 in the middle of the hollow nanoshell. With increasing the inner radius, the difference between the two results in the middle points decreases.

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1. INTRODUCTION

Recently, consideration of the mechanics and physics of nanowires, nanotubes, and nano-particles has been of interest due to their vast applications in electronics, energy conversion, optics, chemical sensing, cancer therapy, and drug delivery, among other fields. In view of the traditional continuum inadequacy in treating the mechanical aspects of nanostructures, resorting to augmented continuum theories especially, Second Strain Gradient Theory (SSGT), seems to be remedial [1-3]. Based on the methodology presented by Shodja et al. [4], the material parameters in SSGT are calculated via quantum computations and lattice dynamics combined with the continuum description of materials. Because of the vast possible applications of the carbon-coated silicon nanospheres in lithium batteries [5, 6], the present work focuses on the physical and mechanical characteristics of these nanostructures. First, The relaxed configuration under the surface effects is obtained. Afterwards, an external symmetric loading is applied to the nanospherical relaxed configuration and SSGT mechanical response is resulted and compared with the pertinent response in the Classic Theory (CT).

2. SECOND STRAIN GRADIENT THEORY IN A MEDIUM WITH SPHERICAL SYMMETRY

The governing equilibrium equation in a medium with spherical symmetry in SSGT in the spherical coordinate system has the following form [3]:

$$\begin{aligned}&r^6 u_r'''''' + 6r^5 u_r''''' - (6r^4 + p_1 r^6) u_r''''\\&-4r^5 p_1 u_r''' + (4 p_1 r^4 + p_2 r^6) u_r''\\&+2 p_2 r^5 u_r' - 2 p_2 r^4 u_r = 0,\end{aligned} \tag{1}$$

where p_1 and p_2 depend on Mindlin characteristic lengths $\{\ell_{11}, \ell_{12}, \ell_{21}, \ell_{22}\}$, r is the radial variable in the spherical domain, and u_r is the radial displacement. The corresponding six independent solutions are

$$\begin{aligned}&u_r(r) = \mathscr{L}\{r, \frac{1}{r}\cosh\frac{r}{\ell_{11}} - \frac{\ell_{11}}{r^2}\sinh\frac{r}{\ell_{11}},\\&\frac{1}{r}\cosh\frac{r}{\ell_{12}} - \frac{\ell_{12}}{r^2}\sinh\frac{r}{\ell_{12}},\\&\frac{1}{r^2}, \frac{\ell_{11}+r}{r^2} e^{-\frac{r}{\ell_{11}}}, \frac{\ell_{12}+r}{r^2} e^{-\frac{r}{\ell_{12}}}\}.\end{aligned} \tag{2}$$

Three of the above solutions are undefined at origin ($r = 0$) and the others are undefined at infinity. The tractions at the boundaries of the spherical domain are obtained in the spherical coordinates, as well. Employing the obtained solution, two problems of spherical Lame-type and coated

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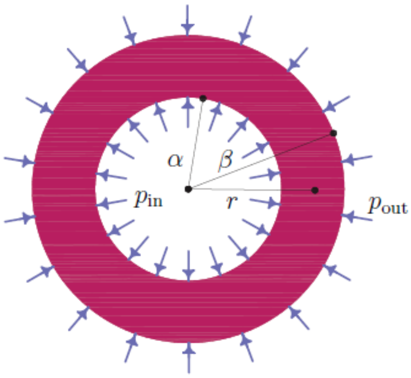

Fig. 1. The spherical Lame-type problem with inner and outer radii α and β under the external pressures p_{in} and p_{out}.

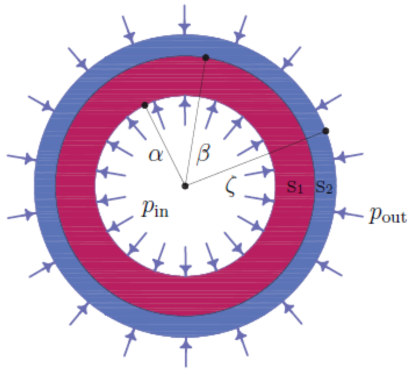

Fig. 2. The spherical coated shell with radii α, β, and ζ under the external pressures p_{in} and p_{out}.

Table 1. Lame constants in terms of $eV/\mathring{A}^3$ and characteristic lengths in terms of $\mathring{A}$ for silicon and carbon

	λ	μ	ℓ_{11}, ℓ_{12}	ℓ_{21}, ℓ_{22}
Si	0.45	0.62	$0.44 \pm 0.71\,i$	$1.19 \pm 1.35\,i$
C	0.94	2.94	$0.67 \pm 0.84\,i$	$0.87 \pm 1.05\,i$

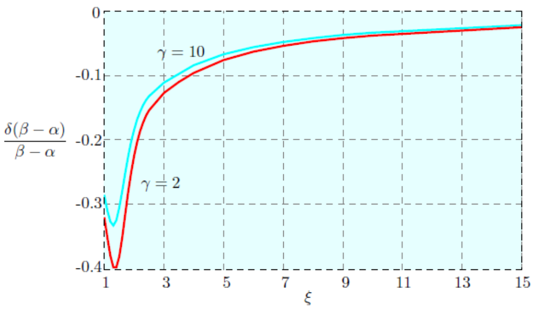

Fig. 3. The average radial strain in the carbon shell due to the surface relaxation versus ξ for two values of γ.

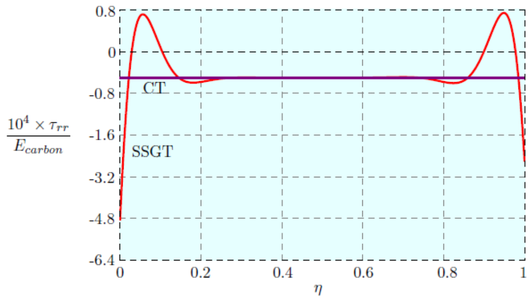

Fig. 4. The normalized radial stress versus η for the carbon shell under external pressure.

spherical shell are examined. In the Lame-type problem depicted in Fig. 1, with inner and outer radii α and β, the external surface loadings are p_{in} and p_{out}. For this problem, there are six unknown coefficients in the displacement field that are determined via the six traction boundary conditions.

In the coated shell problem, Fig. 2, with two material phases (S_1 and S_2), there are twelve unknown coefficients in u_r determined via nine traction and three displacement boundary conditions. It should be noted that at the boundary of S_1 and S_2, the radial components of traction and displacement are assumed to be continuous.

3. RESULTS AND DISCUSSION

To give the numerical results, the material parameters in SSGT should be evaluated. Exploiting the results and methodology of Ojaghnezhad and Shodja [2, 7] and Shodja et al. [4], Lame constants and characteristic lengths are computed as summarized in Table 1.

In a carbon shell, the surface relaxation implies a radial strain causing a thickness change. The average radial strain is plotted in Fig. 3 versus the normalized thickness, ξ for two normalized radii, γ. It is observed that the average strain tends to zero with increasing ξ.

Applying $p_{in} = p_{out} = 0.0001 E_{carbon}$ on the carbon shell ($\gamma = 10$, $\xi = 10$) relaxed configuration implies radial stress plotted versus radial normalized variable η and compared with that of CT in Fig. 4.

Consider a carbon-coated silicon nanosphere in SSGT to obtain its relaxed configuration under the surface effect. For example, the average radial strain in the silicon shell versus its initial normalized thickness ξ_1 is plotted in Fig. 5 for different values of the normalized inner radius γ and coating normalized thickness ξ_2.

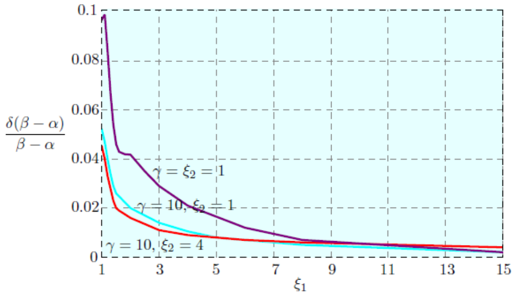

Fig. 5. The average radial strain in the silicon shell versus ξ_1 for some values of γ and ξ_2 under surface effect.

4. CONCLUSION

The surface effect in spherical domains implies a radial strain field causing the thicknesses change. With increasing the dimensions, the effects tend to zero as predicted by CT. Under an external loading, SSGT predictions are different from those of CT, especially near the boundaries.

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