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Effect of residual surface stress and surface elasticity on deformation of nanometer spherical inclusions in an elastic matrix

R.V. Goldstein*, V.A. Gorodtsov and K.B. Ustinov

Ishlinsky Institute for Problems in Mechanics RAS, Moscow, 119526, Russia

The analytical solution of the Eshelby problem, which describes the deformation of an elastic medium inside and outside a spherical inclusion with uniform internal eigenstrain and specified remote stress, is generalized taking into account both surface elasticity and residual surface stress. Expressions are derived for the internal and external Eshelby tensors and stress concentration tensors with regard to the above effects. A characteristic strain field inhomogeneity and its dependence on the inclusion diameter in the nanometer range (the scale effect) are found. It is shown that under certain conditions, the effect of residual surface stress surpasses that of surface elasticity.

Keywords: inclusion, elastic matrix, Eshelby problem, Eshelby tensor, stress concentration tensor, surface strain, eigenstrain, residual surface stress

1. Introduction

As the size of deformed solids is decreased down to nanometers, scale effects of their physical properties come into play. The classical theory of elasticity lacks characteristics of a medium with length dimension such that this theory fails to describe the scale effect. Describing the observed scale effect of mechanical behavior of nanoobjects, such as nanotubes, nanowhiskers (nanowires), nanoinclusions, thin films, atomic clusters, nanoislands, etc., requires one or another generalization of the theory of elasticity.

A possible explanation for the arising scale effect is the impossibility to apply the continuum approximation to nanosizes, i.e., of importance on these scales is the discrete atomic structure of material. The governing factor, in this case, can be peculiar features of the atomic structure of near-surface layers and near-interface regions. The role of these relatively narrow regions can greatly increase in importance where the number of near-surface atoms is no longer too small compared to that of atoms in the rest material.

Numerous ab initio calculations and semiempirical molecular simulations, which take into account the atomic structure of materials, and experimental studies confirm the scale effect in nanoobjects of size from fractions to tens of nanometers. This behavior is found, in particular, in simplified discrete film models (e.g., [1]) and generalized nanotube elasticity models based on molecular simulation (e.g., [2]).

In recent years, there has been a dominant trend toward describing the mechanical behavior of nanoobjects in the framework of generalized theory of elasticity in which a nonstandard characteristic is introduced only for surfaces and interfaces of material, while its bulk is treated using the classical theory. In so doing, anomalous surface elasticity is described by various constitutive relations that supplement ordinary Hooke's law.

A theoretical estimate of the role of surface elasticity peculiarities of nanoparticles is rather easy to obtain using the well-known Eshelby problem [3]. This problem consists in determining the stress-strain state of an infinite elastic medium with a spherical inclusion that differs in material from the matrix and experiences uniform eigenstrain. The eigenstrain can be induced by thermal expansion, phase transformation, incompatible atomic lattices of the matrix and inclusion, residual stress, plastic flow, twinning, etc. The analytical solution of the Eshelby problem with regard to additional surface strains described by two-dimensional Hooke's law and generalized surface elastic moduli is analyzed in detail in [4, 5]. However, the researchers take no account of the so important factor like residual surface stress. In our work, this parameter is taken into account and, using available theoretical estimates of surface elastic moduli and residual stress, it is shown that the latter can be of greater

* *Corresponding author*
Prof. Robert V. Goldstein, e-mail: goldst@ipmnet.ru

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significance than the former. We begin our paper with general relations and solutions of the Eshelby problem for a spherical inclusion with internal eigenstrain and surface effects and analyze kinematics, statics and constitutive equations for its spherical boundary. These data are reported in Sect. 2, 3. In Sect. 4, we present a dependence of the strain fields induced by the spherical inclusion on its eigenstrain with regard to surface effects (Eshelby tensor). This section considers in detail only the internal Eshelby tensor components for the strain field inside the inclusion; certain of cumbersome coefficient functions entered in the solution are given in Appendix. A distinctive feature of the derived solution is a nonuniform strain field and a scale effect (the dependence of the solution on the inclusion diameter). Section 5 provides a solution of the more general problem on the stress-strain state inside and outside the inclusion with specified internal eigenstrain and specified remote stress fields with regard to elastic strain and residual stress at the “elastic matrix – inclusion” interface. Finally, Section 7 discusses the association between the interface constitutive equations used and the known, by and large, more general Gurtin–Murdoch constitutive equations [6, 7]. The effects under consideration, in our viewpoint, are important for the further advances in physical mesomechanics [8, 9] whose main approaches concern, among other things, the description of the processes occurring on various scales at the meso-to-nanolevel transition.

2. Relations for the medium inside and outside the inclusion

In the subsequent discussion we assume that the medium under study can be considered as a piecewise-homogeneous medium in which every subregion is described by equations of the linear theory of elasticity with possible eigenstrain (initial or residual). In this context, due to the problem linearity, the strain ε for the k-th homogeneous region can be expressed as the sum of elastic and inelastic components:

$$\varepsilon_{ij}^{k\mathrm{T}} = \varepsilon_{ij}^{k} + \varepsilon_{ij}^{k0}. \tag{1}$$

Hereinafter the second upper index T stands for total strain, and the second upper index 0 for eigenstrain. If no second upper index is used, it is for elastic strain. The first upper index k characterizes the region under study; this index can go with e (matrix) and i (inclusion). The lower indices denote components of tensor quantities.

In the problem, which is similar to the known Eshelby problem, we assume that the infinite elastic matrix is everywhere free from eigenstrain, and the inclusion experiences homogeneous eigenstrain. The assumption of homogeneity is sufficient to resolve both the strain and the displacements into elastic and inelastic components:

$$\varepsilon_{ij}^{\mathrm{eT}} = \varepsilon_{ij}^{\mathrm{e}},\ \ \varepsilon_{ij}^{\mathrm{iT}} = \varepsilon_{ij}^{\mathrm{i}} + \varepsilon_{ij}^{\mathrm{i0}},$$

$$U_i^{\mathrm{eT}} = U_i^{\mathrm{e}},\ \ U_i^{\mathrm{iT}} = U_i^{\mathrm{i}} + U_i^{\mathrm{i0}}. \tag{2}$$

Here the indices for U are similar to those for the strain.

In view of the problem linearity, it is sufficient to further consider uniaxial eigenstrain, whereupon we can arrive at a general solution by simple superposition of the solutions corresponding to eigenstrain in different directions.

The elastic displacement field inside and outside the spherical inclusion can be represented in spherical coordinates r, θ, φ as follows (see, e.g., [10], Sect. IV, formulae (1.8), (1.10)):

$$\begin{aligned}
U_r^{\mathrm{i}} &= \sum_{n=0}^{N}\left[A_n(n+1)(n-2+4\nu^{\mathrm{i}})r^{n+1} + B_n n r^{n-1}\right]\times \\
&\quad \times P_n(\cos\theta),\ r \le R,\\
U_\theta^{\mathrm{i}} &= \sum_{n=0}^{N}\left[A_n(n+5-4\nu^{\mathrm{i}})r^{n+1} + B_n r^{n-1}\right]\times \\
&\quad \times \frac{\mathrm{d}P_n(\cos\theta)}{\mathrm{d}\theta},\ r \le R,\\
U_r^{\mathrm{e}} &= \sum_{n=0}^{N}\left[C_n n(n+3-4\nu^{\mathrm{e}})r^{-n} + D_n(n+1)r^{-n-2}\right]\times \\
&\quad \times P_n(\cos\theta),\ r \ge R,\\
U_\theta^{\mathrm{e}} &= \sum_{n=0}^{N}\left[C_n(-n+4-4\nu^{\mathrm{e}})r^{-n} + D_n r^{-n-2}\right]\times \\
&\quad \times \frac{\mathrm{d}P_n(\cos\theta)}{\mathrm{d}\theta},\ r \ge R.
\end{aligned} \tag{3}$$

Here R is the inclusion radius; $P_n(x)$ is the Legendre polynomials; ν^{i}, ν^{e} are Poisson’s ratios for the inclusion and matrix, respectively; A_n, B_n, C_n, D_n are the coefficients to be determined. The discussion below makes clear that for the problem under study we suffice to retain the lowest terms with $n \le 2$, while the terms with $n = 1$ should be omitted because they are related to the resultant force vector, which is absent in the problem.

In the inclusion problem with eigenstrain, the total displacements inside the inclusion are elastic displacements (3) and eigendisplacements due to the uniform tensile eigenstrain $\varepsilon^{\mathrm{i0}}$ along the z axis:

$$\begin{aligned}
U_r^{\mathrm{i0}} &= \varepsilon^{\mathrm{i0}} r\cos^2\theta,\\
U_\theta^{\mathrm{i0}} &= -\varepsilon^{\mathrm{i0}} r\sin\theta\cos\theta.
\end{aligned} \tag{4}$$

The elastic strain inside and outside the inclusion is expressed in terms of the elastic displacements in the ordinary way:

$$\begin{aligned}
\varepsilon_{rr}^{k} &= \frac{\partial U_r^k}{\partial r},\ \ \varepsilon_{\theta\theta}^{k} = \frac{1}{r}\frac{\partial U_\theta^k}{\partial\theta} + \frac{U_r^k}{r},\\
\varepsilon_{\varphi\varphi}^{k} &= \frac{U_\theta^k}{r}\mathrm{ctg}\,\theta + \frac{U_r^k}{r},\\
\varepsilon_{r\theta}^{k} &= \frac{1}{2}\left(\frac{\partial U_\theta^k}{\partial r} - \frac{U_\theta^k}{r} + \frac{1}{r}\frac{\partial U_\theta^k}{\partial\theta}\right).
\end{aligned} \tag{5}$$