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Solutions of inhomogeneity problems with graded shells and application to core–shell nanoparticles and composites

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Abstract

This paper first presents the Eshelby tensors and stress concentration tensors for a spherical inhomogeneity with a graded shell embedded in an alien infinite matrix. The solution is then specialized to inhomogeneous inclusions in finite spherical domains with fixed displacement or traction-free boundary conditions. The Eshelby tensors in the infinite and finite domains and the stress concentration tensors are especially useful for solving many problems in mechanics and materials science. This is demonstrated on two examples. In the first example, the strain distributions in core–shell nanoparticles with eigenstrains induced by lattice mismatches are calculated using the Eshelby tensors in the finite domains. In the second example, the Eshelby and stress concentration tensors in the three-phase configuration are used to formulate the generalized self-consistent prediction of the effective moduli of composites containing spherical particles within the framework of the equivalent inclusion method. The advantage of this micromechanical scheme is that, whilst its predictions are almost identical to the classical generalized self-consistent method and the third-order approximation, the expressions for the effective moduli have simple closed forms.

Keywords: Eshelby tensor; Stress concentration tensor; Finite domain; Core–shell nanoparticle; Effective modulus

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1. Introduction

The synthesis and characterization of particles with core–shell structures have attracted a lot of attention in many areas of science and technology. In materials science and engineering, these particles have been used as reinforcements and tougheners in composites. In solid-state physics, core–shell nanoparticles are found to exhibit novel physical effects and properties, such as quantum confinement effect, and novel electronic, magnetic and optical properties (e.g. Zhou et al., 1996; Rockenberger et al., 1998; Brongersma, 2003; Goncharenko, 2004). Core–shell particles can be used as functional devices on their own, besides being a constituent part of a composite medium (e.g. Williamson and Zunger, 1999; Lauhon et al., 2002; Abe and Suwa, 2004; Goncharenko, 2004). Many researchers have studied the strain distributions in heterogeneous electronic structures of fine scale, e.g. quantum dot structures (Gosling and Willis, 1995; Freund and Johnson, 2001; He et al., 2004) and shown that the strain affects the optical properties of these structures by modifying the energies and wave functions of the confined carriers. For core–shell nanoparticles, as pointed out by Little et al. (2001), and Perez-Conde and Bhattacharjee (2003), the misfit strain, the surface stress and the applied external pressure all modify the strain fields in them, which in turn affect the electronic structures, and hence their physical properties.

Core–shell structures also widely exist in conventional particle-reinforced composites and nanocomposites due to complicated interactions between the particle surface and the matrix (e.g. Theocaris, 1987; Tzika et al., 2000) and the need for good bond between the reinforcement and the matrix. The elastic properties of the interphase can be uniform or variable through its thickness (Ostoja-Starzewski et al., 1996). The inhomogeneity problems with graded interphases have attracted a lot of attention (e.g. Lutz and Zimmerman, 1996; Wang and Jasiuk, 1998). However, almost all the existing works on inclusion/inhomogeneity problems with graded (inhomogeneous) interphases are concerned with the solutions of stress fields under special loading conditions or with the predictions of effective elastic moduli. It is noted that Ding and Weng (1998), and Weng (2003) have predicted the effective bulk moduli of composites containing spherical particles and graded matrices using a three-phase model containing a graded interphase.

The Eshelby formalism (Eshelby, 1957, 1959) for an inclusion/inhomogeneity is one of the cornerstones in the solutions of many problems in materials science, solid-state physics and mechanics of composites. The classical Eshelby formalism is for an inclusion/inhomogeneity without an interphase in an infinite matrix. In this paper, we shall give the solution of the Eshelby formalism for a spherical particle with a graded interphase embedded in an infinite medium. The Eshelby tensors in the whole region when an eigenstrain is prescribed in the particle and the stress concentration tensors under remote loading will be presented. When the stiffness of the infinite medium is set to be infinite or zero, the Eshelby tensors in a finite domain with a fixed displacement or traction-free boundary condition are given. The application of the Eshelby formalism in the finite and infinite domains is demonstrated on two examples, namely, the calculation of the strains in core–shell nanoparticles and the prediction of the effective moduli of particle-reinforced composites.

2. Solution of spherical inhomogeneity with graded interphase

Consider a spherical inhomogeneity with a graded interphase embedded in an infinite elastic matrix, as shown in Fig. 1. The radius of the inhomogeneity and the outer radius of