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Inclusion of an arbitrary polygon with graded eigenstrain in an anisotropic piezoelectric half plane

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ABSTRACT

This paper presents an exact closed-form solution for the Eshelby problem of a polygonal inclusion with graded eigenstrains in an anisotropic piezoelectric half plane with traction-free on its surface. Using the line-source Green's function, the line integral is carried out analytically for the linear eigenstrain case, with the final expression involving only elementary functions. The solutions are applied to the semiconductor quantum wire (QWR) of square, triangular, and rectangular shapes, with results clearly illustrating various influencing factors on the induced fields. The exact closed-form solution should be useful to the analysis of nanoscale QWR structures where large strain and electric fields could be induced by the non-uniform misfit strain.

1. Introduction

Eshelby problem (Eshelby, 1957, 1961) has been an interesting topic in various engineering and material fields for more than 50 years, and is the subject of constant studies (Willis, 1981; Mura, 1987). Some of the previous studies include the effective elastoplastic behavior of composites (Ju and Sun, 2001), and dynamic Eshelby tensor of ellipsoidal inclusions (Michelitsch et al., 2003), among others. Although most Eshelby problems in isotropic elasticity can be solved analytically for both two-dimensional (2D) and three-dimensional (3D) deformations (see, e.g. Kouris and Mura, 1989), solution to the corresponding anisotropic elasticity is still a challenging and attractive topic. For a transversely isotropic elasticity problem an analytical solution can be obtained (Yu et al., 1994), whilst in an anisotropic elasticity it is usually solved numerically (Dong et al., 2003). As a typical application of the Eshelby solution, it is effective to study the semiconductor properties for efficient device design. However, different from simple isotropic elastic materials, most semiconductor materials show both anisotropic and piezoelectric properties, with some of them being strongly electromechanically coupled (Pan, 2002). For piezoelectric Eshelby inclusion problems, most reported analytical solutions concerned with elliptical/ellipsoidal shapes only (Wang, 1992; Chung and Ting, 1996). In real applications, however, the Eshelby problem with arbitrarily shaped inclusion is particularly useful in the study of the strained semiconductor quantum devices (Freund and Gosling, 1995; Andreev et al., 1999). In the work of Ru (1999), analytical solutions for Eshelby inclusion of arbitrary shape were derived based on the conformal mapping which maps the exterior of a unit circle onto the exterior of the inclusion. This method is elegant and convenient for the inclusion with smooth boundary. In the work of Pan (2004), the Green's function solutions were adopted with the final solution involving only elementary functions, which is particularly suited for a polygonal inclusion. The perturbation method can also be applied to handle the elastic material anisotropy and arbitrary shape of an inclusion (Wang and Chu, 2006). Zou et al. (2011) applied the extended Stroh formalism to an Eshelby problem of 2D arbitrarily shaped piezoelectric inclusion, which is actually very powerful in treating 2D anisotropic problems. Inclusion of an arbitrary shape with uniform eigenstrains in magnetoelectroelastic bimaterial planes was also investigated (Jiang and Pan, 2004; Zou and Pan, 2012).

We point out that in most of the previous studies, the eigenstrain within the inclusion was assumed to be uniform, which could be very limited because in most semiconductor materials, the eigenstrain shows non-uniform distribution. Thus, the effect of non-uniform eigenstrain on the induced field is particularly interesting. Eshelby (1961) showed that if the eigenstrain inside an ellipsoidal inclusion in an infinite domain is in the form of a polynomial, then the induced-strain field in the inclusion is also characterized by a polynomial of the same order. Other types of

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non-uniform eigenstrain were also considered, including an ellipsoidal inclusion with dilatational Gaussian and exponential eigenstrains (Sharma and Sharma, 2003), and an ellipsoidal or elliptic inclusion with linear and polynomial distributions of eigenstrain (Rahman, 2002; Nie et al., 2007; Guo et al., 2011). Recently, Sun et al. (2012) solved the Eshelby inclusion problem of an arbitrary polygon with a linear eigenstrain in an anisotropic piezoelectric full plane via the Green's function method.

In most engineering applications, the size of the substrate would be finite. Liu (2010) studied the 2D periodic inclusion problem in a finite cell and obtained the solution to the problem in terms of Cauchy-type integrals. Using the Somigliana's identity and Green's functions in classical elasticity, analytical solution of the Eshelby tensors of a spherical inclusion embedded concentrically within a finite sphere can be derived (Li et al., 2007). Mejak (2011) obtained the Eshelby tensors for a spherical inclusion within a finite spherical body by power series approximation. Ma and Gao (2011) extended the classical elasticity to strain gradient elasticity theory. Zou et al. (2012) proposed a general approach based on the principle of superposition to study the problem of a finite elastic body with an arbitrarily shaped inclusion. Although the half-plane piezoelectric problem of an arbitrarily shaped inclusion was investigated before (Ru, 2003; Wang and Pan, 2010), solution to the inclusion problem with non-uniform eigenstrain in an anisotropic piezoelectric half plane remains to be solved.

In this paper, an exact closed-form solution for an arbitrarily shaped polygonal inclusion in an anisotropic piezoelectric half plane is presented, where the eigenstrain within the inclusion can be not only uniform but also graded. Based on the equivalent body force and by means of subdomain division, the eigenstrain can be expressed as a linear graded function in every subregion. Thus, we can express the induced elastic and piezoelectric fields in terms of a line integral on the boundary of the inclusion, with the integrand being the multiplication of the line-source Green's function and the equivalent body force of the piezoelectric solid. The line integral can be carried out analytically assuming that the inclusion is a polygon. The most remarkable feature is that the final exact closed-form solution involves only elementary functions, similar to the corresponding isotropic elastic solutions (Faux et al., 1997; Nozaki and Taya, 1997; Glas, 2002a). Using our present simple solutions, the piezoelectric field due to multiple inclusions or an array of QWRs can be easily obtained by adding the contributions from all the QWRs. As numerical examples, our solution is applied to square, triangular, and rectangular QWRs within a GaAs (001) half-plane substrate. Our numerical results clearly show the obvious effects of graded eigenstrain distribution, depth, and orientation of the embedded inclusion on the induced fields. When a QWR is embedded sufficiently deep, our results reduce to the exact closed-form solutions in a full plane (Sun et al., 2012). Furthermore, the piezoelectric field due to an elliptical inclusion can be calculated by an inscribed polygon with a relatively large side number and thus it should be an efficient and recommended method for the elastic and electric field analysis in nanoscale QWR structures.

This paper is organized as follows: In Section 2, we derive an exact closed-form solution in a piezoelectric half plane for a general polygon under a linear eigenstrain in x and z. In Section 3, we apply our solutions to a couple of inclusion problems within a piezoelectric half-plane substrate with traction-free boundary conditions. The effect of different non-uniform eigenstrains, different orientations of the polygon, and different embedded depths of the QWR, along with certain interesting features in the induced fields are discussed. Conclusions are drawn in Section 4.

2. Solutions of inclusion problems in piezoelectric half-plane

Let us assume that there is a general inclusion with arbitrary shape in an anisotropic piezoelectric half-plane ($z<0$), and an extended general eigenstrain γ^*_{Ij} (i.e., the eigenstrain γ^*_{ij} and eigen-electric field E^*_j) within the domain V bounded by its boundary ∂V (Fig. 1). The eigenstrain is further assumed to be a linear function of the coordinates (x,z). Our task is to find the eigenstrain-induced field within and outside the QWR.

For a general eigenstrain γ^*_{Ij} at $\boldsymbol{x}=(x,z)$ within the domain V, the induced extended displacement at $\boldsymbol{X}=(X,Z)$ can be expressed based on the method of superposition and equivalent body-force concept. In other words, the response is an integral, over V, of the equivalent body force in the square bracket below, multiplied by the line-source Green's function (Pan, 2004), i.e.,

$$u_K(\boldsymbol{X}) = -\int_V u^K_J(\boldsymbol{x};\boldsymbol{X})[C_{iJLm}\gamma^*_{Lm}(\boldsymbol{x})]_{,i}dV(\boldsymbol{x}) \tag{1}$$

where $u^K_J(\boldsymbol{x};\boldsymbol{X})$ is the J-th Green's elastic displacement/electric potential at $\boldsymbol{x}$ due to a line-force/line-charge in the K-th direction applied at $\boldsymbol{X}$. Summation is assumed for repeated lowercase (from 1 to 3) and uppercase (from 1 to 4) indices.

Integrating by parts and noticing that the eigenstrain is nonzero only in V, Eq. (1) can be written alternatively as

$$u_K(\boldsymbol{X}) = \int_V u^K_{J,x_i}(\boldsymbol{x};\boldsymbol{X})C_{iJLm}\gamma^*_{Lm}(\boldsymbol{x})dV(\boldsymbol{x}) \tag{2}$$

Since the eigenstrain can be expressed as a linear function of the coordinates (x,z) (Sun et al., 2012):

$$\gamma^*_{Lm}(\boldsymbol{x}) = \gamma^{*0}_{Lm} + \gamma^{*x}_{Lm}x + \gamma^{*z}_{Lm}z \tag{3}$$

Eq. (2) becomes

$$u_K(\boldsymbol{X}) = \int_V u^K_{J,x_i}(\boldsymbol{x};\boldsymbol{X})C_{iJLm}\left[\gamma^{*0}_{Lm} + \gamma^{*x}_{Lm}x + \gamma^{*z}_{Lm}z\right]dV(\mathbf{x}) \tag{4}$$

or

$$u^0_K(\boldsymbol{X}) + u^x_K(\boldsymbol{X}) + u^z_K(\boldsymbol{X}) \equiv \int_V u^K_{J,x_i}(\boldsymbol{x};\boldsymbol{X})\left[C_{iJLm}\gamma^{*0}_{Lm} + C_{iJLm}\gamma^{*x}_{Lm}x + C_{iJLm}\gamma^{*z}_{Lm}z\right]dV(x) \tag{5}$$

The involved area integrals can be easily transformed to the line integrals along the boundary of the QWR by the Green formula:

$$u^0_K(\boldsymbol{X}) = C_{iJLm}\gamma^{*0}_{Lm}\int_{\partial V} u^K_J(\boldsymbol{x};\boldsymbol{X})n_i(\boldsymbol{x})dS(\boldsymbol{x}) \tag{6}$$

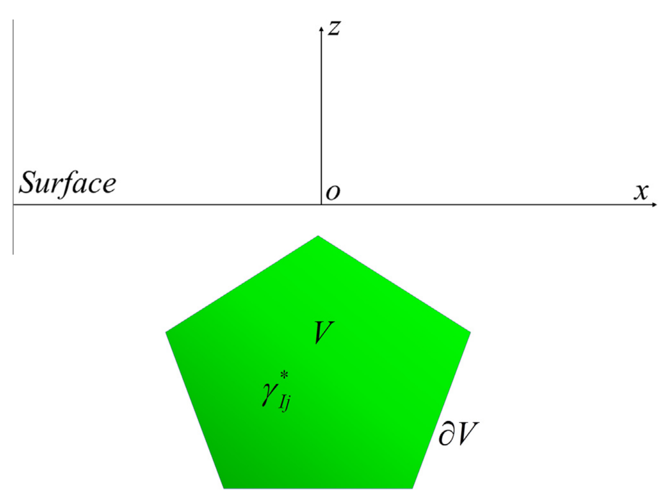

Fig. 1. A general inclusion problem in an anisotropic piezoelectric half-plane ($z<0$): a linear eigenstrain γ^*_{Ij} (γ^*_{ij} and $-E^*_j$) within an arbitrarily shaped polygon.