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# Irregular Inhomogeneities in an Anisotropic Piezoelectric Plane

This paper presents an analytical solution for the Eshelby problem of polygonal inhomogeneity in an anisotropic piezoelectric plane. By virtue of the equivalent body-force concept of eigenstrain, the induced elastic and piezoelectric fields in the corresponding inclusion are first expressed in terms of the line integral along its boundary with the integrand being the Green's functions, which is carried out analytically. The Eshelby inhomogeneity relation for the elliptical shape is then extended to the polygonal inhomogeneity, with the final induced field involving only elementary functions with small steps of iteration. Numerical solutions are compared to the results obtained from other methods, which verified the accuracy of the proposed method. Finally, the solution is applied to a triangular and a rectangular quantum wire made of InAs within the semiconductor GaAs full-plane substrate. [DOI: 10.1115/1.4005557]

Keywords: electromechanical coupling, Green's function, Eshelby problem, polygonal inhomogeneity, iteration

### 1 Introduction

As is widely known, Eshelby problem [1-3] is very important in various engineering and physical fields and is the subject of constant studies [1,4,5]. Although most Eshelby problems concerning isotropic elasticity have been solved analytically for both two-dimensional (2D) and three-dimensional (3D) deformations [6-9], those in the corresponding anisotropic elasticity are still challenging. Since the late 20th century, the Eshelby problem with any shaped inclusion has been found to be useful in the study of the strained semiconductor quantum devices using the straininduced quantum dot (QD) and quantum wire (QWR) [10], where the piezoelectric coupling could also contribute to the electronic and optical properties of the semiconductor structure.

A few of Eshelby problems have been solved for the fully coupled piezoelectric solid materials [5,11–15]. Ru [16,17] further derived the solutions for an arbitrarily shaped inclusion in anisotropic full- and half-planes of elasticity and piezoelectricity using the special conformal mapping method, and Pan [18,19] the corresponding solutions in both full and bimaterial planes using the Green's function methods. Recently, a general solution for the Eshelby problem of arbitrarily shaped piezoelectric inclusions was derived by Zou et al. [20]. However, the corresponding inhomogeneity problem remains to be solved.

Thus, we present an analytical solution for an arbitrarily shaped polygonal inhomogeneity in anisotropic piezoelectric full-planes in this paper. Based on the equivalent body force concept of eigenstrain, we express the induced elastic and piezoelectric fields in the corresponding inclusion in terms of a line integral on its boundary, with the integrand being the line-source Green's functions [18,19]. The most remarkable feature is that the final solution of the inclusion problem involves only elementary functions. For the corresponding inhomogeneity problem, we first extend the classic Eshelby inhomogeneity relation for the elliptical shape to the polygonal inhomogeneity and then propose an iteration approach for evaluating the field inside the inhomogeneity. The field outside the inhomogeneity can be also calculated approxi-

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mately. Due to this simple feature, the elastic and piezoelectric fields due to multiple inhomogeneities or an array of QWRs could be easily obtained by summing all the contributions together. Numerical examples are carried out and compared with existing boundary element method (BEM) results to verify the accuracy of the proposed method. We also apply our solution to triangle-shaped and rectangle-shaped QWRs made of InAs within the GaAs full-plane. Our results clearly show the importance of the material orientation and piezoelectric coupling. Therefore, these results could serve as benchmarks and should be of interests in the analysis of nanoscale quantum-wire structures.

This paper is organized as follows: In Sec. 2, the equivalent body force of the eigenstrain, the governing equations, and the classic Eshelby inhomogeneity relations are presented. In Sec. 3, the proposed method is described where the iteration formula and the inside–outside field conversion are elaborated. It is remarked that the results in Secs. 2 and 3 are applicable to both 2D and 3D deformations. Benchmark numerical examples are presented in Sec. 4, and conclusions are drawn in Sec. 5.

#### 2 Equivalent Body Force of Eigenstrain

At first, we assume that there is an extended general eigenstrain  $\gamma_{Ij}^{p}(\gamma_{Ij}^{p}\&-E_{j}^{p})$  within the domain V bounded by the surface  $\partial V$  (see Fig. 1). We would like to find the equivalent body force of this eigenstrain in V. We first define the extended strain as

$$\gamma_{Ij} = \begin{cases} \gamma_{ij}, & I = 1, 2, 3\\ -E_j, & I = 4 \end{cases}$$
(1)

where  $\gamma_{ij}$  is the total elastic strain and  $E_i$  is the electric field, which are related to the total elastic displacement  $u_i$  and the total electric potential  $\phi$  as

$$\begin{aligned} \gamma_{ij} &= 0.5(u_{i,j} + u_{j,i}) \\ E_i &= -\phi_i \end{aligned} \tag{2}$$

The total extended strain is the sum of

$$\gamma_{II} = \gamma_{II}^e + \gamma_{II}^p \tag{3}$$

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Fig. 1 A general polygonal inhomogeneity problem in an anisotropic piezoelectric plane: An extended eigenstrain  $\gamma^p_{ij}(\gamma^p_{ij}\& - E^p_j)$  within an arbitrarily shaped polygon. The material properties within and outside the polygon are  $C^*_{iJLm}$  and  $C_{iJLm}$ , respectively. If  $C^*_{iJLm}$  equal to  $C_{iJLm}$ , the inhomogeneity problem is then reduced to the inclusion problem.

where  $\gamma_{Ij}^{p}$  is the extended eigenstrain in the inhomogeneity (Fig. 1), and  $\gamma_{Ij}^{e}$  is the extended strain that appears in the constitutive relation [19,20] as

$$\sigma_{iJ} = C_{iJKl} \gamma^e_{Kl} \tag{4a}$$

or

$$\sigma_{iJ} = C_{iJKl}(\gamma_{Kl} - \chi \gamma_{Kl}^p) \tag{4b}$$

Notice that the induced strains  $\gamma_{ij}^e$  satisfy the constitutive relation and again that the total extended strain is the combination of this strain field and the applied eigenstrain field. In Eq. (4*b*),  $\chi$  is equal to 1 if the observation point is within the eigenstrain domain V and to 0 otherwise. The extended stress in Eq. (4) is defined as

$$\sigma_{iJ} = \begin{cases} \sigma_{ij}, & J = j = 1, 2, 3\\ D_i, & J = 4 \end{cases}$$
(5)

where  $\sigma_{ij}$  and  $D_i$  are the stresses and electric displacements, respectively, and

$$C_{iJKl} = \begin{cases} C_{ijkl}, & J, K = j, k = 1, 2, 3\\ e_{lij}, & J = j = 1, 2, 3; K = 4\\ e_{ikl}, & J = 4; K = k = 1, 2, 3\\ -\varepsilon_{il}, & J = K = 4 \end{cases}$$
(6)

with  $C_{ijlm}$ ,  $e_{ijk}$ , and  $\varepsilon_{ij}$  being the elastic moduli, piezoelectric coefficients, and dielectric constants, respectively [21,22].

We also define the extended displacement as

$$u_{I} = \begin{cases} u_{i}, & I = i = 1, 2, 3\\ \phi, & I = 4 \end{cases}$$
(7)

We assume that  $\sigma_{iJ}^0$  is the applied extended stress field at infinity if the material is homogeneous, i.e., without inhomogeneity. The corresponding extended strain field is  $\gamma_{IJ}^0$  by the generalized constitutive relation for the infinite domain, i.e.,  $\sigma_{IJ}^0 = C_{iJLm}\gamma_{Lm}^0$ . Therefore, with an inhomogeneity in the infinite matrix, the generalized constitutive relation in the inhomogeneity V and the matrix is based on the classic Eshelby inhomogeneity relation [1,2], respectively,

$$\sigma_{iJ}^0 + \sigma_{iJ} = C^*_{iJLm}(\gamma_{Lm}^0 + \gamma_{Lm} - \gamma_{Lm}^p) \quad V \tag{8a}$$

$$\sigma_{iJ}^0 + \sigma_{iJ} = C_{iJLm}(\gamma_{Lm}^0 + \gamma_{Lm}) \quad D - V \tag{8b}$$

where  $\sigma_{iJ}$  and  $\gamma_{Ij}$  are the induced extended stress and strain fields, and  $\gamma_{Lm}^{p}$  is again the eigenstrain.

Introducing the equivalent eigenstrain and eigenelectric field concept  $\gamma_{ii}^*$ , Eqs. (8*a*) and (8*b*) can then be expressed equally as

$$\sigma_{iJ}^0 + \sigma_{iJ} = C_{iJLm}(\gamma_{Lm}^0 + \gamma_{Lm} - \gamma_{Lm}^p - \gamma_{Lm}^*) \quad V$$
 (9a)

$$\sigma_{iJ}^0 + \sigma_{iJ} = C_{iJLm}(\gamma_{Lm}^0 + \gamma_{Lm}) \quad D - V \tag{9b}$$

Let

$$\gamma_{Ij}^{**} = \gamma_{Ij}^p + \gamma_{Ij}^* \quad V \tag{10}$$

Eq. (9) can then be rewritten as

$$\sigma_{iJ}^0 + \sigma_{iJ} = C_{iJLm} (\gamma_{Lm}^0 + \gamma_{Lm} - \gamma_{Lm}^{**}) \quad V \tag{11a}$$

$$\sigma_{iJ}^0 + \sigma_{iJ} = C_{iJLm}(\gamma_{Lm}^0 + \gamma_{Lm}) \quad D - V$$
(11b)

It is noted that since the equivalent eigenstrain  $\gamma_{Ij}^*$  in a polygonal inhomogeneity V is not uniform, the new eigenstrain  $\gamma_{Ij}^{**}$  in V is not uniform either; it is a function of the position within V. This is different to the elliptic or ellipsoidal inhomogeneity case.

For the eigenstrain problem described above, the equilibrium equation for the stresses and the balance for the electric displacements in V is [19,20]

$$\sigma_{iJ,i} = 0 \tag{12}$$

Then, substituting Eq. (11a) into Eq. (12), we have

$$C_{iJKl}u_{K,li} = C_{iJKl}\gamma_{Kl,i}^{**} \tag{13}$$

It is clear that the right-hand side of Eq. (13) resembles the extended body force as it would appear on the left-hand side of Eq. (13),

$$f_J = -C_{iJKl}\gamma_{Kl,i}^{**} \tag{14}$$

which is the equivalent body force corresponding to the new eigenstrain.

#### **3** Proposed Calculation Method

Using the equivalent body force (14), the induced total extended displacement  $u_K$  can then be found as

$$u_K(\mathbf{X}) = -\int_V u_J^K(\mathbf{x}; \mathbf{X}) [C_{iJLm} \gamma_{Lm}^{**}(\mathbf{x})]_{,i} dV(\mathbf{x})$$
(15)

where  $u_J^K(x; X)$  is the Green's *J*th elastic displacement/electric potential at *x* due to a line–force/line–charge in the *K*th direction applied at *X*.

Integrating by parts and noticing that the new eigenstrain is nonzero only in V, Eq. (15) can be expressed alternatively as

$$u_K(\boldsymbol{X}) = \int_V u_{J,x_i}^K(\boldsymbol{x};\boldsymbol{X}) C_{iJLm} \gamma_{Lm}^{**}(\boldsymbol{x}) dV(\boldsymbol{x})$$
(16)

The total extended strain  $\gamma_{Ij}$  can be obtained by taking the derivative of  $u_K(X)$ .

$$u_{K,p}(\boldsymbol{X}) = \int_{V} u_{J,x_{i}X_{p}}^{K}(\boldsymbol{x};\boldsymbol{X}) C_{iJLm} \gamma_{Lm}^{**}(\boldsymbol{x}) dV(\boldsymbol{x})$$
(17)

We now write Eq. (17) symbolically and equivalently as

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$$\gamma_{Ii}(\boldsymbol{X}) = S_{IjLm}(\boldsymbol{x}; \boldsymbol{X}) \otimes \gamma_{Lm}^{**}(\boldsymbol{x})$$
(18)

where  $S_{IJLm} \otimes$  is an integral operation tensor over  $\gamma_{Ij}^{**}$ , and for the elliptic or ellipsoidal inhomogeneity, it reduces to the well-known Eshelby tensor [1,2] being a function of the field point *X* only (extended to the piezoelectric case).

To carry out the integration, we assume that the boundary of the eigenstrain domain is composed of piecewise straight line segments. We define an arbitrary line segment in the (x,z)-plane starting from point 1  $(x_1, z_1)$  and ending at point 2  $(x_2, z_2)$ , in terms of the parameter  $t(0 \le t \le 1)$ , as  $x = x_1 + (x_2 - x_1)t$ ,  $z = z_1 + (z_2 - z_1)t$ . The outward normal component  $n_i(x)$  along the line segment is constant, given by  $n_1 = (z_2 - z_1)/l$ ;  $n_2 = -(x_2 - x_1)/l$ , with  $l = \sqrt{(x_2 - x_1)^2 + (z_2 - z_1)^2}$ . Under this assumption, the integration can be carried out and expressed in terms of the elementary functions for the corresponding inclusion problem [18,19].

Now, letting Eq. (8a) equals to Eq. (11a) gives, in the inhomogeneity domain V,

$$C_{iJLm}^{*}(\gamma_{Lm}^{0} + \gamma_{Lm} - \gamma_{Lm}^{p}) = C_{iJLm}(\gamma_{Lm}^{0} + \gamma_{Lm} - \gamma_{Lm}^{**}) \quad V$$
(19)

Substitution of Eq. (18) into Eq. (19) gives, for any point X in V,

$$C^*_{iJLm}[\gamma^0_{Lm} + S_{Lmlj}(\boldsymbol{x}; \boldsymbol{X}) \otimes \gamma^{**}_{lj}(\boldsymbol{x}) - \gamma^{\nu}_{Lm}(\boldsymbol{X})]$$
  
=  $C_{iJLm}[\gamma^0_{Lm} + S_{Lmlj}(\boldsymbol{x}; \boldsymbol{X}) \otimes \gamma^{**}_{lj}(\boldsymbol{x}) - \gamma^{**}_{Lm}(\boldsymbol{X})]$  (20)

However, it is clear that for a general polygonal geometry, the general eigenstrain  $\gamma_{lj}^{**}$  is nonuniform. Thus, Eq. (20) would require a domain integration of x over V for the unknown  $\gamma_{lj}^{**}$ , as given in Eqs. (17) and (18). The direct domain discrete approach was employed by Ref. [23] for the isotropic elastic case with polygonal inhomogeneity.

Here, we propose a new approach to solve Eq. (20). We first assume that  $\gamma_{lj}^{**}(x)$  are uniform in the inhomogeneity taking the values at point X so that the "Eshelby tensor"  $S_{ljLm}(x; X)$ , which is a two-point function tensor, can be found exactly (by carrying out the integration for the variable x) as a function of X only. In so doing, we are approximating the "operational Eshelby tensor" by its average value. Then Eq. (20) can be solved for  $\gamma_{lj}^{**}$  as a function of X. In other words, we can solve  $\gamma_{lj}^{**}$  at all points of the inhomogeneity domain V. It is striking that the solution based on this approximation, named as the first-order solution  $\gamma_{lj}^{**(1)}$ , is already





Fig. 2 (a) A triangular QWR (SiC) in an isotropic elastic fullplane under a far-field stress  $\sigma_0$  (Young modulus = 210 GPa, Poisson's ratio = 0.3). (b) Stress  $\sigma_{zz}$  along the *x*-axis.

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Fig. 3 (a) A triangular QWR (Ti-6Al-4V) in an isotropic elastic full-plane under a far-field stress  $\sigma_0$  (Young modulus = 210 GPa, Poisson's ratio = 0.3). (b) Stress  $\sigma_{zz}$  along the *x*-axis.

Table 1 Elastic properties of the matrix and inhomogeneity materials used in the triangle model (Figs. 2(*a*), 2(*b*), 3(*a*), and 3(*b*))

		Inclusion materials		
	Matrix	SiC	Ti-6Al-4V	
Young's modulus $E$ (GPa)	210	410	110	
Poisson's ratio $\nu$	0.30	0.16	0.34	

very accurate as compared to the direct method (based on the BEM, see comparison in the Figs. 2(*b*), 3(*b*), and 4(*b*)). Furthermore, the unknown eigenstrain  $\gamma_{ij}^{**}$  can be further refined if needed by using the following iteration for *i* = 1, 2, 3...:

$$C_{iJLm}^{*}[\gamma_{Lm}^{0} + S_{Lmlj}(\mathbf{x}; \mathbf{X}) \otimes \gamma_{lj}^{**(i)}(\mathbf{x}) - \gamma_{Lm}^{p}(\mathbf{X})] = C_{iJLm}[\gamma_{Lm}^{0} + S_{Lmlj}(\mathbf{x}; \mathbf{X}) \otimes \gamma_{lj}^{**(i)}(\mathbf{x}) - \gamma_{Lm}^{**(i+1)}(\mathbf{X})]$$
(21)

This solution is valid for the field inside the inhomogeneity of an arbitrary shape in an infinite plane and its convergence can be indirectly observed by comparing with the BEM results and by checking the results at different iteration steps. With the calculated field inside, the stress immediately outside the inhomogeneity can be evaluated approximately by the following relation [2]:

$$\sigma_{iJ}^{out} = \sigma_{iJ}^{in} + C_{iJKl} [-C_{pQMn} \gamma_{Mn}^{**} n_p n_l N_{QK}(\boldsymbol{n}) / D(\boldsymbol{n}) + \gamma_{Kl}^{**}]$$
(22)

where  $N_{II}(n)$  and D(n) are the cofactor and determinant of the matrix  $K_{II}(n)$  defined as

$$K_{JK}(\boldsymbol{n}) = C_{iJKl}n_in_l \tag{23}$$

with  $n_p$  being the unit outward normal on the interface. Using relation (22), the iteration for the outside points close to the interface between the inhomogeneity and matrix can be carried out using the iteration results at the corresponding inside points.

It should be pointed out that since the iteration results for outside points are obtained from the iteration results at the inside points near the interface, the results in the matrix could contain some errors due to this approximation.

#### 4 Numerical Examples

We point out that the solutions developed in Sec. 3 can be applied to both 2D and 3D problems. In this paper, we will concentrate on the 2D case. Furthermore, before using our analytical solution to the general inhomogeneity in the piezoelectric InAs/GaAs system, we first apply it to a triangular QWR (Fig. 2(*a*)) and a rectangular QWR (Fig. 3(*a*)) in the elastic matrix to verify our method. These two systems are both under the remote uniaxial stress  $\sigma_0 = 0.2$  GPa. The triangular QWR is an isosceles with the base-



Fig. 4 (a) A rectangular QWR (ZrO<sub>2</sub>) in an isotropic elastic Al<sub>2</sub>O<sub>3</sub> full-plane under a far-field stress  $\sigma_0$ . (b) Stress  $\sigma_{zz}/\sigma_0$  along the x-axis.

line length being b = 10 nm and its height being a = 20 nm. The elastic properties of the matrix and inclusion are listed in Table 1. In both examples, the matrix is made of the same isotropic material. Our analytical solutions with different iterations are compared with the BEM results [24], as shown in Figs. 2(*b*) and 3(*b*). The rectangular QWR has a length of b = 20 nm and a width of a = 10 nm. The matrix is Al<sub>2</sub>O<sub>3</sub> with the Young's modulus E = 345 GPa, Poisson's ratio  $\nu = 0.131$ . The inclusion is ZrO<sub>2</sub> with E = 192 GPa,  $\nu = 0.3$ . The results are also compared with those obtained by the BEM (Fig. 4(*b*)). It is seen from Figs. 2(*b*), 3(*b*), and 4(*b*) that our

Table 2 The maximum relative errors of the stress component  $\sigma_{zz}$  between the fifth-order/six-order iteration and BEM [24] results for inhomogeneities SiC, Ti-6AI-4V, and ZrO2 in the matrix under a far-field stress  $\sigma_0 = 0.2$  GPa. The matrix corresponding to inhomogeneities SiC and Ti-6AI-4V is made of isotropic material (Young modulus = 210 GPa, Poisson's ratio = 0.3 as given in Table 1) (relative error = abs (iteration result – BEM)/BEM \* 100%).

Inhomogeneity materials	Matrix	First order (%)		Fifth order (%)	
		Inside	Outside	Inside	Outside
Triangle SiC	$E = 210 \text{ GPa}$ $\nu = 0.3$	5.26	7.06	2.03	6.12
Triangle Ti-6Al-4V	$E = 210 \text{ GPa}$ $\nu = 0.3$	1.28	7.28	0.18	3.10
Rectangle ZrO <sub>2</sub>	Al <sub>2</sub> O <sub>3</sub>	1.57	3.32	0.27	1.84

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solutions inside the QWRs are almost the same as the previously published results and that the accuracy of the iteration is apparent. However, the solutions outside the QWR show some error which may be caused by the approximate formula (22).

Table 2 lists the maximum relative errors between our iteration and BEM for the stresses both inside and outside the inhomogeneity shown in Figs. 2(b), 3(b), and 4(b). It is clear that the maximum relative error inside is much smaller than that outside and



Fig. 5 (a) Triangular QWR of InAs (001) within the GaAs (001) full plane (under a hydrostatic eigenstrain in QWR). (b) Stress  $\sigma_{xx}$  along the *x*-axis. (c) Stress  $\sigma_{xx}$  along the *z*-axis. (d) Stress  $\sigma_{zz}$  along the *x*-axis. (e) Stress  $\sigma_{zz}$  along the *z*-axis. (f) Stress  $\sigma_{xz}$  along the *z*-axis. (g) Electric displacement  $D_z$  along the *z*-axis.

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that this error decreases with increasing iteration steps. Furthermore, the maximum error occurs at the point near the interface. We would like to point out that since the interface between the inhomogeneity and matrix is a singular line, in our numerical cal-

culation, we use points near the interface. For example, if the coordinate for the interface is at (x,z) = (-10.0 nm, 0), we then use (x,z) = (-9.75 nm, 0) and (x,z) = (-10.25 nm, 0) for the inhomogeneity and matrix sides, respectively.



Fig. 6 (a) Triangular QWR of InAs (111) within the GaAs (111) full plane (under a hydrostatic eigenstrain in QWR). (b) Stress  $\sigma_{xx}$  along the x-axis. (c) Stress  $\sigma_{xx}$  along the z-axis. (d) Stress  $\sigma_{zz}$  along the x-axis. (e) Stress  $\sigma_{zz}$  along the z-axis. (f) Stress  $\sigma_{xz}$  along the z-axis. (g) Electric displacement  $D_x$  along the x-axis. (h) Electric displacement  $D_x$  along the z-axis.

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Fig. 7 (a) Rectangular QWR of InAs (001) within the GaAs (001) full plane (under a hydrostatic eigenstrain in QWR). (b) Stress  $\sigma_{xx}$  along the x-axis. (c) Stress  $\sigma_{xx}$  along the z-axis. (d) Stress  $\sigma_{zz}$  along the x-axis. (e) Stress  $\sigma_{zz}$  along the z-axis.

The method above is now applied to the mechanical–electrical coupling systems. There will be no remote uniaxial stress in the numerical examples below. The triangular QWR has the dimension of a = 20 nm and b = 10 nm (Figs. 5(*a*) and 6(*a*)), and the rectangular QWR has a size of  $a \times b = 30$  nm  $\times 20$  nm (Figs. 7(*a*) and 8(*a*)). The misfit-strain is hydrostatic, i.e.,  $\gamma_{xx}^* = \gamma_{zz}^* = 0.07$  and the elastic properties for the matrix GaAs (001) are  $C_{11} = 118 \times 10^9$  N/m<sup>2</sup>,  $C_{12} = 53.8 \times 10^9$  N/m<sup>2</sup>, and  $C_{44} = 59.4 \times 10^9$  N/m<sup>2</sup> [25]. The piezoelectric constant and relative permeability for GaAs (001) are, respectively,  $e_{14} = 0.16$  C/m<sup>2</sup> and  $\varepsilon_r = 12.5 \times 10^{-9}$  [25]. For the

inhomogeneity InAs (001), we have  $C_{11} = 83.29 \times 10^9$  N/m<sup>2</sup>,  $C_{12} = 45.26 \times 10^9$  N/m<sup>2</sup>, and  $C_{44} = 39.59 \times 10^9$  N/m<sup>2</sup>. The piezoelectric constant and relative permeability for InAs (001) are, respectively,  $e_{14} = 0.0456$  C/m<sup>2</sup> and  $\varepsilon_r = 0.1346 \times 10^{-9}$ . We obtain the material properties for GaAs (111) and InAs (111) by coordinate transform as in Ref. [25].

Some numerical results are discussed below and the maximum relative errors along the selected lines (include both inside and outside points) between the fourth and fifth order of iterations are listed in Table 3. Actually, the results for inside points are very accurate,

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Fig. 8 (a) Rectangular QWR of InAs (111) within the GaAs (111) full plane (under a hydrostatic eigenstrain in QWR). (b) Stress  $\sigma_{xx}$  along the x-axis. (c) Stress  $\sigma_{xx}$  along the z-axis. (d) Stress  $\sigma_{zz}$  along the x-axis. (e) Stress  $\sigma_{zz}$  along the z-axis. (f) Electric displacement  $D_x$  along the z-axis.

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Table 3 The maximum relative errors of the field quantities between the fourth-order and fifth-order iterations for results presented in Figs. 5–8 (relative error = abs (fourth-order iteration–fifth-order iteration)/fifth-order iteration \* 100%)

Inhomogeneities	Matrix		Fourth order	Fifth order	Maximum error (%)
Triangle InAs(001)	GaAs(001)	$\sigma_{xx} (x-axis)$ $\sigma_{xx} (z-axis)$ $\sigma_{zz} (x-axis)$ $\sigma_{zz} (z-axis)$ $\sigma_{xz} (z-axis)$ $D_{z} (z-axis)$	$\begin{array}{r} -0.87612 \times 10^8 \\ 1.68768 \times 10^9 \\ 0.3602 \times 10^9 \\ -1.1469 \times 10^9 \\ -2.20323 \times 10^9 \\ -6.05364 \end{array}$	$\begin{array}{c} -0.82606 \times 10^8 \\ 1.70771 \times 10^9 \\ 0.3483 \times 10^9 \\ -1.0172 \times 10^9 \\ -2.17312 \times 10^9 \\ -5.85352 \end{array}$	6.06 1.17 3.4 12.75 1.4 3.4
Triangle InAs(111)	GaAs(111)	$\sigma_{xx} (x-axis)$ $\sigma_{xx} (z-axis)$ $\sigma_{zz} (x-axis)$ $\sigma_{zz} (z-axis)$ $\sigma_{xz} (z-axis)$ $D_x (x-axis)$ $D_x (z-axis)$	$\begin{array}{c} -14.0031\times10^{10}\\ -6.90889\times10^9\\ -9.682\times10^{10}\\ -8.30697\times10^9\\ \textbf{0.22698\times10^9}\\ 0.00852\\ -0.00583\end{array}$	$\begin{array}{c} -14.5023\times10^{10}\\ -7.00895\times10^9\\ -10.679\times10^{10}\\ -8.53714\times10^9\\ \textbf{0.17704}\times10^9\\ 0.00949\\ -0.00602\end{array}$	3.44 1.43 9.33 2.7 <b>28.2</b> 10.2 3.16
Rectangle InAs(001)	GaAs(001)	$\sigma_{xx} (x-axis) \sigma_{xx} (z-axis) \sigma_{zz} (x-axis) \sigma_{zz} (z-axis) \sigma_{zz} (z-axis)$	$\begin{array}{c} -2.46491 \times 10^9 \\ 2.04622 \times 10^9 \\ 1.62011 \times 10^9 \\ -2.28361 \times 10^9 \end{array}$	$\begin{array}{c} -2.40489 \times 10^9 \\ 2.14618 \times 10^9 \\ 1.59008 \times 10^9 \\ -2.23355 \times 10^9 \end{array}$	2.5 4.66 1.89 2.24
Rectangle InAs(111)	GaAs(111)	$ \begin{aligned} \sigma_{xx} & (x\text{-axis}) \\ \sigma_{xx} & (z\text{-axis}) \\ \sigma_{zz} & (x\text{-axis}) \\ \sigma_{zz} & (z\text{-axis}) \\ D_x & (x\text{-axis}) \\ D_x & (z\text{-axis}) \end{aligned} $	$\begin{array}{c} -2.24003 \times 10^9 \\ 1.92126 \times 10^9 \\ -9.20411 \times 10^9 \\ -9.38096 \times 10^9 \\ 0.00597 \\ 0.00106 \end{array}$	$\begin{array}{c} -2.13981 \times 10^9 \\ 1.76956 \times 10^9 \\ -9.39512 \times 10^9 \\ -9.57843 \times 10^9 \\ 0.00631 \\ 0.00094 \end{array}$	4.7 8.57 2.03 2.06 5.39 12.8

and the maximum relative errors in the table correspond to the points outside. We have tested that the maximum relative errors continuously decrease with increasing orders of iteration. For example, in Fig. 6(*f*), the maximum relative error for  $\sigma_{xz}$  is 28.2% at (x,z) = (0.0, -4.75) nm, as highlighted in Table 3. With increasing iteration steps, the error is then reduced to 8.3% for sixth order, 2.1% for seventh order, and 0.2% for eighth order. This further shows indirectly that our iteration approach is convergent.

Shown in Figs. 5(b)-5(f) are the stress distributions in the system of a triangular InAs (001) QWR within the GaAs (001) matrix (Fig. 5(a)) using different orders of iteration. The corresponding electric displacement  $D_z$  along the z-axis is shown in Fig. 5(g). From these figures, it is observed that the calculated field quantities inside the QWR are almost independent of the iteration steps, showing that the first-order iteration is already accurate enough (to  $10^{-4}$ ). On the other hand, outside in the matrix, we observe obviously more accurate results with increasing iteration steps. Therefore, iteration is essential especially for the outside field. Concerned with Fig. 5(g), the electric displacement  $D_z$  is antisymmetric about the central point, especially after iteration. This is a very interesting electric phenomenon.

Figures 6(b)-6(h) show the stress and electric displacement fields in the system where a triangular InAs (111) QWR is in the GaAs (111) full-plane matrix (Fig. 6(a)). The most impressive phenomenon in Figs. 6(b) and 6(d) are the stress concentration at the corner of the triangle inhomogeneity. It is observed from Fig. 6(c) that the stress  $\sigma_{xx}$  along the z-axis is symmetric. However, the stress  $\sigma_{zz}$  along the z-axis is asymmetric particularly after iteration (Fig. 6(e)), which may be caused by the electromechanical coupling. Figure 6(f) shows the distribution of the stress  $\sigma_{xz}$  along the z-axis, which is similar but different to Fig. 5(f) in the corresponding InAs/GaAs (001) system, due to the material anisotropy (caused by material property transform). Figures 6(g) and 6(h)show the variation of the electric component  $D_x$  along the x- and z-axes. The refinement of the solutions via iteration can be obviously observed from these figures. Figures 7(b)-7(e) shows the stress distributions in the corresponding InAs/GaAs (001) system with a rectangular QWR (Fig. 7(a)).

Finally, Figs. 8(b)-8(g) show the field quantity variation in the system of a rectangular InAs (111) QWR within the GaAs (111) matrix (Fig. 8(a)). Figures 8(b)-8(c) demonstrate clearly the im-

portance of the iteration for the stress component  $\sigma_{xx}$  in the matrix, especially in the vicinity of the interface. The iteration refinement on the stress component  $\sigma_{zz}$  within the QWR is shown in Fig. 8(*d*). Also, the stress component  $\sigma_{zz}$  is continuous across the interface between the QWR and matrix (shown by Fig. 8(*e*)). Finally, the magnitude of the electric displacement  $D_x$  along the *z*-axis becomes smaller after iteration (shown by Fig. 8(*f*)).

#### **5** Conclusions

In this paper, we have derived an analytical solution for the Eshelby problem of polygonal inhomogeneity in an anisotropic piezoelectric full-plane. Based on the equivalent body-force concept of eigenstrain, we first expressed the induced elastic and piezoelectric fields in the corresponding inclusion in terms of a line integral on the boundary of the inclusion with the integrand being the linesource Green's functions. Using the recently derived exact closedform Green's functions, the line integral is carried out analytically by assuming a piecewise straight-line boundary for the inhomogeneity, i.e., an arbitrarily shaped polygon. The most remarkable feature is that the final result involves only very simple elementary functions. For the corresponding inhomogeneity problem, the classic Eshelby inhomogeneity relation is extended to the polygonal inhomogeneity so that the inhomogeneity problem can be solved by a simple iteration algorithm. The proposed method is first validated to be accurate by comparing with existing results for the isotropic elastic inhomogeneity case. It is demonstrated that with only a few iterations, very accurate field results inside the inhomogeneity can be obtained whilst the solution outside contains some errors due to the approximation used. The developed solution is then applied to triangular and rectangular piezoelectric InAs QWRs within GaAs full-planes, with results clearly showing the importance of the material orientation and piezoelectric coupling. While our numerical results can serve as benchmarks and could be useful to the analysis of nanoscale QWR structures, multiple inclusion/inhomogeneity problems in elastic and piezoelectric matrices (i.e., Ref. [26]) could be performed readily using the proposed analytical approach.

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