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Singularity analysis at the vertex of polygonal quantum wire inclusions

E. Pan *, X. Jiang

Department of Civil Engineering, The University of Akron, Akron, OH 44325-3905, USA

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Abstract

Singular behavior near the vertex/corner of polygonal inclusions in anisotropic piezoelectric planes is identified and investigated. Using a recently derived exact closed-form solution, the elastic and electric fields associated with regular polygon-shaped quantum wires are analyzed in detail, revealing the effect of factors such as material orientation, type of eigenstrain, and number of sides of polygons on the singular behavior. Our study shows that by adjusting these factors properly, one could avoid the singular behavior or reduce the level of singularity, which could be of significance in the design and fabrication of the semiconductor devices.

Keywords: Singular behavior at vertex; Polygonal inclusion; Analytical solution; Quantum wire

1. Introduction

Elastic singularity occurs when there is a discontinuity including significant variation in geometry, interface of dissimilar material (Koguchi and Muramoto, 2000), or an abrupt change in the boundary conditions (Huang, 2003). Previously, various stress/strain singularity problems were addressed (Mantic et al., 1997; Savruk and Shkarayev, 2001; Apel et al., 2002; Dimitrov et al., 2002; Huang, 2003). As far as the geometric change is concerned, elastic singularity has been reported and investigated in both two-dimensional (2D) and three-dimensional (3D) dislocation analyses (Tong and Zhang, 1996; Apel et al., 2002), in polygonal inclusion with corner or vertex (Rodin, 1996; Nakasone et al., 2000; Dimitrov et al., 2001; Savruk and

* Corresponding author. Tel.: +330 972 6739; fax: +330 972 6020.
E-mail address: pan2@uakron.edu (E. Pan).

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Shkarayev, 2001; Apel et al., 2002), in problems associated with notches or laminated composite wedges (Pageau and Biggers, 1996; Dimitrov et al., 2002; Helsing and Jonsson, 2002), and for edges of thick plates (Kohno and Ishikawa, 1995; Huang, 2003). As to the material discontinuity, bimaterial crack front (Kohno and Ishikawa, 1995; Xie and Chaudhuri, 1998), order of stress singularity at 3D joints and interface or interface corner (Koguchi, 1997; Yosibash, 1997; Liu et al., 1999; Koguchi and Muramoto, 2000), and compound piezoceramic wedge (Fil'shtinskii and Matvienko, 2001) are examples of the research that have been carried out. Knowledge of singular behavior is most important since singularity could initiate local failure thus essential to the failure criteria (Dunn et al., 1997; Mantic et al., 1997). Furthermore, numerical study of any complex structure involving sharp geometry and material discontinuity requires the information on singularity (Huang, 2003).

In light of its significance, various methods have been proposed to the study of singularity near the vertices, among which are finite element method (FEM) (Apel et al., 2002), boundary element method (BEM) (Koguchi, 1997; Savruk and Shkarayev, 2001) and their coupling (Li and Lu, 2000), Galerkin-Petrov finite-element approximation technique (Dimitrov et al., 2001), conformal mapping (Kohno and Ishikawa, 1995) in addition to the equivalent inclusion method (Nakasone et al., 2000). Many factors or conditions have been identified which can affect either the singular behavior or the level of singularity. For example, the effect of the material orientation on singularity has been discussed particularly in the cases of isotropy (Tong and Zhang, 1996; Koguchi and Muramoto, 2000), orthotropy (Mantic et al., 1997), and general anisotropy (Apel et al., 2002).

Low dimensional quantum structures including quantum well/wire/dot nowadays are subject to intensive research in semiconductor physics community and are attracting increasing attention due to their novel electronic and optical features associated with the strain field (Gosling and Willis, 1995). Under certain assumptions, a strained quantum structure can be treated as an elastic inclusion (Gosling and Willis, 1995) where an eigenstrain inside is induced due to the lattice mismatch between the inclusion and its surrounding matrix. Therefore the Eshelby inclusion model can be applied in the examination of these structures. Again, singular behavior in the elastic field distribution associated with these structures has been reported in the vicinity of the corner/vertex of isotropic quantum wires (QWR) of different shapes (Caro et al., 1996; Niquet et al., 1998). However complete understanding in elastic singularity particularly in anisotropic elasticity, is needed in the design and fabrication process because strain, on one hand, provides freedom of tailoring the band structure and modify optical/transport properties of semiconductors (Jain et al., 1996), and on the other hand, could lead to, for example, structural problems causing accelerated degradation of the devices (Bangert, 1994; Downes et al., 1995).

Nozaki et al. (2001) studied the stress field associated with polygonal inclusion in an elastic homogeneous and isotropic domain using the Green's function. He found that there is no stress singularity at the corner of the square inclusion where the sides of the square are parallel to the coordinate axes and the eigenstrain has no shear component (Nozaki et al., 2001). Investigation of singular behavior in a more realistic system with material anisotropy is still lack; yet, a large variety of semiconductor materials are anisotropic, which requires a detailed investigation on this matter.

Utilizing an exact close-form solution to 2D piezoelectric inclusion problems, we study, in this paper, the model systems of the QWR with regular polygonal shapes embedded in an anisotropic plane. We identify and examine the factors that influence the singular behavior close to the vertex of the polygons. Those factors include material orientation, corner angle (the sides of the regular polygon), and the prescribed eigenstrain inside the QWR. Representative isotropic, cubic, transversely isotropic and generally anisotropic semiconductor materials are selected while dilatational and uniaxial eigenstrain are prescribed inside the inclusion of the polygon. In what follows, after briefly reviewing the analytical solution we derived previously, we employ this solution to the analysis of singular behaviors in the QWR structure. Results are discussed and certain conclusions are drawn.

2. Analytical solution to the 2D inclusion problem

With the help of the fundamental solution, the inclusion problem in a piezoelectric full-plane can be solved analytically (Pan, 2004a,b). Assume that there is an N-sided arbitrarily shaped polygonal inclusion in an anisotropic piezoelectric full-plane with a prescribed extended eigenstrain $\gamma_{Ij}^*(\gamma_{ij}^*; -E_j^*)$ inside, then the induced extended displacement u_K (elastic displacement u_k and electric potential ϕ) can be expressed in the form (Pan, 2004a)

$$u_K(\boldsymbol{X}) = C_{iJLm}\gamma_{Lm}^* \int_{\partial V} u_J^K(\boldsymbol{x};\boldsymbol{X}) n_i(\boldsymbol{x})\,\mathrm{d}S(\boldsymbol{x}) \tag{1}$$

where C_{iJKl} is the extended material properties, γ_{Ij}^* the extended eigenstrain in the inclusion, $n_i(\boldsymbol{x})$ the outward normal on the boundary of the inclusion, and $u_J^K(\boldsymbol{x};\boldsymbol{X})$ the Green's Jth elastic displacement/electric potential at $\boldsymbol{x}$ due to a line-force/line-charge in the Kth direction applied at $\boldsymbol{X}$.

Substituting the 2D piezoelectric Green's functions (Ting, 1996; Pan, 2002) in the Stroh formalism and making use of the equivalent body-force concept (Mura, 1987; Pan, 2004a), the extended displacement has the simple form as

$$u_K(\boldsymbol{X}) = \sum_{s=1}^{N} n_i^{(s)} C_{iJLm}\gamma_{Lm}^* \frac{l^{(s)}}{\pi} \mathrm{Im}\left\{A_{JR} h_R^{(s)}(X,Z) A_{KR}\right\} \tag{2}$$

in which superscript (s) indicates the sth line segment of the boundary, l the length of the line segment, $h_R^{(s)}$ a simple function of the coordinate $\boldsymbol{X} = (X, Z)$, and p_J (in the expression of $h_R^{(s)}$) and $\boldsymbol{A}$ the Stroh eigenvalues and eigenvectors.

Taking the derivatives of Eq. (2) gives the extended strain (elastic strain and electric field), and making use of the constitutive law gives the extended stress (stress and electric displacement).

3. Numerical examples

With the analytical solution (2) for the elastic displacement/electric potential and the corresponding extended strain/stress available, we examine, in the following, the elastic/electric fields due to a polygonal inclusion in a full-plane.

We assume that there is a regular polygonal inclusion in a semiconductor full-plane as shown in Fig. 1 where one vertex is fixed on the x-axis for all the polygons. We concentrate on the elastic and electric fields along the x-axis passing this vertex (line OA) (Nozaki et al., 2001). The material properties selected in our study are: transversely isotropic AlN with the z-axis being the poling direction (along 0001) (Singh, 1993; Pan, 2003); cubic GaAs(001) with material orientations along the coordinate axes (Pan, 2004a); anisotropic GaAs(111) where the z-axis of the coordinates is along the (111)-direction of the cubic GaAs material (Pan, 2004a); and finally, an isotropic semiconductor material with Young's modulus of 2.6×10^7 kN/m^2 and Poisson's ratio of 0.3. Two eigenstrain fields are described inside the inclusions: a dilatational eigenstrain $(\gamma_{xx}^*, \gamma_{yy}^*, \gamma_{zz}^*) = (1.0, 1.0, 1.0)$ and a uniaxial eigenstrain $(\gamma_{xx}^*, \gamma_{yy}^*, \gamma_{zz}^*) = (1.0, 0.0, 0.0)$ (Nozaki et al., 2001). N-sided regular polygons with $N = 3, 4, 5, 6, 10, 20$ are chosen with a triangular, rectangular, and square cross-section of the quantum wires being under intensive study (Freund and Gosling, 1995; Ogawa et al., 1998).

The calculated stress component σ_{zz} for the N-sided polygonal inclusion with a uniaxial eigenstrain in an elastic isotropic full-plane is plotted in Fig. 2, which is similar to the result in Nozaki et al. (2001). The most striking feature is that in contrast to that in other polygonal shapes, the stress σ_{zz} due to a square inclusion does not have logarithmic singularity at the vertex. Additionally, along the x-axis from the center point to

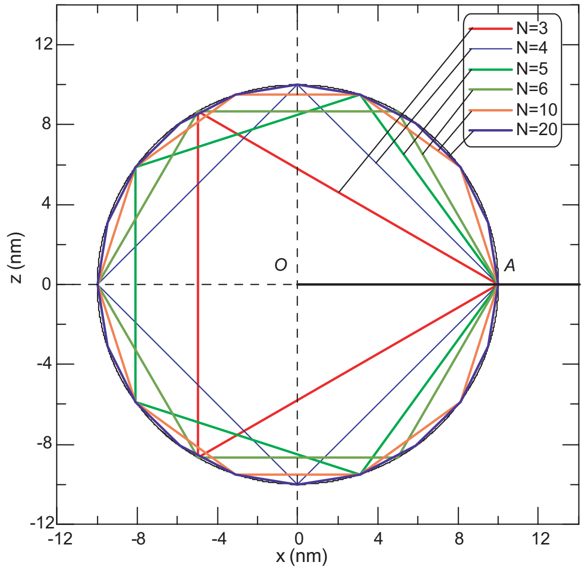

Fig. 1. N-sided regular polygon inclusion embedded in the semiconductor full-plane with the radius of the circumscribed circle of 10 nm and with one vertex on the x-axis ($N = 3, 4, 5, 6, 10, 20$).

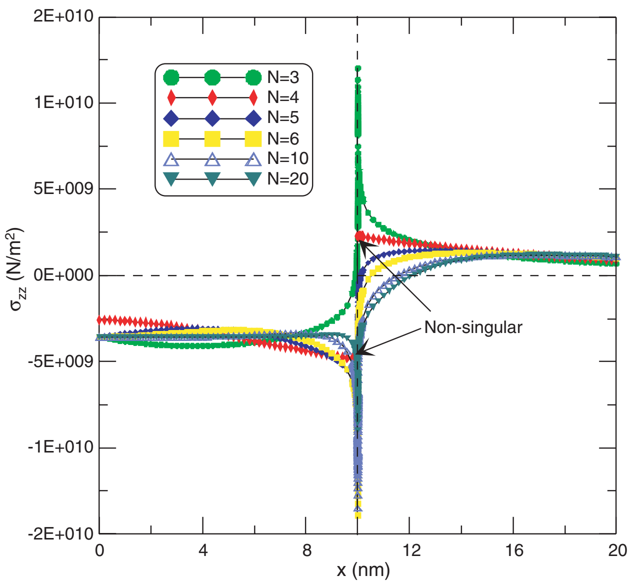

Fig. 2. Stress component σ_{zz} along x-axis due to an N-sided polygonal inclusion with a uniaxial eigenstrain, embedded in an isotropic full-plane.

the outside, σ_{zz} inside the triangle exhibits a different trend from that of the other shapes, where a slight decrease starts from the center followed by an abrupt increase to the vertex.

Shown in Fig. 3 are hydrostatic strains ($\gamma_{xx} + \gamma_{zz}$) in an N-sided polygonal inclusion with different eigen-strain conditions in the domain of cubic materials, e.g., GaAs(001). As expected, the more the polygon

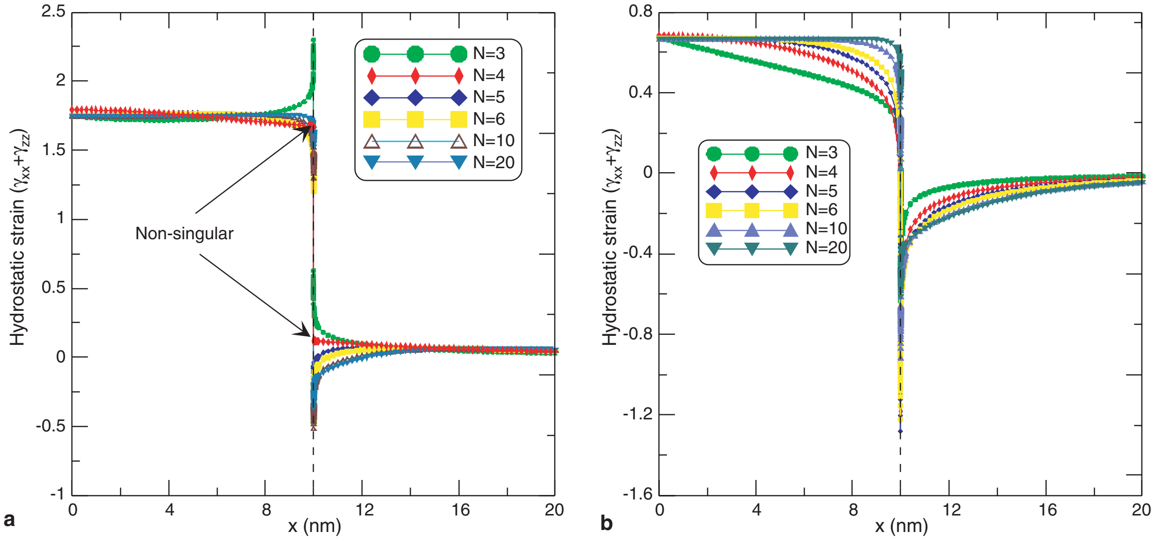

Fig. 3. Hydrostatic strain $\gamma_{xx} + \gamma_{zz}$ along x-axis due to an N-sided polygonal inclusion with a dilatational eigenstrain (a) and a uniaxial eigenstrain (b), embedded in cubic semiconductor GaAs(001).

resembles the circle, the more uniform the inside fields are, which is the well-known results (Pan, 2004a). All of these again prove the validity and accuracy of our method. The difference in the prescribed eigenstrain leads to not only the difference in the inside strain field (starting with 1.8 for dilatational eigenstrain case in Fig. 3a versus 0.7 for uniaxial eigenstrain case in Fig. 3b) but also the difference in the trend of hydrostatic strain in and outside the triangular quantum wire. Meanwhile singularity of the elastic fields in and outside square inclusions occurs for the uniaxial eigenstrain case (Fig. 3b) but not for the dilatational case (Fig. 3a).

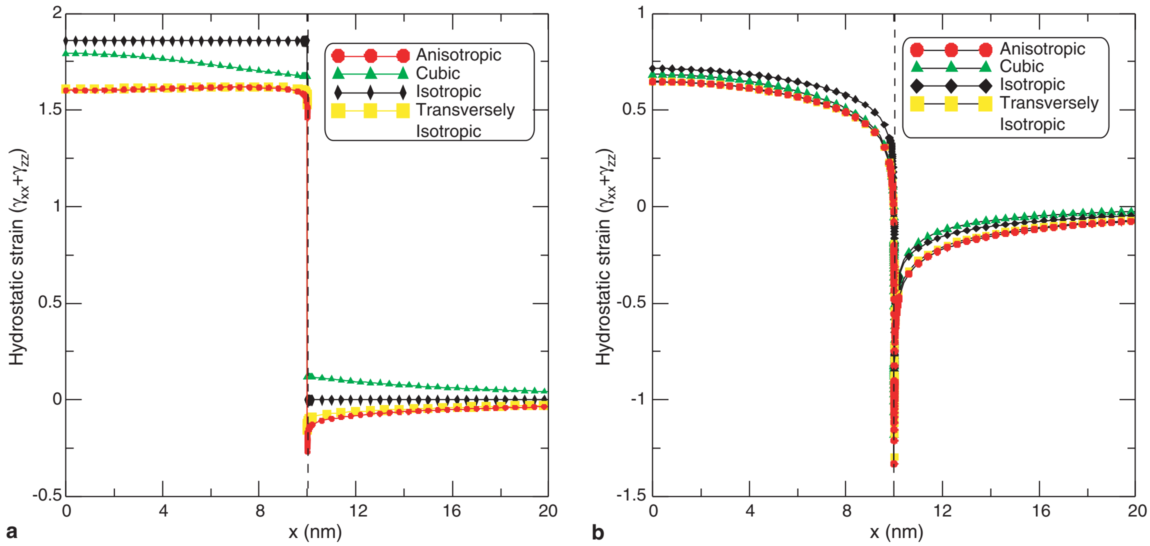

Fig. 4. Hydrostatic strain $\gamma_{xx} + \gamma_{zz}$ along x-axis due to a square inclusion with a dilatational eigenstrain (a) and a uniaxial eigenstrain (b), embedded in a semiconductor full-planes of isotropic, cubic, transversely isotropic, and generally anisotropic materials.

Fig. 4 shows the hydrostatic strain ($\gamma_{xx} + \gamma_{zz}$) along the x-axis in and outside a square inclusion within four different material planes. While results due to a dilatational eigenstrain are plotted in Fig. 4a, those due to a uniaxial eigenstrain are presented in Fig. 4b. Apparently singular behavior is observed for all the materials when a uniaxial eigenstrain is applied. For the dilatational eigenstrain case, however, singularity is

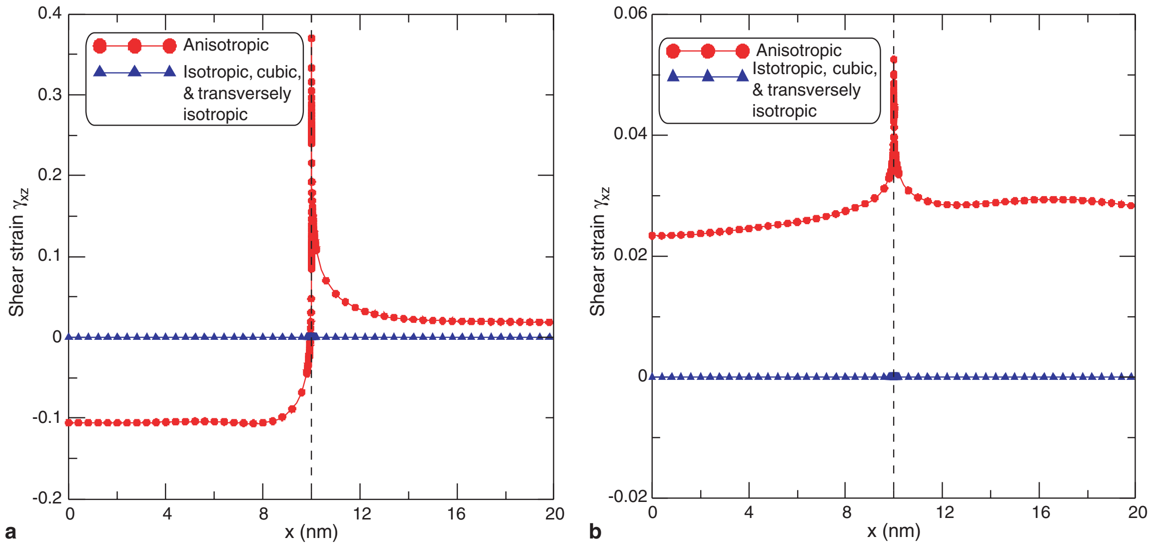

Fig. 5. Shear strain γ_{xz} along x-axis due to a 10-sided polygonal inclusion with a dilatational eigenstrain (a) and a uniaxial eigenstrain (b), embedded in a semiconductor full-planes of isotropic, cubic, transversely isotropic, and generally anisotropic materials.

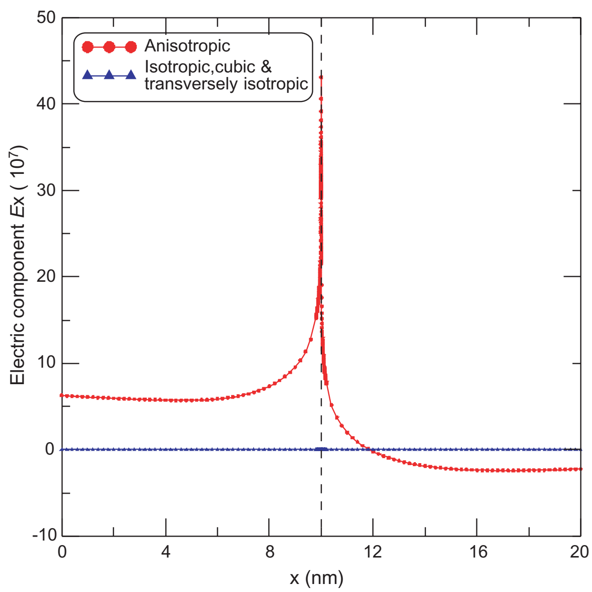

Fig. 6. Electric component E_x due to a pentagonal inclusion with a uniaxial eigenstrain, embedded in isotropic, cubic, transversely isotropic, and generally anisotropic full-plane.

associated only with anisotropic and transversely isotropic materials. The elastic fields due to inclusions of other regular polygons also follow the same feature. This suggests that for materials with higher material symmetry, i.e., isotropic and cubic, the hydrostatic strain field under a dilatational eigenstrain can be finite.

Shear strain γ_{xz} along the x-axis due to a 10-sided polygonal inclusion is presented in Fig. 5. Again, results due to a dilatational eigenstrain are in Fig. 5a, whilst those due to a uniaxial eigenstrain are plotted in Fig. 5b. It is obvious that except for the anisotropic case, γ_{xz} is identically zero. Also we find that for a dilatational eigenstrain the shear strain is negative (i.e., compressive) inside and positive (i.e., tensile) outside. Under uniaxial eigenstrain, however, the shear strain is positive both inside and outside the inclusion. Knowledge of this interesting point could contribute to better utilization of strains in obtaining desirable quantum heterostructures.

Finally Fig. 6 shows the electric component E_x due to a pentagonal inclusion with a uniaxial eigenstrain embedded in different materials. Similar to the shear strain case, E_x is identically zero in isotropic, cubic, and transversely isotropic materials, whilst in the anisotropic GaAs(1 1 1), a singularity exists at the vertex.

4. Concluding remarks

An exact closed-form solution derived previously is utilized to investigate the stress singularity at vertices of regular polygonal inclusions. By selecting four different materials (isotropic, cubic, transversely isotropic, and generally anisotropic), two prescribed eigenstrains (dilatational and uniaxial), and regular polygonal inclusions with various numbers of sides, the effect of material orientation, prescribed eigenstrain, and corner angle at the vertex on the elastic singularity is revealed. A summary on this effect is given below:

(1) Under uniaxial eigenstrain inside the QWR of polygons with different number of sides, the hydrostatic strain ($\gamma_{xx} + \gamma_{zz}$) usually shows a singularity at the corner; under dilatational eigenstrain, however, the singularity of hydrostatic strain at the corner disappears for a square inclusion within an isotropic or cubic material.
(2) For a QWR with a square cross-section in an isotropic semiconductor material under a uniaxial eigenstrain, the stress component σ_{zz} at the corner is non-singular.
(3) The elastic field due to a QWR with a triangular cross-section exhibits different features as compared to those associated with other regular polygons.
(4) Shear strain and electric fields can be induced by the polygonal QWR with both eigenstrain conditions if the material is anisotropic, i.e., GaAs(1 1 1).

We finally remark that the present work is the initial step towards the understanding of the impact of the various factors on the singular behavior of the induced stress and electric fields. Further investigation taking into account of more realistic situations, including half space, quantum arrays, and 3D singularity, is needed.

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