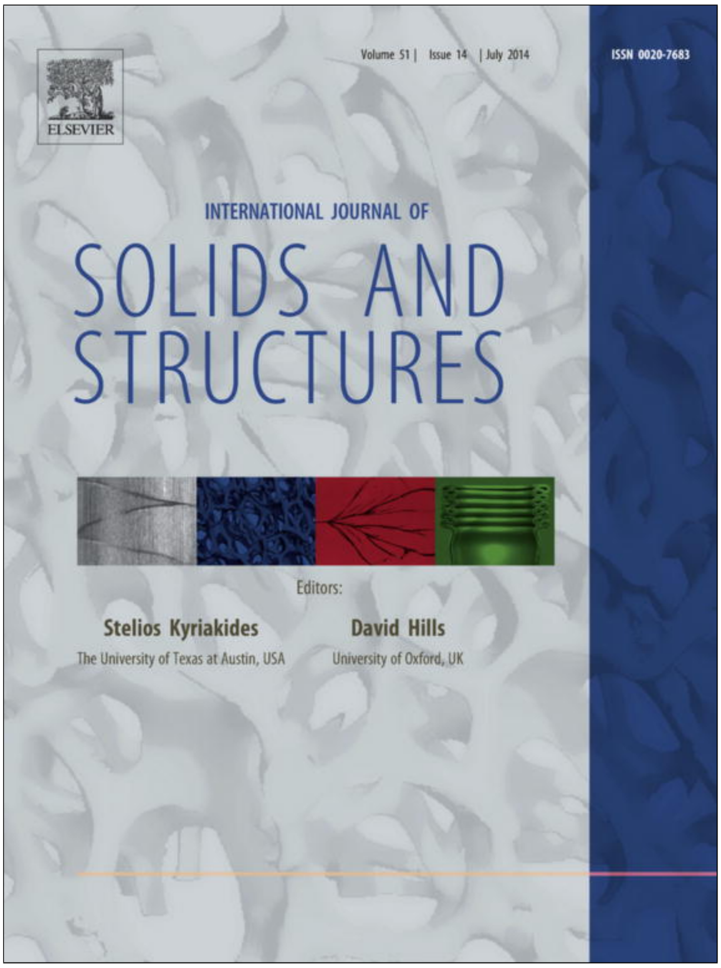
Volume 51 | Issue 14 | July 2014
ISSN 0020-7683
ELSEVIER
INTERNATIONAL JOURNAL OF
SOLIDS AND STRUCTURES
Editors:
Stelios Kyriakides
The University of Texas at Austin, USA
David Hills
University of Oxford, UK

International Journal of Solids and Structures 51 (2014) 2648–2655

Contents lists available at ScienceDirect

International Journal of Solids and Structures

journal homepage: www.elsevier.com/locate/ijsolstr

Charged dislocations in piezoelectric bimaterials

Xueli Han [a], Ernie Pan [b,*], Ali Sangghaleh [b], John Albrecht [c]

[a] School of Aerospace, Beijing Institute of Technology, Beijing 100081, China
[b] Computer Modeling and Simulation Group, University of Akron, Akron, OH 44325, USA
[c] Department of Electrical and Computing Engineering, Michigan State University, East Lansing, MI 48824, USA

ARTICLE INFO

Article history:
Received 6 September 2013
Received in revised form 26 March 2014
Available online 5 April 2014

Keywords:
Charged dislocation
Anisotropic bimaterial
Piezoelectricity
Polarization

ABSTRACT

In some piezoelectric semiconductors and ceramic materials, dislocations can be electrically active and could be even highly charged. However, the impact of dislocation charges on the strain and electric fields in piezoelectric and layered structures has not been presently understood. Thus, in this paper, we develop, for the first time, a charged three-dimensional dislocation loop model in an anisotropic piezoelectric bimaterial space to study the physical and mechanical characteristics which are essential to the design of novel layered structures. We first develop the analytical model based on which a line-integral solution can be derived for the coupled elastic and electric fields induced by an arbitrarily shaped and charged three-dimensional dislocation loop. As numerical examples, we apply our solutions to the typical piezoelectric AlGaN/GaN bimaterial to analyze the fields induced by charged square and elliptic dislocation loops. Our numerical results show that, except for the induced elastic (mechanical) displacement, charges along the dislocation loop could substantially perturb other induced fields. In other words, charges on the dislocation loop could significantly affect the traditional dislocation-induced stress/strain, electric displacement, and polarization fields in piezoelectric bimaterials.

1. Introduction

Piezoelectric (PE) materials are applied to various electronic devices due to their ability to direct electronic signals, to amplify electrical power, and to conserve energy. Recently, semiconductor materials including gallium nitride (GaN) and related heterostructures become the subject of considerable research due to their unique physical properties appropriate for applications in optical and electronic devices (Asbeck et al., 1997; Alessio Marino et al., 2010; Liu et al., 2012; Manuel et al., 2012; Wong et al., 2013). However, dislocation defects are common in this and many other piezoelectric (bilayer) materials. For instance, threading dislocation (TD) has been observed by transmission electron microscope (TEM) for many years in piezoelectric AlGaN/GaN (Cordier et al., 2005). While screw threading dislocations provide a conducting path in the AlGaN layer for the leakage current (Wong et al., 2010), the majority of dislocations in GaN are of the edge and mixed types (Cordier et al., 2005). Furthermore, misfit dislocation (MD) can also be created due to the lattice constant mismatch of involved bimaterials. In terms of modeling the interaction between the dislocations and interface, while Wang et al. (2011) studied the influence of interface shear strength on the interaction of lattice glide dislocations with fcc/bcc interfaces, the interaction of a screw dislocation with a coated nanowire containing interface effects was investigated by Fang et al. (2009). The analytical solution for the interaction between a piezoelectric screw dislocation and a piezoelectric interface was also derived by Wang and Pan (2008).

Besides the local deformation in the crystal lattice induced by various types of dislocations, the accumulation of charge along the dislocation lines affects the transport phenomena by dislocation–electron interaction (Cherns and Jiao, 2001; Muller et al., 2006). In one hand, dislocations can be charged upon irradiation by ions and electrons in metals and ceramics. Ryazanov and Klaptsov (2005) investigated the instability of charged dislocation loops in dielectric materials and demonstrated the formation of very strong elastic field near interstitial dislocation loops caused by the accumulation of charges on the loops. They also found that the dislocation loops become unstable when the loop radius reaches a certain critical value. On the other hand, dislocations in piezoelectric semiconductors can be highly charged and act as lines of Coulomb scattering centers, reducing the carrier mobility (Wong et al., 2010; Ambacher et al., 2000), and degrading the performance of these nitride-based devices (Joshi et al., 2003). More recently, Greco et al. (2011) experimentally showed that

* Corresponding author. Tel.: +1 330 972 6739.
E-mail addresses: hanxl@bit.edu.cn (X. Han), pan2@uakron.edu (E. Pan), as147@zips.uakron.edu (A. Sangghaleh), jalbrech@msu.edu (J. Albrecht).

http://dx.doi.org/10.1016/j.ijsolstr.2014.03.035
0020-7683/

dislocation defects and/or negative charges in AlGaN/GaN heterostructure are the main cause of the depletion of the two-dimensional electron gas (2DEG) and shift of the threshold voltage in high electron mobility transistor (HEMT) devices. Thus, in order to ultimately understand the impacts of the charged dislocations in piezoelectric materials on the performance and reliability of the corresponding structures, it is essential to understand the fundamental behavior of the charged dislocations.

In previous theoretical analyses of dislocations in piezoelectric crystals, the dislocations were usually assumed to be simple lines in an infinite 2D plane, with the materials being assumed to be electrically insulators (e.g. Pak, 1990; Wang and Pan, 2008). In reality, however, dislocations usually form three-dimensional (3D) loops, which poses great challenge due to the increased complexity (Minagawa, 2003). To investigate the possible contributions from the charge, some charged dislocation models were proposed. In general, charges on the dislocation loop could be modeled as charged lines (Look and Sizelove, 1999; Miller et al., 2011; Liu et al., 2012). However, in these charged dislocation models, the dislocation problems were assumed to be under simple 2D plane deformation.

Recently, based on the point-force Green's functions (Pan and Yuan 2000a,b), Chu et al. (2012) and Han and Pan (2012) were able to solve the elastic and electric fields due to 3D dislocation loops in anisotropic elastic and piezoelectric bimaterials. In this paper, we study the effect of the three-dimensional (3D) charged dislocations in piezoelectric bimaterial systems. We first present the basic formulae and solutions in terms of simple line integrals for the fields induced by an arbitrary 3D dislocation loop with charges in a piezoelectric bimaterial. The fields predicted from our model include the elastic displacement, electrical potential, stress/strain, electric displacement, and polarization fields (and also polarization charge density). The contributions from both uncharged-dislocation loop and charge-only sources are clearly separated so that one can easily address the relative importance of these two different types of sources. Our solutions are analytical in the sense that only line integrals along the dislocation loop are involved and that for some special dislocation segments, such as a 3D straight dislocation segment, the integrals can be carried out analytically so that the corresponding solutions are in exact closed form (Han et al., 2013). As numerical examples, the fields induced by charged vertical square and horizontal elliptic dislocation loops in the piezoelectric AlGaN/GaN bimaterial space are presented, showing the important contribution of charges to the induced fields.

2. Problem description and formulae

The problem of interest consists of a dislocation loop in two joined half spaces with dissimilar PE material properties as illustrated in Fig. 1. We consider an anisotropic piezoelectric bimaterial space where $x_3 > 0$ and $x_3 < 0$ are occupied by materials 1 and 2, respectively, with interface at $x_3 = 0$ plane. We first write the governing equations for a linear anisotropic PE solid. Then, based on the Green's function in PE bimaterials, we derive the dislocation-induced fields.

For PE materials, the extended equilibrium equations in terms of the extended stresses σ_{iJ} can be expressed as follows.

$$\sigma_{iJ,i} + f_J = 0 \tag{1}$$

where f_J is the extended body force, and a repeated lowercase (uppercase) index takes the summation from 1 to 3 (4). An index following the subprime "i" denotes the derivative with respect to the coordinate x_i. The linear constitutive relations for the coupled PE media can be written as follows.

$$\begin{cases} \sigma_{ij} = c_{ijlm}\gamma_{lm} - e_{kij}E_k \\ D_i = e_{ijk}\gamma_{jk} + \varepsilon_{ij}E_j \end{cases} \tag{2}$$

where D_i are the electric displacements; γ_{ij} and E_i are the strain and electric field, respectively; c_{ijlm} and e_{ijk} are the elastic and piezoelectric coefficients, respectively; and ε_{ij} are the dielectric permittivities. Using the extended notation of Barnett and Lothe (1975), Eq. (2) can be rewritten in a compact form as follows.

$$\sigma_{iJ} = C_{iJKl}\gamma_{Kl} \tag{3}$$

where C_{iJKl} and γ_{Kl} are the extended elastic constants and strains, respectively. The governing equations in terms of the extended dispalcements u_K can then be expressed.

$$C_{iJKl}u_{K,li} + f_J = 0 \tag{4}$$

We consider the following general boundary value problem in the domain V bounded by ∂V. On its boundary ∂V, the extended displacements $u_J(\mathbf{x})$ (elastic displacement u_j and electric potential ϕ) or extended tractions (elastic traction $\sigma_{ij}n_i$ and normal component of the electric displacements $D_i n_i$) are given. Within the domain V, the extended body force f_J (elastic body force f_j and electric charge density f_e) is described. Then, making use of the extended Betti's reciprocal theorem (Pan, 1999; Han and Pan, 2012), the extended displacement field can be expressed by

$$u_M(\mathbf{y}) = \int_{\partial V} \left[G_{JM}(\mathbf{y};\mathbf{x})\sigma_{iJ}(\mathbf{x}) - C_{iJKl}(\mathbf{x})G_{KM,x_l}(\mathbf{y};\mathbf{x})u_J(\mathbf{x})\right]n_i(\mathbf{x})\mathrm{d}S(\mathbf{x}) + \int_V G_{JM}(\mathbf{y};\mathbf{x})f_J(\mathbf{x})\mathrm{d}V(\mathbf{x}) \tag{5}$$

where n_i are the components of the unit normal to boundary ∂V, $f_{,x_i} = \partial f/\partial x_i$, and $G_{KM}(\mathbf{y};\mathbf{x})$ (4×4 tensor) are the extended Green's functions in piezoelectric solids, defined as the extended displacement component $u_K(\mathbf{x})$ at field point $\mathbf{x}$ due to an extended point force f_M of unit magnitude at source point $\mathbf{y}$. Eq. (5) is an integral

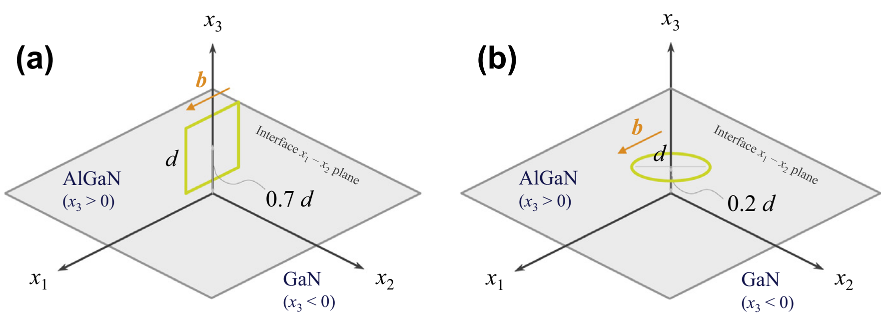

Fig. 1. Schematics of (a) a vertical square dislocation loop of side length d and (b) a horizontal elliptic dislocation loop of major-axis length d in AlGaN/GaN heterostructure. The Burgers vector is assumed along x_1-axis.

expression of the extended displacement in terms of the extended point-force Green's functions.

Using the 2D Fourier transform method, the extended Green's functions in piezoelectric bimaterials were obtained by Pan and Yuan (2000b). Thus, the extended Green's function tensor $\mathbf{G}(\mathbf{y};\mathbf{x})$ and their derivatives for a general anisotropic bimaterial space can also be found (Pan and Yuan, 2000a). Based on these point-force Green's functions, the coupled elastic and electric fields produced by an arbitrarily shaped extended dislocation loop in an anisotropic piezoelectric bimaterial space can be derived. This is done as described below.

The dislocation loop L is defined as the boundary of an internal surface S across which the elastic displacement and electric potential experience discontinuities, which can be described by an extended Burgers vector $\mathbf{b} = [b_1, b_2, b_3, \Delta\phi]^{\mathrm{T}}$. The elastic displacement jump is the traditional dislocation while $\Delta\phi$ corresponds to an electric dipole layer along the surface S (Barnett and Lothe, 1975) and is called the electric potential dislocation (Pak, 1990). The tractions and the normal component of the electric displacement are continuous across this internal surface, assuming that there is no force and no electric charge. Based on these conditions, the boundary conditions on the dislocation surface S can be expressed by the extended components as

$$[u_J] = b_J; \quad [\sigma_{iJ} n_i] = 0 \quad J = 1 \sim 4 \tag{6}$$

Besides the discontinuity across the dislocation surface S, there exist electric charges accumulated on the dislocation core in many piezoelectric semiconductors and ceramic materials under irradiation (Leung et al., 1999; Ryazanov et al., 2003). Assuming an electric charge with density f_e along the dislocation loop core L, then the extended body force can be expressed as

$$f_J = -f_e \delta_{J4} \delta(\mathbf{x}, L) \tag{7}$$

Substituting Eqs. (6) and (7) into Eq. (5), the extended displacement field produced by a charged dislocation loop is reduced to

$$\begin{aligned} u_M(\mathbf{y}) = & \int_S C_{iJKl}(\mathbf{x}) G_{KM,x_l}(\mathbf{y};\mathbf{x}) b_J(\mathbf{x}) n_i(\mathbf{x}) \mathrm{d}S(\mathbf{x}) \\ & - \int_L G_{4M}(\mathbf{y};\mathbf{x}) f_e(\mathbf{x}) \mathrm{d}L(\mathbf{x}) \end{aligned} \tag{8}$$

Besides the extended displacement field, other fields such as the stress/strain and electric displacement fields, are also important. These fields require the derivative of the extended displacement field, which can be expressed as

$$\begin{aligned} u_{M,y_p\ldots}(\mathbf{y}) = & \int_S C_{iJKl}(\mathbf{x}) G_{KM,x_l y_p \ldots}(\mathbf{y};\mathbf{x}) b_J(\mathbf{x}) n_i(\mathbf{x}) \mathrm{d}S(\mathbf{x}) \\ & - \int_L G_{4M,y_p\ldots}(\mathbf{y};\mathbf{x}) f_e(\mathbf{x}) \mathrm{d}L(\mathbf{x}) \end{aligned} \tag{9}$$

It is noted that the surface integral in Eqs. (8) and (9) corresponds to the contribution from the extended dislocation $\mathbf{b}$ on the dislocation surface S without electric charges along the dislocation core L, and thus it is the *uncharged-dislocation*-induced field. The line integral in Eqs. (8) and (9) corresponds to the contribution from the electric charge with density f_e along the loop L, and is called the *charge-only*-induced field. The *total* induced field due to both sources can be simply superposed together.

It should be also noticed that in piezoelectric materials, a strain field will induce piezoelectric polarization field $\mathbf{P}^{Pz}$ as

$$P_i^{Pz} = e_{ijk} \gamma_{jk} = e_{ijk} u_{j,k} \tag{10}$$

Furthermore, the gradient of $\mathbf{P}^{Pz}$ will induce a piezoelectric polarization (volume) charge density ρ^{Pz}, and an abrupt change in $\mathbf{P}^{Pz}$ across the interface will also induce a piezoelectric polarization surface charge density σ^{Pz}. These charge densities are important to the electronic device analysis.

It is pointed out that if the dislocation loop lies on a plane and that the material properties and dislocation charge density f_e on the loop plane are constants or piecewise constants, then the total induced fields in Eqs. (8) and (9) can be simplified into

$$u_M(\mathbf{y}) = C_{iJKl} b_J n_i \int_S G_{KM,x_l}(\mathbf{y};\mathbf{x}) \mathrm{d}S(\mathbf{x}) - f_e \int_L G_{4M}(\mathbf{y};\mathbf{x}) \mathrm{d}L(\mathbf{x}) \tag{11}$$

$$\begin{aligned} u_{M,y_p\ldots}(\mathbf{y}) = & C_{iJKl} b_J n_i \int_S G_{KM,x_l y_p\ldots}(\mathbf{y};\mathbf{x}) \mathrm{d}S(\mathbf{x}) - f_e \\ & \times \int_L G_{4M,y_p\ldots}(\mathbf{y};\mathbf{x}) \mathrm{d}L(\mathbf{x}) \end{aligned} \tag{12}$$

Therefore, when the charge distribution f_e along the loop is constant or piecewise constant, the charge-only-induced field is a simple line integral of the Green's functions along the dislocation loop L. Furthermore, the field due to the uncharged dislocation in the first term of Eqs. (11) and (12) can be also converted into simple line integrals of the Green's functions by following the approach in Han and Pan (2012) and Han et al. (2013).

3. Numerical results

While the formulation can be applied to any PE bimaterial system with charged dislocations, we use the piezoelectric AlGaN/GaN bimaterial as an example where all three types of dislocation loops (edge, screw, and mixed) have been observed experimentally (Follstaedt et al., 2008; Wong et al., 2010; Manuel et al., 2012). We consider a vertical square and a horizontal elliptic dislocation loops in the piezoelectric bimaterial system as shown in Fig. 1a and b where the orientation of the Burgers vector is fixed in the x_1-direction for both dislocations. The AlGaN material has 50% Al and 50% GaN, and both AlGaN and GaN are transversely isotropic with poling direction along x_3-axis. The material properties for AlGaN and GaN are presented in the Appendix (Han and Pan, 2012), with the properties of AlGaN being calculated by linear interpolation between AlN and GaN (Ambacher et al., 2000; Morkoc and Leach, 2007).

In numerical calculations, d is assumed to be the character length of the dislocation loop (side length of the square or major axis length of the ellipse, which is along x_2-axis) and it is taken as the unit length of the coordinates. The uncharged-dislocation-induced (by b and $\Delta\phi$) and charge-only-induced (by $f_e \equiv fe/a$) fields have, respectively, the following dimension relations.

$$\begin{aligned} & \mathbf{U}(\mathbf{u}, \phi) \propto b(b, \Delta\phi) \\ & \mathbf{U}_{,i} \boldsymbol{\Sigma}(\sigma, \mathbf{D}), \boldsymbol{\Gamma}(\gamma, \mathbf{E}), \mathbf{P} \propto b/d(b/d, \Delta\phi/d) \\ & \mathbf{U}_{,ij} \rho(D_{i,i}) \propto b/d^2(b/d^2, \Delta\phi/d^2) \end{aligned} \tag{13}$$

$$\begin{aligned} & \mathbf{U}(\mathbf{u}, \phi) \propto fe/a \propto b[fe/(ab)] \\ & \mathbf{U}_{,i} \boldsymbol{\Sigma}(\sigma, \mathbf{D}), \boldsymbol{\Gamma}(\gamma, \mathbf{E}), \mathbf{P} \propto (fe/a)/d \propto b/d[fe/(ab)] \\ & \mathbf{U}_{,ij} \rho(D_{i,i}) \propto (fe/a)/d^2 \propto b/d^2[fe/(ab)] \end{aligned} \tag{14}$$

For instance, $\mathbf{U}(\mathbf{u}, \phi)$ in Eq. (13) means the extended displacement $\mathbf{U}$ which includes the elastic displacement $\mathbf{u}$ and electric potential ϕ. These quantities are proportional to the Burgers value b for a traditional dislocation or proportional to $\Delta\phi$ for an electric dislocation. Thus in our numerical calculation, these field quantities are normalized accordingly. Similar relations can be found in Eqs. (13) and (14) for other important quantities.

The charge density for charged-only loops along a-axis (c-axis) is given as $f_e = fe/a$ ($f_e = fe/c$) with a (c) being the distance between adjacent possible charge points (considered as lattice constants). We point out that, in this paper, the material a- and c-axes in the two half spaces are oriented to be along the global x_1- and x_3-axes (or x- and z-axes). Also in Eqs. (13) and (14), f is the fraction of the occupied site ($f \leqslant 1$), and e is the unit charge ($\pm 1.6 \times 10^{-19}$ C). The magnitude of f in this study is considered as unity (1 electron/c) while Cherns and Jiao (2001) even estimated a dislocation line of charge 2 electrons/c in GaN. It is noted that f_e is positive (negative) for a positively (negatively) charged dislocation.

In summary, based on Eqs. (13) and (14), the field quantities induced by the uncharged dislocation, charge-only, or charged dislocation can be uniformly normalized as

$$\mathbf{U}/b;\quad \mathbf{U}_{,i}/(b/d);\quad \mathbf{U}_{,ij}/(b/d^2) \tag{15}$$

In the numerical analysis, the following quantities along with the polarization are analyzed: The magnitude of the elastic displacement u, the magnitude of the electric displacement D, and the effective stress σ_e, defined as

$$u=\sqrt{u_x^2+u_y^2+u_z^2};\;\; D=\sqrt{D_x^2+D_y^2+D_z^2}$$
$$\sigma_e=\sqrt{\frac{1}{2}[(\sigma_{xx}-\sigma_{yy})^2+(\sigma_{yy}-\sigma_{zz})^2+(\sigma_{zz}-\sigma_{xx})^2]+3(\sigma_{xy}^2+\sigma_{yz}^2+\sigma_{xz}^2)} \tag{16}$$

It is also noticed that in Eq. (16) and also in all figures presented, the coordinates (x, y, z) are identical to (x_1, x_2, x_3) with normalized coordinates $(X, Y, Z) = (x/d, y/d, z/d)$.

In the first numerical example, the dislocation loop is assumed to be a square on the vertical x_1–x_3 plane with Burgers vector $\mathbf{b} = b[1000]^{\mathrm{T}}$ along x_1-axis. The side length of the square is d and the distance of the loop center to the interface is $h = 0.7d$. We assume that the dislocation is placed in the upper half-space AlGaN with GaN in the lower half-space (Fig. 1a).

The uncharged-dislocation- and charge-only-induced displacement field u on the vertical plane X(x/d) = −0.5 and at the interface are illustrated in Fig. 2. It is observed that although the induced field is symmetric on both sides of the square loop due to both sources, the displacement patterns induced by them are completely different. Furthermore, the charge-only-induced displacement field (Fig. 2b) is about one-order smaller as compared to the uncharged-dislocation-induced field (Fig. 2a). Thus, under the given conditions, the charge effect on the induced displacement can be neglected.

Contours of uncharged-dislocation- and charge-only-induced stress field σ_e at the interface (on the GaN side) are shown in Fig. 3. The features from both sources are different and the field induced by uncharged-dislocation is about five times larger than that by charge-only dislocation (Fig. 3a and b). The field concentrations are directly below the square dislocation loop, with those due to uncharged-dislocation being at the center (coming from the screw dislocation section) and those due to charge-only being at both ends (coming from the edge dislocation section). Since both fields do not reach their maximums at the same location, the charge-only-induced stress will perturb the uncharged-dislocation-induced one, particularly directly below the dislocation loop. This implies that in terms of stress analysis, which is an important quantity in device reliability design, charge-induced field may need to be carefully studied and be included for the safety analysis of the structures made of piezoelectric bimaterials.

Fig. 4 shows the contours of the electric displacement D on the vertical plane $X(x/d) = 0$ and on the horizontal plane $Z(z/d) = 0.68$ due to uncharged-dislocation (4a) and charge-only (4b) of the vertical square dislocation loop. In contrary to the elastic field, the electric displacement due to both sources have the same magnitude with field concentrations from both edge and screw dislocations. Thus contributions from both sources have to be considered if one is interested in the induced electric field of a charged dislocation. It is worth noting that the electron mobility in AlGaN/GaN heterostructures depends on the electric field, layer thickness, and the charge on the dislocation lines (Liu et al., 2012; Ji et al., 2013). In addition, polarization induced electric fields lead to a significant increase of the sheet carrier concentration in AlGaN/GaN semiconductors (Ambacher et al., 2000).

Contours of the induced polarization field |**P**| on the vertical plane $X(x/d) = 0$ and horizontal plane $Z(z/d) = 0.68$ induced by the vertical square dislocation loop are shown in Fig. 5 – uncharged-dislocation induced in Fig. 5a and charge-only induced in Fig. 5b. While the intensity due to uncharged-dislocation is higher for edge dislocation than screw dislocation (Fig. 5a), the intensity due to charge only is higher in screw dislocation with concentration outside the dislocation loop (Fig. 5b). Since the magnitudes of the polarization due to both sources are comparable, the contribution of charge along the dislocation loop needs to be considered in calculating the total polarization field. The strong polarization due to the induction of high electron density at AlGaN/GaN structure (Miyoshi et al., 2008) confirms the importance of both sources in

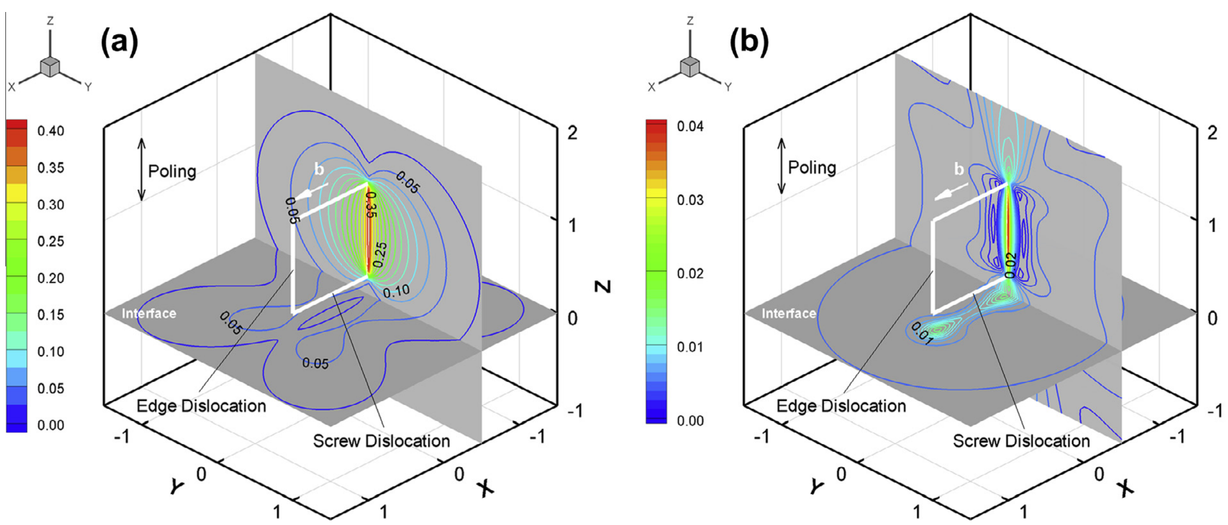

Fig. 2. Contours of (a) uncharged-dislocation-induced and (b) charge-only-induced displacement u (normalized by b) on plane $X(x/d) = -0.5$ and at the interface, by the vertical square dislocation loop as shown in Fig. 1a.

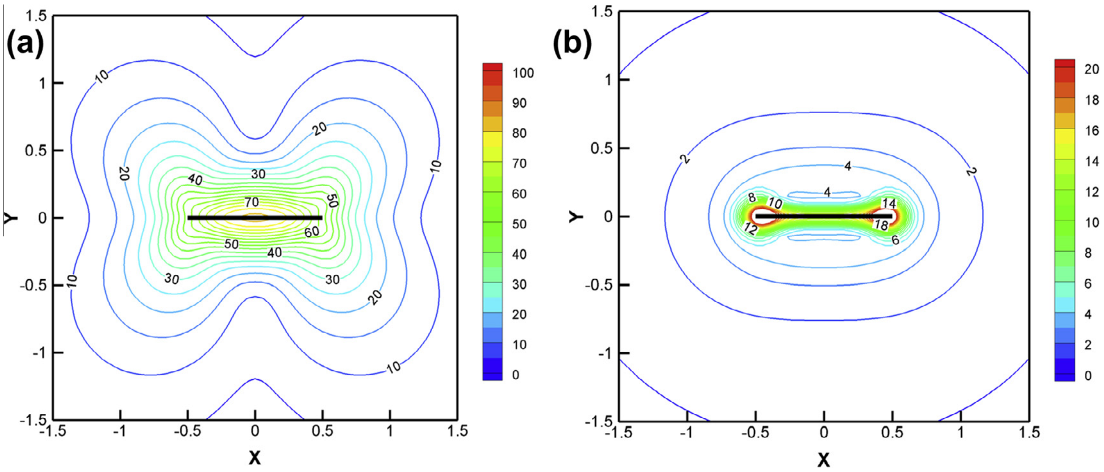

Fig. 3. Contours of (a) uncharged-dislocation-induced and (b) charge-only-induced stress field σ_e (normalized by b/d and in GPa) at the interface (on the GaN side), by the vertical square dislocation loop as shown in Fig. 1a.

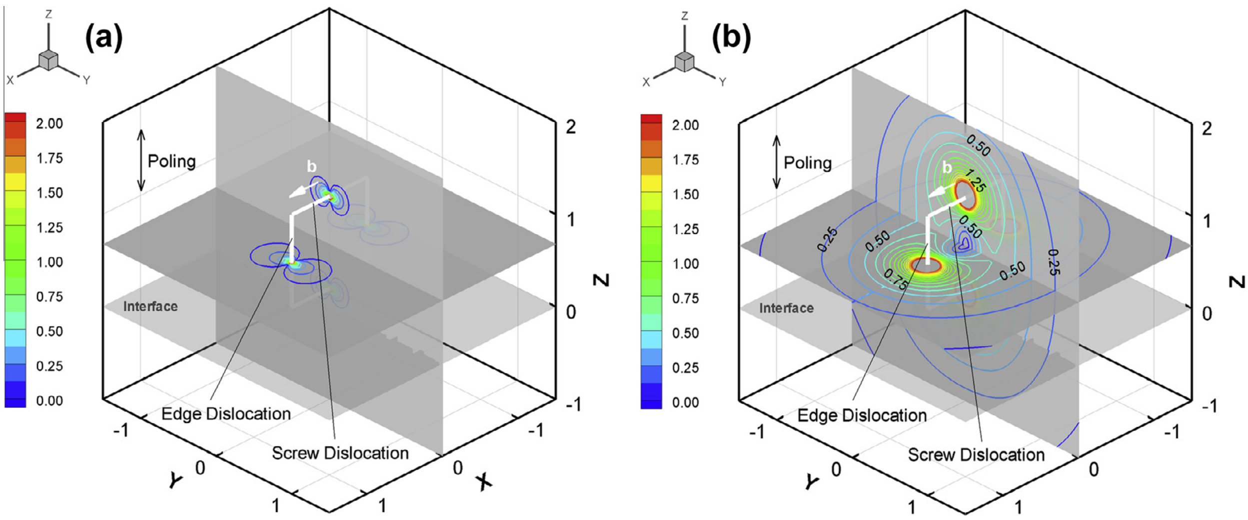

Fig. 4. Contours of (a) uncharged-dislocation-induced and (b) charge-only-induced electric displacement D (normalized by b/d in C m^{-2}) on vertical plane $X(x/d) = 0$ and on horizontal plane $Z(z/d) = 0.68$, by the vertical square dislocation loop as shown in Fig. 1a.

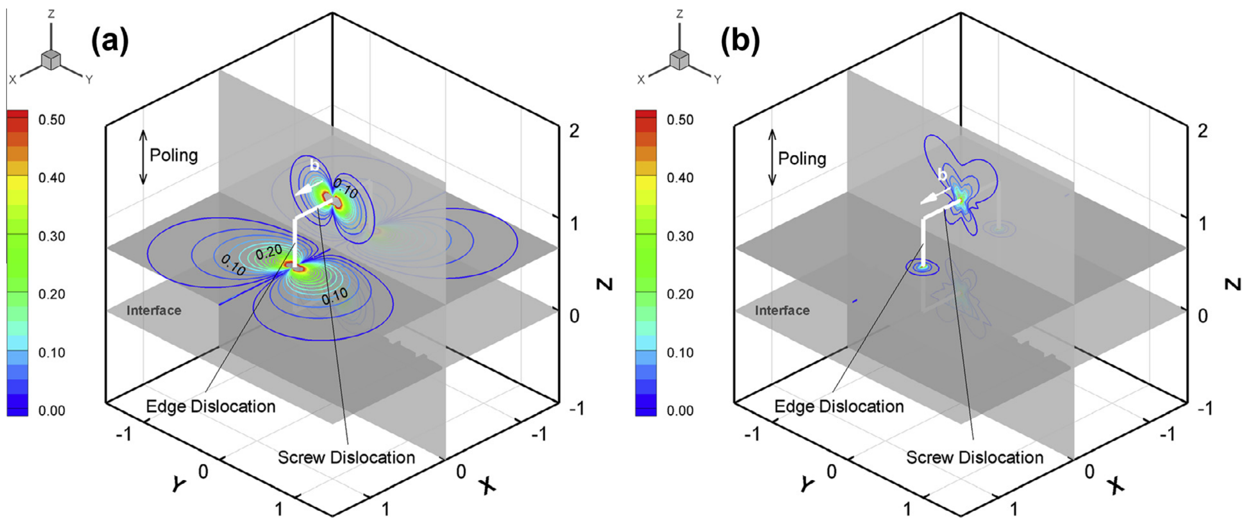

Fig. 5. Contours of (a) uncharged-dislocation-induced and (b) charge-only-induced polarization field $|\mathbf{P}|$ (normalized by b/d and in C m^{-2}) on vertical plane $X(x/d) = 0$ and on horizontal plane $Z(z/d) = 0.68$, by the vertical square dislocation loop as shown in Fig. 1a.

the induced fields and could be actually responsible for the 2DEG (Ambacher et al., 2000). In addition, the calculation of polarization fields due to the effects of misfit dislocations can be used to understand the ferroelectric properties in thin-film substrate systems (Zheng et al., 2006).

In the second numerical example, we consider an elliptic dislocation loop lies on the horizontal plane $Z(z/d) = 0.2$ (Fig. 1b). The major axis of the dislocation loop is along x_2-direction with length d (the character length of the ellipse), and the minor axis is along x_1-direction with length equals to $0.712d$. Again the extended Burgers vector is $\mathbf{b} = b[1000]^{\mathrm{T}}$, along x_1-direction.

Fig. 6 shows the contours of the elastic displacement u on the vertical plane $Y(y/d) = 0$ induced by the horizontal elliptic dislocation loop: Those by uncharged dislocation and charge-only sources are shown respectively in Fig. 6a and b. Similar to the square dislocation case, although their contour patterns are different for the two sources, the charge-only-induced field is much smaller compared to that due to the uncharged dislocation and thus its contribution to the total elastic displacement field is negligible.

The contours of the dislocation-induced stress field σ_e at the interface (on the lower GaN side) by the horizontal elliptic dislocation loop are shown in Fig. 7 – uncharged-dislocation-induced in Fig. 7a and charge-only-induced in Fig. 7b. Comparing both results, we notice that not only the induced field patterns are completely different, but also the magnitude by uncharged dislocation is about ten times larger than that by charge only. As such, near the interface, the stress field is dominated by the uncharged dislocation.

In contrast to the stress field, the induced electric displacement fields by both sources of the horizontal elliptic dislocation loop are comparable, as shown in Fig. 8 where the contours of the induced field on the vertical plane $Y(y/d) = 0$ due to uncharged-dislocation and charge-only are shown, respectively, in Fig. 8a and b. It is observed that while the contour patterns due to uncharged dislocation are very complicated, those by charge-only source are simple.

Fig. 9 shows the contours of the polarization field $|\mathbf{P}|$ on the vertical plane $Y(y/d) = -0.5$ induced by the horizontal elliptic dislocation loop. It is obvious that the fields are concentrated near the dislocation plane. It can also be observed that the uncharged-dislocation-induced field is large around the edge dislocation (Fig. 9a), whilst the field due to charge only is concentrated near the screw dislocation (Fig. 9b). Even though their magnitudes differ about two times, the charge-only induced field could still contribute to the total response due to the fact that both fields do not reach their maximums at the same location. In other words, in the neighborhood of the dislocation plane, the charge-only-induced polarization could substantially contribute to the total induced field.

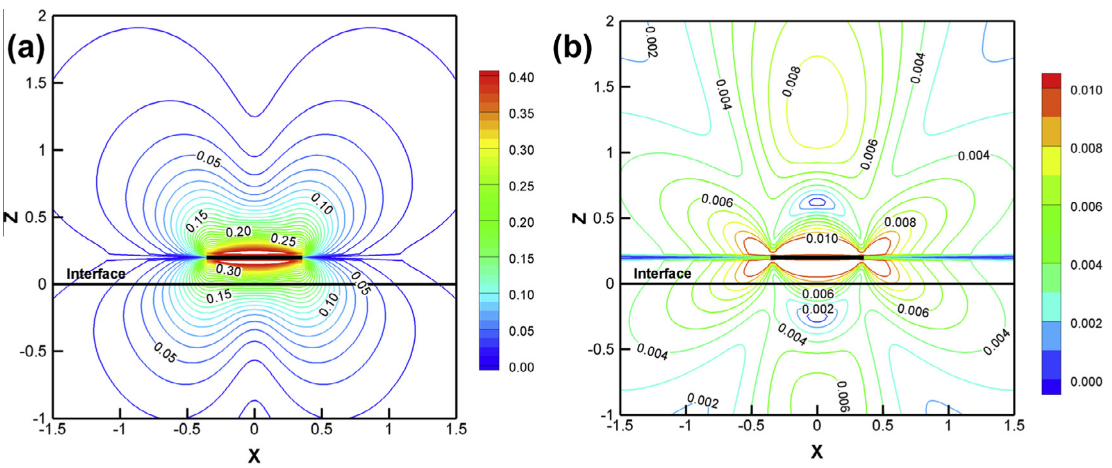

Fig. 6. Contours of (a) uncharged-dislocation-induced and (b) charge-only-induced displacement u (normalized by b) on vertical plane $Y(y/d) = 0$, by the horizontal elliptic dislocation loop as shown in Fig. 1b.

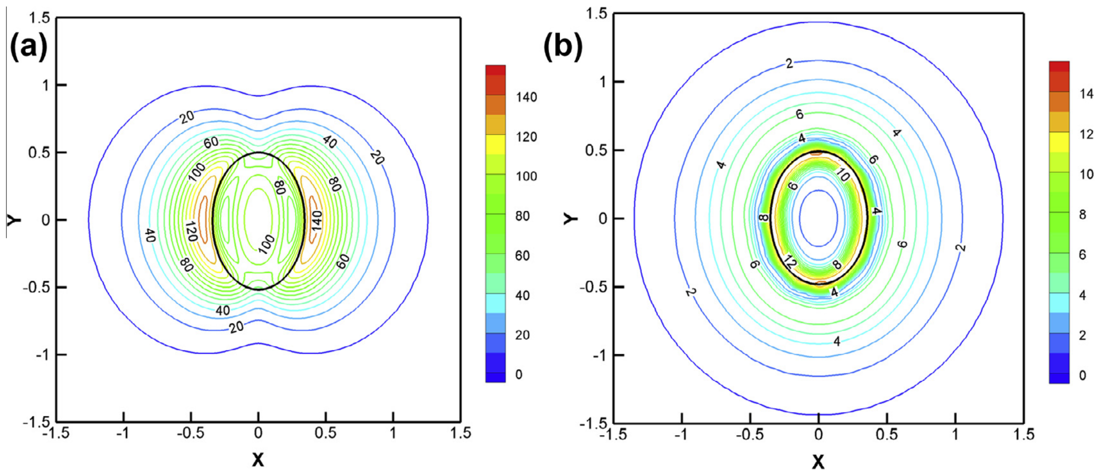

Fig. 7. Contours of (a) uncharged-dislocation-induced and (b) charge-only-induced stress field σ_e (normalized by b/d and in GPa) at the interface (on the GaN side), by the horizontal elliptic dislocation loop as shown in Fig. 1b.

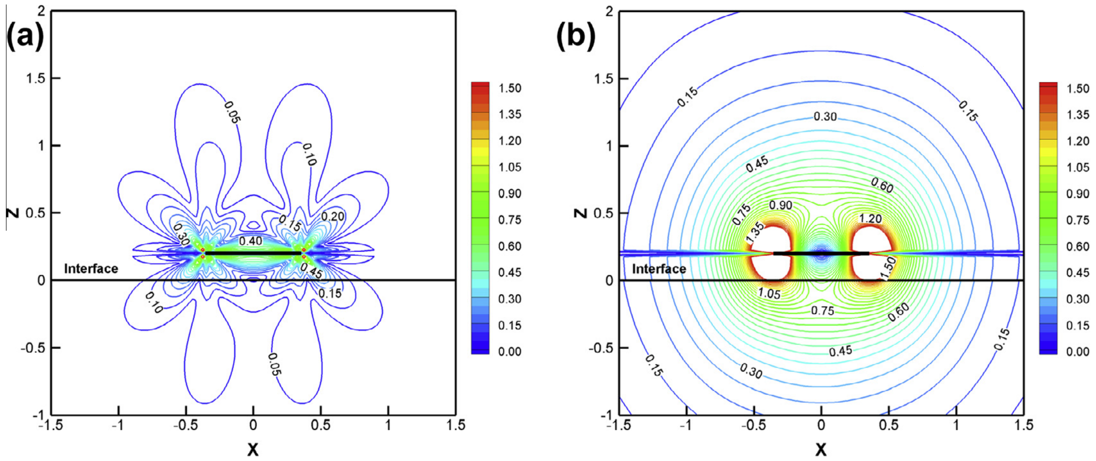

Fig. 8. Contours of (a) uncharged-dislocation-induced and (b) charge-only-induced electric displacement D (normalized by b/d in C m^{-2}) on vertical plane $Y(y/d) = 0$, by the horizontal elliptic dislocation loop as shown in Fig. 1b.

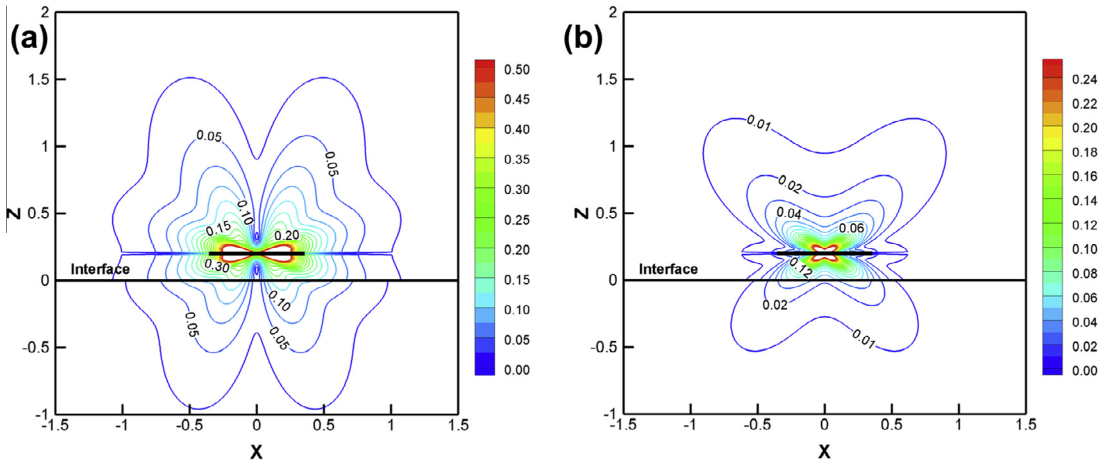

Fig. 9. Contours of (a) uncharged-dislocation-induced and (b) charge-only-induced polarization field |**P**| (normalized by b/d and in C m^{-2}) on vertical plane $Y(y/d) = -0.5$, by the horizontal elliptic dislocation loop as shown in Fig. 1b.

Understanding the elastic and electric fields as well as polarization induced by threading and misfit dislocations in semiconductor bimaterials is necessary in order to produce powerful and high efficiency transistors. Our analytical model together with numerical analyses of vertical square and horizontal elliptic loops confirm the significance of charged dislocations in AlGaN/GaN bimaterials.

4. Conclusions

An analytical solution is developed, for the first time, to study the fields induced by an arbitrary 3D charged dislocation loop in a general anisotropic piezoelectric bimaterial system. The solution is expressed in terms of simple line integrals along the dislocation loop with the integrand being the corresponding point-force Green's functions. The solution is then applied to vertical square and horizontal elliptic dislocation loops within AlGaN/GaN bimaterial spaces. Our numerical results demonstrate clearly the importance of the charge on the dislocation-induced elastic, electric, and piezoelectric polarization fields. More specifically, while the dislocation-induced elastic displacement may not be altered by the charge, all other fields including the stress, electric displacement, and polarization (thus the charge density) can be significantly influenced due to the existence of the charge on the dislocation loop. These observations imply that should a dislocation be charged, the induced fields (including the stress/strain, electric displacement/field, and electric polarization) must include those from both the charges and the uncharged conventional dislocation calculations. The presented analytical model can be utilized to quantitatively predict the behavior of threading and misfit dislocations in novel piezoelectric bimaterial structures and it can be further applied to analyze the growth and instability of charged dislocation loops under irradiation in nuclear materials such as insulating ceramics (Ryazanov et al., 2002,2003).

Acknowledgments

The work was supported by National Natural Science Foundation of China (Nos. 10872179, 11172273 and 11272052). The first author is also grateful for the support from the China Scholarship Council. The authors would like to thank both reviewers for their constructive comments on the original version of the article.

Appendix A. Material properties

Material properties of GaN and AlGaN (with 50% Al) with poling direction along x_3-axis (Han and Pan, 2012).

	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	e_{31}	e_{33}	e_{15}	ε_{11}	ε_{33}
GaN	367	135	103	405	95	−0.36	1.0	−0.3	0.084	0.0921
AlGaN	381.5	136	105.5	389	105.5	−0.47	1.275	−0.39	0.082	0.0934

Elastic constants C_{ij} are in GPa, piezoelectric constants e_{ij} in C/m^2, and dielectric constants ε_{ij} in 10^{-9} F/m (or 10^{-9} C^2/Nm^2).

References

Alessio Marino, F., Faralli, N., Palacios, T., Ferry, D.K., Goodnick, S.M., Saraniti, M., 2010. Effects of threading dislocations on AlGaN/GaN high-electron mobility transistors. IEEE Trans. Electron Dev. 57, 353.

Ambacher, O., Foutz, B., Smart, J., Shealy, J.R., Weimann, N.G., Chu, K., Murphy, M., Sierakowski, A.J., Schaff, W.J., Eastman, L.F., Dimitrov, R., Mitchell, A., Stutzmann, M., 2000. Two dimensional electron gases induced by spontaneous and piezoelectric polarization in undoped and doped AlGaN/GaN heterostructures. J. Appl. Phys. 87, 334.

Asbeck, P.M., Yu, E.T., Lau, S.S., Sullivan, G.J., Van Hove, J., Redwing, J., 1997. Piezoelectric charge densities in AlGaN/GaN HFETs. Electron. Lett. 33, 1230.

Barnett, D.M., Lothe, J., 1975. Dislocations and line charges in anisotropic piezoelectric insulators. Phys. Status Solidi B 67, 105.

Cherns, D., Jiao, C.G., 2001. Electron holography studies of the charge on dislocations in GaN. Phys. Rev. Lett. 87, 205504.

Chu, H.J., Pan, E., Wang, J., Beyerlein, I.J., 2012. Three-dimensional elastic displacement induced by a dislocation of polygonal shape in anisotropic elastic crystals. Int. J. Solids Struct. 48, 1164.

Cordier, Y., Hugues, M., Semond, F., Natali, F., Lorenzini, P., Bougrioua, Z., Massies, J., Frayssinet, E., Beaumont, B., Gibart, B., Faurie, J.P., 2005. AlGaN/GaN/AlGaN DH-HEMTs grown by MBE on Si(1 1 1). J. Cryst. Growth 278, 383.

Fang, Q.H., Liu, Y.W., Jin, B., Wen, P.H., 2009. Interaction between a dislocation and a core-shell nanowire with interface effects. Int. J. Solids Struct. 46, 1539.

Follstaedt, D.M., Allerman, A.A., Lee, S.R., Michael, J.R., Bogart, K.H.A., Crawford, M.H., Missert, N.A., 2008. Dislocation reduction in AlGaN grown on patterned GaN. J. Cryst. Growth 310, 766.

Greco, G., Giannazzo, F., Frazzetto, A., Raineri, V., Roccaforte, F., 2011. Near-surface processing on AlGaN/GaN heterostructures: a nanoscale electrical and structural characterization. Nanoscale Res. Lett. 6, 132.

Han, X., Pan, E., 2012. Dislocation-induced fields in piezoelectric AlGaN/GaN bimaterial heterostructures. J. Appl. Phys. 112, 103501.

Han, X., Pan, E., Sangghaleh, A., 2013. Fields induced by three-dimensional dislocation loops in anisotropic magneto-electro-elastic bimaterials. Philos. Mag. 93, 3291.

Ji, D., Lu, Y., Liu, B., Liu, J., 2013. Converse piezoelectric effect induced misfit dislocation scattering in metal/AlGaN/GaN heterostructures. Appl. Phys. Lett. 102, 132106.

Joshi, R.P., Viswanadha, S., Jogai, B., Shah, P., del Rosario, R.D., 2003. Analysis of dislocation scattering on electron mobility in GaN high electron mobility transistors. J. Appl. Phys. 93, 10046.

Leung, K., Wright, A.F., Stechel, E.B., 1999. Charged accumulation at a threading edge dislocation in gallium nitride. Appl. Phys. Lett. 74, 2495.

Liu, G., Wu, J., Zhao, G., Liu, S., Mao, W., Hao, Y., Liu, C., Yang, S., Liu, X., Zhu, Q., Wang, Z., 2012. Impact of the misfit dislocations on two-dimensional electron gas mobility in semi-polar AlGaN/GaN heterostructures. Appl. Phys. Lett. 100, 082101.

Look, D.C., Sizelove, J.R., 1999. Dislocation scattering in GaN. Phys. Rev. Lett. 82, 1237.

Manuel, J.M., Morales, F.M., Garcia, R., Aidam, R., Kirste, L., Ambacher, O., 2012. Threading dislocation propagation in AlGaN/GaN based HEMT structures grown on Si (111) by plasma assisted molecular beam epitaxy. J. Cryst. Growth 357, 35.

Miller, N., Haller, E.E., Koblmüller, G., Gallinat, C., Speck, J.S., Schaff, W.J., Hawkridge, M.E., Yu, K.M., Ager, J.W., 2011. Effect of charged dislocation scattering on electrical and electrothermal transport in n-type InN. Phys. Rev. B 84, 075315.

Minagawa, S., 2003. On the stress and electric field produced by dislocations in anisotropic piezoelectric crystals with special attention to the stress function. Mech. Mater. 35, 453.

Miyoshi, M., Kuraoka, Y., Tanaka, M., Egawa, T., 2008. Metalorganic chemical vapor deposition and material characterization of lattice-matched InAlN/GaN two-dimensional electron gas heterostructures. Appl. Phys. Express 1, 081102.

Morkoc, H., Leach, J., 2007. Polarization in GaN Based heterostructures and heterojunction field effect transistors (HFETs). In: Wood, Colin, Jena, Debdeep (Eds.), Polarization Effects in Semiconductors: From Ab Initio Theory to Device Applications, vol. 373. Springer.

Muller, E., Gerthsen, D., Brückner, P., Scholz, F., Gruber, T.H., Waag, A., 2006. Probing the electrostatic potential of charged dislocations in n-GaN and n-ZnO epilayers by transmission electron holography. Phys. Rev. B 73, 245316.

Pak, Y.E., 1990. Force on a piezoelectric screw dislocation. ASME J. Appl. Mech. 57, 863.

Pan, E., 1999. A BEM analysis of fracture mechanics in 2D anisotropic piezoelectric solids. Eng. Anal. Boundary Elem. 23, 67.

Pan, E., Yuan, F.G., 2000a. Three-dimensional Green's functions in anisotropic bimaterials. Int. J. Solids Struct. 37, 5329.

Pan, E., Yuan, F.G., 2000b. Three-dimensional Green's functions in anisotropic piezoelectric bimaterials. Int. J. Eng. Sci. 38, 1939.

Ryazanov, A.I., Klaptsov, A.V., 2005. Instability of interstitial dislocation loops in electron-irradiated dielectrics. J. Exp. Theor. Phys. Lett. 81, 383.

Ryazanov, A.I., Yasuda, K., Kinoshita, C., Klaptsov, A.V., 2002. Growth and instability of charged dislocation loops under irradiation in ceramic materials. J. Nucl. Mater. 307, 918.

Ryazanov, A.I., Yasuda, K., Kinoshita, C., Klaptsov, A.V., 2003. Instability of interstitial clusters under ion and electron irradiations in ceramic materials. J. Nucl. Mater. 323, 372.

Wang, J., Hoagland, R.G., Liu, X.Y., Misra, A., 2011. The influence of interface shear strength on the glide dislocation-interface interactions. Acta Mater. 59, 3164.

Wang, X., Pan, E., 2008. Interaction between a screw dislocation and a viscoelastic piezoelectric bimaterial interface. Int. J. Solid Struct. 45, 245.

Wong, Y.Y., Chang, E.Y., Yang, T.H., Chang, J.R., Ku, J.T., Hudait, M.K., Chou, W.C., Chen, M., Lin, K.L., 2010. The roles of threading dislocations on electrical properties of AlGaN/GaN heterostructure grown by MBE. J. Electrochem. Soc. 157, H746.

Wong, M.H., Keller, S., Dasgupta, N.S., Denninghoff, D.J., Kolluri, S., Brown, D.F., Lu, J., Fichtenbaum, N.A., Ahmadi, E., Singisetti, U., Chini, A., Rajan, S., DenBaars, S.P., Speck, J.S., Mishra, U.K., Umesh, K., 2013. N-polar GaN epitaxy and high electron mobility transistors. Semicond. Sci. Technol. 28, 074009.

Zheng, Y., Wang, B., Woo, C.H., 2006. Simulation of interface dislocations effect on polarization distribution of ferroelectric thin films. Appl. Phys. Lett. 88, 092903.