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Near-interface charged dislocations in AlGaN/GaN bilayer heterostructures

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Understanding the behavior of semiconductor dislocation defects in AlGaN/GaN heterostructures is necessary in order to produce powerful and efficient transistors. This letter presents a straightforward technique to characterize dislocation defects with charges along their loops in a bilayer system. This is important regarding the behavior of near-interface dislocations in order to obtain an insight of the mechanical and physical responses. We characterize piezoelectric polarization and emphasize on the importance of dislocation-core electric charge. The results elaborate the variations of the dislocation force by the accumulation of charge and provide an explanation for the dominant dislocation types in nitride semiconductors. © *2014 AIP Publishing LLC*. [http://dx.doi.org/10.1063/1.4895511]

Nitride-based semiconductor materials including gallium nitride and related heterostructures are the subject of considerable research due to their unique physical properties appropriate for applications in optical and electronic devices.[1] GaN development has been extensively fast in the market due to high breakdown field and wide-bandgap for micro/nano-electronics and photovoltaic applications.[2,3] AlGaN/GaN is well known for the application in high electron mobility transistors (HEMTs) and for the ability of achieving two-dimensional electron gas (2DEG) with a high-sheet-carrier density required for the design of field-effect transistors (FETs).[4,5] Epitaxial growth of these semiconducting materials on sapphire or Si/SiC substrates are routinely performed despite the fact that lattice mismatch create high density of crystal imperfections. This exposes the countless efforts on the reduction of defects in semiconducting materials bearing in mind that the elimination of the entire network of defects is unattainable.

Misfit dislocations (MDs) and threading dislocations (TDs) are the common defects in AlGaN/GaN heterostructures.[6,7] The internal stress due to the lattice mismatch is the driving force for the formation of MDs.[8,9] TDs, however, are generated as a result of coalescence of adjacent grains during epitaxial growth at high temperatures with density ranging between 10^8 and $10^{11}\,\mathrm{cm}^{-2}$.[4,10] The observation of different types of dislocation in AlGaN/GaN heterostructures demonstrates that most dislocations are of threading straight type which persuade researchers to simulate those as threading lines.[5,11] However, TDs can be entangled with misfit dislocations to form closed or open dislocation loops, arousing the engagement with dislocation loops in nitride heterostructures.

Dislocations in AlGaN/GaN heterostructures can be highly charged and act as lines of Coulomb scattering centers, reducing the carrier mobility, and degrading the device performance.[12] However, the lack of theoretical analyses on charged dislocations is perceptible. In this letter, we have presented an analytical study to characterize electromechanical coupling force applying to charged dislocations in AlGaN/GaN heterostructures. Explicit analytical solution for different fields of dislocations in piezoelectric and magneto-electro-elastic bimaterial heterostructures have been already presented by Han and his colleagues.[13–16] Despite the fact that the analysis is static, it will provide good understanding on the behavior of dislocations near the interface in nitride heterostructures.

To model the AlGaN/GaN heterostructure, we consider a piezoelectric bimaterial space in a Cartesian coordinate system (x,y,z), where $z>0$ and $z<0$ are occupied by transversely isotropic AlGaN and GaN, respectively, with interface at $z=0$ plane. The AlGaN material has 50% Al and 50% GaN with poling direction along z-axis. The material properties for AlGaN and GaN are presented by Han *et al.*[16] An extended dislocation loop L defined as the boundary of a dislocation surface S can be described by an extended Burgers vector $\mathbf{b}=[b_1,b_2,b_3,\Delta\varphi]^{\mathrm{T}}$ with b_i $(i=1,2,3)$ as the components of the dislocation's Burgers vector and $b_4=\Delta\varphi$ as the electric potential dislocation corresponding to an electric dipole layer along the surface S.[17] The size of the dislocation loop is assumed to be much smaller than the thickness of the bilayer system in the way that the effect of the free surface can be neglected. The presumed dislocation loop in piezoelectric medium will induce coupled elastic and electric fields. The strain field will induce a piezoelectric polarization field $\boldsymbol{P}^{pz}$ in the domain as follows:

$$P_i^{pz}=e_{ijk}\gamma_{jk}=e_{ijk}u_{j,k}, \tag{1}$$

where γ_{ij} and u_i are, respectively, the strain and displacement fields and e_{ijk} represents the piezoelectric coefficients. A sub index after the subprime denotes the derivative with respect to the coordinate. The analytical solution for the displacement and its derivatives has been verified with the classical theory of elastic fields around dislocations[18] and has been compared to the results by Minagawa for the electric fields.[19] The corresponding elastic and electric fields (stress and electric displacement) will apply a force back on the dislocation loop. This force known as the Peach-Koehler (PK) force for elastic materials represents the barrier by the change in interatomic potential across the interface and it is extended here to the piezoelectric material case. The magnitude of the

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PK force is proportional to the local stress field and its direction is a function of the position of the dislocation in the domain. The work done by the extended stress field σ_{iJ} (elastic stress field σ_{ij} and electric displacement D_i) can be written as follows:

$$W = -\int_S (b_j\sigma_{ij} + \Delta\varphi D_i)\mathrm{d}S_i \equiv -\int_S b_J\sigma_{iJ}\mathrm{d}S_i, \tag{2}$$

where $b_J\sigma_{iJ}$ is a vector with i ($i = 1,2,3$) being the free index and the summation over J is from 1 to 4. We assume that every line element d$\mathbf{l}$ on the loop L has a virtual displacement $\delta\mathbf{r}$. When the dislocation expands, the loop area S will be increased by $\delta\mathbf{r} \times \mathrm{d}\mathbf{l}$ due to the virtual displacement of d$\mathbf{l}$, and consequently, the variation of the work by σ_{iJ} becomes as follows:

$$\delta W = \int_L \mathrm{d}\mathbf{F}\cdot\delta\mathbf{r} = -\int_L b_J\sigma_{iJ}(\delta\mathbf{r}\times\mathrm{d}\mathbf{l})_i = \int_L [(b_J\sigma_{iJ})\times\mathrm{d}\mathbf{l}]\cdot\delta\mathbf{r}, \tag{3}$$

where d$\mathbf{F}$ is the change of the extended PK force acting on a dislocation element d$\mathbf{l}$, defined obviously as

$$\mathrm{d}\mathbf{F} = (b_J\sigma_{iJ})\times\mathrm{d}\mathbf{l}. \tag{4}$$

We consider the force acting on a dislocation element d$\mathbf{l}$ due to the electric charge along the dislocation line $\mathbf{F}^e = f_e\mathbf{E}\,\mathrm{d}l$ with f_e being the electric charge density, $\mathbf{E}$ the stimulated electric field, and dl the length of the element d$\mathbf{l}$. The electric charge density for charged dislocation loops along a (along c) is defined as $f_e = fe/a$ ($f_e = fe/c$), with a and c being the lattice constants equal to the distance between the adjacent possible charge points, f the fraction of the occupied sites ($f \leq 1$), and e the unit charge ($\pm1.6\times10^{-19}$ C for positive and negative charged particles). The total force acting on a unit length charged dislocation element in component form becomes

$$F_l = \varepsilon_{ikl}b_J\sigma_{iJ}\nu_k + f_eE_l, \tag{5}$$

where ε_{ikl} is the permutation tensor and ν_k corresponds to the components of unit tangent vector $\boldsymbol{\nu}$ along the dislocation loop.

The interface and free surfaces disturb the stress fields of dislocations and thus contributes not only to the mobility of dislocations but also to the polarization charge variations in semiconductor heterostructures. Analytical research is available focusing on the image force acting on edge and screw dislocations in materials along with numerical methods.[9,17,20–23] When a dislocation lies within a solid with surfaces/interfaces, the extended stress fields induced by dislocation are divided into the full-space fields σ_{iJ}^{∞} and E_l^{∞}, and the complementary (image) fields σ_{iJ}^{Image} and E_l^{Image}. The full-space fields induced by the dislocation in a homogeneous and infinite space are due to the perturbation of atomic crystals. These fields will induce a self-force on the dislocation line called the core field.[13,22] The extra force on the dislocation (image force) is induced by the image fields σ_{iJ}^{Image} and E_l^{Image} reflecting surface/interface effects. The PK force presented in Eq. (5) is the combination of full-space field and the image force thus it can be calculated from the elastic stress and electric fields. It is noted that the high magnitude of the image force in nanoscale is the consequence of the large ratio of surface/interface region and thus controls the mechanics and physics of dislocations. However, classical elasticity solutions should be carefully considered in small scales and any constraint on the surface or interface can significantly change the nature of the image force.[21] Recent advancements in molecular dynamics and kinetic Monte Carlo of defect interactions provide a meaningful connection between the atomistic simulations in small scales and elastic continuum.[24]

Experimental observation of grown epitaxial GaN layers shows that the TD line direction is along $\langle 0001\rangle$ direction for edge and screw dislocations.[25] Additionally, the Burgers vector of MDs in AlGaN/GaN system is found to be along $\langle 11\bar{2}0\rangle$ direction.[8] Floro *et al.*[8] have shown that $1/3\langle\bar{1}\bar{1}23\rangle/\{11\bar{2}2\}$ is believed to be the predominant slip system (direction and plane) producing misfit dislocations in AlGaN/GaN heterostructures. Thus, we adopt a Cartesian coordinate system with x-axis along $[1\bar{1}00]$, y-axis along $[11\bar{2}0]$, and z-axis along $[0001]$ in the hexagonal system with the origin at the interface. An inclined elliptic loop on $(11\bar{2}2)$ plane is considered with its major and minor axes equal d and $0.712d$, placed in the upper AlGaN material with its center located at (0, 0, 0.7d). The Burgers vector is along $[\bar{1}\bar{1}23]$ direction and thus the direction of the mixed dislocation lines varies depending on the lattice parameters.[8,10,25]

The electrostatic field in nitride heterostructures is controlled by the total polarization at the interface while the discontinuity of polarization between layers forms the 2DEG of trapped electrons.[26] The spontaneous polarization occurs due to the polar-atomic arrangement of Ga and N atoms and it is not explored in this letter. The piezoelectric polarization occurs, however, due to the strain induced by the lattice mismatch of GaN and AlGaN at the interface. Contours of the piezoelectric polarization around the inclined dislocation loop placed near the interface of AlGaN/GaN bilayer system are plotted in x-z plane as shown in Fig. 1. The polarization field is normalized with respect to the d/b ratio. The field pattern is concentrated at locations where the dislocation loop intersects the x-z plane. There is a discontinuity in the polarization at the interface due to the change in piezoelectric properties. This can also be noticed by the inset diagram where the components of the piezoelectric polarization are plotted along the vertical line that passes through the center of the dislocation loop. The vertical polarization P_z is clearly dominant since the piezoelectric layers are oriented in (0001) c-plane direction. The maximum normalized polarization is about $1\,\mathrm{Cm}^{-2}$ which occurs around the same vertical coordinates that the dislocation is located. This occurs by only one dislocation loop near the interface. However, there is a huge density of dislocation ensembles containing 2DEG density of about $10^{13}\,\mathrm{cm}^{-2}$ at the AlGaN/GaN interface.[26] Additionally, the polarization field will induce local stress and electric fields. The effective stress (which is proportional to the second invariant of the stress tensor) and electric displacement fields along the vertical line corresponding to $x = 0$ and $y = 0$ in AlGaN/GaN bilayer system are presented in Fig. 2. The amount of $1\,\mathrm{Cm}^{-2}$ normalized polarization at the center of the dislocation loop corresponds to a maximum electric displacement of about $1.8\,\mathrm{Cm}^{-2}$. This diagram also

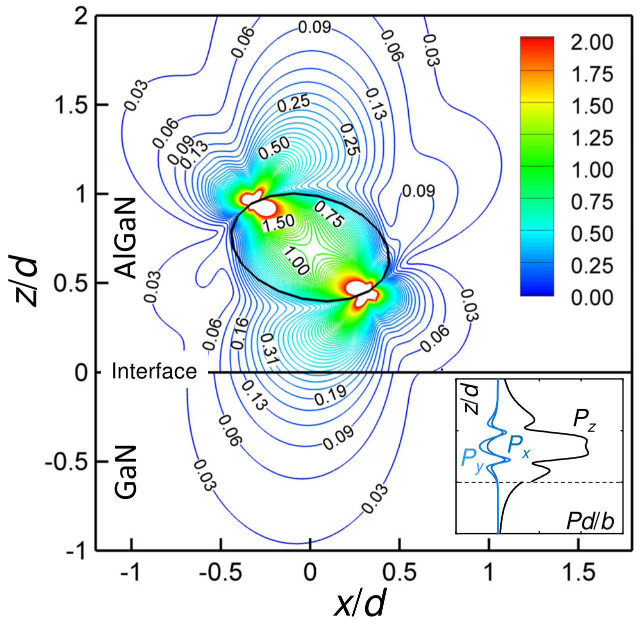

FIG. 1. Contour plot of piezoelectric polarization field in x-z plane around an inclined dislocation loop placed near the interface of AlGaN/GaN bilayer system. The polarization is in Cm^{-2} and it is normalized by the ratio of Burgers vector b and the dislocation size d. The normal direction of the dislocation loop is [0.43, 0.74, 0.53] and the direction of the major axis of the elliptic loop is [−0.87, 0.5, 0]. The x and z axes are normalized by the dislocation size d and 1 e/c electric charge is accumulated on the dislocation core. The inset shows the line plot of the components of the polarization along the vertical line with x and y equal to zero.

implies that a dislocation loop of size 100b will induce effective stress of about 3.2 GPa around the dislocation loop center. It can be seen from the animation in Fig. 2 of supplementary material[34] that the iso-stress surface expands into the lower GaN layer with softer material properties.

Experimental results by electron emission microscopy and electron holography on GaN indicate, respectively, the charge of up to 0.25 e/c on TDs[27] and up to 2 e/c on edge

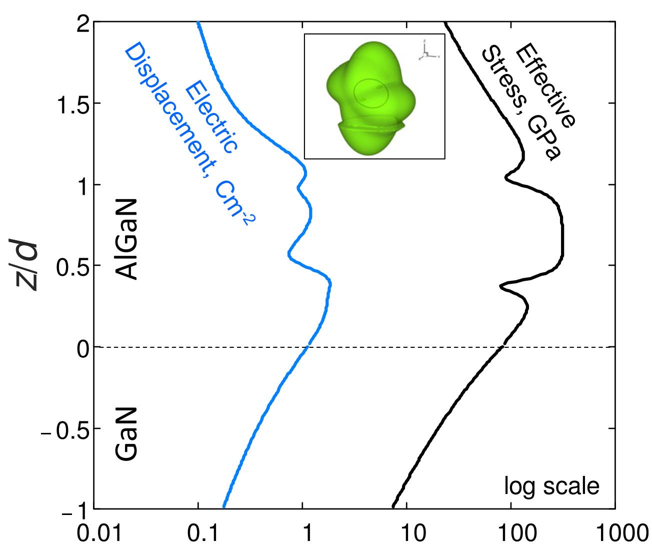

FIG. 2. The effective stress (in GPa) and electric displacement (in Cm^{-2}) induced by the polarization field close to the interface of an AlGaN/GaN bilayer system along the vertical line with x and y equal to zero. These fields are responsible for the acting force on the dislocation loop in the domain. The inset shows the 3D iso-stress surface of 12 GPa around the dislocation core. (Multimedia view) [URL: http://dx.doi.org/10.1063/1.4895511.1].

dislocations.[28] However, calculations and modeling of measured electron mobility in GaN films have verified significant trapped electron charge density up to 1 e/c in III-nitrides.[29,30] We here consider 1 e/c charge on the dislocation core and show that this amount of charge can significantly change the acting force on the dislocation and thus might affect the earlier theories and experiments on polarization and dislocation behavior in nitride semiconductors. The normalized PK force acting on the dislocation loop is depicted in Fig. 3 for AlGaN/GaN bimaterial with uncharged and charged dislocation loops. It can be seen that strong PK force is applied to the lower edge-type segment of the dislocation close to the interface. The magnitude of the total PK force for an assumed dislocation loop of size 100b increases from about 0.32 mN/m for screw-type segments to about 1 mN/m for lower edge-type segment. The upper edge-type segment of the dislocation feels a repulsive force toward the interface. This result accommodating with the results by Khanikar *et al.*[21] supports that the attractive or repulsive nature of dislocation force depends on the dislocation core distance from the interface. Conclusively, the nature of the interfacial image force can only be observed in the three-dimensional (3D) space as shown in the animation in Fig. 3 of supplementary material[34] pointing out that both glide and climb components are to be accounted for near-interface phenomena. It can be seen that with only 1 e/c charge on the dislocation core, the direction of the acting force changes dramatically while the magnitude changes about 33% for the lower edge dislocation segment. We have also noticed that the direction of the PK force induced by charge only points away from the interface for the whole edge, screw, and mixed dislocation segments and it will balance the elastic-induced field into the force vector field shown in Fig. 3(b). The resultant acting force indicates the tendency of the dislocation loop to expand in all directions, to become close to the interface, and to rotate in a fashion that screw-type dislocations eliminate, provided that the acting force is greater than the Peierls stress required to move the dislocation by shear. This further indicates that the dislocations in nitride-based semiconductors are mainly of edge and mixed types since the energy per unit length to generate screw MDs or TDs is much higher than edge or mixed ones.

Figure 4 shows the glide and climb components of normalized PK force versus the accumulated charge on the dislocation core for one screw and two edge segments of the dislocation loop. Both glide and climb components are decreased with increasing charge for the upper edge dislocation segment. However, the charge increases the tendency of the dislocation to glide rather than climb for the screw segment. At the lower edge segment, the glide component of force is dominant and for a dislocation loop of size 100b it will decrease with charge from about 1 mN/m down to 0.6 mN/m. The climb component however may decrease or increase depending on the amount of accumulated charge on the dislocation core. Near the interface, due to the image stress, glide component is larger than climb about 5–9 times for different accumulated electric charge. We only show in this letter that the dislocation force varies by charge significantly which can perturb the polarization charge in nitride heterostructures and the stress/electric fields in piezoelectric-

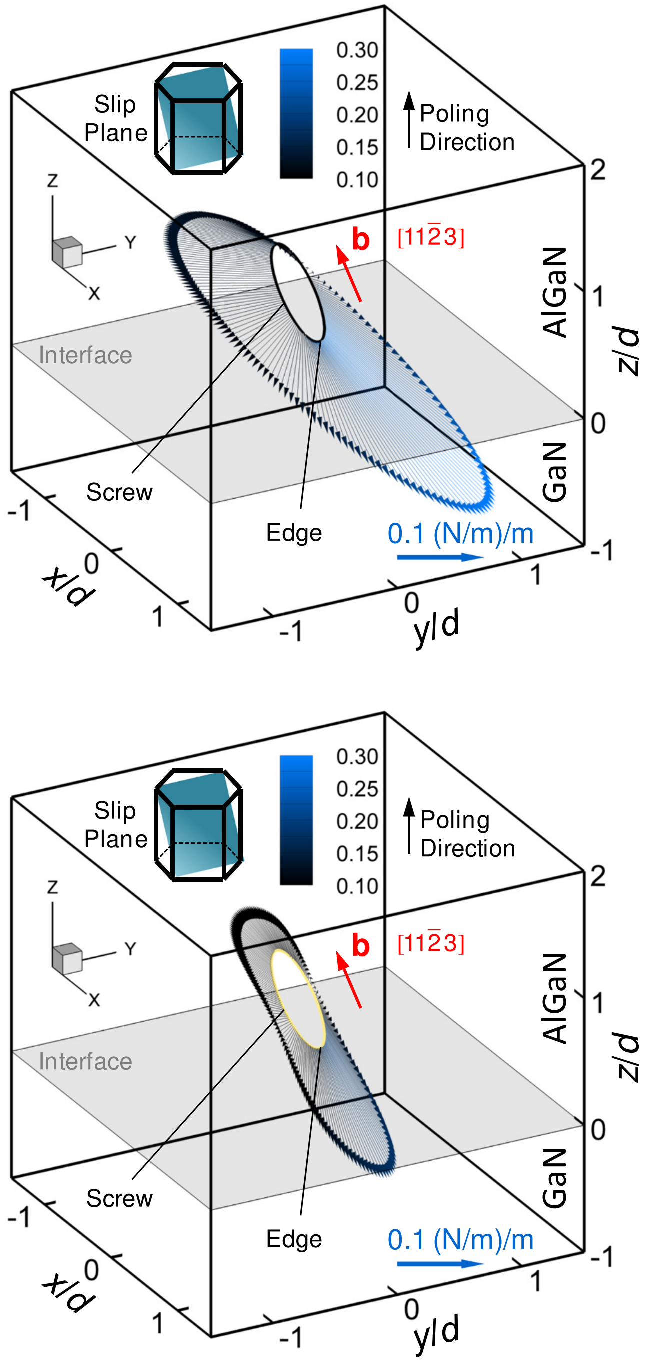

FIG. 3. Peach-Koehler force vector field (normalized by $10^9 b^2/d$ and in unit (N/m)/m) along an inclined elliptic dislocation loop with (a) dislocation loop without charge and (b) 1 e/c charged dislocation loop. The poling direction is along [0001] direction and the reference vector 0.1 (N/m)/m represents the magnitude scale of the force. The elliptic loop is considered to be on $(1\,1\,\bar{2}\,2)$ plane with Burgers vector along $[\bar{1}\,\bar{1}\,2\,3]$ direction. The ratio of the lattice parameters c/a equals 1.613. (Multimedia view) [URL: http://dx.doi.org/10.1063/1.4895511.2].

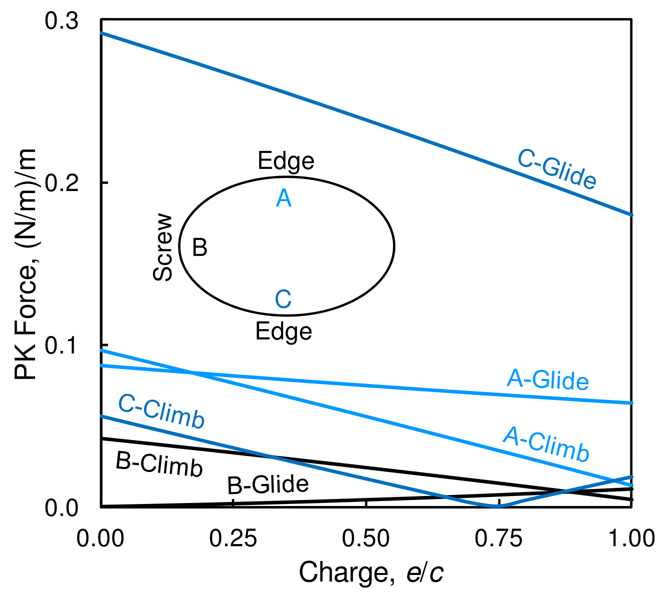

FIG. 4. The force glide and climb components (normalized by $10^9 b^2/d$ and in unit (N/m)/m) at three segments of the inclined elliptic dislocation loop. Segments A and C represent the edge-type dislocation and segment B represents the screw-type dislocation.

based electronic devices. Any further predictions of dislocation motion require dynamic analysis of ensembles of dislocations with discrete Burgers vector or continuous distribution of disregistry[31] using discrete/continuum models and field theories[32] as well as utilizing the dislocation density-based model to account for the dislocation interactions.[33]

The presented analytical method characterizes the piezoelectric polarization in a bilayer system while emphasizes on the importance of charge and its effect on the dislocation force. This is important regarding the dislocation dynamics and plastic deformation, the design of novel semiconductor heterostructures, and the irradiation of metals and ceramics. We conclude that strong piezoelectric polarization concentrates around the dislocation area in polar AlGaN/GaN bilayer system while it passes through the interface into the lower GaN material with an expected jump related to different piezoelectric properties at sides of the interface. The presented model reveals the significant changes in the dislocation force by the accumulation of electric charge. The extended Peach-Koehler force analysis in this letter confirms that the majority of dislocations have edge and mixed characters, while the resultant force on the dislocation has a tendency to eliminate the screw dislocations which are energetically unstable in comparison to edge and mixed dislocations.

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[34]See supplementary material at http://dx.doi.org/10.1063/1.4895511 for brief description of the multimedia animations.