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Paweł Dłużewski[1], **Toby D. Young**[1], **Gregorz Jurczak**[1], and **Jacek A. Majewski**[2]

[1] Interdisciplinary Center of Materials Modeling, Institute of Fundamental Technological Research, PAS, Świętokrzyska 21, 00-049 Warsaw, Poland

[2] Institute of Theoretical Physics, Interdisciplinary Center of Materials Modeling, Warsaw University, ul. Hoża 69, 00-681 Warszawa, Poland

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It was observed experimentally by Rouviere et al. that GaN/AlN Quantum Dots (QDs) nucleate at the edge of threading dislocations (Appl. Phys. Lett. **75**, 2632 (1999) [1]). The preferred nucleation of QDs in this way is generally assumed to be due to the influence of the stress/strain field around the dislocation core, which in turn, gives the chemical and geometric conditions for nucleation of the QDs. We solve the finite element problem for QDs situated at the edge of threading dislocations where different lattice parameters, piezoelectric and spontaneous polarisation coefficients are assumed for the QD and its matrix. By solving the elastic and electric equilibrium problems we obtain both the residual stress and electric fields. The computational scheme employed here was obtained by linking two previous finite element algorithms described inreferences (P. Dłużewski et al., Comput. Mater. Sci. **29**, 379 (2004) [2]) and (G. Jurczak et al., phys. stat. sol. (c) **2**, 972 (2005) and S.P. Łepkowski et al., Phys. Rev. B **73**, 245201 (2005) [3, 4], respectively). This approach allows us to get a deeper physical insight into the mechanics and electrical properties of QDs and ultimately determine the efficiency of light emission from these objects.

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It was observed experimentally by Rouviere et al. that GaN/AlN Quantum Dots (QDs) nucleate at the edge of threading dislocations (Appl. Phys. Lett. **75**, 2632 (1999) [1]). The preferred nucleation of QDs in this way is generally assumed to be due to the influence of the stress/strain field around the dislocation core, which in turn, gives the chemical and geometric conditions for nucleation of the QDs. We solve the finite element problem for QDs situated at the edge of threading dislocations where different lattice parameters, piezoelectric and spontaneous polarisation coefficients are assumed for the QD and its matrix. By solving the elastic and electric equilibrium problems we obtain both the residual stress and electric fields. The computational scheme employed here was obtained by linking two previous finite element algorithms described inreferences (P. Dłużewski et al., Comput. Mater. Sci. **29**, 379 (2004) [2]) and (G. Jurczak et al., phys. stat. sol. (c) **2**, 972 (2005) and S.P. Łepkowski et al., Phys. Rev. B **73**, 245201 (2005) [3, 4], respectively). This approach allows us to get a deeper physical insight into the mechanics and electrical properties of QDs and ultimately determine the efficiency of light emission from these objects.

Type III-N semiconductor materials are of significant interest for their potential as electronic and optical devices, though it is well known that wurtzite III-N materials have a relatively high dislocation density and that, from the lattice mismatch between GaN/AlN and dislocations in the GaN substrate, are induced local tension at the surface of the AlN film. This can augment the physical properties and thus the efficency of technological GaN/AlN devices. It is therefore meaningful to consider the affect strain fields have on the elastic and piezoelectric properties of the QD itself. The typical radius of self-assembling quantum dots is reported to be $\sim$ 16 nm [1]. While smaller QDs can have a radius of $\sim$ 2 nm, larger QDs have a radius as large as $\sim$ 25 nm in diameter and contain millions of atoms within its volume. An appropriate method with which to simulate medium-large QDs, and while including its immediate surroundings, is within Finite Element (FE) analysis where the simplifying assumption is made that the system is composed of a continuous bulk of material. Our FE model is based on constitutive equations for nonlinear anisotropic hyperelasticity [5] where coupling between the elastic and and electric fields has been incorporated.

The investigative procedure followed here involves a two-step routine. First we construct the two-fold matrix for QDs at edge dislocations where the continuous field of the dislocation core is taken from the computer processing of high resolution transmission elecron microscopy images of threading dislocations (TDs) observed in wurtzite GaN [2, 6–8]. Here, we assume the anticipated [9] and observed [1] geometry of the QD as a capped hexagonal-based pyramid; illustrated in Fig. 1. Second, by solving the elastic and electric problems we find both the residual stress and electric potential at equilibrium.

* Corresponding author: e-mail: tyoung@ippt.gov.pl, Phone: +48 022 826 9833, Fax:+48 022 826 9815
** Currently at: Faculté des Sciences et Techniques, Université Paul Cezanne, Av. Escadrille Normandie Niemen, 13397 Marseille Cedex 20, France

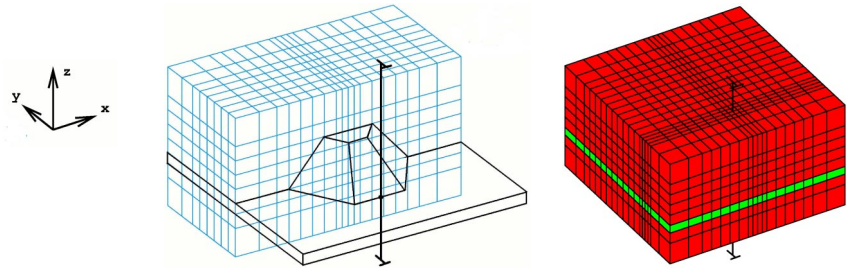

Fig. 1 Schematic diagram of the QD geometry with height 4 nm and radius 11.5 nm, where the black vertical line (parallel to z-axis) indicates the location of the TD. The volume of the whole sample is $(22 \times 22 \times 13)$ nm.

Since the core of QDs are generally believed to be charge free, we have assumed that there are no free charges in the dot and calculate the electric potential from the condition div $\boldsymbol{D}(\boldsymbol{r}) = 0$, where the electric displacement $\boldsymbol{D}$ contains contributions from the spontaneous $\boldsymbol{P}_{\text{spont}}$ and piezoelectic $\boldsymbol{P}_{\text{piezo}}$ polarizations [9]

$$\boldsymbol{D}(\boldsymbol{r}) = \varepsilon_r(\boldsymbol{r})\nabla\phi(\boldsymbol{r}) + \boldsymbol{P}_{\text{piezo}}(\boldsymbol{r}) + \boldsymbol{P}_{\text{spont}}(\boldsymbol{r}) \quad . \tag{1}$$

Following reference [9], we use locally anisotropic static dielectric constant ε_r. Since the strain tensor $\hat{\epsilon}$ is not trace free, we have local hydrostatic pressure in the system. The pressure dependence of elastic modulus was predetermined in *ab initio* calculations [10] and these pressure dependent moduli were used to determine stress and later on electrostatic potential. To take into account piezoelectric nonlinearity we adopted a model following Ref. [10] which assumes strain dependency of the piezoelectric coefficients.

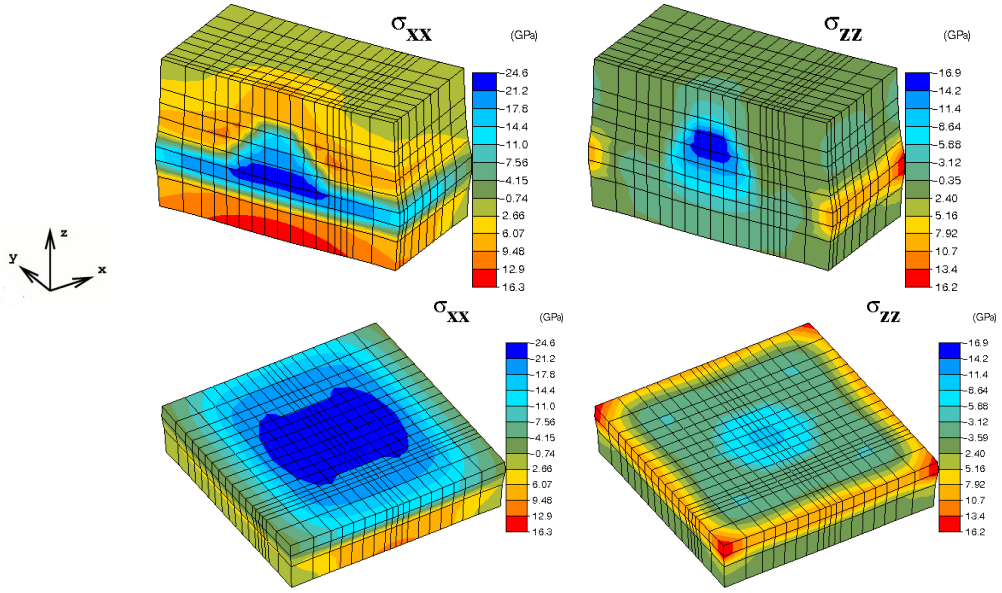

Fig. 2 Cross-sectional images of the residual stress distribution in GaN/AlN QDs. On the left column in the yz-plane and on the right column in the xy-plane; c.f. Fig. 1.

1 Results The residual stress distribution σ_{ii} $\forall i \in \{x, z\}$ in cross-section for GaN/AlN QDs without and with threading dislocations is given in Figs. 2 and 3, respectively. A straightforward comparison

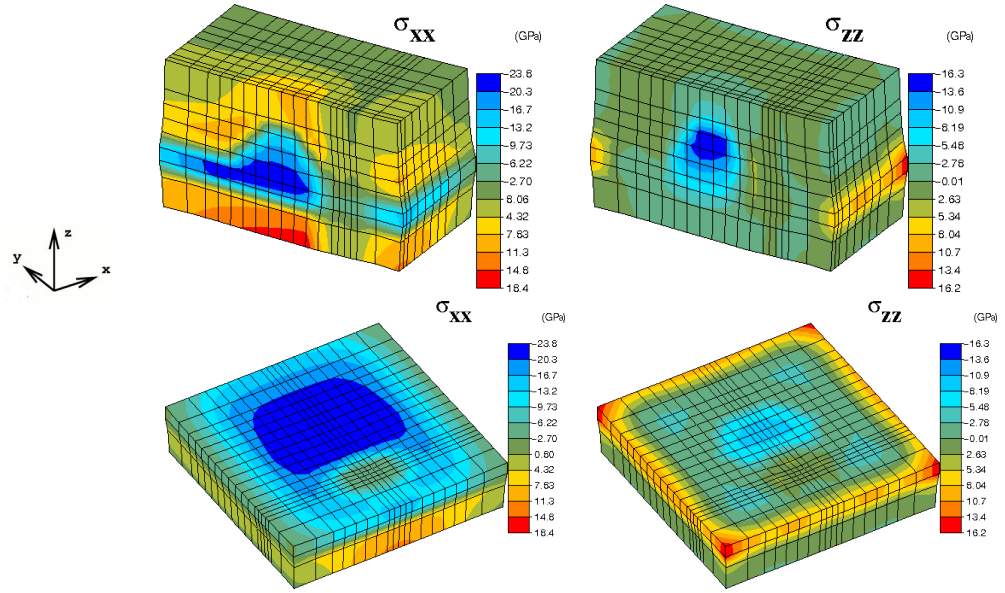

Fig. 3 Same as in Fig. 2 but for GaN/AlN QDs located at the edge of a TD.

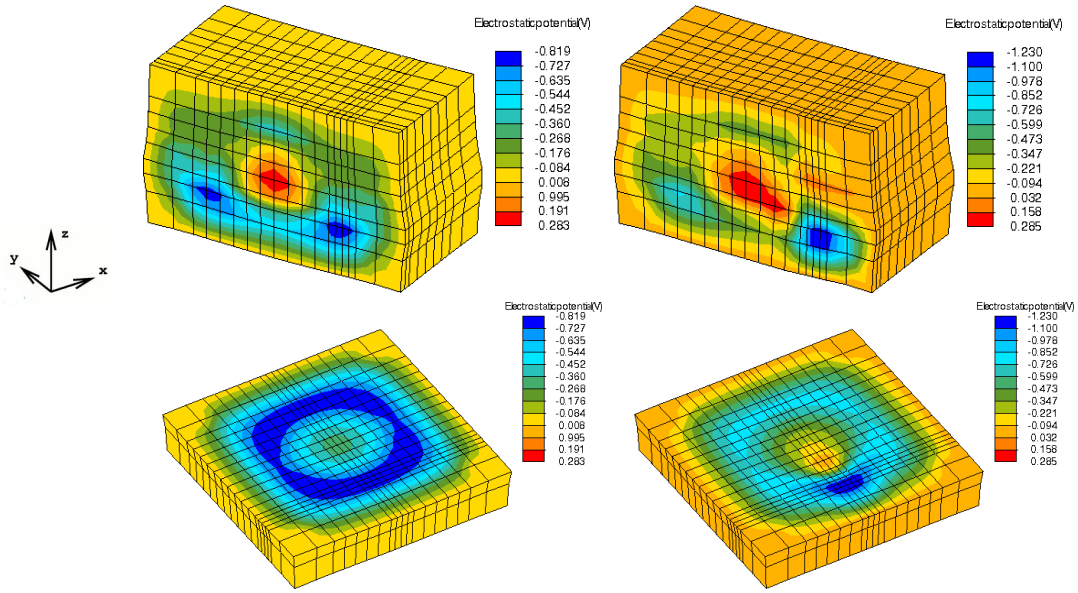

Fig. 4 Cross-sectional images of the electrostatic potential in GaN/AlN QDs. On the top row in the yz-plane and on the bottom row on the xy-plane; both without and with TD for the left and right columns, respectively.

of these two figures clearly show a modification of the stress within the QD in regions of local tension surrounding the TD and is most evident for in-plane residual stresses. A contour plot of the variation in the built-in electrostatic potential is given in Fig. 4 and is in close agreement to that found in Ref. [9]. A straightforward comparison of these results show that coexistence of TDs has a dramatic symmetry

breaking effect on the built-in electrostatic potential of the system. In particular, there is a a significant drop in the electrostatic potential within the QD/TD region induced by the local strain field of the TD; see also Fig. 5. The difference between the electrostatic potential drop for the two cases presented is most fortuitous in the AlN buffer/QD region; depicted between dashed lines in Figs. 5b, 5d.

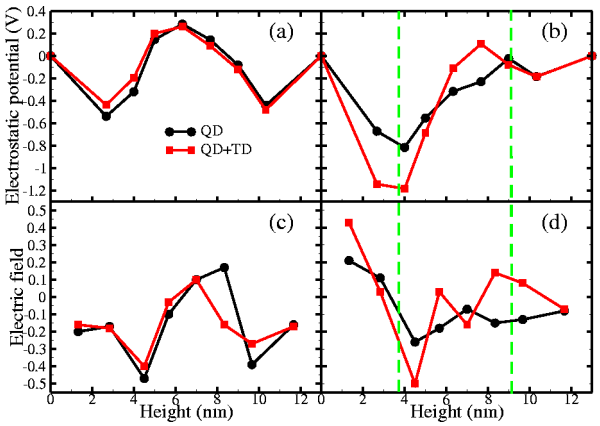

Fig. 5 Electrostatic potential drop and electric field drop through two points of the QD. Figures (a) and (c) through the centre of the dot and figures (b) and (d) through the TD. The meaning of the lines is given in the main text.

2 Summary The elastic and piezoelectric properties of wurtzite GaN/AlN QDs nucleated at the edge of TDs has been investigated. It has been shown that the residual stress arising from TDs affects mainly the in-plane stress/strain fields within the QD. The coexistence of TDs have been shown to have a large symmetry-breaking effect on stress fields and, moreover, on the electrostatic potential. We have measured a drop in the electrostatic potential and distortion of the electric field in the QD region induced by residual stresses surrounding TDs. Furthermore, from the effects shown here in QDs nucleated on the edge of TDs, we would expect to observe a marked shift in the band-to-band transition energy, or equivalently, a red-shift in the optical spectra. The quantification of this phenomena is the aim of future work.

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