Finite element modelling of threading dislocation effect on GaN/AlN quantum dot

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III-nitride based heterostructures have been studied for decades, however commercial success of the GaN, AlN, InN and their compounds arisen lately, notably from applications in blue light emitting diodes for Information Technology. Optically active, III-N layers contain many threading dislocations (TD) resulting from huge lattice mismatch between nitride layers and commonly used substrates. Group III-N semiconductors seems to be less sensitive to the presence of crystal defects, however their affect is still important e.g. in the form of non-radiative recombination of the carriers or thermal degradation of the optical performance. The initial density of TDs in polar III-nitrides reaches 10^9-10^{11} cm^{-2} and corresponds to planar density of the self-assembled quantum dots (QDs) [1]. During growth process, local lattice deformation near the core of TD seems to create energetically favourable position in AlN matrix for GaN QD formation while later on, for capped QD, it reduces residual stresses build-in the dot as well as modify (via piezoelectric coupling) piezoelectric component of the electric field. Except that, several reports advocate the position that local electric charge carriers are trapped by broken atomic bonds along dislocation line [2]. Electric charges localised along dislocation line generate axisymmetric electrostatic potential field affecting piezoelectric and spontaneous potential build-in QD. Finally, shift in optoelectronic band edge structure caused by total electrostatic potential is observed. Unfortunately, effect of electrically active dislocations is usually ignored because precise measurements of the electric charges or the value of the electrostatic potential and its spatial distribution are very difficult. In addition, it seems that they are strongly dependent on doping level and type.

To investigate that phenomena, a models of a hexagonal-based GaN/AlN QDs of a different size (3.5-4.0-4.5nm) nucleated at the edge of a TD (pure edge or screw type) are studied. The boundary-value problem for fully coupled piezoelectricity is then solved by use of a finite element method. Results are presented in terms of the quantitative and qualitative differences in terms of elastic and electric fields caused by the presence of the electrically charged dislocation line. Calculated elastic strain field and total electrostatic potential are used to estimate a band edge structure of the QD-TD system and predict the optoelectronic affect of the charged dislocation on the band-to-band transition energy of that complex system.

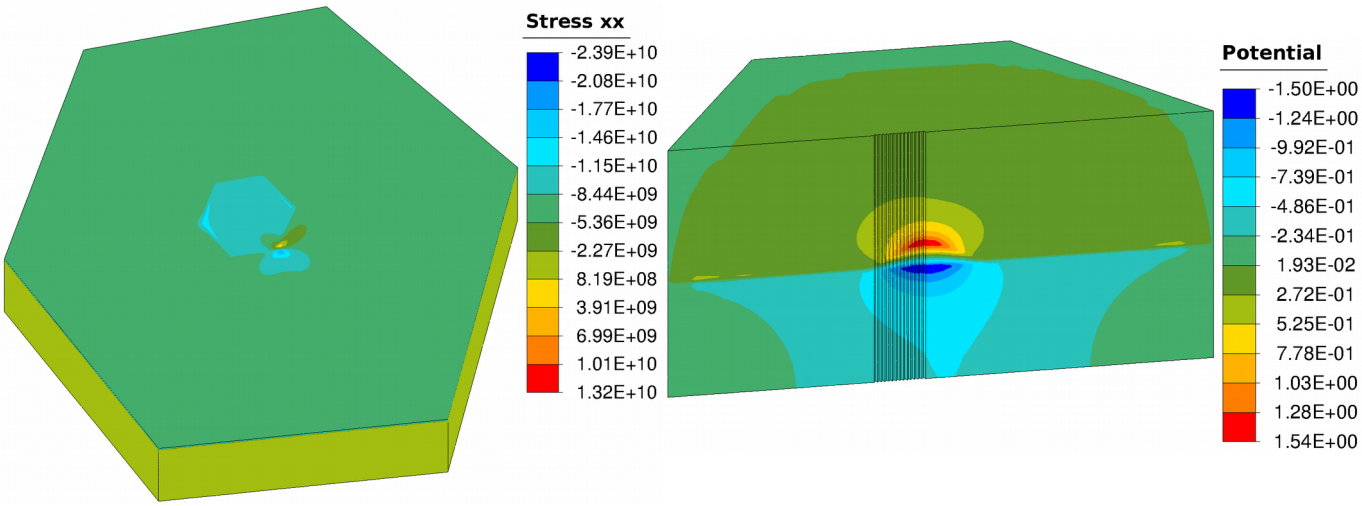

Fig. Elastic stress (xx component) and electrostatic potential fields around GaN/AlN QD nucleated at the edge type TD.

[1] J. L. Rouviere et al., Appl. Phys. Lett. **75**, 2632. (1999).
[2] J. Cai et al., phys. stat. sol. (a) **192**, No. 2, 407–411. (2002).