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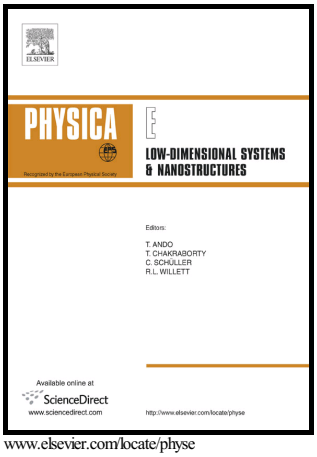

www.elsevier.com/locate/physe

PII: S1386-9477(17)30934-7
DOI: http://dx.doi.org/10.1016/j.physe.2017.08.018
Reference: PHYSE12898

To appear in: *Physica E: Low-dimensional Systems and Nanostructures*

Received date: 28 June 2017
Accepted date: 25 August 2017

Cite this article as: Grzegorz Jurczak and Paweł Dłużewski, Finite Element Modelling of Threading Dislocation Effect on Polar GaN/AlN Quantum Dot, *Physica E: Low-dimensional Systems and Nanostructures,* http://dx.doi.org/10.1016/j.physe.2017.08.018

Finite Element Modelling of Threading Dislocation Effect on Polar GaN/AlN Quantum Dot

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Abstract

In this paper the effect of adjacent threading dislocation at the edge of the GaN/AlN quantum dot is analysed by use of the finite element analysis. Elastic as well electric effects related to dislocation core are taken into account. Two types of threading dislocations: edge- and screw-type, common for III-nitride epitaxial layers, are considered. Also, three different QD geometries are considered to estimate the impact of the threading dislocation on quantum heterostructure. It is demonstrated that the local elastic and electric fields around dislocation affect local piezoelectric fields built-in the quantum dot. Local lattice deformation near the dislocation core reduce residual strains in the quantum dot. It is prominent in the case of edge-type dislocation. The presence of an electric charge along dislocation line provides significant shift of the total potential towards the negative values. However, estimated difference in band-to-band transition energy for edge- and screw-type dislocations are rather small, what suggest low sensitivity to the charge density along dislocation line. Unexpectedly, local strain field around the edge-type dislocation, slightly compensate the negative affect of the electrostatic potential.

Keywords: Quantum dot, Threading dislocation, Piezoelectricity, Finite element modelling

1. Introduction

Successful application of III-Nitride semiconductors in blue light emitting diodes for Information Technology caused a upsurge of research concerning these crystals in mid 1990s [1, 2]. The continuous exert on power efficiency and power density by manipulation of growth parameters, chemical composition, morphology, strain state led to a significant technological progress for GaN, AlN, InN crystals and their compounds. Nowadays, III-N semiconductors are commonly used in various branches of consumer electronics, for example in optoelectronic devices operating in wide range of wavelengths from UV up to green light [2, 3, 4, 5, 6]. Simultaneously with technological advances, a progression in theoretical modelling of the heterostructures took place. By the use of various numerical methods, e.g. Finite Element Method (FEM) or Density Functional Theory (DFT) we are able to accurately predict the strain state, potential, electric field or band edge structure for various morphologies observed in III-nitride heterostructures [7, 8, 9, 10, 11, 12].

Huge lattice mismatch between nitride layers and commonly used substrates (Al_2O_3, SiC) is the source of many defects observed in the III-N epitaxial layers. Typical defects are Basal-plane Stacking Faults and Threading Dislocations (TD) [13, 14]. Wurtzite III-N semiconductors seems to be less sensitive to the presence of crystal defects and electronic or optoelectronic devices may successfully operate with defect density unacceptable in the case of devices based on classical semiconductors, e.g. GaAs, CdTe. Nevertheless, the affect of crystal defects is still important and reduce performance and lifetime of the semiconducting devices. In the case of optoelectronic devices such affect manifests, among others, as the non-radiative recombination of the carriers on TD line and the thermal degradation of the heterostructure performance [15, 16]. The initial density of TDs in polar III-nitride heterostructure reaches $10^9 - 10^{11}\,\mathrm{cm}^{-2}$ [17, 18] and corresponds to planar density of the self-assembled quantum dots (QDs).

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