# DISLOCATIONS IN ATOMISTIC/CONTINUUM MODELLING OF SEMICONDUCTOR STRUCTURES

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Dislocations and interfacial structures formed by different chemical components of crystal lattice result the residual stresses and coupled physical fields. The fieds are crucial for understanding the conditions in which the semiconductor devices grow up and work. The question is: why, in some cases, the growth results the flat layers while in others the channels, clusters, quantum dots, nanowires and other geometric objects nucleate. Such complex technological problems of crystal growth compose a new challenge for computer modelling.

In the present paper, the atomistic model with dislocations and interfacial layers of crystal lattice is embedded in a 3D finite element mesh. Thanks to such a multiscale approach the tensor fields (residual stresses, electric fields, concentration gradients of chemical and electronic elements) sharing the model of crystal lattice can be considered both in the FE and molecular methods. The advantages of such approach is shown in examples.

In the first example, we consider the GaN/AlN Quantum Dots (QDs) nucleated at the edge of threading dislocations (TDs), see Fig. 1. This phenomenon was observed first by Rouviere et al. [1]. It was caused by the fact that TDs induce local tension in certain regions of crystal lattice. This, in turn, gives the preferable geometric condition for nucleation of QDs.

Concerning the FE part, as an example, we consider the interdiffusion induced by the residual stresses and chemical potential force in semiconductor layers. The constitutive equations are based on the transport of chemical components induced by the gradient of residual stresses [GPa/nm] and chemical potentials [2.3].

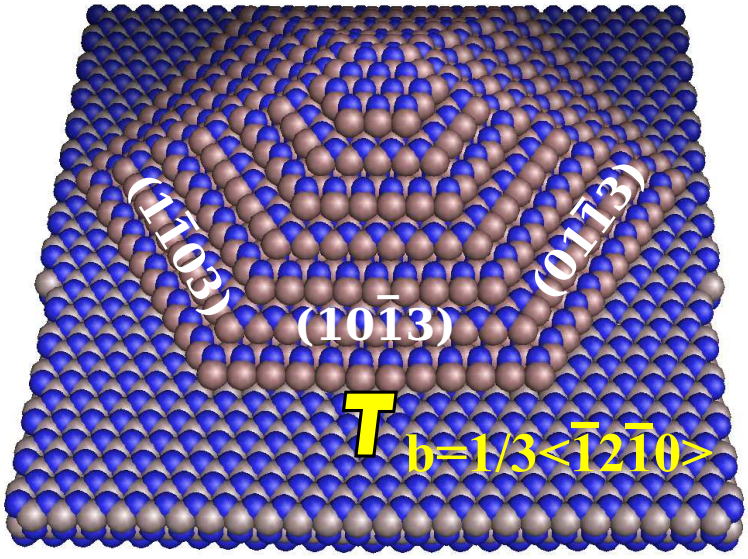


**Figure 1.** Atomistic model of GaN quantum dot formed on the border of edge dislocation pierceing AlN layer.

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Concerning the atomistic part, a 3D atomic model of a system of QDs situated on the edges of threading dislocations is considered. The resultant chemical segregation obtained from our FE simulation is next reconstructed at the atomic scale.

In the next example, the residual stresses, piezoelectric field and optoelectronic properties of QDs are considered by using the nonlinear FE method. As the input data we assume the geometry of the observed hexagonal pyramid-shape QDs [1]. Our finite element constitutive equations are based on the nonlinear anisotropic hyperelasticity [5] where the interaction with electric field is incorporated. The composition and pressure dependence of the elastic constants of AlGaN alloys have been determined from ab-initio calculations.

At the first step the piezoelectric FE problem for QDs situated at the edge of TDs is solved. The different piezoelectric coefficients and spontaneous polarization are used for the QD and the host matrix. Finally, using the such derived electrostatic potential and stress distribution, the optical matrix elements of the QDs are calculated within the framework of k·p perturbation theory. The influence of dislocation on the properties of QDs are discussed [6].

## REFERENCES

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