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1 Introduction It is generally accepted that in nitrides and in many others semiconductors the formation of chemical clusters can be induced by residual stresses. For example, it was obseved experimentally [1] that quantum dots (QDs) form on the edge of threading dislocation (TD) where the lattice spacing is larger and fit better to the lattice of the deposited layer. The dislocation density in InGaN layers often reaches the value $10^8 \mathrm{cm}^3$. Therefore in the current investigation we analyze how far the residual stresses from threading dislocation can be responsible for formation of QDs. In recent years we have investigated the residual stresses induced by a pattern of threading dislocations in GaN [4]. The novel method applied there was based on a few steps. In the first step the lattice distortion field was extracted by computer processing of High Resolution Transmission Electron Microscopy (HRTEM) image of TDs in GaN, see Fig. 1a. Second, the extracted distortion field was used as input to Finite Element (FE) code to find the stress distribution corresponding to the nonlinear hyperelastic behaviour of GaN crystal lattice. In the current investigation we analyze the chemical segregation induced by the residual stresses to estimate how far the stress field induced by threading dislocations can be considered as the thermodynamic driving force for the formation of QDs at the edge of TDs. We consider $In_{0.25}Ga_{0.75}N$ layer deposited on GaN.

The process of chemical segregation induced by stress field can be divided into a few main parts:

1. Deformation of the crystal lattice as a whole (its rotation, strain and displacement),
2. Chemical segregation (interdiffusion of chemical components),
3. Ordered transport of all chemical constituents in crystal lattice (drift of tracers),
   - Within the bulk — movement of vacancies,
   - Surface movement of atoms (interdiffusion of atoms with free lattice sites).

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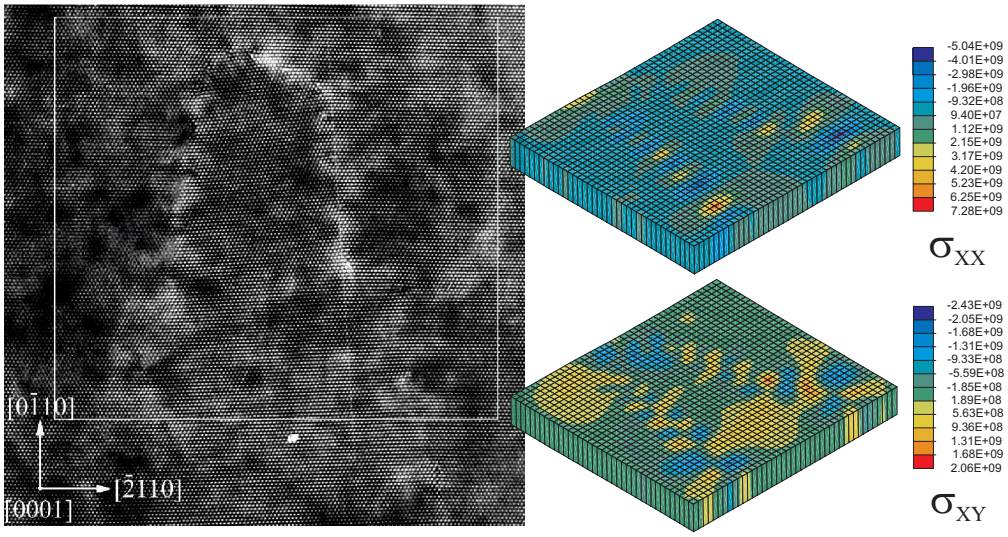

Fig. 1 HRTEM image of TDs in GaN and residual stresses determined by means 3D nonlinear FEM [4].

In our FE simulations only two first parts are taken into account. The respective FE Method (FEM) algorithm to take mass transport into account is currently under construction. In our case the process is governed by the driving force induced by the gradient of residual stresses operating in an anisotropic nonlinear elastic structure [3]. The source of stresses we consider is a set of threading dislocations observed in the HRTEM image of wurtzite GaN deposited on sapphire [4, 5]. A single dislocation was extracted for computer analysis.

2 Constitutive equations We assume that the molar density of chemo-mechanical energy of the crystal is governed by the following function:

$$\psi = \frac{1}{2\widehat{c}}(\widehat{\varepsilon} - \widehat{\varepsilon}_{\rm ch}) : \widehat{\mathbf{c}} : (\widehat{\varepsilon} - \widehat{\varepsilon}_{\rm ch}) + \Delta\psi_{\rm ch}(n) \tag{1}$$

where $\widehat{\varepsilon}$ is the Hencky strain measure of lattice deformation, [2]. The elastic stiffness and chemical strain referred to the perfect lattice are governed by a multi-linear (Vegard) law

$$\widehat{\mathbf{c}} = \widehat{\mathbf{c}}_{\mathsf{GaN}}\,(1-n) + \widehat{\mathbf{c}}_{\mathsf{InN}}\,n \qquad \text{and} \qquad \widehat{\varepsilon}_{\rm ch} = \widehat{\mathbf{a}}_{\mathsf{GaN}}\,(1-n) + \widehat{\mathbf{a}}_{\mathsf{InN}}\,n \tag{2}$$

Substitution of (1-2) into balance laws gives the following formulas for the Cauchy stress and driving force in the actual (deformed) configuration

$$\boldsymbol{\sigma} = \mathbf{c}\,\vdots\,(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_{\rm ch}), \qquad \mathbf{f} = -\mathrm{grad}\,\mu \tag{3}$$

where the stiffness in the current configuration is dependent on lattice rotation tensor $\mathbf{R}$ and deformation gradient $\mathbf{F}$. It gives the following transformation rule for stiffness tensor in the actual configuration: $c^{ijkl} = R^i{}_{\widehat{I}} R^j{}_{\widehat{J}} R^k{}_{\widehat{K}} R^l{}_{\widehat{L}} \big(\widehat{\mathcal{A}}^{\widehat{I}\widehat{J}}{}_{\widehat{M}\widehat{N}}\, \widehat{c}^{\widehat{M}\widehat{N}\widehat{K}\widehat{L}}\big)\,\det \mathbf{F}^{-1}$. More mathematical details on nonlinear elasticity applied here are in [2, 6, 7]. The chemical potential is given by $\mu = \frac{\partial\psi}{\partial n}$. It leads to the following equation for the driving force for interdiffusion

$$\boxed{\mathbf{f} = (\widehat{\mathbf{a}}_{\mathsf{InN}} - \widehat{\mathbf{a}}_{\mathsf{GaN}})\,\vdots\,\widehat{\mathbf{c}}\,\vdots\,\mathrm{grad}\,(\widehat{\varepsilon} - \widehat{\varepsilon}_{\rm ch}) - \mathrm{grad}\,\mu_{\rm ch}} \tag{4}$$

where $\mu_{\rm ch} = \frac{\partial \Delta \psi_{\rm ch}}{\partial n}$ is a pure chemical part of the chemical potential (without mechano-chemical coupling); see [3]. We assumed that the velocity of interdiffusion is governed by the equation $\mathbf{v} = D\,\mathbf{f}$. In our FE calculations we neglect the pure chemical (unknown) part of the driving force in order to check how the gradient of the stress field [GPa/nm] effect on chemical segregation. We assume also that the mobility of atoms in the bulk is negligible and, due to the large mobility of atoms on the free surface, segregation develops only in the surface layers.

Our FEM algorithm is based on the integration of two balance equations

$$\operatorname{div} \boldsymbol{\sigma} = \mathbf{0} \qquad\qquad c\,\dot{n} + \operatorname{div}(c\,n\mathbf{v}) = 0 \tag{5}$$

where $\boldsymbol{\sigma} = \boldsymbol{\sigma}(\nabla \mathbf{u}, n)$ and $\mathbf{v} = \mathbf{v}(\nabla \mathbf{u}, \nabla^2 \mathbf{u}, n, \nabla n)$. We have used 27-node brick finite elements in which the shape function for displacements was spread on all 27 nodes and based on the second-order Lagrangian polynomials, while for Indium fraction we used the first order Lagrangian polynomials spread on the corner 8 nodes (multilinear) only.

3 Results In our FE simulation we have scaled the time of the process to obtain a final stress equilibrium of Indium concentrations in 10 time units. To this aim we have applied the following diffusivity coefficients: for the InGaN (surface) 3D finite elements $D = 10^{-28}$ and for the GaN (bulk) elements $D = 10^{-38}$ and the time step was $\Delta t = 0.1$. The diffusivity and FE results can be rescaled to any other (real) time scale of the process. All other parameters was assumed to be the same as those from our previous FE calculations [4] . The results are presented in Figs. 2 and 3.

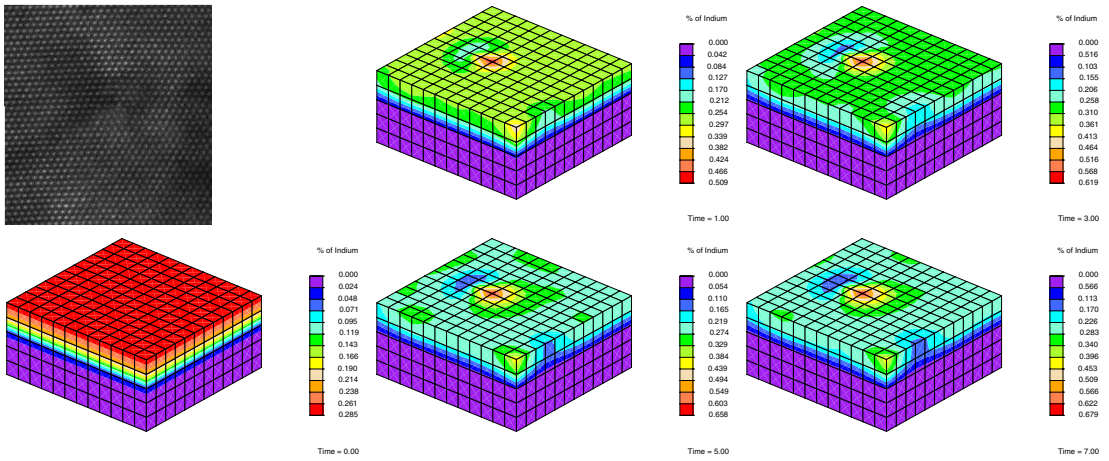

Fig. 2 Fragment of HRTEM image showing a single threading dislocation for subsequent time frames illustrating indium concentrations around TD.

4 Conclusions For the last time step we see the highest concentration of Indium (with a concentration of $\sim$ 70%) which, due to another chemical composition, accommodated all residual stresses induced by TD, c.f. residual stress field corresponding to the initial and final In distribution. The results show that the residual stresses induced by threading dislocations are too small a driving force to form QDs with Indium concentrations greater than 70-80%. In other words the residual stresses induced TD can be treated as the dominant driving force which can nucleate QDs but to form a QD with concentration higher than 70-80% $\frac{\rm In}{\rm Ga+In}$ fraction an additional driving force must be taken into account. As it is easy to guess this additional driving force responsible for Indium segregation over 80% can be the osmotic force induced by a pure chemical part of chemical potential $\mu_{\rm ch}(n)$ which was neglected in the present calculations. Summing up,

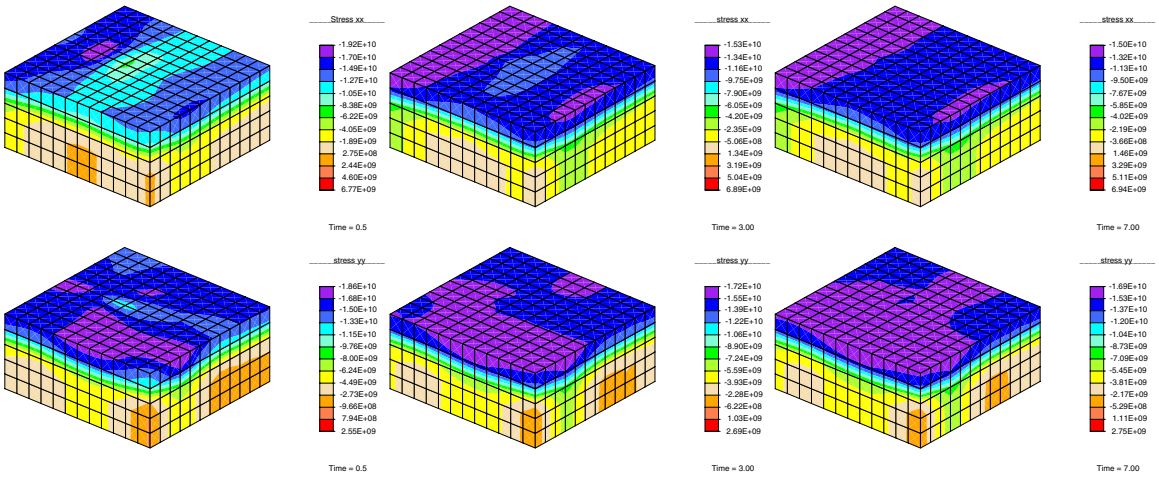

Fig. 3 Similar as Fig. 2 but for residual stresses.

we have demonstrated how far the segregation of Indium in InGaN layer can be interpreted in terms of residual stresses induced by threading dislocation.

A more complete 3D FE simulation of QD formation should take into account not only interdiffusion but also: (a) Surface mass transport towards QD and (b) an additional driving force induced by the gradient of chemical potential. This will be the topic of a future publication.

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