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The dislocation of low-angle grain boundaries in GaN epilayers: a HRTEM quantitative study and finite element stress state calculation

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Abstract

During epitaxy of GaN on sapphire grains form a mosaic structure. The distance between edge dislocations in these boundaries is from 2 to 15 nm. The strain around the dislocations is quantitatively measured by processing of HRTEM images. The dislocation core distribution maps and in plane Burgers vectors components are derived from the experimental strain tensor by applying the continuum dislocation theory. Experimental results were compared with the atomic models of edge dislocations calculated using a modified Stillinger–Weber potential for different atomic configurations of the cores. It is concluded that the strain field extracted from simulated images matches with that of observed dislocations. Starting from experimental distortion distribution data, the finite element calculations are used to estimate the stress around the boundaries. © 2002 Published by Elsevier Science B.V.

Keywords: Nitrides; Electron microscopy; Dislocations; Stress

1. Introduction

The knowledge of local strain fields associated with defects is important for understanding and modelling the properties of semiconductor devices, as well as for optimising the growth of heterostructures. This is particularly necessary in GaN based heterostructures where the density of defects is very high. The interference maxima of high resolution electron microscopy images give information about atomic positions in deformed crystals. Image processing and image simulations help to extract quantitative information. In the case of the strain field around a defect, one useful technique of image processing is the 'geometric phase method' proposed by Hytch et al. [1]. The dislocation core distribution measurement can be applied to determine the dislocation core type and Burgers vectors in an automatic way [2]. In this work we determine the stress fields in subgrains present in GaN layers grown on (0001) sapphire by using the experimentally measured distortion on the HRTEM images.

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2. Experimental details and numerical processing

The planar-view TEM samples of GaN epilayers on sapphire substrate were prepared in the conventional way by mechanical polishing followed by ion milling. HRTEM was carried out on a Topcon 002B microscope operating at 200 KV, with a point resolution of 0.18 nm. The HRTEM images were formed by using $01\bar{1}0$ diffracted beams, with a weak contribution of $11\bar{2}0$ ones. The images were recorded on photographic films and digitised by sampling of 0.15 Å/pixel with 8 bits dynamic. Processing of experimental and simulated images was performed using routines written in ALI (Analytical Language for Images) of Optimas graphical environment [3]. In our procedure, the phase images $P_{gi}(x,y)$ are calculated for $10\bar{1}0$, $01\bar{1}0$ or $1\bar{1}00$ lattice periodicities and z is perpendicular to the image plane. The lattice displacement field $\hat{u}(x,y)$ is calculated using the following vector relationship:

$$P_{gi}(x,y) = -2\pi g_i \cdot \hat{u}(x,y) \quad (1)$$

Differentiation of the displacement field $\hat{u}(x,y)$ followed by smoothing procedure gives possibility to deduce a continuous tensor field of lattice distortions

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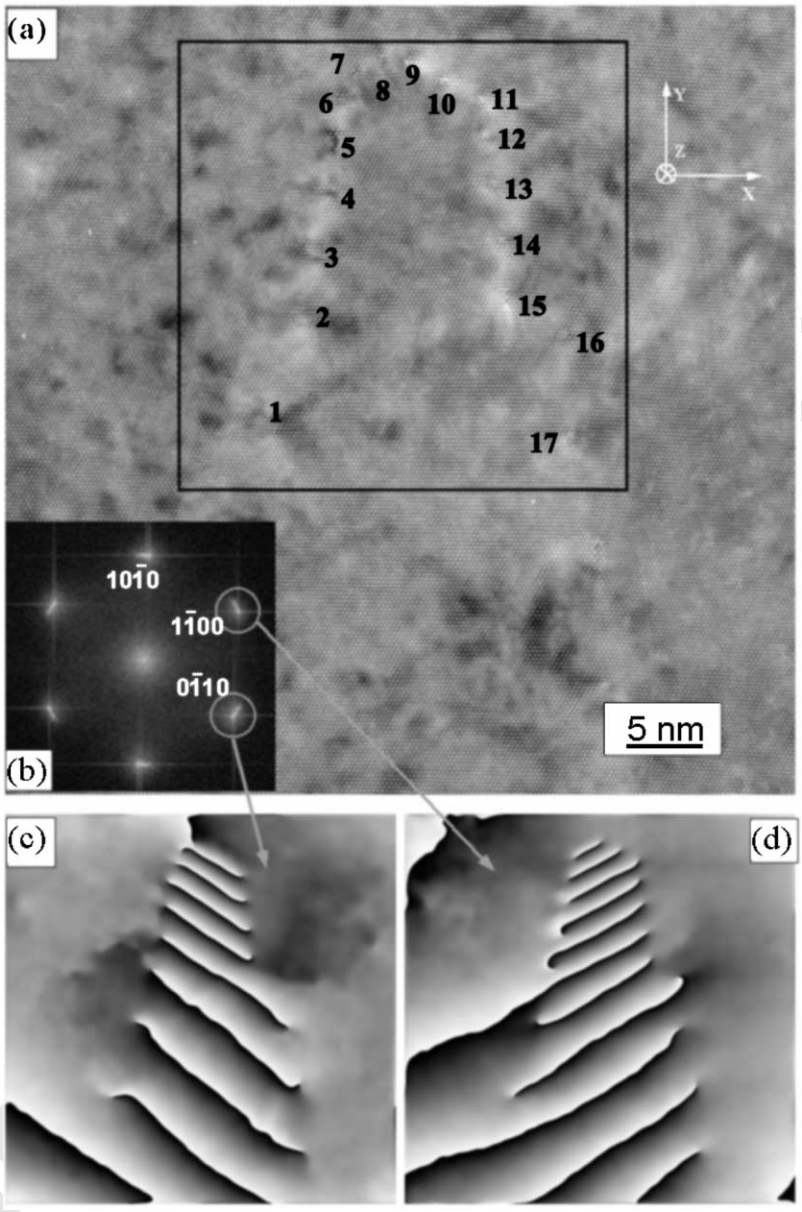

Fig. 1. (a) HRTEM image of a subgrain; (b) FFT of (a); (c),(d) phase images $P_{gi}(x,y)$ obtained respectively for $\breve{g}=1\bar{1}00$ and $\breve{g}=01\bar{1}0$.

$\beta_{ij}(x,y)$. According to the continuum theory of dislocations [2] the further differentiation of the lattice distortion leads to determine the dislocation core distribution tensor.

$$\tilde{\alpha} \overset{df}{=} -curl\beta \tag{2}$$

The tensor $\tilde{\alpha}$ vanishes in the whole region excepting insides of the core where it forms characteristic peaks. By integration of these $\alpha_{ij}(x,y)$ values the in-plane Burgers vector $b_i = -\int_{Sc} \alpha_{ij} ds$ (Sc: dislocation core surface) is calculated. The invariant of the dislocation density tensor id defined by:

$$\rho_d(x,y) = \sqrt{\alpha(x,y)_{xz}^2 + \alpha(x,y)_{yz}^2} \tag{3}$$

where the components α_{xz} and α_{yz} of the dislocation core distribution tensor contribute respectively to the in-plane components of Burgers vector, b_x and b_y.

The Finite Element Method (FEM) is used to determine the stress distribution. As large values of distortions take place the finite deformation approach is performed, i.e. difference between the initial and deformed configurations is included in a algorithm. We use Finite Element calculation by with Taylor's FEAP program [4] which is modified to take into account the finite deformation of anisotropic crystals [5]. In the procedure applied the lattice distortion measured from

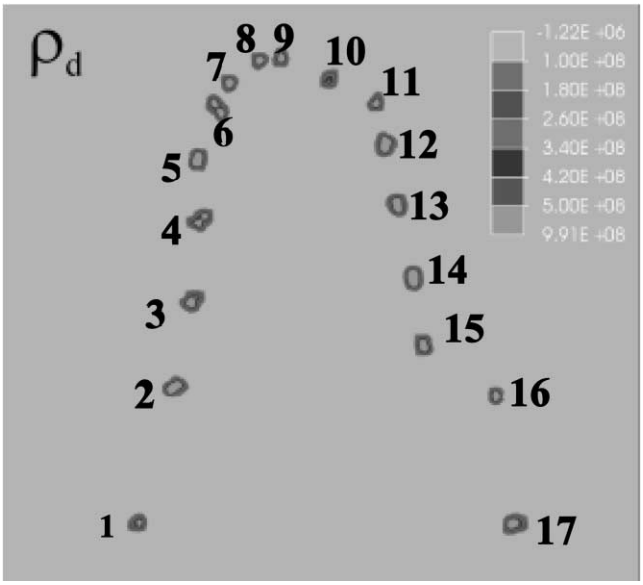

Fig. 2. Invariant of dislocation density tensor $\rho(x,y)$calculated from HRTEM image (Fig. 1) used to reduce the stiffness near dislocation cores.

HRTEM image are stored in the nodes of the mesh. The dimensions of elements are changed in two ways: initial deformation–induced by the imposed distortions and elastic relaxation–due to elastic behaviour of material. The boundary conditions for FEM are taken to be free; the left lower node has been constrained in *xy*-directions and right-lower node in *y*-direction.

The core region of dislocations is treated in a different way; the modules of elasticity which are function of the position *x,y* as stiffness are softened through the equation:

$$c_{ij}(x,y) = c_{ij}e^{-R\rho_d(x,y)} \quad (4)$$

where *R* is the factor reducing stiffness. The factor *R* allows the stiffness reduction in lattice disordered regions, the width and shape of dislocation cores corresponds to the spatial distribution of $\rho_d(x,y)$. The details of the method are published elsewhere [6]. Fig. 1 shows the used distribution $\rho_d(x,y)$ to calculate $c_{ij}(x,y)$.

3. Results and discussion

The image processing was first checked on simulated images of super cells ($14\times14\times0.5$ nm^3) containing approximately 10000 atoms generated by anisotropic elasticity calculation in 2D for a $1/3\ \langle 2\bar{1}\bar{1}0\rangle$ edge dislocation. Different core configurations of the dislocations are made of 4, 8, 5/7 atom cycles in agreement with the experimental HRTEM images [7]. These supercells used in image simulation were first relaxed using a modified Stillinger–Weber potential [8]. Images were

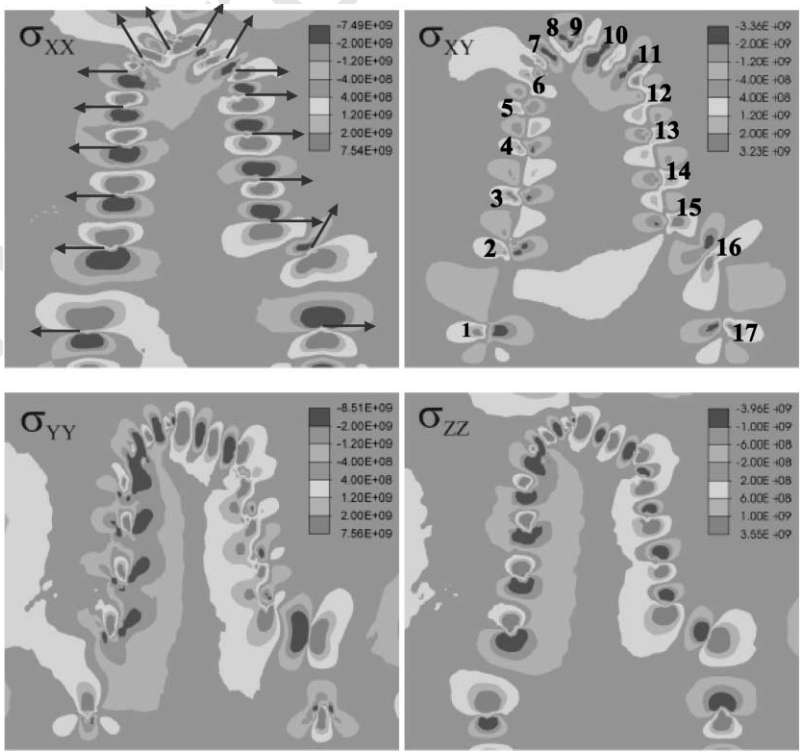

Fig. 3. The stress fields obtained from the experimentally measured distortion by FE calculation. The arrows show orientation of the Burgers vector.

calculated for thicknesses (2–15 nm) and defocus (0–100 nm) series, using the multislice package of the electron microscopy software [9]. Simulation shows that for foil thicknes $t=5$–15 nm and defocus windows $df=-10\ldots-30$ nm the strain fields extracted from HREM images are in agreement with the distortion calculated by atomistic relaxation [10].

The above procedure was applied to a HRTEM image of a sub-grain boundary in which the distance between the dislocations is variable. The lattice distortion distribution tensor $\beta_{ij}(x,y)$ and dislocation core distribution $\alpha_{ij}(x,y)$ were calculated using the two phase images shown on Fig. 1b,c and using Eqs. (1) and (2). The $\beta_{ij}(x,y)$ distribution which is determined in this way in thin TEM sample was read by finite element program as initial values of distortion. FE iteration with border condition corresponding to the bulk sample material was performed to obtain stable solution and finally the stress field was calculated as shown on Fig. 3. Fig. 2 shows the $\rho(x,y)$ used to reduce stiffness.

All the dislocations in Fig. 3 have the same Burgers vector $1/3\ \langle 2\bar{1}\bar{1}0\rangle$, but for some of them, this vector is not parallel to the x axis. Only the dislocations marked: 1,2,3,4,5,6 have a similar distribution of σ_{ij}. For dislocations 12,13,14,15,17 which have Burgers vectors oriented in opposite direction the stress field has inverted positive and negatives lobes. For the other dislocations 7,8,9,10,16 it is necessary to rotate the co-ordinate system by 60° to obtain a corresponding stress field distribution. The maximal values of calculated stress reach ± 7–8 GPa in the case of the σ_{xx} and σ_{yy} component and ± 4 Gpa for σ_{xy} and σ_{zz} component. These maximal values depend on the stiffness reduction parameters and influence of this parameter needs to be studied and discussed in the future.

Anyway, the R parameter influences only the stress level inside the core of dislocations so the long range stress fields are estimated correctly and the interactions between dislocation can be analysed. It is clear that interaction between these dislocations is very high. Only dislocations separated by 7–9 nm can be considered as independent (1,17,16).

Presented methods of the stress estimation at atomic scale in GaN based epilayers is general and can be use to study energetical stability of many nanoscopic systems.

4. Summary

The finite element method applied here has many additional advantages. For example it gives potential ability to 3D simulation of the stress/strain behaviour of HRTEM specimens. Another ability is the possible division of the specimen into crystallographic FE cells. This can be used to link atomic models for unit cells with FE method. On the other hand, the well investigated non-linear elastic behaviour of crystal lattice allows also the prediction of the higher order elastic effects like e.g. the volume expansion of crystal lattice induced by the presence of dislocations. This expansion is responsible for the interfacial surface tension induced by the presence of misfit dislocations which often leads to bending or fracture of epitaxial layers.

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