Stress analysis of $Al_xGa_{1-x}N$ films with microcracks

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(Received 22 July 2002; accepted 11 November 2002)

Thick $Al_xGa_{1-x}N$ epilayer with microcracks grown by metalorganic vapor-phase epitaxy on a GaN buffer above a (0001) sapphire substrate was comprehensively characterized by spatially and spectrally resolved cathodoluminescence (CL) and micro-Raman (μ-Raman) spectroscopy. The variation of the CL line shift and the μ-Raman measurements between the microcracks are consistent with the interpretation that AlGaN is to a large extent stressed like a two dimensional film between the microcracks with nearly full relaxation close to the cracks. A satisfactory theoretical confirmation of this stress distribution was obtained by a three-dimensional finite-element application of the elasticity theory. © *2002 American Institute of Physics.*
[DOI: 10.1063/1.1534408]

In the film growth of $Al_xGa_{1-x}N$ and $Al_xGa_{1-x}N$/GaN heteroepitaxial quantum well structures for short-wavelength optoelectronic devices[1,2] and high-power applications,[3] Al modifies the stress distributions in the films caused by the lattice mismatch between the nitrides and the buffer/substrates. When the epilayer exceeds a certain critical thickness catastrophic flaws appear in the $Al_xGa_{1-x}N$ film in the form of micro-cracks (called cracks in this letter) in the growth plane.[4–6]

We have comprehensively characterized, using spatially and spectrally resolved CL and μ-Raman spectroscopy, a particular sample of thick $Al_xGa_{1-x}N$ epilayers with cracks. The findings and their interpretations are compared with the theoretical results obtained from the elasticity theory using the three-dimensional (3D) finite-element (FE) method.[7]

The sample under investigation was a 0.56 μm thick $Al_{0.17}Ga_{0.83}N$ (labeled AlGaN in this letter) epilayer grown by metalorganic vapor-phase epitaxy (MOVPE) on a 1.9 μm thick GaN buffer on top of a sapphire substrate. It is one in a series of sample grown for investigation by x-ray diffraction (XRD).[8–10] The material quality is considered to be typical when compared with those from others groups. The Al content x was determined by XRD that led to an estimate of the critical thickness of 0.45 μm for $x=0.17$.[9] Al segregation after the formation of cracks has also been discussed.[5]

Cracks forming a hexagonal (trigonal) network are observed in the epilayer. The most frequent and recognizable pattern of the cracks are parallelograms. For later comparison with 3D FE calculations, we have zeroed in on one typical parallelogram of sides 30.4 and 13.1 μm, with the longer side in the {11-20} direction and the shorter side rotated 120°.

The experimental detail of the low temperature CL and RT μ-Raman spectroscopy have been reported elsewhere.[11,12] For our discussion, a CL wavelength image (CLWI) maps the CL wavelength λ of the maximum local intensity at each sampling point. The details of the depth resolved CL spectroscopy can be found in the literature,[6] where the relationship between the electron accelerating voltage and the penetration depth is given.

We show in the left-hand side column of Fig. 1 the CLWIs scanned for different accelerating voltages. The CLWI from the surface clearly shows that the main emission line is progressively blueshifted as one moves from the crack-free center of the parallelogram towards the cracks. This contrast diminishes with increasing accelerating voltage, strongly suggesting that the blueshift described above decreases with increasing depth. This is more explicitly displayed in the right-hand side column of Fig. 1. The horizontal scanning path was chosen as shown in the left-hand side column. It spans two cracks 13 μm apart. Along this path the peak energy of the CL spectral line as a function of the lateral position is plotted. At the surface a monotonic blueshift is detected from the center towards the cracks, reaching its maximum emission energy at the crack positions. In contrast to the surface case, close to the AlGaN/GaN interface, a blueshift towards the cracks is followed by a redshift in the vicinity of the cracks. In the middle region between the cracks, fairly uniform stress distributions are found.

A CLWI of the near-band-gap luminescence of the underlying GaN buffer is shown in the left-hand side of Fig. 2. A CL linescan along the same path as shown in the left-hand side of Fig. 1 is chosen. A redshift from the center in direc-

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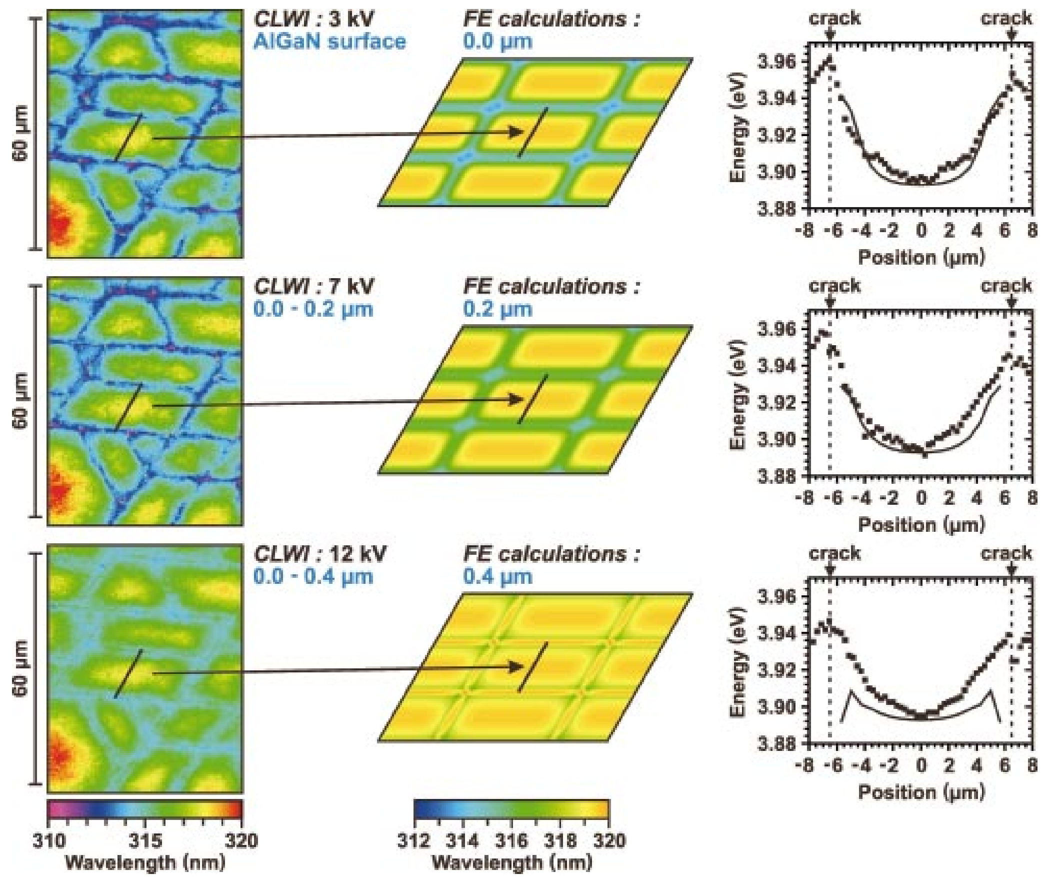

FIG. 1. (Color) Left-hand side: CLWIs of the AlGaN film for different electron accelerating voltages. Center: FE results at different depths. Right-hand side: Comparison of the CLWIs along the line scan with the converted results from FE calculations (solid lines).

tion to the cracks and a strong blueshift near the crack are observed, right-hand side column of Fig. 2.

We performed a stress analysis of the sample with elasticity theory using the FE method. We will show that the CL wavelength shifts are strongly correlated with the stress distributions obtained from 3D FE calculations.

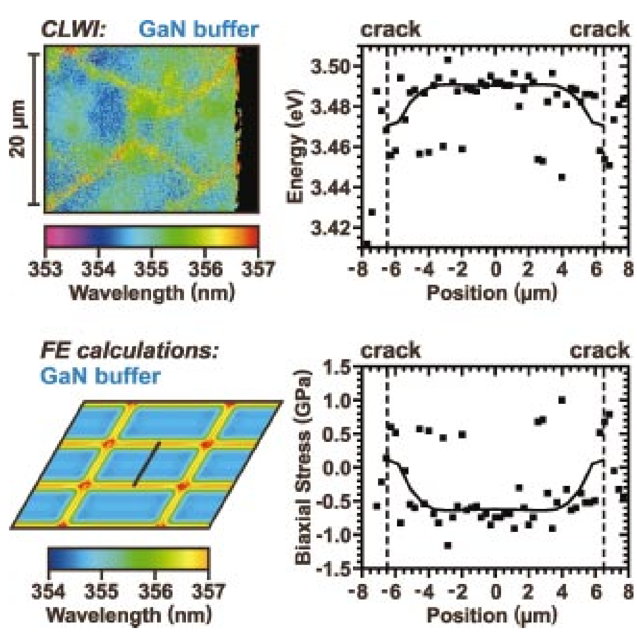

FIG. 2. (Color) Left-hand side: CLWIs of the GaN buffer. Right-hand side: comparison of the stresses along the line scan with the stresses from FE calculations (solid lines).

The sample size for the FE simulation has dimensions specified earlier, with the cracks penetrating as far as the AlGaN/GaN interface, although the crack depth is not known experimentally. The nodes of the FEs that are on the side-faces (only in GaN, in our construction) of the theoretical sample in Fig. 3 obey periodic boundary conditions. We have taken the anisotropic moduli of elasticity from the literature.[13] Without loss of accuracy, one could assume that AlGaN has the same moduli of elasticity as GaN.

The effective lattice mismatch parameters between the sapphire/GaN, $(a_{\mathrm{sapphire}}-a_{\mathrm{GaN}})/a_{\mathrm{GaN}}$, and GaN/AlGaN, $(a_{\mathrm{GaN}}-a_{\mathrm{AlGaN}})/a_{\mathrm{AlGaN}}$, are adjusted to be -0.04% and 0.26%, respectively. These implicitly encompass the effects

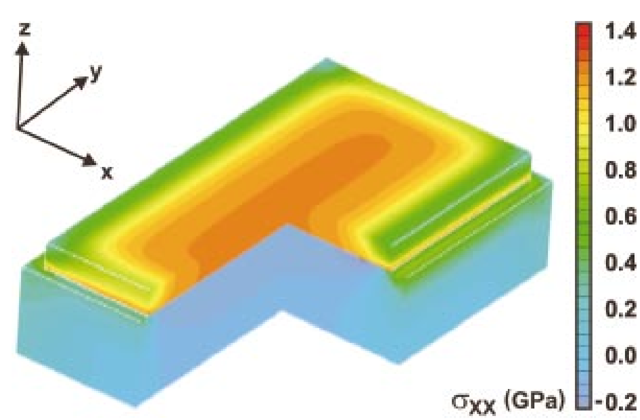

FIG. 3. (Color) Overview of the results from FE simulation of the stresses in the AlGaN film and the GaN buffer.

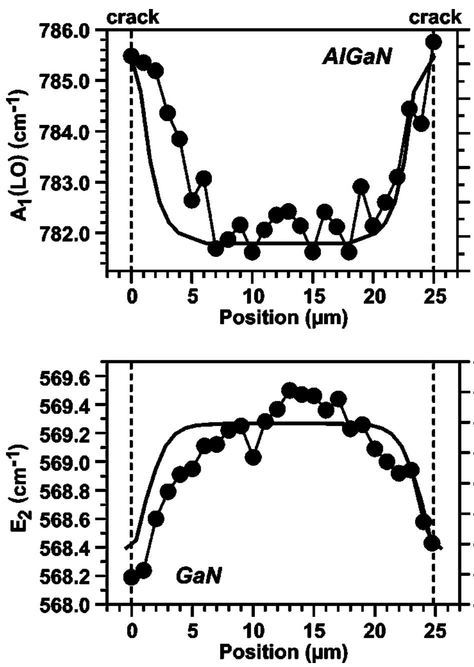

FIG. 4. A_1(LO) mode of AlGaN and E_2 mode of GaN from μ-Raman spectroscopy. Their converted stresses are compared with the results from FE calculations (solid lines).

of impurities, dislocations, etc., in the material, and their magnitudes are consistent with previous studies.[12] The sapphire/GaN effective mismatch leads to a reproduction of the compressive biaxial stress measured in the GaN buffer by μ-Raman spectroscopy. This will be discussed further in Fig. 4. The GaN/AlGaN effective mismatch produces a good agreement between the theoretical tensile stress distribution of the top surface of AlGaN and the CL shift, when we use an approximate parametrization of the shift of 30 meV/GPa, see top of the right-hand side column in Fig. 1. This is quite close to 27 meV/GPa that was derived for GaN.[14]

A general overview of the results from simulation is displayed in Fig. 3. The stress distribution in AlGaN is dominated by biaxial (film-like) tensile stress in most of the volume surrounded by the cracks. The stresses relax noticeably in the vicinity of the cracks. In contrast, in the GaN buffer directly underneath the AlGaN epilayer, one sees mostly biaxial (film-like) compressive stresses. It is reasonable to discuss the results in the areas not too close to the cracks in terms of biaxial stresses because the respective stress tensors are very much dominated by the two approximately equal diagonal elements σ_{xx} and σ_{yy}, while all the other elements have small absolute values, reminiscent of a two-dimensionally stretched (compressed) film.

We should point out that at the cracks, in the absence of any AlGaN material, we find tensile stress in GaN. The reason is that the compressive stresses in GaN described in the previous paragraph are pulling the GaN underneath the crack in opposite directions. This mechanism might have implication for eventual cracks forming in the buffer.[5]

We compare in the right-hand side column of Fig. 1 stresses from simulation converted to wavelength shifts with some typical experimental CL results at different depths inside the AlGaN film. The agreements are quite satisfactory. Similar agreement is found for the GaN buffer (Fig. 2). One should note that close to the AlGaN/GaN interface where the cracks terminate, the stress tensor becomes more complicated and loses its easy interpretation in terms of stressed film.

The overall consistent interpretation of the CL spectroscopy by stress distribution, as supported by simulation, is also confirmed by μ-Raman spectroscopy. In Fig. 4 we show Raman results between two cracks 25 μm apart, exposed after cracking of the sample. The stress in the GaN buffer is calculated from the Raman E_2 mode.[14] The results show generally compressive stresses that relax towards the cracks.

As the E_2 mode of the AlGaN layer appeared as a broad shoulder of the E_2 mode of the GaN buffer, the A_1(LO) mode of AlGaN is used instead for the discussion of the stress distribution, although it is not quite optimal for the estimation of the stress due to the polar character. The AlGaN layer shows the contrasting tensile stresses between the cracks that also relax as one approaches the cracks. The 3D FE simulation is able to reproduce the stress distributions quite satisfactorily.

In conclusion, we reported on CL and μ-Raman spectroscopy on thick AlGaN epilayers with cracks. The shift of the local near-band-gap emission line and the A_1(LO) mode of the AlGaN layer follows the strain profile between the cracks. 3D FE application of the elasticity theory can produce a consistent description of the stress profile of the AlGaN film and the GaN buffer, and support the interpretation that the AlGaN surrounded by cracks behaves for the most part like a biaxially stretched film. The tensile stress in the GaN buffer underneath the cracks could cause cracks formation in the buffer under suitable circumstances.

The authors gratefully acknowledge the financial support of the Deutsche Forschungsgemeinschaft (DFG).

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