Stress analysis of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ films with microcracks

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Thick $\text{Al}_x\text{Ga}_{1-x}\text{N}$ 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 ($\mu$-Raman) spectroscopy. The variation of the CL line shift and the $\mu$-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 $\text{Al}_x\text{Ga}_{1-x}\text{N}$ and $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ 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 $\text{Al}_x\text{Ga}_{1-x}\text{N}$ 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 $\mu$-Raman spectroscopy, a particular sample of thick $\text{Al}_x\text{Ga}_{1-x}\text{N}$ 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 $\mu$m thick $\text{Al}_{0.17}\text{Ga}_{0.83}\text{N}$ (labeled AlGaN in this letter) epilayer grown by metalorganic vapor-phase epitaxy (MOVPE) on a 1.9 $\mu$m 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 $\mu$m 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 $\mu$m, 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 $\mu$-Raman spectroscopy have been reported elsewhere. 11,12 For our discussion, a CL wavelength image (CLWI) maps the CL wavelength $\lambda$ 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 $\mu$m 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 blue-shift 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-
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.

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 FE 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. 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, \((a_{\text{sapphire}} - a_{\text{GaN}})/a_{\text{GaN}}\), and GaN/AlGaN, \((a_{\text{GaN}} - a_{\text{AlGaN}})/a_{\text{AlGaN}}\), are adjusted to be \(-0.04\%\) and \(0.26\%\), respectively. These implicitly encompass the effects...
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tions for AlGaN material, we find tensile stress in GaN. The rea-
tionedly stretched elements have small absolute values, reminiscent of a two-
axial film.

In the vicinity of the cracks, in the GaN buffer we see mostly bi-
agonal elements $\sigma_{xx}$ and $\sigma_{yy}$, 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 rea-
son 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 implica-
tions for eventual cracks forming in the buffer.

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 in-
side 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 complica-
ted and loses its easy interpretation in terms of stressed film.

The overall consistent interpretation of the CL spectro-
copy by stress distribution, as supported by simulation, is also confirmed by $\mu$-Raman spectroscopy. In Fig. 4 we show Raman results between two cracks 25 $\mu$m apart, exposed after cracking of the sample. The stress in the GaN buffer is calculated from the Raman $E_2$ mode. 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 Al-
GaN 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 $\mu$-Raman spectros-
copy 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 Al-
GaN 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 forma-
tion in the buffer under suitable circumstances.

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

\begin{itemize}
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