

In-plane strain anisotropy and lattice parameters of GaN films grown on a-plane sapphire by metalorganic vapor phase epitaxy

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Due to the lack of native substrate the III–V nitrides are typically grown on foreign substrates such as sapphire, SiC and Si. As a result of the different thermal expansion coefficients and lattice parameters of the substrate and the film, the film is strained. The effect of strain on the fundamental properties of III–V nitrides, in particular GaN, has been extensively studied in the case of growth on c-plane sapphire [1], while little is known in the case of growth on a-plane sapphire. The in-plane strain of III–V nitride layers grown on a-plane sapphire is expected to be anisotropic due to the different thermal expansion coefficients of sapphire in the directions parallel and perpendicular to its *c*-axis [2], as well as to the nonequal lattice mismatches along the two directions. Manifestations of anisotropic strain have been reported so far in the emission and reflectance spectra of GaN layers [3, 4].

In this work we report on the effect of the anisotropic strain on the lattice parameters of GaN layers grown on a-plane sapphire by metalorganic vapor phase epitaxy (MOVPE). High resolution x-ray diffraction (HRXRD) is used to determine the lattice parameters and the epitaxial relationships between the films and the substrates. The in-plane lattice parameter was determined from sets of equivalent interplanar distances in six different directions. It is found that the obtained six values of the in-plane lattice parameter can be discriminated into two groups. It is suggested that this result is a consequence of the presence of anisotropic in-plane strain in the films. The in-plane strain anisotropy in the films is determined in the crystal coordinate system, and it is compared with a theoretical estimation.

GaN layers with thickness of 2 μm were grown on a-plane sapphire in an Aixtron planetary reactor at 1170 °C using a low temperature GaN buffer layers. The *a* and *c* lattice parameters of the GaN films and the epitaxial relationship between the layers and the sapphire substrate were determined by using a Philips triple axis diffractometer.

The asymmetric {10–12} reflections of GaN and {11–23} of the sapphire substrate were measured in order to determine the epitaxial relationships. Figure 1 (a) shows azimuthal ϕ -scans of GaN {10–12} and sapphire {11–23} planes for one representative sample. It is seen that there is a coincidence of the sapphire peaks with two of the six GaN reflections. Since the normal to the projection of the sapphire (11–23) plane includes an angle of 30° with the sapphire [1–100] direction, and the normal to the projection of the GaN (10–12) plane is parallel to the GaN [1–100] direction, the angle between the two normals is 30°. It means that the GaN [1–100] is parallel to the sapphire [0001] and the GaN [11–20] is parallel to the sapphire [1–100]. Such epitaxial relationships have been reported by Bai *et al.* for MOVPE–GaN layers on a-plane sapphire [5]. The thermal expansion coefficient along the sapphire *c*-axis is known to be larger than that one along its *a*-axis [2]. Therefore, the thermal strain in the GaN layers will be higher along the GaN [1–100] than in the perpendicular direction. This is illustrated in Fig. 1(b), where the distortion of the GaN basal plane under anisotropic strain is schematically shown. The presence of anisotropic in-plane strain would result in a distortion of the hexagonal symmetry, reflected by two different lattice parameters *a'* and *a''*. In contrast, the undistorted hexagon has two equal lattice parameters *a* (Fig. 1 (b)).

The distortion of the GaN basal plane under anisotropic strain (see Fig. 1 (b)) should be reflected in the 2 θ – ω asymmetric peak positions, since the interplanar distance *d* i.e. the values of the lattice parameters are directly related to the scattering angle 2 θ via the Bragg law $n\lambda = 2d\sin(\theta)$, where λ is the x-ray radiation wavelength and *n* is an integer.

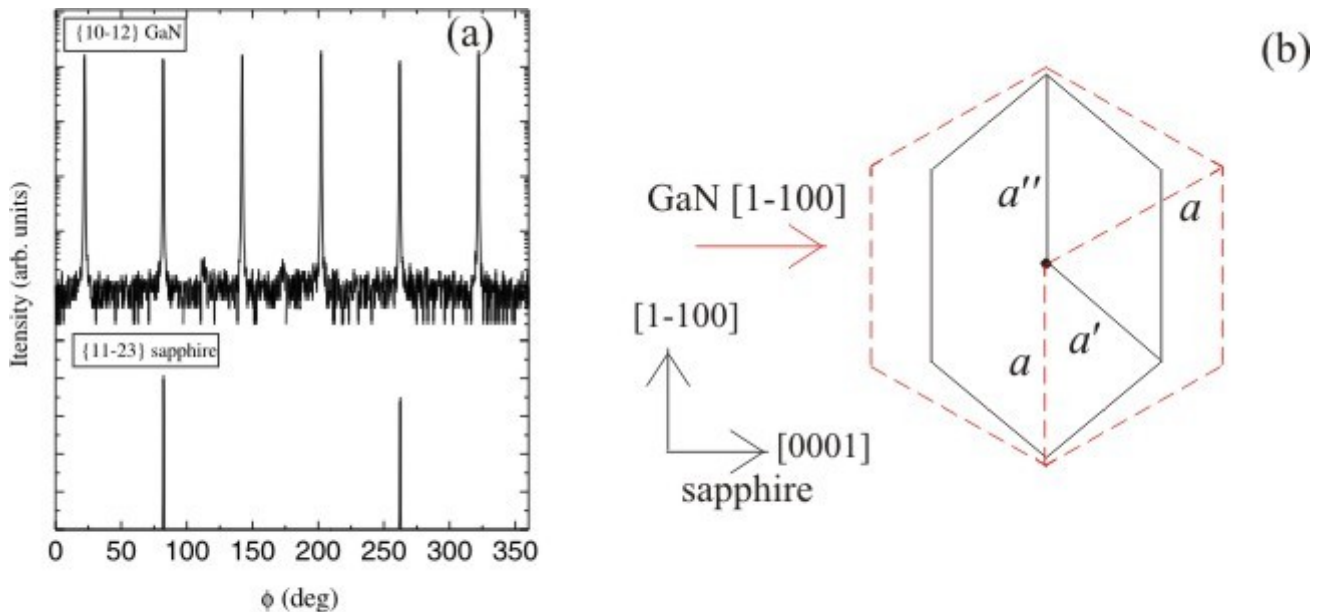


Fig.1 Azimuthal phi-scans of GaN {10-12} and sapphire {11-23} planes - (a) and a schematic drawing of the basal plane distortion under anisotropic strain - (b). The directions of higher strain in the GaN layer and the sapphire orientation are indicated. The undistorted basal plane is shown with scattered red lines.

Therefore, we measured 2θ – ω for the asymmetric peaks at each six phi positions, since in this way the interplanar distances of all six equivalent planes were obtained. The 10–15 2θ – ω diffraction peak positions of the representative MOVPE–GaN layer at each of the phi positions are shown in Fig. 2. It is clearly seen that the 2θ – ω peak appears at different positions reflecting a distortion of the hexagonal symmetry – two of the 2θ – ω positions appear at higher (squares) and four at lower (dots) scattering angles and the same trend is observed for all asymmetric peaks measured. The values of the interplanar distances derived from these peak positions can be discriminated accordingly into two groups (two smaller and four larger). Consequently, the in–plane lattice parameter also has two values: a smaller value – a' and a larger value – a'' .

The c lattice parameter of the films was determined from the 0002, 0004 and 0006 2θ – ω diffraction peaks for four different azimuthal positions. Each azimuthal position is achieved by a rotation of the sample around its normal by 90° . The asymmetric 10–14, 10–15, 20–24 and 20–25 reflections and the average value of the c lattice parameter were used for the determination of the a lattice parameter. The c and a lattice parameters of the films were calculated taking the refraction correction into account (for calculation details see Ref. 6). As a result we obtained the following values for the lattice parameters: $c = 5.18973(2) \text{ \AA}$, $a' = 3.1820(1) \text{ \AA}$ and $a'' = 3.1841(2) \text{ \AA}$. The values of the lattice parameters of the GaN film show that the films are compressively strained, as can be expected due to the difference in thermal expansion coefficients and lattice mismatch of sapphire and GaN. We note that the two in–plane lattice parameters – a' and a'' appear smaller than the unstrained one a_0 . The determination of two different values for the in–plane lattice parameter can be related to the presence of in–plain strain anisotropy (see Fig. 1(a)). The same result has been obtained for hydride vapor phase epitaxial (HVPE) GaN films grown on a–plane sapphire [6]. We note that the distortion of the hexagonal symmetry is also manifested in the polarized photoluminescence spectra of the MOVPE– and HVPE– GaN films grown on a–plane sapphire (not shown here) and as a result a splitting of the A free exciton peak has been observed [3]. The A free exciton peak position in the MOVPE–GaN films appear at higher energy in [1–100] polarization implying a higher compressive strain in this direction. This finding is in agreement with the determined epitaxial relationships. It is worth noting that for GaN films grown on c–plane sapphire (isotropically stressed) only one a –lattice parameter is determined when the above described HRXRD procedure is applied, and no splitting in the polarized PL spectra

from these films is observed [3, 7].

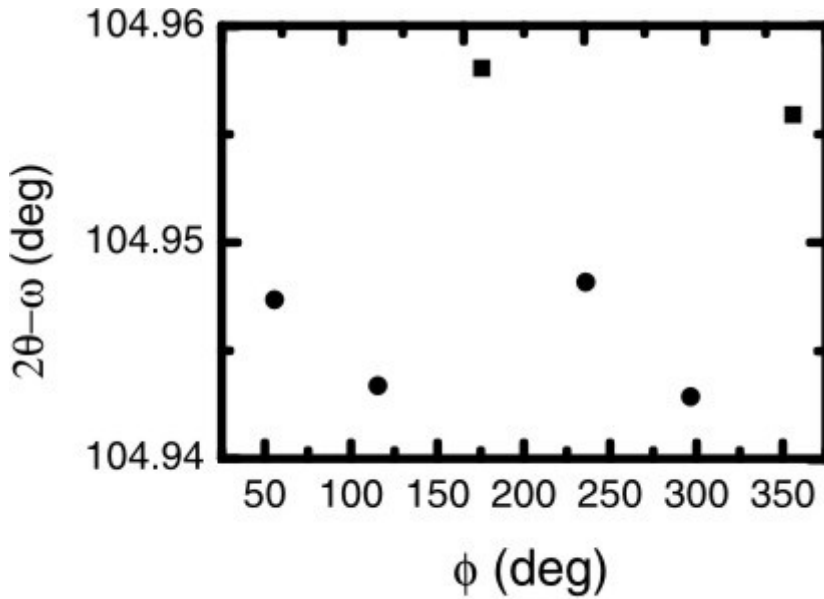


Fig. 2 2θ-ω 10-15 peak positions versus azimuthal φ positions. Dots and squares represent different groups of interplanar distances

We also estimated the in-plane strain anisotropy $\left| \frac{a' - a''}{a_0} \right|$ in the films to be $6.6(5) \times 10^{-4}$. As unstrained in-plane

lattice parameters we used $a_0 = 3.18935 \text{ \AA}$ determined for a 130 μm-thick GaN layer grown by HVPE on c-plane sapphire [7]. In principle, the strain anisotropy in GaN films on a-plane sapphire could originate from: (i) different lattice mismatches between the film and the substrate in the [1-100] and [11-20] directions; (ii) a difference in the thermal expansion coefficients of sapphire in the two directions which will result in different thermal strain, and (iii) an anisotropic distribution of defects in the film which will lead to different film elasticity in the two perpendicular directions and a different ability to release the strain.

We estimated lattice mismatches of -6.3% and -16% along the GaN [11-20] and [1-100] directions for the obtained epitaxial relationships (Fig. 1 (b)) and using the values for the sapphire lattice constants reported in Ref. 8. It is believed that the lattice mismatch induced strain is relieved during the initial stage of growth [9], however there are some reports that MOVPE-GaN films are strained at the growth temperature [10]. In order to infer which is the dominant distribution to the strain anisotropy we estimated its value in the case of thermal strain. It can be easily shown that on the assumption of total relaxation of the lattice mismatch induced strain before the cooling down starts, the strain anisotropy at room temperature, T_{RT} is determined by $\left| \frac{a' - a''}{a_0} \right| = \left| \sqrt{\frac{1}{4} \alpha_a^2 + \frac{3}{2} \alpha_c^2} - \alpha_a \right| (T_{gr} - T_{RT})$, where α_a and α_c are the sapphire thermal expansion

coefficients in the [1-100] and [0001] directions, respectively and T_{gr} is the growth temperature. We note that in the calculations it is assumed that the distortion of the hexagonal symmetry is not very large and the angles are kept close to their non-distorted values of 120°. Using the values for the thermal expansion coefficients reported by Maruska and Tietjen [2] we obtained a value of 1.10×10^{-3} for the strain anisotropy in the film, being somewhat larger than the experimentally determined value. The estimated value is in a very good agreement with the experimentally determined strain anisotropy, having in mind that there is a considerable uncertainty in the values of the thermal expansion coefficients of sapphire. Moreover, the unstrained lattice parameter of GaN is also not

well established. This agreement shows that the strain anisotropy is mainly governed by the difference in the thermal expansion coefficients of sapphire. However, a contribution to the strain anisotropy from the lattice mismatch induced strain in [1–100] and [11–20] directions and from an anisotropic defect distribution can not be excluded. In this respect it is worth mentioning that recently we have reported that the strain anisotropy has different values in HVPE– and MOVPE–GaN films [6].

In conclusion, we have reported on the HRXRD determination of two different values of the in–plane lattice parameter of MOVPE–GaN layers grown on a–plane sapphire. We suggest that the observed distortion of the hexagonal symmetry can be attributed to the presence of anisotropic in–plane strain in the films. The strain anisotropy is determined in the crystal coordinate system, and it is compared with a estimation in the case of thermal strain. It is suggested that the difference in the thermal strain in the [1–100] and [11–20] directions has a dominant contribution to the strain anisotropy, although the lattice mismatch induced strain and an anisotropic defect distribution can also affect its value.

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