DIELECTRIC FUNCTION OF AlN GROWN ON Si (111) BY MBE

Stefan Zollner *, Atul Konkar *, R.B. Gregory *, S.R. Wilson *, S.A. Nikishin **, H. Temkin **
*Motorola Semiconductor Products Sector, Embedded Systems Technology Laboratories, MD M360, 2200 West Broadway Road, Mesa, AZ 85202
**Texas Tech University, Dept. of Electrical Engineering, Box 43102, Lubbock, TX 79409

ABSTRACT

We measured the ellipsometric response from 0.7-5.4 eV of *c*-axis oriented AlN on Si (111) grown by molecular beam epitaxy. We determine the film thicknesses and find that for our AlN the refractive index is about 5-10% lower than in bulk AlN single crystals. Most likely, this discrepancy is due to a low film density (compared to bulk AlN), based on measurements using Rutherford backscattering. The films were also characterized using atomic force microscopy and x-ray diffraction to study the growth morphology. We find that AlN can be grown on Si (111) without buffer layers resulting in truely two-dimensional growth, low surface roughness, and relatively narrow x-ray peak widths.

INTRODUCTION

AlN, like all group-III nitrides, has recently received much attention because of its potential applications in high-power and high-frequency electronics, optoelectronics, electronic packaging, and deep-UV lithography. The resulting flurry of activities in this area, however, does not mean that AlN is a new material. Publications on the physical properties of AlN go back more than 35 years [1]. Much of the early results are based on pioneering work by Slack, who synthesized high-purity AlN single-crystals and studied their properties, particularly the high thermal conductivity [2,3]. Recent interest in AlN has shifted to thin films prepared on different substrates (Si, SiC, sapphire) using a variety of techniques, such as molecular beam epitaxy (MBE), chemical vapor deposition [4], and RF sputtering [5].

The optical properties of AlN, i.e., the refractive index n and extinction coefficient k, have recently been reviewed by Loughin and French [3]. Below the band gap of about 6.1 eV, the material is essentially transparent, allowing the determination of n using bulk crystals. Such measurements are usually carried out employing the minimum-deviation prism method with extremely high accuracy, not achieveable on thin films. Bulk measurements are not affected much by surfaces and interfaces, although the chemical composition is important. It is generally assumed that the crystals grown by Slack contain a very little oxygen or other impurities [3].

Therefore, the purpose of our work is not to determine the refractive index of AlN, but rather to compare the refractive index of AlN thin films grown by MBE with that of bulk crystals and to draw conclusions about the properties of the film. Our work is similar to that of Jones *et al.* [5], except that their films were prepared by RF sputtering. Our AlN films were grown using MBE on low-resistivity Si (111), cut 3° off towards (110), at 860°C with ammonia as the nitrogen source, therefore they might contain some hydrogen or silicon, which tend to reduce n. Because of the high affinity of AlN for oxygen, contamination with oxygen is a possibility [4], which would also reduce the value of n. Infrared transmission measurements of AlN on high-resistivity two-side polished Si are planned to determine the impurity content. Two films were studied here, one displaying predominantly 2-D growth (#1, nominal thickness 1500 Å), the other mixed 2-D and 3-D growth (#2, nominal thickness 2000 Å).

AlN FILM PROPERTIES BY X-RAY DIFFRACTION, RUTHERFORD BACKSCATTERING, AND ATOMIC FORCE MICROSCOPY

Since the AlN films are grown on Si (111), the crystal structure template defined by the substrate encourages growth of wurtzite AlN with the hexagonal axis along the growth direction. This is confirmed by a ϑ-2ϑ x-ray diffraction scan using a D-MAXB single-axis goniometer with a Rigaku RU-200BH rotating-anode x-ray generator, see Fig. 2 (a). Because of the substrate miscut, which cannot be compensated by our experimental arrangement, the Si (111) peak is broad and weak. The AlN (0002) peak for film #1 is found at $2\vartheta=36.05°$ corresponding to a lattice constant $c=4.98$ Å, in agreement with the literature for bulk AlN [1]. Therefore, the strain in the film due to the lattice mismatch between AlN and Si is completely relaxed by misfit dislocations. The width of the 2θ peak is 0.3-0.4°, slightly larger than the instrumental resolution of 0.2°. A rocking curve with the detector fixed at $2\vartheta=36.05°$ shows a peak at 16.2°, indicating a tilt between the c-axis of the film and the surface normal because of the substrate miscut. The magnitude of the tilt cannot easily be determined with our goniometer. The width of the AlN (0002) rocking curve peak, see Fig. 2 (b), is slightly less than 1°, giving an estimate of the mosaic spread due to dislocations. The width of the AlN (0004) rocking curve peak is 0.86° (not shown). Film #2 shows similar x-ray diffraction results.

Atomic force microscopy (AFM) analysis of the AlN films were carried out on a Dimension 3000 instrument in tapping mode. The surface roughness of the two AlN films was substantially different. Whereas the film #2 with mixed 2-D and 3-D growth mode had a surface roughness of about 142 Å, film #1 with 2-D growth mode was much smoother and had surface roughness of about 10 Å. Shown in Fig. 1 is a perspective view AFM image of the AlN film #1 evidencing the high growth quality. The film exhibits a clear terrace and step structure that is typical of films with layer-by-layer 2-D growth on tilted substrates. The angle subtended by the terraces with the average film surface is about 2°. Assuming that the terraces are the AlN (0001) planes the miscut angle for AlN would be 2° which compares favorably with the intended miscut of the Si substrate of 3°. The average step height measured by AFM is greater than 30 Å. Since the thickness of 1 ML of AlN is 2.49 Å, the AFM results show that there is significant step bunching during AlN growth resulting in steps that are greater than 10 MLs high.

Rutherford backscattering (RBS) finds that the density of the AlN film #1 is 3.0 g/cm^3, about 10% lower than the published density of 3.26 g/cm^3 [1]. For film #2, the density is 2.9 g/cm^3, i.e., somewhat lower. Most likely, the differences in density are due to hydrogen (possibly saturating dangling bonds at structural defects) or other impurities (such as oxygen) propagating along dislocations or other growth defects (particularly in film #2). There is also a very small RBS yield due to a contaminant with a mass similar to that of Ga (less than 0.1% by composition), which is not expected to have a measureable influence on the optical properties.

ELLIPSOMETRY MEASUREMENTS

Ellipsometry measurements were carried out using a Woollam variable-angle ellipsometer with compensator in the 0.74 to 5.4 eV spectral range at three angles of incidence $\phi=65°$, 70°, and 75°. We obtained the ellipsometric angles ψ and Δ, which are defined by $r_p/r_s=\tan\psi\exp(i\Delta)$, where r_p and r_s are the complex Fresnel reflection coefficients (amplitude and phase) for p- and s-polarized light. The finite bandwidth of our monochromator (about 1.5 nm) leads to a depolarization with an amplitude of no more than 6%. There is no additional depolarization due

to thickness nonuniformities, which is also evident by the uniform coloration of the films across the wafer surface. The ellipsometric angles for film #1 are shown in Fig. 3 (dashed lines).
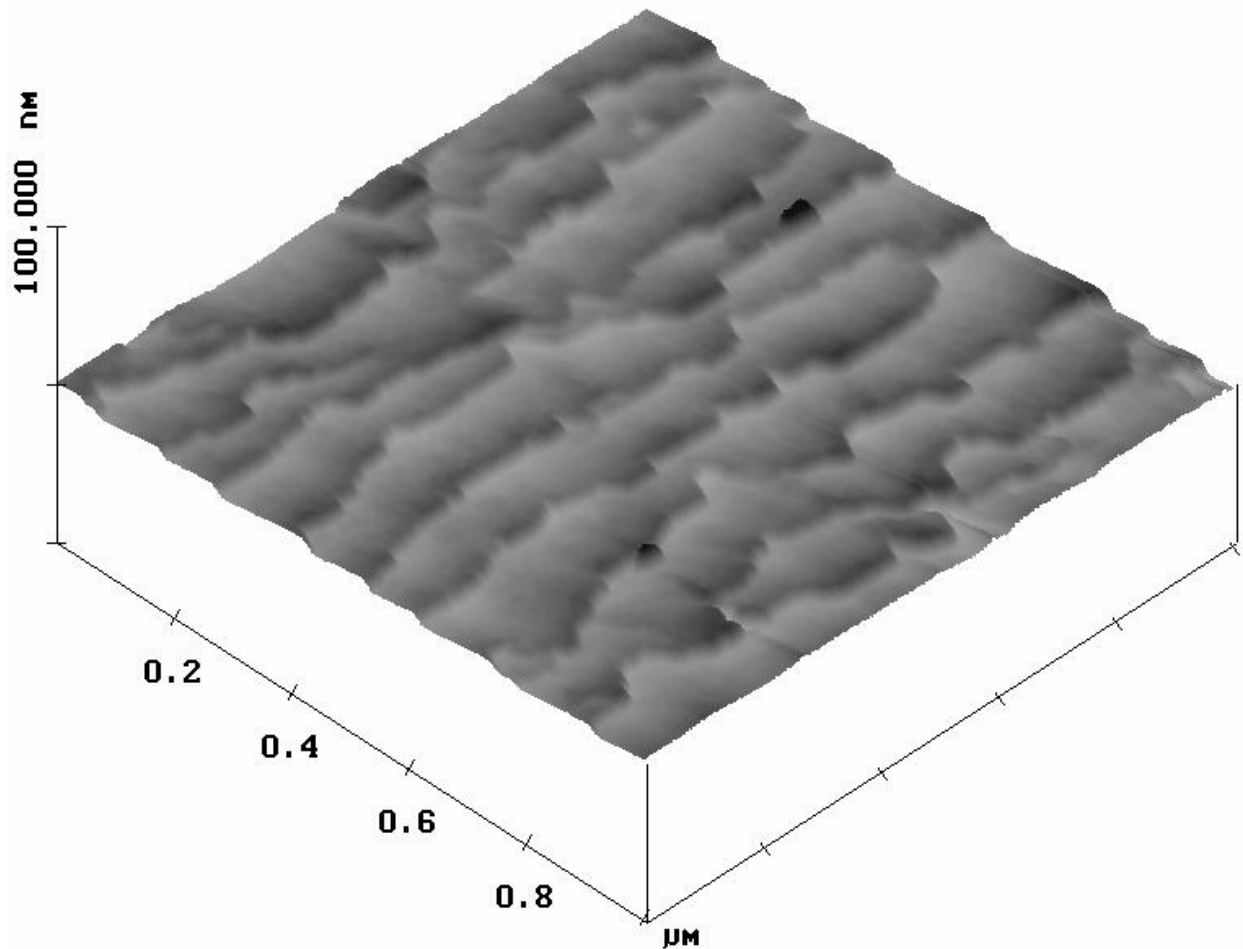

Figure 1: Perspective view atomic force microscopy image of AlN film #1 with 2-D growth by the terrace and step structure of the film.

We describe our data using a four-layer (ambient/surface/AlN film/substrate) model. An interface layer between the AlN film and the substrate does not improve the agreement between the data and the model. (In contrast to the work described in [4], no buffer was grown between the substrate and the AlN film.) We first ignore the birefringence of AlN and describe n with a Cauchy equation $n=A+B/\lambda+C/\lambda^2$, where λ is the wavelength. (Similar results are obtained with a Sellmeier equation or using a Lorentz oscillator.) The extinction coefficient k of the film is assumed to be given by an exponential Urbach tail. The absorption in the film is very small and might be located at the AlN/Si interface. The surface layer is modeled within the Bruggeman effective medium theory as a 50/50 mix of AlN and voids. (An oxide with properties similar to those of SiO_2 or Al_2O_3 gives a similar description.) Our model thus contains five parameters for the optical constants of the film plus the thicknesses of the film and the surface layer. These eight parameters are varied using the Marquardt-Levenberg algorithm to minimize the least-square deviation between the data and the model. The calculated ellipsometric angles, shown by the solid lines in Fig. 3, are in good agreement with the measured data. This agreement can be improved slightly by taking into account the small difference Δn between the ordinary and

extraordinary refractive index of wurtzite AlN, also described with a Cauchy model. The anisotropy effects are small, on the order of 2% of n, see Ref. [3].
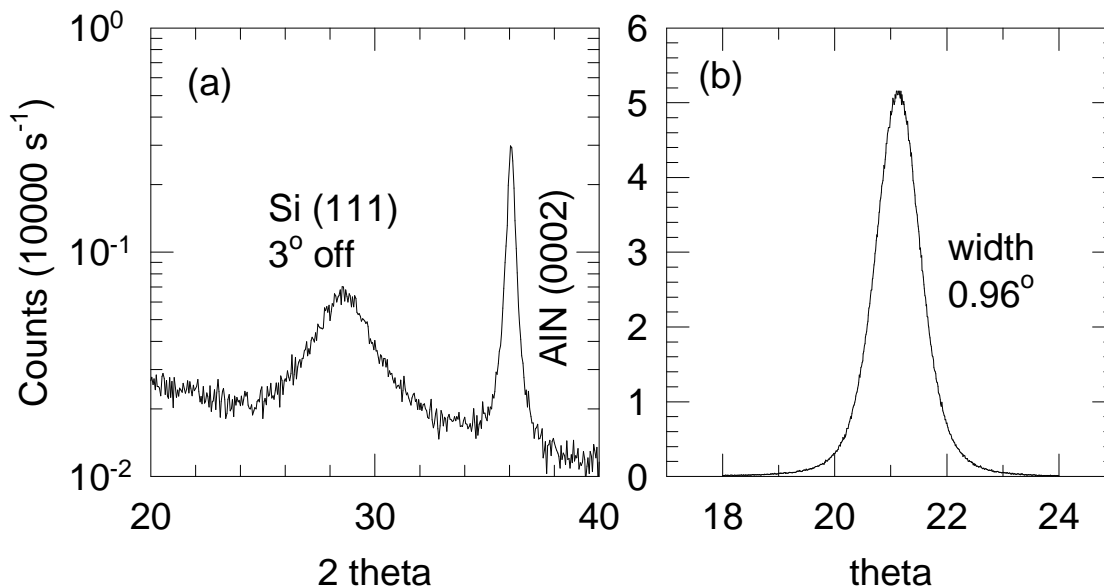

Figure 2: X-ray diffraction results of AlN on Si (111), film #1. (a) θ-2θ scan. (b) Rocking curve of the AlN (0002) peak. Data for film #2 are essentially the same.

For film #1 (see data in Fig. 3), we obtain thicknesses of the surface and AlN layers equal to 17 Å and 1500 Å, respectively, and a refractive index n=2.05 at 2 eV for AlN with a probable error on the order of 2%. AlN film #2 (data not shown) is found to have a thickness of 2026 Å, a surface layer thickness of 124 Å, and n=1.98 at 2 eV, slightly smaller than for #1, which we would expect due to the slightly smaller density found from RBS. The rms surface roughness found by AFM is 10 Å for film #1 and 142 Å for film #2, in reasonable agreement with the ellipsometry results.

DISCUSSION OF OPTICAL CONSTANTS

In Fig. 4, the ordinary refractive index determined from the Cauchy parameters and the extinction coefficient from the Urbach tail of the AlN film #1 are given by solid and the dash-double dotted lines, respectively. By fixing the thicknesses to their values determined in the model and solving the ellipsometric angles for n at each wavelength without any assumption about the dispersion model, we obtain n given by the dotted line, which is basically the same as in the Cauchy model. This confirms that the Cauchy description for n is adequate in our spectral range. The figure also shows the extraordinary refractive index found by the model (dashed line). We compare our results with the data of Ref. [3] for bulk AlN and of Refs. [6-7] for thin films, given by the symbols. The refractive index for the AlN film #2 is 3% lower (not shown).

DISCUSSION AND SUMMARY

It was shown that the refractive index of our AlN films grown on Si (111) by MBE is about 5-10% lower than that of bulk AlN single crystals [3]. Since RBS finds a density of our films that is about 10% lower than the density of bulk AlN [1], the difference in density is the most likely culprit for the low *n*. Impurities in the film (oxygen, hydrogen, or silicon) are also a possible explanation, although their presence has not been demonstrated. The different refractive index between two films is also due to density differences, as shown by RBS.

REFERENCES

1. O. Madelung, *Semiconductors - Basic Data*, 2nd ed. (Springer, Berlin, 1996), p. 69.
2. G.A. Slack, J. Phys. Chem. Solids **34**, 321 (1973).
3. S. Loughin and R.H. French, in *Handbook of Optical Properties of Solids*, edited by E.D. Palik, (Academic, Orlando, 1998), p. 373, and references therein.
4. S.Q. Hong, H.M. Liaw, K. Linthicum, R.F. Davis, P. Fejes, S. Zollner, M. Kottke, S.R. Wilson, this volume.
5. D.J. Jones, R.H. French, H. Müllejans, S. Loughin, A.D. Dorneich, P.F. Carcia, (in print).
6. O. Ambacher, M. Arzberger, D. Brunner, H. Angerer, F. Freudenberg, N. Esser, T. Weth-kamp, K. Wilmers, W. Richter, M. Stutzmann, MRS Internet Journal of Nitride Semiconductor Research **2**, Article 22 (1997).
7. N.V. Edwards, M.D. Bremser, T.W. Weeks, R.S. Kern, R.F. Davis, and D.E. Aspnes, Appl. Phys. Lett. **69**, 2065 (1996).
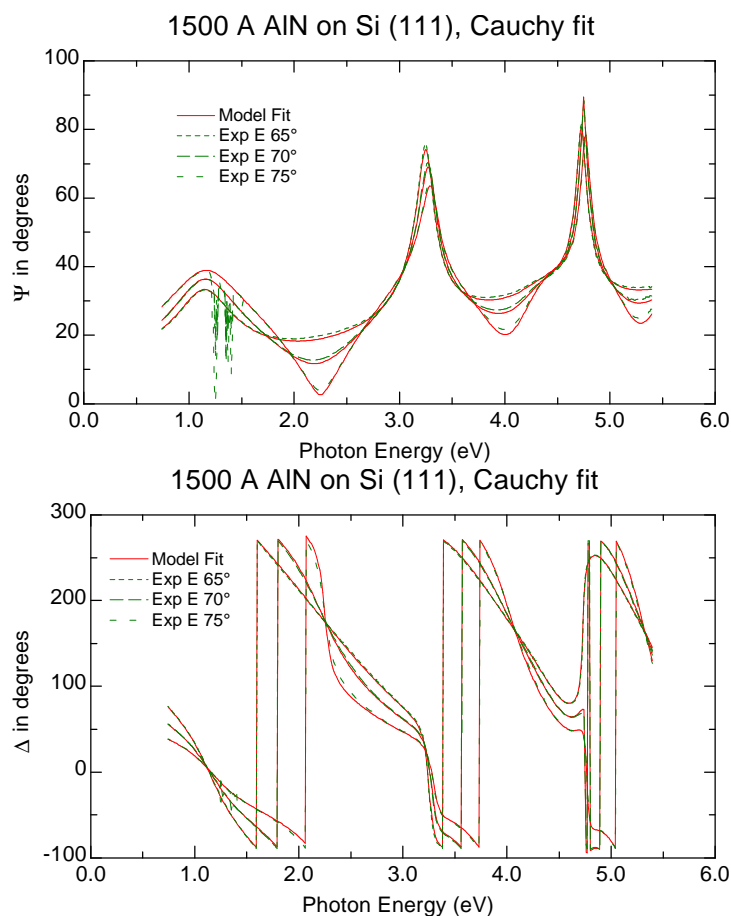
Figure 3: Ellipsometric angles for AlN on Si (111) grown by MBE (film #1). The dashed lines show the experimental data at three angles of incidence. The solid lines are the results of a calculation, based on (i) a Cauchy model with an Urbach tail for absorption to describe the AlN layer, (ii) a thin surface layer due to surface roughness or a native oxide, (iii) optical anisotropy due to the wurtzite crystal structure of GaN, (iv) finite bandwidth of the monochromator (1.5 nm).
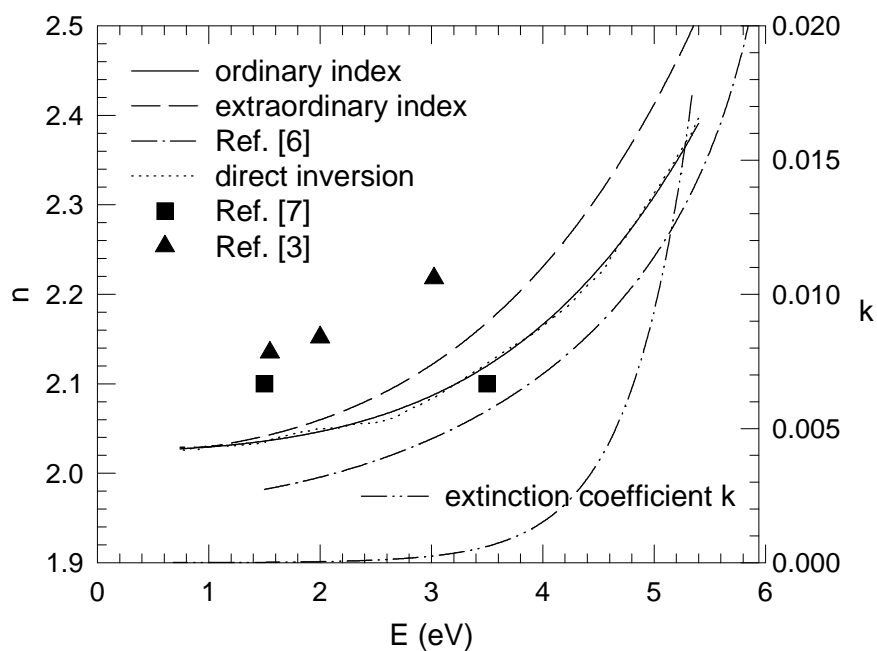
Figure 4: Ordinary (solid) and extraordinary (dashed) refractive index n and extinction coefficient k (double dot-dashed) of AlN film #1 based on the data and model calculation from Fig. 3. The dotted line shows n calculated at each wavelength from the ellipsometric angles, without assuming a specific model for the dispersion of AlN. Data from the literature are given for comparison.