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N- and Al-K-Edge EXAFS of AlN Grown on GaAs by MBE

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Abstract: Hexagonal AlN, epitaxially grown on GaAs, is studied with X-ray absorption measurements at the N- and Al-K-edges. The measured nearest neighbour (nn) distances are found shorter than expected by 0.04 Å to 0.13 Å for the 1st to 3rd nn shells, respectively, while there is no evidence of undercoordination for the N or Al atoms. The reduction in the nn distances is attributed to the presence of oxygen contamination. The characteristic angular dependence of the N-K-edge NEXAFS spectra verifies the hexagonal structure of the AlN film while the N-Al-N bond angle, determined from the angular dependence of the NEXAFS spectra, is found equal to $53.8 \pm 5.7^\circ$ indicating that the oxygen does not distort significantly the local symmetry around the N atom.

1. Introduction

AlN has some attractive physical properties, such as high hardness and thermal conductivity, which render it suitable for applications in microelectronics. The current emphasis in AlN research stems primarily from the properties of its alloys with GaN which permit bandgap engineering and the fabrication of AlGa_xN based optical devices active in the blue and UV [1]. The main problems in AlN technology are related to the reactivity of Al and more specifically to the formation of AlN_xO_y compounds. The O-related defect, which consists of an O_N and a V_{Al} created at a ratio O_N/V_{Al} = 3, is reported to cause a reduction of the lattice parameters [2].

Here we present an EXAFS study, at the N-, Al- and O-K-edges, of AlN grown on Si (001) GaAs in a molecular beam epitaxy system equipped with an rf activated plasma source. The AlN film was grown at 650°C and is 1 μm thick. The AlN surface was protected against oxidation by an in-situ deposited 7 nm thick GaN layer. The X-ray absorption data revealed that the GaN cap is not providing sufficient protection against Al oxidation and from a comparison of the N and O edge jumps it is estimated that the O concentration amounts to nearly 20% of the N concentration. The EXAFS spectra were recorded at the N- and Al-K-edges, using the SX-700-I plane grating monochromator at the electron storage ring BESSY in Berlin. Detection was in the fluorescence mode (angle of incidence 35°), using a high purity Ge detector. The data recording system permitted simultaneous recording of two energy windows at the N- and O-K-edges and thus the two edges could be electronically isolated [3]. The angle-resolved N-K-edge NEXAFS measurements were recorded for five values of the angle of incidence ϑ , $20^\circ \leq \vartheta \leq 80^\circ$, where ϑ is measured with respect to the sample surface.

2. Results and Discussion

The EXAFS analysis at the N-K-edge was done with EXCURV90 [4] assuming a hexagonal AlN model. The data were fitted by iterations for the nearest neighbour (nn) distances (R_i) and coordination numbers (N_i) over the 6 nn shells, consisting of Al and N atoms, alternatively. The Debye-Waller factors (σ^2) were determined from the correlated Debye model. The background subtraction induced error was determined by analysis with different spline functions. The results from the EXAFS analysis for the nn distances and coordination numbers for the well separated 3 nn shells are listed in Table 1. The $\chi(k)$ versus k spectrum from the N-K-edge and the corresponding Fourier transform (FT) are shown in Fig. 1. The data shown in the figure have not been subjected to Fourier filtering and the FT has been calculated in the k -range $4.3 \cdot 10 \text{ \AA}^{-1}$. Attempts to include N-O paths have not improved the fitting. The N-Al distance is found to be 1.85 Å which is smaller by 0.04 Å from the value predicted by the AlN model. This distance reduction could be attributed to the O-defect which results in a contraction of the unit cell [2]. The coordination of the N atom is tetrahedral, as expected from the hexagonal AlN model.

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The Al- EXAFS spectra were analysed with the FEFF code (FEFFIT 3.23) [5] over the k-range 4.8-9.6Å⁻¹ while the O-edge was analysed with both EXCURV and FEFFIT, which gave identical results. The measured N_i and R_i at the Al-K-edge are also listed in Table 1 while the χ(k) spectra and the FT are shown in Fig.2. At the Al-K-edge the iteration was done for the 4 nn shells (fixed Al-N and Al-O distances to the values derived from the N- and O-K-edges respectively and fixed total coordination numbers in the 1st and 2nd nn shells) while at the O edge only the Al nn was included. The effective coordination of the Al atom in the 1st nn shell is 4.1 ("subshells" consisting of O and N atoms) and that of the 2nd nn shell is 11.2 ("subshells" consisting of Al atoms bonded to N and Al' atoms bonded to O). The EXAFS results from the O-K-edge show that O has 2.5 Al atoms as nn at a distance of 1.67Å (σ_i²=0,005). The fact that O is bonded only to Al was verified by a comparison of the envelope functions for the 1st nn shells using Al₂O₃ and NO₂ models. As shown in the Table, the distances affected strongly by the presence of O are those involving bonded O while the Al-N-Al nn distance is not affected significantly.

The angular dependent NEXAFS measurements were analysed as reported previously [6]. The energy position and full width at half maximum of the NEXAFS resonances do not depend on θ and this is a characteristic property of a crystal with hexagonal (C_{6v}) symmetry. From the angular dependence of the resonance intensities the Al-N-Al bond angles were found equal to 53.8±5.7°.

Table 1 : EXAFS analysis results from the N- and Al-K-edges. The 3rd nn of the absorbing Al atom (Al') is bonded to O. The values shown in parenthesis correspond to the hexagonal AlN model.

N-K-edge					Al-K-edge				
shell #	N _i	atom	R _i	σ _i ² (Å ²)	N _i	atom	R _i	σ _i ² (Å ²)	
1	4,3 ±0.4 (4)	Al	1,85± 0,01 (1,89)	0,009	1,2±0.1	O	1,67± 0,01	0,011	
2	12,1 ±2.0 (12)	N	3,02 ±0,02 (3,09)	0,013	2,9±0.3	N	1,84± 0,01	0,015	
3	9,7 ± 2.5 (10)	Al	3,52 ±0,03 (3,65)	0,014	3,7±0.8	Al'	2,53±0,02	0,015	
					7,5±1.5	Al	2,84±0,02	0,016

Fig. 1 : FT and χ(k) - k spectrum from the N-K-edge

Fig. 2 : FT and χ(k) - k spectrum from the Al-K-edge

IV. Conclusions

The EXAFS measurements at the N- Al- and O-K-edges reveal that in the presence of O-contamination the nn distances in AlN are reduced, in accordance with previously reported XRD results, while the effect of O is stronger around the Al atom with which it is preferentially bonded. The Al-N-Al bond angle, determined from the angular dependence of the N-NEXAFS spectra, is found equal to 53.8±5.7°. This value agrees well with that determined from XRD measurements [7] and indicates that the local symmetry around the N-atom, as determined by the nn distance and the bond angle, is not significantly distorted by the presence of oxygen.

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