Polarized XAFS study of Al K-edge for m-plane AlGaN films

T.Miyanaga^{*1}, T.Azuhata¹, K.Nakajima¹, H.Nagoya¹, K.Hazu² and S.F.Chichibu² ¹Department of Advanced Physics, Hirosaki University, Hirosaki, Aomori 036-8561, Japan ² Institute of Multidisciplinary Research for Advanced Materials and Dept. Appl. Phys., Tohoku University, Aoba, Sendai 980-8577, Japan

The abstract is optional; if your report is long and an abstract is necessary, please include it here. If an abstract is not necessary, please delete this sentence.

1 Introduction

III-nitrides have attracted much attention as materials for blue and ultraviolet light emitters [1]. The most studied member of this group, wurtzite GaN, has a direct band gap of 3.5eV, while pseudo-binary alloy, $Al_xGa_{1-x}N$, provides a direct gap up to 6.0eV. It is attractive that it covers the wide range of ultraviolet rays. However, its basic physical properties are not fully understood. In this paper, polarized XAFS studies have been carried out for the Al *K*-edge of *m*-plane $Al_xGa_{1-x}N$ thin films. The films (140nm thick, *x*=0.58, 0.32) have been grown up by the NH₃ source molecular beam epitaxy method on *m*-plane GaN substrates [2].

2 Experiment

Al *K*-edge (1560eV) XAFS was measured on BL11A at Photon Factory, KEK, in fluorescence mode using SDD. To measure the polarization dependence XAFS, we set the sample in three alignments: (1) the electric field vector of X ray is parallel to the *a*-axis [11-20], (2) to the *c*-axis [0001], and (3) to the *m*-axis [1-100], respectively.

3 Results and Discussion

Figure 1 and 2 show the Fourier transforms for a-, c-, m-Al_{0.32}Ga_{0.68}N and Al_{0.58}Ga_{0.42}N film, respectively. We analyzed polarization depending XAFS data individually. The step-by-step procedure has been proposed for more precise polarization analyses [3], but in this paper we applied simple two-shell fitting for Al-Al and Al-Ga pairs. The structural parameters are listed in Table.1. For both films, the interatomic distances of Al-Al and Al-Ga for the *a*-axis-polarized spectra are about 3.17 A which is close to Ga-Ga distance in GaN. On the other hand, those for the m-axis spectra are about 3.10 A which is close to Al-Al distance in AlN. It is suggested that local structures along the *a*-axis of the films are strongly affected by GaN substrates. Next, we estimated the proportion of the second nearest neighbor Al atoms around Al atoms in the films($N_{\rm Al}/N_{\rm Al+Ga}$). Those for $Al_{0.32}Ga_{0.68}N$ and Al_{0.58}Ga_{0.42}N films are around 0.6 for each direction, suggesting that Al atoms are almost randomly distributed in the Al_{0.58}Ga_{0.42}N film and are localized in the $Al_{0.32}Ga_{0.68}N$ film within the simple model.



Fig. 1: Fourier transforms for a-, c-, m-, Al_{0.32}Ga_{0.68}N film.



Fig. 2 Fourier transforms for *a*-, *c*-, *m*-, Al_{0.58}Ga_{0.42}N film.

Table 1. Structural	parameters for A	l _x Ga _{1-x} N EXAFS
---------------------	------------------	--

	$r_{ m Al-Al}/ m \AA$	r _{Al-Ga} Å	$N_{\rm Al}/N_{\rm Al+Ga}$
$a-Al_{0.32}Ga_{0.68}N$	3.17	3.17	0.63
<i>c</i> -Al _{0.32} Ga _{0.68} N	3.11	3.18	0.67
$m-Al_{0.32}Ga_{0.68}N$	3.09	3.10	0.67
a-Al _{0.58} Ga _{0.42} N	3.17	3.18	0.58
$c-Al_{0.58}Ga_{0.42}N$	3.10	3.11	0.67
m-Al _{0.58} Ga _{0.42} N	3.11	3.12	0.59

References

[1] F,H.Morkoc and S.N.Mohammad, Science **267**, 51(1995).

[2] K.Hazu et al., J. Appl. Phys. 107, 033701 (2010).

[3] T.Miyanaga et al. unpublished.

* takaf@cc.hirosaki-u.ac.jp