Materials Science

11A/2004G306

Characterization of nanotextured AlN thin films by x-ray absorption near-edge structures

Isao TANAKA[1*], Takeo SUGA[2], Satoru YOSHIOKA[1], and Teruyasu MIZOGUCHI[3]
[1] Dept. of Mat. Sci. & Eng., Kyoto University, Yoshida, Sakyo, Kyoto 606-8501, Japan.
[2] FIFC, Kyoto University, 34-4 Nishihirakicho, Takano, Sakyo, Kyoto 606-8501, Japan.
[3] Institute of Eng. Inn., The University of Tokyo, 2-11-16 Yayoi, Bunkyo, Tokyo 113-8656, Japan.

Introduction

III-V nitrides based light emitting devices have been massively used in modern technology. Pulsed-laser deposition (PLD) is an emerging technique, which has some advantages compared to other techniques. Basically PLD can avoid impurity to incorporate into the film. Microstructure and stoichiometry of the film can be controlled by deposition parameters such as substrate temperature, deposition rate, atmosphere, laser power, etc. In the present study, we report a technique to quantitatively characterize nanotexture of the film using x-ray absorption near-edge structure (XANES) technique. The method is extremely useful when the crystallite size is too small or too much faulted/strained to be analyzed by conventional XRD technique.

Methodology

The thin films were made by PLD using a KrF* excimer laser($\lambda = 248$ nm, Lambda Physik COMPex205) with pulse rate of 5 Hz and laser power of 600 mJ (9 J/cm^2). Sintered AlN compact was used as a target. Sample was deposited on substrate of *c*-cut sapphire without N_2 gas backfill.

XANES were obtained at KEK-PF BL-11A by total electron yield method with 1200 line/mm grating monochromators. All measurements of XANES spectra were carried out in vacuum at room temperature.

In order to interpret experimental spectra, first-principles orthogonalized linear combination of atomic orbitals (OLCAO) method was employed [1]. This is a band structure calculation based on the density functional theory within local density approximation. In the calculation, the initial state and final state were calculated separately. A core hole was included in an Al 1*s* orbital. Matrix elements of electric dipole transition between the initial state and final states were rigorously computed using wave functions of the two states. In order to minimize artificial interactions among core holes under periodic boundary condition, a large supercell composed of 108 atoms has been adopted.

Results and Discussion

Crystalline quality and texture of the deposited film was investigated by XRD. The AlN film is epitaxially grown on the substrate with the relationship of AlN(1 0$\bar{1}$ 0) / / Al_2O_3(1 1 $\bar{2}$ 0).

The left panel of Fig. 1 shows experimental XANES of sample in comparison to that of w-AlN powder. Sample was mounted in two different geometries with its surface 90° and 50° to the incident x-ray beam. When measured with the 50°-geometry, XANES of sample is identical to that of w-AlN powder. The angle is close to $\cos^{-1}(1/\sqrt{3})$=54.7°, which should provide averaged XANES of all crystallographic directions [2]. When measured with the 90° geometry, however, peaks B_2, C, and D_2, as denoted in Fig. 1(b), remarkably lost their intensity. Given the fact that the sample exhibits a high degree of texturing along the *c* axis normal to the substrate, peaks B_2, C, and D_2 should be ascribed to the XANES components that appears only when measured with ***E*** / /***c*** condition where ***E*** is the electric field vector and ***c*** is the *c* axis of the hexagonal crystal. The right panel of Fig. 1 shows theoretical XANES with ***E*** // ***c***, ***E***⊥***c*** and average conditions. The averaged theoretical XANES satisfactory reproduces the spectrum from the w-AlN powder. Increase in intensity of peaks B_2, C, and D_2 is evident in the ***E*** // ***c*** condition, which is also in good agreement with the experimental spectra. We can therefore conclude that the absence of peaks B_2, C, and D_2 can be a good fingerprint to the preferred orientation of c perpendicular to the film surface.

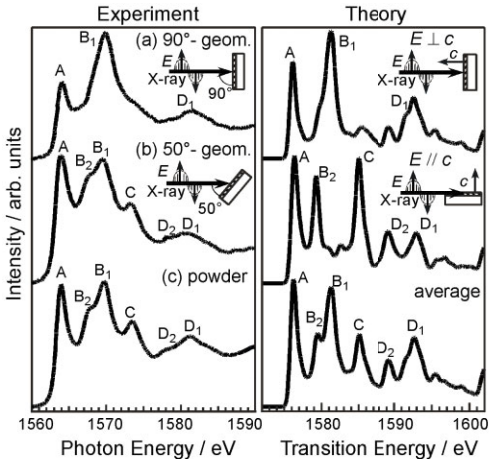

Fig. 1 Experimental XANES (left) and theoretical XANES calculated by first-principles OLCAO method (right).

References

[1] S. D. Mo and W. Y. Ching, Phys. Rev. B 62, 7901 (2000).
[2] E. Tegeler, Phys. Status Solidi B 84, 561 (1977).
* isao.tanaka@materials.mbox.media.kyoto-u.ac.jp