

Identification of the Vacancy Site in GaN:Gd

Shuichi Emura^{1,*}, Akihiro Koike², and Takashi Fujikawa²

¹ISIR, Osaka University, Mihoga-oka 8-1, Ibaraki, Osaka 567-0047

² Graduate School of Advanced Integration Science, Chiba University, Yayoi-cho 1-33, Inage, Chiba, 263-8522,

Utilizing X-ray absorption near edge structure (XANES), the three-dimensional structure of the vacancy environment is determined in the Gd-doped GaN crystal. We observed two different XANES spectra corresponding to the different crystal growth conditions. The crystals prepared under the nitrogen rich condition involve the nitrogen vacancies, which adjoin the dopant ion Gd. The analysis of the XANES spectra is carried out by multi-scattering theory.

1 Introduction

The identification of vacancy site is the biggest highlight problem in the crystal analysis research filed nowadays. Fine structures appearing at the higher energy than the absorption edge in X-ray absorption spectra are well understood and widely applied to examine the structure around the specific element in solid and liquid phase [1-3]. The local structure analysis using the fine structures establishes the position in a complementary viewpoint with diffractometry. Meanwhile, we still more catch fine structures in the X-ray absorption spectra around the absorption very-near-edge, we call whole structures “X-ray absorption edge region structure (XAERS)” including the pre-peaks, the pre-edge structures and near edge structure just after the absorption edge (X-ray absorption near edge structure = XANES), which is not yet understood so much, and the efforts to elucidate physical phenomena observed are still nominal. We tried to utilize XAERS (especially pre-peaks) for the local structure analysis around Cr ions in GaN. We found the Jahn – Teller distortion of the CrN₄ cage in GaN, supported by X-ray absorption fine structure (XAFS) analysis [4].

Light elements, especially hydrogen, are very hard to decide their exact sites in structure analysis because of very weak scattering strength. Besides the identification of vacancy coordinates and the decision of their coordination environment look like impossibility. We have no suitable and direct methods for those. At present, a positron annihilation method can detect empty lattice points, but cannot give the information of its coordinates and the coordination environment of those. XAERS spectra involve richer information than XAFS one. In particular, as the fine structure just after the absorption edge reflects a multiple scattering process, it is of high potentiality to obtain the precise position of the vacancy, which neighbours on the specific element. Moreover, it is strongly expected that even slight deviation in the three-dimensional structure draw a change to XANES spectra. Vacancies at the neighbourhood especially alter the XANES shape largely.

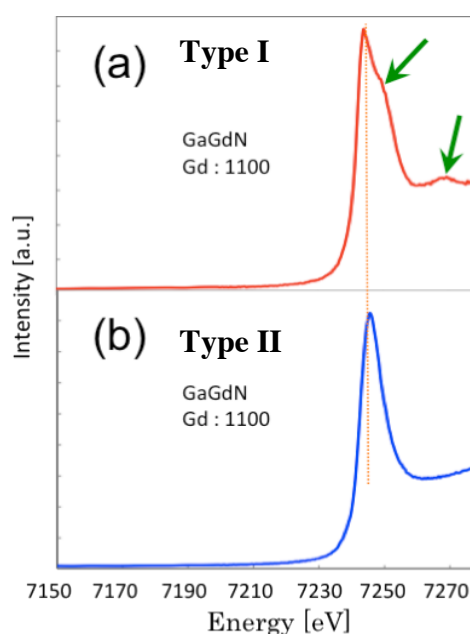
In this report, we demonstrate for local three-dimensional structure analysis the availability of XAERS at the Gd *L*_{III}-edge in the Gd-doped GaN thin layer crystals.

2 Experiment

X-ray absorption spectroscopic (XAS) measurements of XAERS and XAFS were performed at a beamline BL9A at room temperature. A fluorescence mode is employed to obtain the XAERS spectra of Gd *L*_{III}-edge because the number of the Gd ion is $\sim 10^{14}$ in the area exposed by X-rays. A high purity (99.95%) aluminum pipe was set just before the crystal to block detector reception of elastic and inelastic scattering by air in the X-ray path to the crystal. The crystal was mounted on a stand prepared in particular with about 7 degrees to the incident X-ray beam to expose widely the specimen with X-rays. The typical specimen size is 5 mm in width and 10 mm in length.

3 Results and Discussion

Figures given below show the XAERS spectra of the different types. The upper part is taken in the crystal prepared under the stoichiometric III/V ratio condition (Type I), and the lower part is taken the crystal prepared under nitrogen-rich III/V ratio condition (Type II).



The XRD profiles observed in two types (not shown) apparently correspond to each type. The sharp peak at 7248eV is characteristic in rare earths, so-called, white peak. Type I spectrum shows a shoulder and a small hump, which are indicated by arrows, while Type II spectrum has no additional peaks.

We analysed the both observed spectra by modeling, using multi-scattering code developed by Fujikawa [5,6]. The simulation well explains both different spectra. Type I spectrum is reproduced by a model without any nitrogen vacancies, and Type II spectrum is simulated by a model with one nitrogen vacancy. The further detailed analysis gives the site of the nitrogen vacancy, which locate on the apex site of the triangle in wurtzite structure but at one of equivalent three legs.

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