

Extended Abstract of PSA-19

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# Chemical-state-discriminated hard X-ray photoelectron diffraction study for polar InN

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Near-surface structures of polar InN films were investigated by laboratory-based hard x-ray photoelectron diffraction (HXPd) with chemical-state-discrimination. HXPd patterns from In 3d<sub>5/2</sub> and N 1s core levels of the In-polar and N-polar InN films were different from each other and compared with the simulation results using a multiple-scattering cluster model. It was found that the near-surface structure of the In-polar InN film was close to the ideal wurtzite structure. On the other hand, on the N-polar InN film, defects-rich surface was formed. In addition, the existence of the In-polar domains was observed in the HXPd patterns.

## 1. Introduction

With the small band gap ( $\sim 0.7$  eV) and superior electrical transport properties, InN is attracting great attention for potential region optoelectronic devices such as emitters spanning a wider wavelength range and high-efficiency photovoltaic devices.[1] For InN single crystal, as a wurtzite crystal lacks inversion symmetry along the c-axis direction, In-polar and N-polar InN exhibit different properties. For example, the maximum growth temperature for N-polar InN is about 100 °C higher than In-polar InN. The N-polar InN shows better bulk crystalline quality. However, an atomically flat surface can be observed for the In-polar InN but not for the N-polar one yet.[2]

The critical issue of InN is that PN junction has not been realized yet. Therefore, in order to fully realize the potential of InN, a fundamental understanding of structures near surface are required. For the near surface structures, photoelectron diffraction (PED) is powerful tool to investigate the structures. In addition, PED is the element and chemical state specificity so as to elucidate a local atomic structure. [3] Hard x-ray photoelectron diffraction (HXPd) is expected to open up additional analytical possibilities for materials because of the larger probing depth. In this study, we

employed high energy angle resolved spectroscopy for laboratory (HEARP Lab,  $h\nu=5414.7$  eV). [4] HEARP provides hard x-ray photoelectron spectroscopy (HAXES) and HXPd, which enables us to elucidate local atomic structures. In the present study, we have investigated near surface structures of polar InN using HEARP lab.

## 2. Experimental

Two kinds of InN films were prepared by radio-frequency plasma-assisted MBE. For In-polar, in situ In droplet elimination by radical beam irradiation was employed. An N-polar InN film with a thickness of about 750 nm was grown directly on a nitrided sapphire. The two samples were cleaned using acetone, methanol, 35% hydrochloric acid, and deionized water before measurement.

The HXPd system consists of a monochromatic Cr K $\alpha$  source (5414.7 eV), a high energy version of the VG SCIENTA R4000 10 kV analyzer with wide acceptance objective lens. The angle acceptance of the combined objective lens and the analyzer is  $\pm 35^\circ$  with an angular resolution of  $0.5^\circ$ . The total energy resolution was 1 eV. In this study, the polar angle  $\theta$  is defined to be zero for the photoemission direction normal to a sample surface.

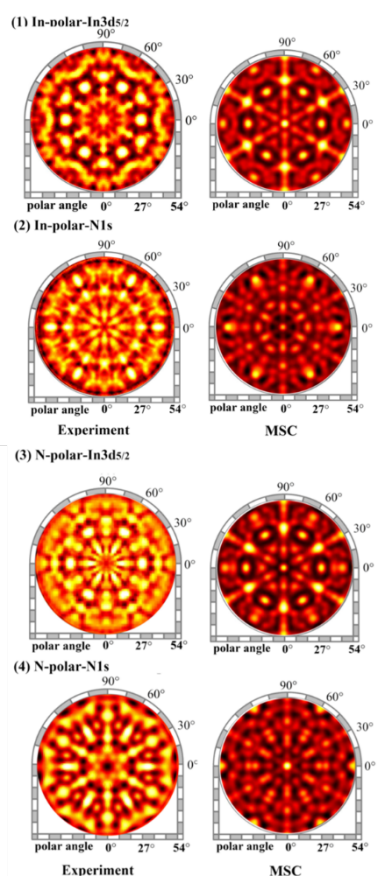


Fig.1 Experimental (left) and multiple scattering cluster (MSC) calculations (right) HXPDP patterns

The  $\theta$ -dependent sensitivity of the analyzer, was calibrated using an amorphous GeSbTe sample.

### 3. Results and discussion

Figure 1 shows HXPDP patterns of In-polar and N-polar InN. For structural analysis, we found that the diffraction patterns were dominated by forward scattering of nearest-neighbor In atoms. This is because the strong forward focusing was dominant in this energy range.

In the case of In-polar InN, In 3d<sub>5/2</sub> pattern to (10-10) M-plane ((11-20) A-plane) exhibited the strong spots of 30° (17°), 40° (30°), and 50° (40°) while N 1s patterns in M plane (A plane) for In-polar InN exhibited the strong spots of 20°, 30° (30°), and 45° (45°). These patterns were good agreements with the diffraction patterns of the ideal wurtzite structure.

In the case of N-polar InN, two components for both In 3d<sub>5/2</sub> and N 1s existed. the chemical-state-discriminated N-polar In 3d<sub>5/2</sub> and N1s HXPDP patterns indicated that main component of the core levels

exhibited clear diffraction patterns. On the other hand, the patterns of the satellite component were unclear. Angle resolved core levels analysis indicated that main component was come from bulk while the satellite component was surface origin. Thus, the surface exhibited defect rich and/or amorphous structure. Comparison of the main components diffraction patterns with the simulation results based on a multiple-scattering cluster model exhibited an additional structure. We found that N-polar InN may be mixed with In-polar InN domain in a near-surface area of the N-polar InN film. Thus, in the N-polar InN film, the existence of In-polar domains in the near surface region was observed, and the defect atoms of N-polar InN film were located on the surface.

### 4. References

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