

# X-ray Photoelectron Spectroscopy of Aluminum Gallium Nitride

Nathan Bishop  
Ohio University

Mentor: Leonard Brillson  
The Ohio State University

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**Abstract:** Aluminum Gallium Nitride is an exciting new semiconductor that is not yet fully understood. Detailed electrical analysis can be undertaken using cathodoluminescence spectroscopy, and the results correlated to the relative abundance of the aluminum, gallium, and nitrogen, as well as oxygen impurities.

## I. Introduction

Semiconductors are used everywhere in electrical engineering. Most are silicon, with some other very specialized components used for special purposes. Aluminum Gallium Nitride (AlGaN) aims to fill one of those niches, those requiring high power output while also maintaining high efficiency. For this reason, much work has been done on the compound.

However, it has proved very difficult to manufacture acceptable devices using this material. While metal contacts have been successfully constructed, consistency has not been achieved.

A variety of aluminum to gallium ratios and gallium to

nitrogen ratios have been tried. The sample that I have analyzed contains such variations across its surface. My purpose is to discover the correlation of these ratios to the observed cathodoluminescence (CL) spectra, and to integrate the resulting data into the previously acquired data set. For this purpose X-ray photoelectron spectroscopy (XPS or ESCA) was used to identify the relative concentrations of all elements present.

## II. Background

Materials may be described as belonging to one of three classes: insulators, such as ceramics; conductors, such as most metals, and semiconductors, which can have both conducting and

insulating properties depending on applied voltages and other circumstances. Semiconductors are valued because of their ability to be either a conductor or an insulator.

The origin of the differences between conductors and insulators has to do with the state of the outermost occupied electron shell in the material. This shell is known as the valence band, and the shell in which electrons are free to move is called the conduction band. The distance between the valence and conduction bands is known as the “band gap.”

Another important concept is the Fermi level of the material. This is defined as the highest occupied level in the valence band at 0K. The position of the Fermi level determines the properties of the material.

In metals, the Fermi level lies inside the valence band, leaving room for electrons to move about freely and still obey the Pauli exclusion principle. Thus, the valence band and the conduction band are the same in metals. This is illustrated in the top part of Figure 1.

In insulators, the Fermi level is above the valence band and the conduction band is separated from it by a large gap. It takes a comparatively large amount of

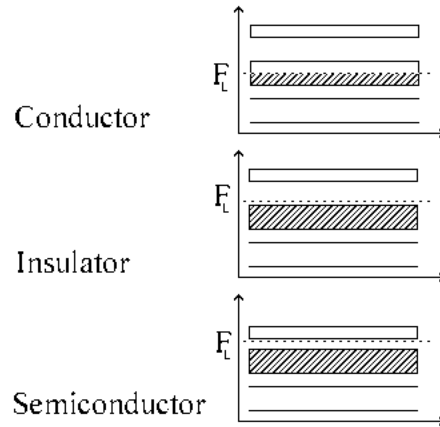


Figure 1

energy to transport an electron to the conduction band, and so very few electrons are free to carry current. This is illustrated in the middle part of Figure 1.

In semiconductors, the Fermi level lies above the valence band, but close to the conduction band. This means that according to Fermi-Dirac statistics, there is a small but meaningful chance of an electron escaping into the conduction band and being free to carry current. However, any small negative bias can decrease this probability to as low a level as desired. This is how a semiconductor may have the properties of a conductor or insulator. See the bottom part of Figure 1.

Semiconductors themselves come in two types: n-type, which has an excess of electrons, and p-type, which has an excess of “holes” or absence of electrons. N-type semiconductors conduct current well, almost as well as metals. P-type semiconductors do

not conduct. Whether a semiconductor is n-type or p-type depends on the process used to manufacture it. Impurities, or dopants, are used to control this. In fact, the same semiconductor crystal may have both n-type and p-type regions in it. GaN is p-type, and AlGaN is n-type. This fact is used to our advantage when manufacturing transistors.

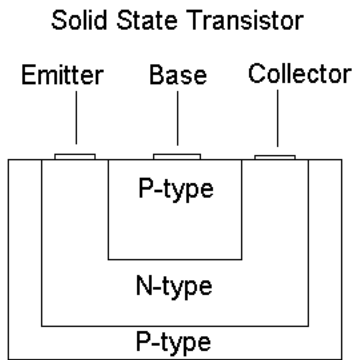


Figure 2

When a semiconductor is arranged as shown in Figure 2, it becomes a metal oxide semiconductor field effect transistor (MOSFET). Current flows through a limited area of n-type semiconductor, and avoids the PN junction. The zone of n-type where current does not flow is known as the area of avoidance. When a negative voltage is applied to the base, the electrons are driven away, into the p-type transistor, and the current decreases. With a large enough negative voltage, no current will flow at all. With a positive voltage applied the area of

avoidance decreases, and current increases, up to a point.

### III. Experimental Aspects

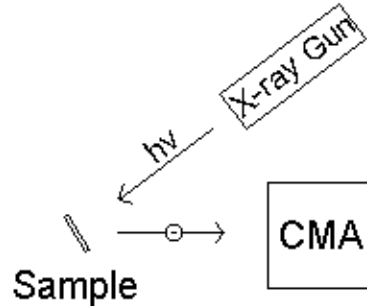


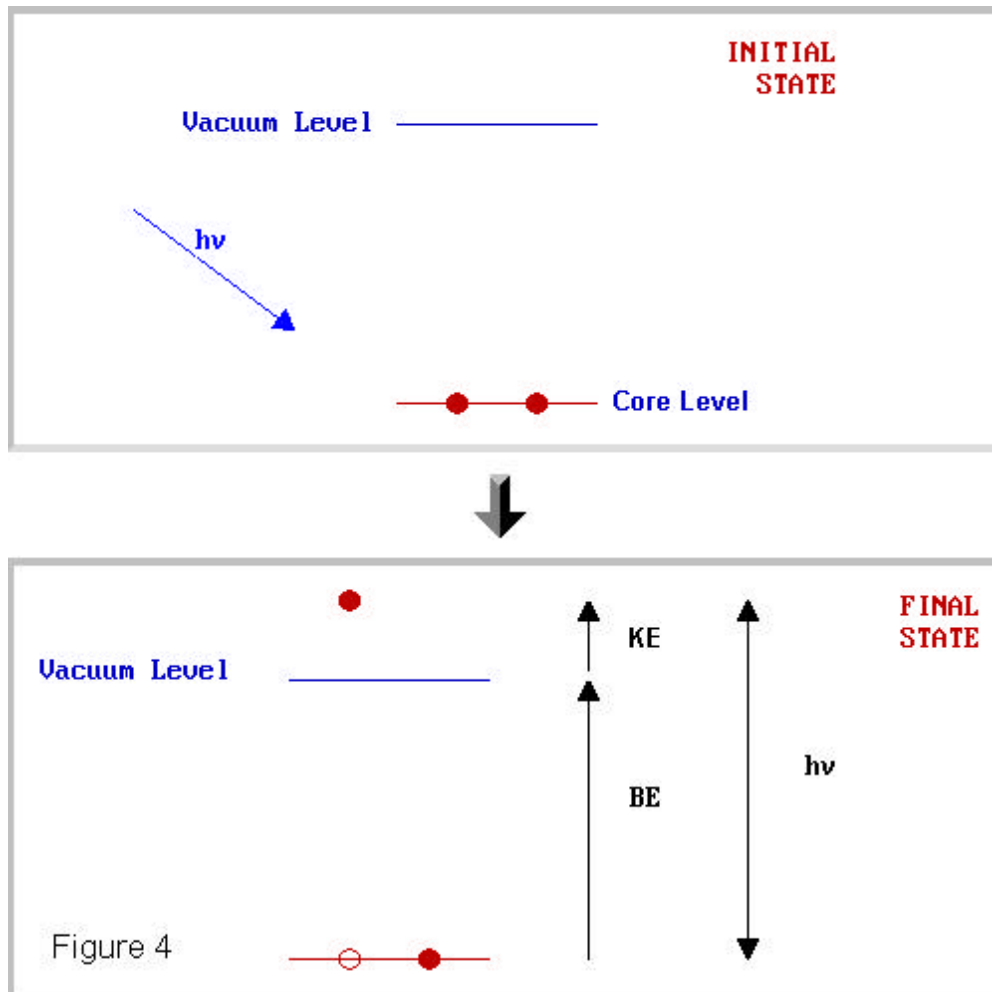
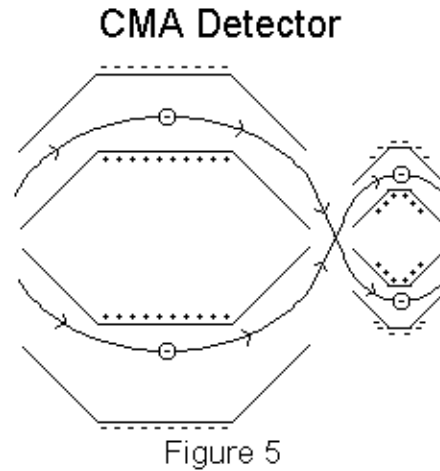
Figure 3

X-ray photoelectron spectroscopy works by accelerating electrons through a certain voltage, typically 10 kV, into a metal anode. In this experiment, the anode is magnesium. The electrons, in turn, decelerate and emit x-rays in the characteristic Brehmstrahlung spectrum. A thin sheet of aluminum foil screens out all but the x-rays. The X-rays are then incident on the sample, mounted in ultra-high vacuum.

Via the photoelectric effect, electrons are ejected from the sample with a definite energy. See Figure 4. These electrons are incident on the detector, in this case a CMA, or cylindrical mass analyzer. The CMA can be tuned to only allow electrons of a certain energy to pass through, where they are counted. In this case, a double pass CMA was used. This is basically two CMAs in series,

separated by an aperture which can be adjusted to control the selectivity of the detector. See Figure 5.

From these results, a histogram can be constructed. Each core level of every element present leaves a distinct peak in the resulting curve. From quantum mechanics, a cross section for each core level can be calculated, and the raw data adjusted by the sensitivity of each orbital. From this adjusted data, the relative proportions of each element may be determined.

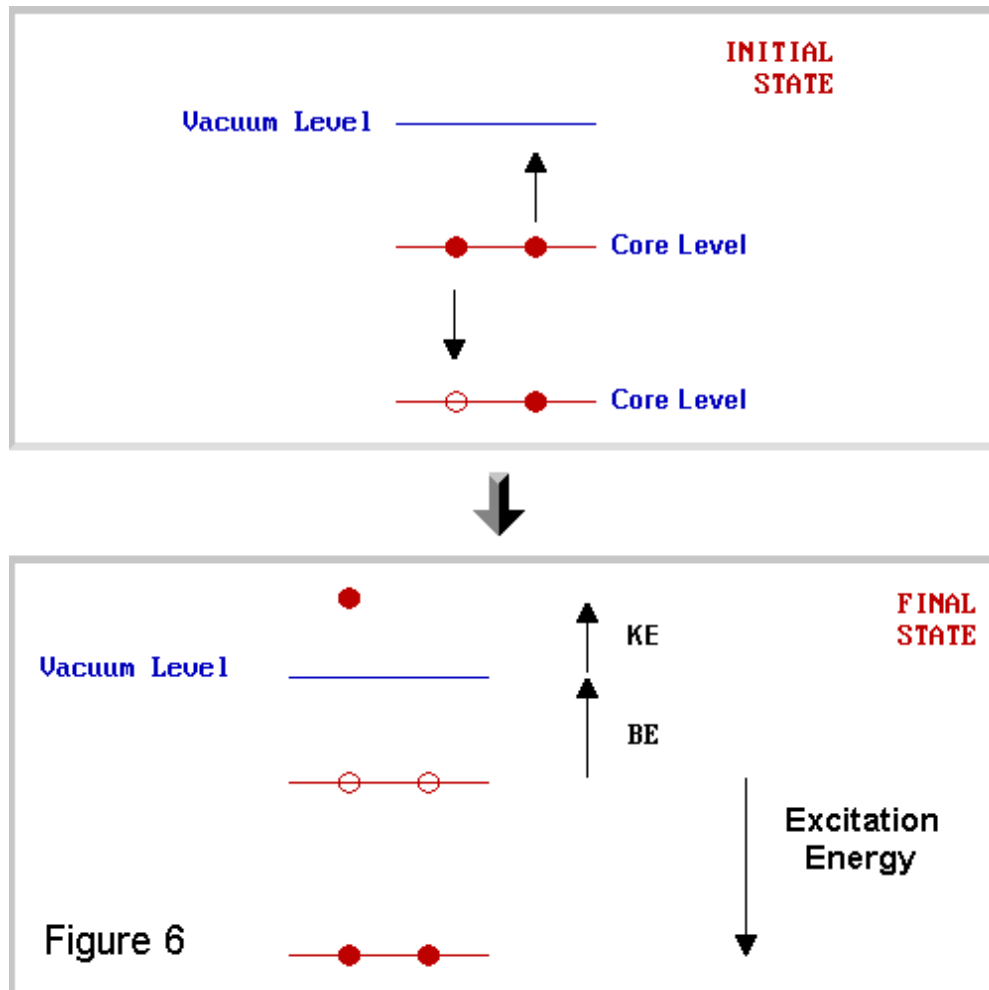


Also present in the resulting histogram are extraneous peaks resulting from the ejection of Auger electrons from the excited atoms. After the photoelectric effect ejects a core level electron, the resulting ion is in an excited state. An outer level electron will then jump inward to fill the vacancy, leaving it with an excess of energy. Sometimes this excess energy is carried off by a photon and other times by an additional electron. This process is illustrated in Figure 6.

Other data taken for this project was done with

cathodoluminescence. For this method, electrons at a specific energy, typically 2 keV, are incident on the sample in vacuum, which then emits visible light photons. These photons are then passed through a monochromator, and counted with a photomultiplier tube. When a histogram is constructed, obvious peaks are observed. These peaks correlate with the structure of the valence and conduction bands in the sample.

Of particular interest are so called “isolated states”, or electron states inside the band gap between



the conduction and valence bands. The presence or absence of these states and their relative intensity is indicative of the presence of dopants in the sample. In the case of AlGaN, aluminum is the dopant and adds peaks in the vicinity of 2.18 and 2.35 eV.

All of this takes place in ultra-high vacuum, or UHV. UHV is characterized by pressures below  $1 \times 10^{-9}$  torr (mm Hg). This allows ultra-clean surfaces to be studied for several days in vacuo before significant contamination results. At pressures such as this, only one particle per second strikes each square millimeter of the

surface, on average. In addition, the mean free path of a free particle in such a vacuum is  $>10^5$  meters, if collisions with the chamber walls are ignored. The usual operating pressure for the chamber on which these experiments were carried out is  $1-2 \times 10^{-10}$  torr.

All data was taken using equipment from Physical Electronics Co (PHI). Data acquisition software used was AugerScan V2.0, in XPS mode. All data analysis was performed in Oriol Origin graphing software.

The chamber is depicted below.

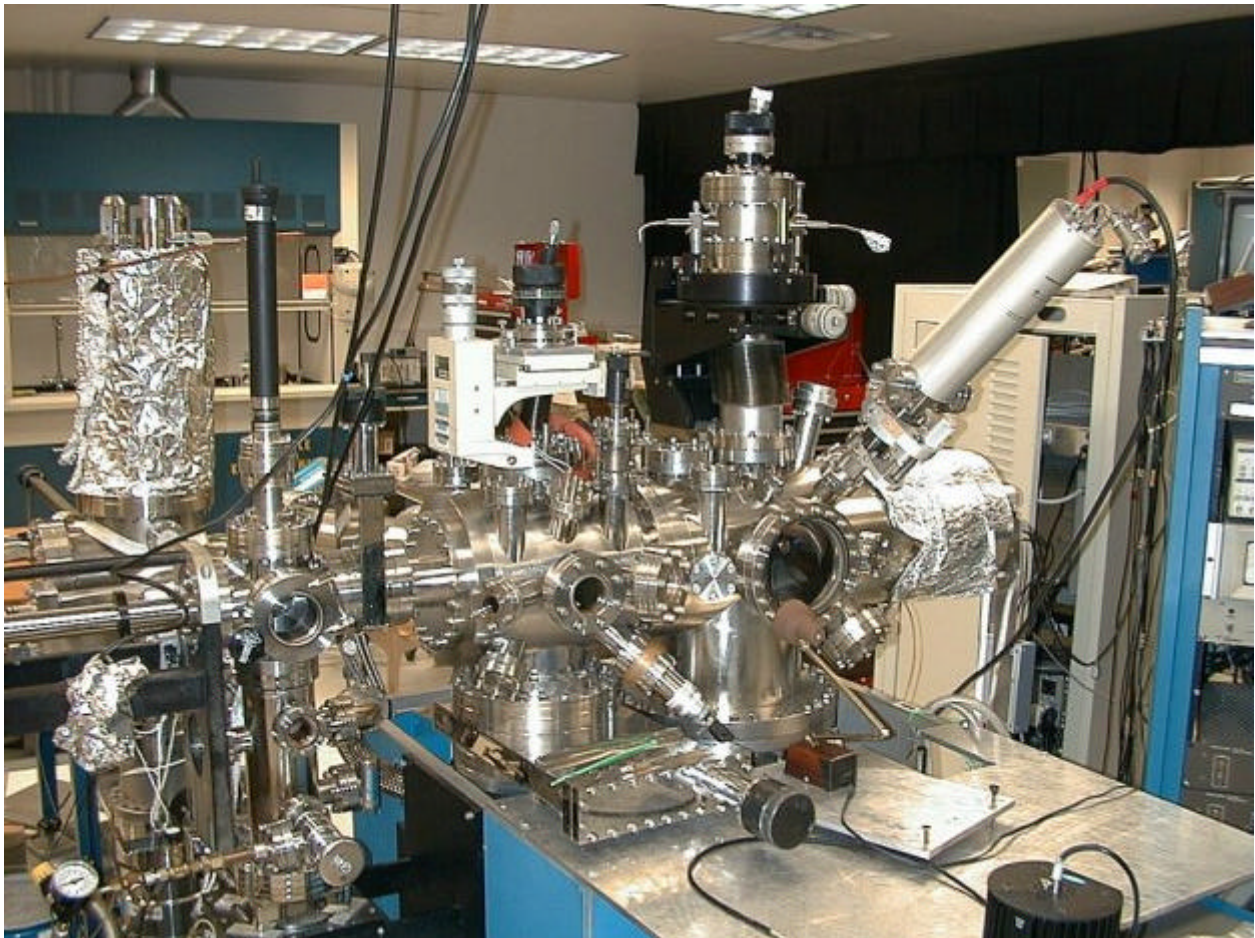
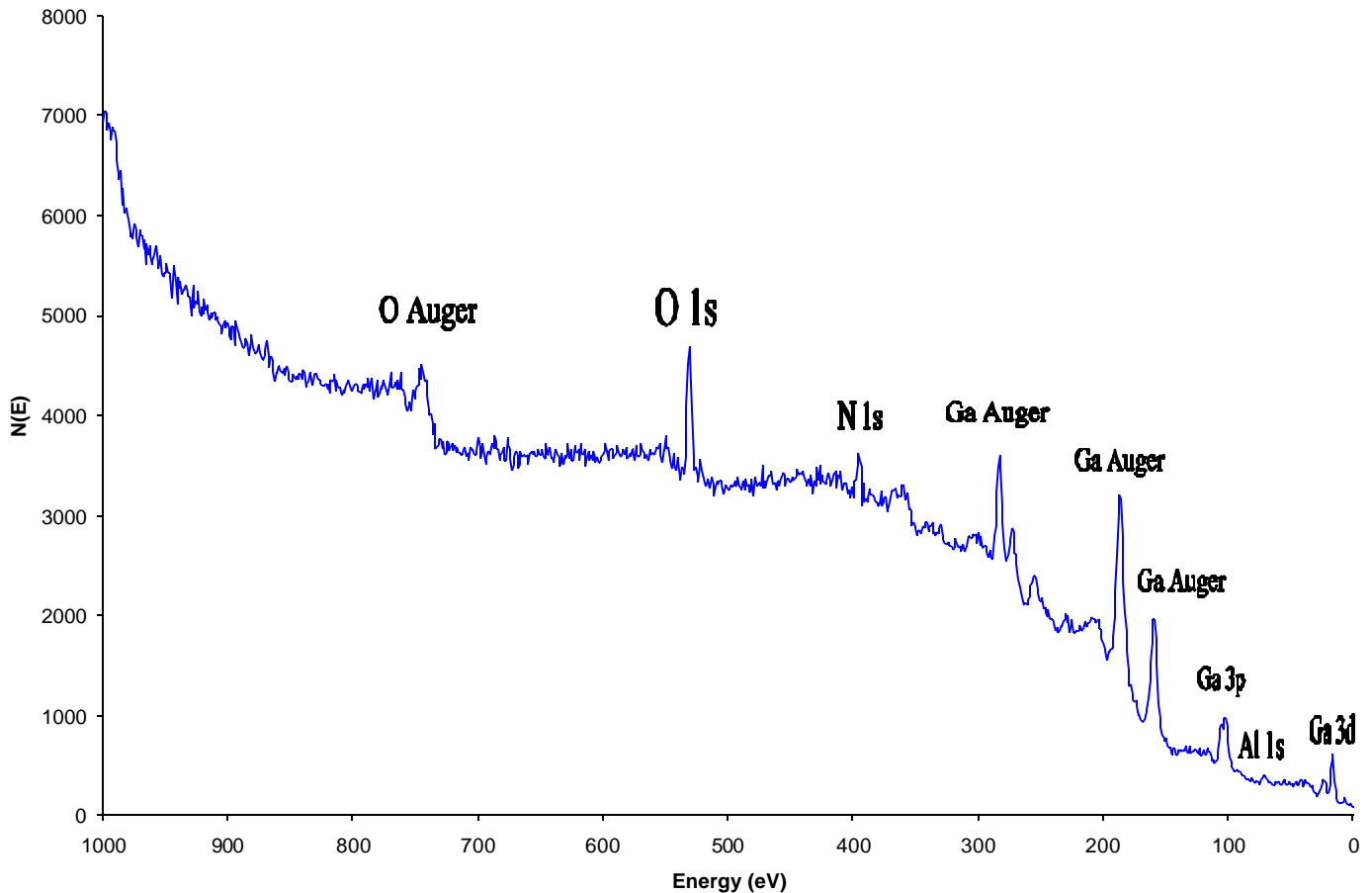


Figure 7



The sample observed is  $\text{Al}_{0.3}\text{Ga}_{0.7}\text{N}$  grown by molecular beam epitaxy and sputter cleaned using an argon active-ion sputter gun.

#### IV. Results

The data taken from the XPS system seems to fit well with the cathodoluminescence data. A sample scan from the data is included above, see Figure 7.

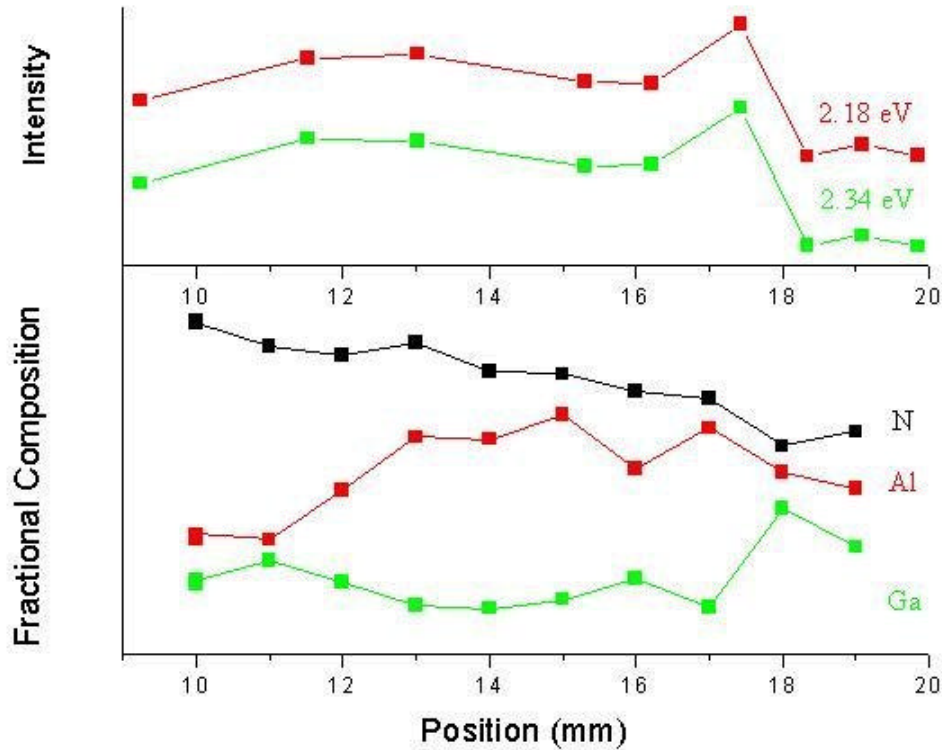
Scans were taken at various points across the wafer, to observe variations in aluminum content. This data was then correlated to the cathodoluminescence data and

the 2.18 and 2.34 eV peaks. A large variation in these peaks is observed between 16-18 mm from the center of the wafer.

The addition of XPS data to the previously acquired CL data provides the missing composition information. In this case, a large change in the gallium / nitrogen ratio is observed near the large change in the 2.18 and 2.34 eV peaks. This is shown in Figure 8.

It is obvious that the relationships between the observed peaks in the CL spectrum and the composition of the wafer,

Figure 8



specifically the aluminum dopant, is complex. My part in this experiment is primarily to acquire the data and integrate it into the existing data set. Therefore, I feel unqualified to draw concrete conclusions from these results. I leave the detailed analysis of this to my excellent colleagues in Brillson Labs.

### V. Conclusions

AlGa<sub>x</sub>N and GaN are very interesting semiconductors with high potential to be very useful. Because of this, it is important to understand how the composition and processing of the material affects the electrical properties of the wafer.

XPS and CL allow us to ascertain these important facts and correlate them together.

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