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Environment About Indium in $\text{Ga}_{1-x}\text{In}_x\text{N}$ from In and Ga K-Edge XAFS

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Abstract. GaN doped with various amounts of In can be used to make diodes with colors from blue to green. In order to determine the effect of the In on the local nitrogen and gallium environment, we have collected both In and Ga K-edge XAFS data on films of $\text{Ga}_{1-x}\text{In}_x\text{N}$. The distribution of In in the GaN matrix was found to be random both by plotting the amplitude of the In-Ga/In peak vs. x and from more detailed fits, although small clusters of three or fewer In atoms cannot be ruled out. In-In and In-Ga atom pairs are of comparable bond length, increasing approximately linearly with concentration x . These atom-pair distances are between the Ga-Ga distance in GaN (3.18 Å) and the In-In distance in InN (3.52 Å). Ga edge data is consistent with this distribution, but further distortions make detailed fits more difficult.

1. INTRODUCTION

$\text{Ga}_{1-x}\text{In}_x\text{N}$ has received a lot of attention recently because it can be made into a light-emitting diode with colors from blue and green. Together with red diodes, $\text{Ga}_{1-x}\text{In}_x\text{N}$ offers the possibility of ultra-high-resolution color displays. These devices behave roughly like standard semiconductors. However, if accurate band structure calculations are to be performed, the distortions around and the distribution of the In atoms must be understood. The local environment is expected to behave like $\text{Ga}_{1-x}\text{In}_x\text{As}$. Previous work by Mikkelsen and Boyce[1] shows that the In is distributed randomly and the nearest neighbor environment around the Ga and In behaves roughly like the end-compounds (that is, the Ga-As pair looks like GaAs and the In-As pair looks like InAs). These measurements run contrary to Vegard's law[2], which states that the structure of an intermediately substituted compound is simply the weighted average of the end-structures. Interestingly, Vegard's law does roughly apply to the second-nearest neighbors in $\text{Ga}_{1-x}\text{In}_x\text{As}$. Our XAFS measurements demonstrate that $\text{Ga}_{1-x}\text{In}_x\text{N}$ behaves similarly.

2. EXPERIMENTAL

In order to determine the effect of the indium on the local nitrogen and gallium environment, we have collected both In and Ga K-edge XAFS data on films of $\text{Ga}_{1-x}\text{In}_x\text{N}$ with samples grown using MOCVD and MBE. Data were collected on BL 4-3 at SSRL using Si(220) monochromator crystals. The films were placed at a 55° angle to the incident beam, and the fluorescent photons were collected with the 13-element Ge detector. Data were corrected for dead-time and self-absorption[3,4], although the exact film thickness was not known. Indium fluorescence yield data confirm the nominal concentrations. Data are reduced using our standard procedures[4,5]; r -space data are shown for the In K-edge in Fig. 1.

3. RESULTS

Fig. 2 and Fig. 3 show the amplitude of the peaks centered at ~1.7 Å and 2.9 Å in Fig. 1 vs. nominal In concentration. The first peak is due to the In-N atom pairs and the second peak is a combination of the In-Ga and In-In atom pairs. Fits indicate that the In-N bond length remains fairly constant with concentration at 2.09 Å, which is somewhat lower than 2.15 Å for InN. The decreasing peak height (Fig. 2) does demonstrate increasing disorder.

The effect of the overlap of the In-In peak on the In-Ga peak is to rapidly reduce the overall amplitude. In fact, the In-In and In-Ga signals are nearly out-of-phase. Fits to this peak that assume that the two paths are the same length give proportions of In to Ga that is consistent with the nominal concentrations (Fig. 4), and also give bond lengths in between 3.17 Å (GaN) and 3.52 Å (InN) proportional to x . These fits do not include the 8% sample because the fits were unreliable. However, the peak heights in Fig. 3 indicate that it follows the same trend as the other data. Therefore we conclude that the In is randomly distributed in the sample. Small clusters of three or fewer In atoms cannot be ruled out.

FIG. 1. Fourier Transform (FT) of $k\chi(k)$ vs. r for $\text{Ga}_{1-x}\text{In}_x\text{N}$ with various x . The first peak at ~ 1.7 Å is due to the In-N scattering path. The second peak at ~ 2.9 Å is due to a combination of the In-In and In-Ga scattering paths.

FIG. 2. Amplitude of the FT for the In-N peak vs. In concentration.

FIG. 3. Amplitude of the FT for the In-In/Ga peak vs. In concentration.

FIG. 4. Estimated concentration (from the relative contributions of In-In paths and In-Ga paths) vs. the nominal concentration. These numbers should be the same only if the indium does not cluster in the sample and the nominal concentrations are the actual average concentration of the sample.

Ga K -edge data (not shown) are consistent with the above conclusions. The Ga-In/Ga peak height data show the same trend as in Fig. 3. Interestingly, the Ga-N peak height increases linearly with concentration; we do not have a good model for this behavior. Reliable fits were not obtained; fits to the GaN data (no In) were improved by a significant In amplitude, and therefore fits to all other concentrations were suspect. Some extra distortion in the Ga-Ga pair may be responsible. The nearest neighbor Ga-N pair could be fit reasonably with a bond length of 1.94 Å, which is the same as diffraction measurements.

4. Conclusion

Although good fits to the data were only obtained for the In K -edge XAFS on $\text{Ga}_{1-x}\text{In}_x\text{N}$, these fits together with the raw data are consistent with a random In distribution and distortions that are similar to $\text{Ga}_{1-x}\text{In}_x\text{As}$.

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