

# X-ray Absorption and Emission Spectroscopy at the Nitrogen K-Edge in Dilute GaAs<sub>1-x</sub>N<sub>x</sub>

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GaAs<sub>1-x</sub>N<sub>x</sub> and In<sub>y</sub>Ga<sub>1-y</sub>As<sub>1-x</sub>N<sub>x</sub> alloys containing a few percent nitrogen have attracted attention in recent years due to their potential use in 1.3 micron emitters on GaAs substrates. The incorporation of nitrogen at low concentrations in these III/V materials results in a large band gap bowing parameter and a sharp decrease of the band gap with increasing nitrogen [1]. A wide range of lattice constants can be obtained by varying the N content. For example In<sub>0.3</sub>Ga<sub>0.7</sub>As<sub>0.98</sub>N<sub>0.02</sub> quantum wells are pseudomorphic to GaAs and emit at 1.3 micron. In the present work, we have studied the density of states in the valence and conduction bands of dilute GaAs<sub>1-x</sub>N<sub>x</sub> using soft x-ray emission and absorption at the nitrogen K-edge. The emission spectrum is compared to a tight binding band structure calculation for the electronic structure of GaAs<sub>1-x</sub>N<sub>x</sub>.

The GaAs<sub>1-x</sub>N<sub>x</sub> samples were grown by Molecular Beam Epitaxy (MBE) at a substrate temperature in the 500-600°C range using a RF plasma source for the dissociation of molecular nitrogen. The nitrogen content ranged from 0.02% to 2%. Nitrogen concentrations were obtained using X-ray diffraction and SIMS. The samples were cleaved in two pieces; one piece was annealed at 850° for 1 min. Nitrogen K-edge absorption and emission spectra were measured at beamline 8.0.1. The absorption spectra were obtained in the fluorescence yield mode. The emission spectra were measured using a 600 lines/mm diffraction grating providing an energy resolution of 0.8eV (FWHM) as determined from the scattered primary beam.

Emission and absorption spectra at the nitrogen K-edge are shown in Fig. 1 for a GaAs<sub>1-x</sub>N<sub>x</sub> sample with a 2% N content, together with calculated nitrogen 2p density of states. The emission spectrum (lower spectrum in the figure) was excited at a photon energy of 402.1 eV corresponding to the peak absorption in the upper spectrum in Fig. 1. The small peak at 402.1 eV in the emission spectrum is the elastically scattered excitation radiation which is not completely rejected by the soft x-ray spectrometer. This peak serves as an energy calibration for the emission spectrometer. The emission and absorption spectra show a band gap of about 1 eV in agreement with optical measurements.

Absorption at the nitrogen K-edge probes the unoccupied density of states in the conduction band with p-symmetry at the nitrogen sites. The spectrum shows a strong

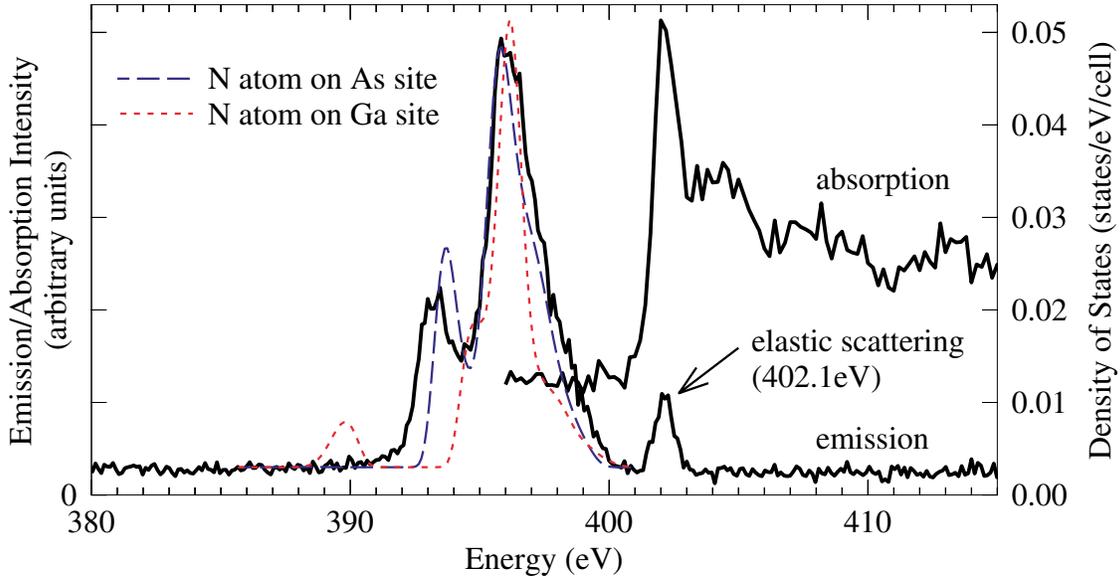


Figure 1: Emission and absorption curves for  $\text{GaAs}_{1-x}\text{N}_x$  with 2% N and calculated local DOS on the Nitrogen 2P state. Orthogonal (random) noise of 0.003 states/eV/cell has been added to the calculated spectra. The origin of the energy scale in the calculations is arbitrary.

excitonic type peak just above the bottom of the conduction band which we attribute to the well known nitrogen resonance in the conduction band. The shape of the absorption spectrum was independent of the nitrogen content.

The emission spectrum in Fig. 1 at the nitrogen K-edge is due to transitions from valence band states on nitrogen sites with p-symmetry to the nitrogen 1s core hole. The spectrum has two peaks located at 393.2 eV and 396.1 eV. No changes in the shape of the spectrum were observed as a function of nitrogen content in the 0.02% - 2% range. Similarly no changes were observed with annealing at 850°C. Annealing is expected to substantially reduce the number of nitrogen interstitials. The absence of a change in the emission spectrum with annealing suggests that the fraction of interstitial nitrogen is low. Emission spectra were measured as a function of excitation energy through the absorption edge and no resonant effects were observed in the soft x-ray emission.

Emission spectra were calculated in a tight binding model in which a single nitrogen atom is located on a Ga or an As site in a  $2 \times 2 \times 2$  supercell containing 64 atoms. The model spectra are the p-projected densities of states on the nitrogen atom. The energies for the atomic orbitals and interatomic overlap matrix elements for the Ga and As 4s and 4p orbitals were taken from Harrison [2]. The energy level for the nitrogen 2p orbital was taken to be an adjustable parameter and was used to fit the experimental spectrum. The spectra were convolved with a 0.8 eV Gaussian window in accordance with the experimental resolution. The lifetime broadening of the emission band is ignored. A best fit was obtained with the nitrogen 2p orbital energy  $\epsilon_p$  equal to -8.5 eV which compares with the -11.47 eV recommended by Harrison. For  $\epsilon_p < -9.5$  eV the nitrogen 2p orbital forms a bound state in the valence band and the shape of the emission spectrum changes. The good agreement with the experimental data in Fig. 1 suggests that there is

no nitrogen p-like bound state in the valence band. When the nitrogen is located on a Ga site a deep bound state is obtained in the model as indicated by the peak in the dotted curve in Fig. 1 at 389.8 eV. The good fit with the calculated spectrum for nitrogen on the As site suggests that most of the nitrogen is on the group V site, as expected. No emission was detected from the lower part of the GaAs valence band, which is dominated by As 4s, in good agreement with the model.

## Acknowledgments

We thank Tony Van Buuren for his help and the Natural Sciences and Engineering Research Council of Canada (NSERC) for financial support.

## References

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