ESRF	**Experiment title:** Local structure and magnetic properties of Cu dopands in group III nitrides grown by molecular beam epitaxy investigated by XLD and XMCD	**Experiment number**: HE-3297
Beamline: ID12	**Date of experiment**: from: 16/06/2010 to: 22/06/2010	**Date of report**: 31/08/2010
Shifts: 18	**Local contact(s)**: A. Rogalev, F. Wilhelm	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Philipp R. Ganz*, Ralf Schuber*, Daniel M. Schaadt*

DFG-Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology (KIT)

Report:

Abstract

We report on the local structure of Cu-doped group-III nitrides. We measured x-ray absorption spectra of Cu-doped nitrides with nominal Cu concentrations from 0.0% to 2.3% before and after etching with HNO_3 for 5 minutes. The local structure of the incorporated Cu atoms, their effect on the nitride host lattice as well as the influence of the Cu-Ga islands on top of the surface (Fig. 1) was investigated. The XLD signal, measured at the Cu K-edge, indicates that only a small amount of Cu atoms is incorporated on lattice sites in the wurzite crystal structure of group-III nitrides. Due to a small XAS Cu signal on the etched samples, XMCD measurements were not feasibel and therefore not performed. However, this gave us the opportunity to obtain a more complete picture of the XLD studies on Cu-doped nitrides.

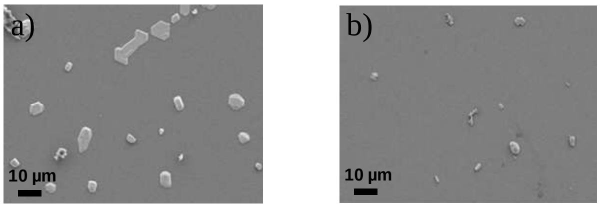

Fig. 1: SEM picture of the surface of 1.2% Cu-doped GaN before (a) and after etching (b)

Results

All samples were mesured as grown and after etching with HNO_3 for 5 minutes. Etching was necessary to remove the Cu-Ga islands from the surface of the Cu-doped GaN. The influence of etching on the Ga K-edge is shown in Fig. 1. The normalized XANES spectra are look similar for the as grown and etched sample. The normalized XLD signal indicates clearly for both spectra the wurtzite crystal structure of GaN. However, the XLD signal for the etched sample is significantly higher and reaches almost the theoretical maximum of 0.63 units. This indicates a high crystalline quality of the GaN. TEM studies show, that the Cu-Ga compounds (Cu_9Ga_4), which have a cubic crytsal structure, grew epitaxially on the Cu-doped, which results in a strained Cu_9Ga_4 lattice. A contribution to the XLD signal is therefore also given by the Ga bound in the Cu_9Ga_4 crystal overlapping with the signal from the Ga in

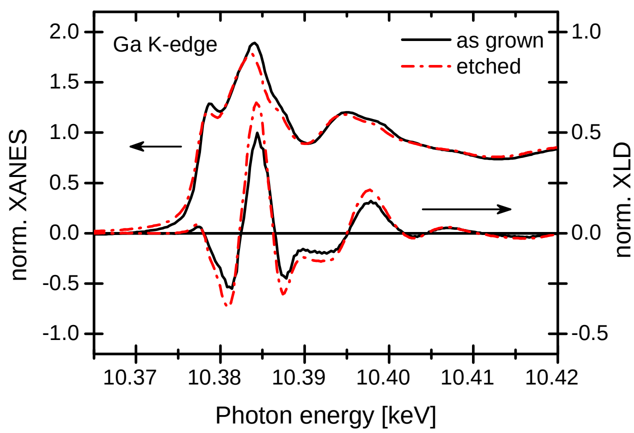

Fig. 2: Normalized XANES and XLD at the Ga K-edge before and after etching for the 1.2% nominal doped sample

the wurtzite crystal structure. All samples from 0.5% to 2.3% nominal Cu doping showed a similar behavior in the XANES and XLD spectra for the Ga K-edge.

For the Cu K-edge, a clear influence of the etching on the XANES spectra is visible (Fig. 3). After etching, the intensity of the spectra decreased by more than a factor of 5. The islands on the surface consist of a high amount of Cu (60%) and Ga (40%). X-ray diffraction spectra showed that about 90% of the islands were removed after etching. Therefore, the main contribution to the XANES and XLD spectra after etching is attributed to the Cu incorporated in the film. The normalized XANES and XLD spectra for the Cu K-edge are shown in Figure 4. These normalized XANES spectra look quite similar for the as grown and etched sample, indicating, that Cu is also incorporated in the GaN host. However, the XLD spectra are different. The spectra for the etched sample shows a different shape and a higher intensity. However, the strong variation of the XLD signal in the etched sample around 9.004 keV can be ascribed to a diffraction peak. Compared to the XLD for the Ga K-edge, the intensity for the Cu K-edge is more than 10 times lower. Therefore, the etched samples were measured several times at the Cu K-edge in order to obtain a good signal to noise ratio. Because of the small XLD signal, we cannot conclude yet if Cu is incoporated on substitunional lattice sites in the wurtzite crystal structure. Theoretical calculations with the FDMNES code, which we are currently performing, will help us to evaluate the Cu configuration. Initial data from the calculation show, that only a small amount of Cu is incorporated on Ga sites in the wurtzite crystal structure. In Figure 5, the normalized XLD spectra for different Cu concentrations are shown. The shape and intensity is independent of the nominal Cu supply. The Cu content in the film must be therefore very similar. From recent TEM measurements, we can conclude, that the Cu concentration in the film is less than 0.2% and decrease slightly with the nominal Cu supply.

We also measured XANES for as grown and etched Cu-doped AlN and InN. In the case of Cu-doped AlN, similar results as for Cu-doped GaN are obtained. For Cu-doped InN, only the as grown sample was measured. In the case of Cu-doped InN, the main layer consiting the Cu-doping was removed by etching. This explains, that we could not detect any Cu signal on the Cu-doped InN sample after etching.

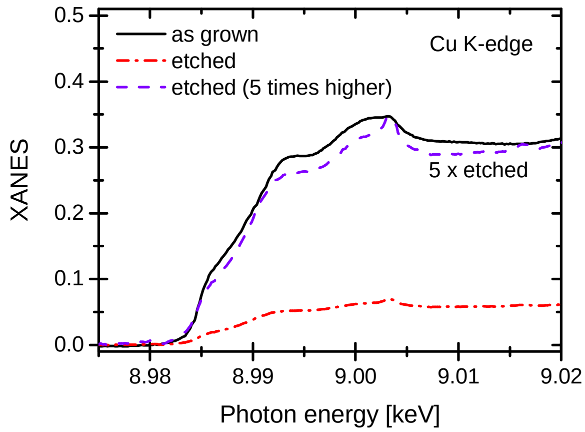

Fig. 3: XANES at the Cu K-edge before and after etching for the 1.2% nominal doped GaN:Cu

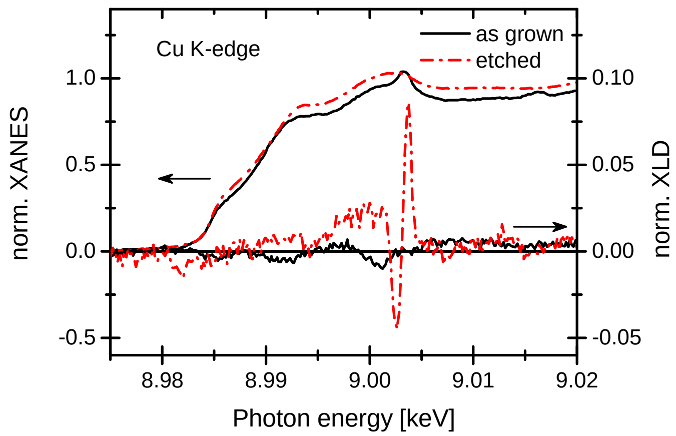

Fig. 4: Cu K-edge XANES and XLD for the 1.2% nominal doped sample

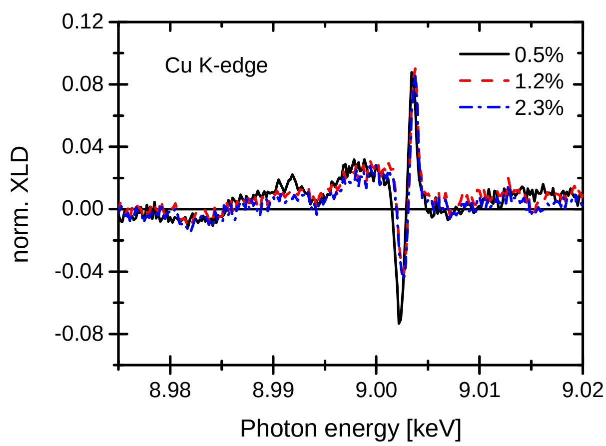

Fig. 5: XLD at the Cu K-edge for different nominal Cu concentrations

Conclusion

The XLD spectra at the Ga K-edge for all samples showed clearly a wurtzite typical shape, indicating a high purity of GaN. Cu is incorporated in the nitride host. However, calculations indicate only a small amount of Cu is sitting on Ga sites in the nitride matrix.

The results of this work will be published as soon as the calculations are performed for several Cu configuration in the GaN host. This allows us to conclude, how Cu is incoprorated in the GaN host.