ESRF	**Experiment title:** XSW analysis of Si and Mg dopants in GaN	**Experiment number:** SI-1115
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Report:

Magnesium and silicon are the materials most commonly used for p- and n-type doping of GaN films. The quality of doped films is known to significantly depend on the doping concentration. In order to determe the incorporation sites, and especially the fractions of the dopants on non-substitional sites, we performed XSW measurements in backscattering geometry on Mg and Si doped GaN films grown by MOVPE on sapphire (0001) substrates.

As we demonstrated in earlier experiments [1], the GaN crystal quality of thicker films degrades drastically with increasing Mg concentration. The presence of different lattice constants inhibit XSW experiments even in back-scattering geometry. In order to avoid such effects, a 3.5 μm thick undoped GaN film was used to establish a standing wave field which was used for the investigation of 100 nm thin Mg doped films on top. As secondary signal we recorded the Mg KLL Auger electron intensity. As the measurements were performed in (002) backscattering geometry at an incident photon energy of 2.4 keV, influences of secondary channels on the Mg KLL signal can be neglected.

Exemplarily, the results of XSW measurements performed on samples with a Mg doping concentration of a) $1\times10^{19}\,\mathrm{cm}^{-3}$ and b) $2\times10^{19}\,\mathrm{cm}^{-3}$ are shown in Fig. 1. The reflectivity signal is nicely fitted by the reflectivity expected for a perfect GaN single crystal convoluted with the monochromator instrumental function. In order to obtain well defined reference data, XSW measurements were performed with Ga $2p$ photoelectron secondary signal on the same samples. These measurements yielded values of a) Φ_c=0.96 and b) Φ_c=0.95, which virtually equals the bulk position.

The obtained coherent fractions of a) f_c=0.83 and b) f_c=0.81 reflect a slight surface degradation and oxidation of the samples resulting from air exposure during transport. XSW measurements with Mg KLL secondary signal yield coherent positions of a) Φ_c=1.06 and b) Φ_c=1.04, which points to the substitution of Ga atoms. The difference of the obtained Φ_c lies within the accuracy of the measurements of $\Delta\Phi_c$=Δf_c=0.02. The values for the coherent fractions are a) f_c=0.64 and b) f_c=0.45. From a comparison to the results for the Ga signal, we conclude that at higher dopant concentration non-substitutional sites are occupied to a larger extent. More detailed information on the non-substitutional sites may be obtained by XSW investigations in asymmetric Bragg conditions in backscattering geometry, e. g. in (101) Bragg reflection. Such measurements were performed, but due to technical problems during the experiment the data can hardly be evaluated.

XSW measurements on 3.5 μm thick Si doped samples were performed in (002) and (101) backscattering geometry with both surface and bulk sensitive probes, i. e. photoelectrons and fluorescence. The homogenous Si doping of the thick GaN films has lead to a significant broadening of the reflectivity width to 1.83 eV as compared to the width of the Mg doped samples discussed above of 0.63 eV. Therefore, the evaluation of the data is difficult, requiring convolutions with asymmetric lattice parameter distribution functions in order to fit the reflectivity. For further experiments —as successfully shown above for Mg doped samples— it is planned to investigate thin Si doped layers on top of undoped GaN films. The Si K fluorescence was observed even after sputtering of the sample surface, whereas the Si 1s photoelectron signal vanished after sputtering.

In the experiments presented here, XSW measurements on light trace elements in GaN films were performed successfully for the first time and we observed a systematic variation of the Mg incorporation in dependence of the dopant concentration.

[1] M. Siebert et al., Hasylab Annual Report 2004

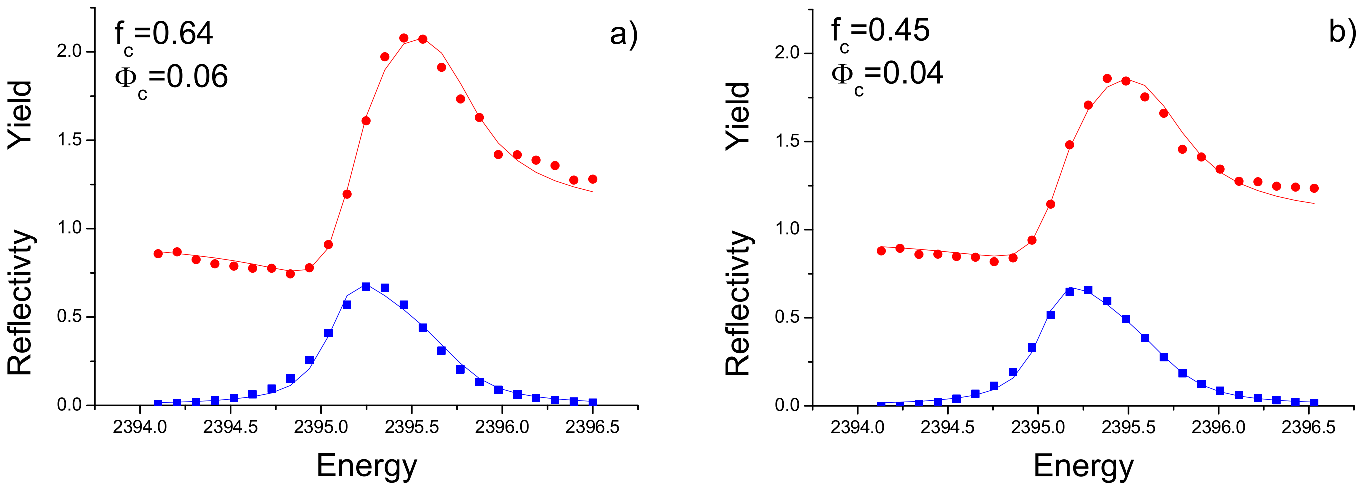

Fig. 1: XSW data and fit (solid lines) of reflectivities (□) and Mg KLL yield (○) at a photon energy of E = 2.4 keV in (002) backscattering geometry at a Mg dopant concentration of a) 1×10^{19}cm^{-3} and b) 2×10^{19}cm^{-3}.