ESRF	**Experiment title:** Spatially resolved study of InN films by sotf and hard X-ray microprobes	**Experiment number:** HS3742
Beamline: ID21	**Date of experiment:** from: July 11th to: July 14st 2009	**Date of report:** January 11th 2011
Shifts:	**Local contact(s):** Jakub Szlachetko	*Received at ESRF:*

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Three non-intentionally doped InN films (500 nm thickness) grown on sapphire substrates by PIMBE with different buffer layers of AlN and GaN have been studied by means of XAS and μ-X ray fluorescence at the microprobe beamlines ID21 and ID22. The purposes of the work were: to analyze the local arrangement of In in the InN with different polarities (In- and N-face), as well as Mg doping concentrations; to clarify the existence of polytype mixing (cubic and hexagonal); and to study spatially the structural disorder, elemental traces, and dopant variations. All these are relevant factors which could contribute to clarify the effect of polarity and Mg on the local atomic structure and chemical characteristics of InN films.

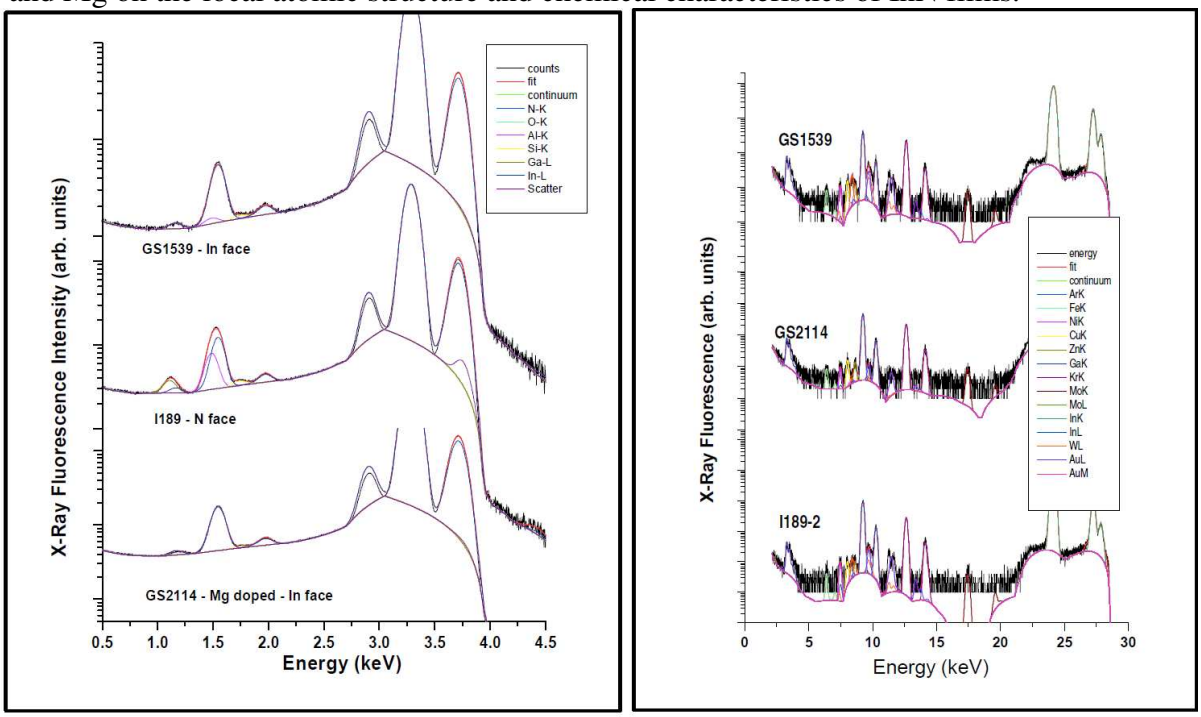

Fig. 1 XRF spectra from InN samples with In- and N-face polarities as well as from a Mg doped InN layer .

In Fig. 1 the XRF data acquired on ID21 at low excitation energy (on the left side) show the L and K shell lines of In, Al and Ga, as well as Si. On ID22 at 28.2 keV excitation energy (on the right side) the presence of elemental traces such as Fe, Ni, Cu, and Zn is also revealed. There is no evidence of field-driven electrodiffusion effects or clear influence of lattice polarity on the content of the elemental traces. By setting

examined. Uniform patterns with no intensity changes were observed, showing a homogeneous distribution of all samples. Whereas impurity aggregation effects are expected and observed in InGaN alloys, in the length scale of the beam size our results suggest no tendency to agglomerate residual impurities at those low concentration levels.

The XANES data at the In L3 and K edges are plotted in Fig. 2. Since the electronic transitions responsible for both XANES follow the dipole selection rules, K and L3 edges reflect the p- and (s+d)-partial density of states (PDOS), respectively. On the left, the L3-related spectra exhibit the typical data of fourfold In in InN.[1] The main features of InN XANES spectrum is composed of two shoulders and three peaks labeled as s_1, s_2, p_1, p_2, and p_3. In general, all five features present similar spectral characteristics in both positions and shapes. However, slight differences in peak areas and half widths can be found between the N-face and In-face InN layers. The In K-edge XANES, on the right, shows remarkable resemblance with the Ga *K*-edge XANES measured in wurtzite-type GaN under similar measurement conditions (Ref. 2), suggesting the preservation of the main hexagonal crystal structure. For the case of Mg doped InN, although it could be expected the coexistence of cubic and hexagonal polytypes, here there is no indication on the XANES data of In on any other highly lattice symmetry other than the hexagonal on a tetrahedral site. In the case of group III nitrides, structural difference between wurtzite and zinc blende polytypes is known to be small with differences in the layer stacking sequence. The wurtzite phase has A,B,A,B,., stacking with a hexagonal unit cell, namely, 2H structure, whereas the zinc blende phase has A,B,C,A,B,C,., stacking with a cubic unit cell, namely, 3C structure. The point symmetry of the tetrahedral unit [AB_4] is also different. [AB_4] in the wurtzite structure has a C_{3v} symmetry which is lower symmetry than that in the zinc blende structure T_d. The coordination number of all atoms in the two phases is 4, whereas in the rock-salt phase it is 6. In addition, among these polymorphs, the c crystallographic orientation dependence of the XANES can be expected only in the wurtzite phase because of its hexagonal lattice. However, contrary to those in K edges, the spectral changes due to the different incidence orientations are found to be small in the L3 edge. The reason can be ascribed to

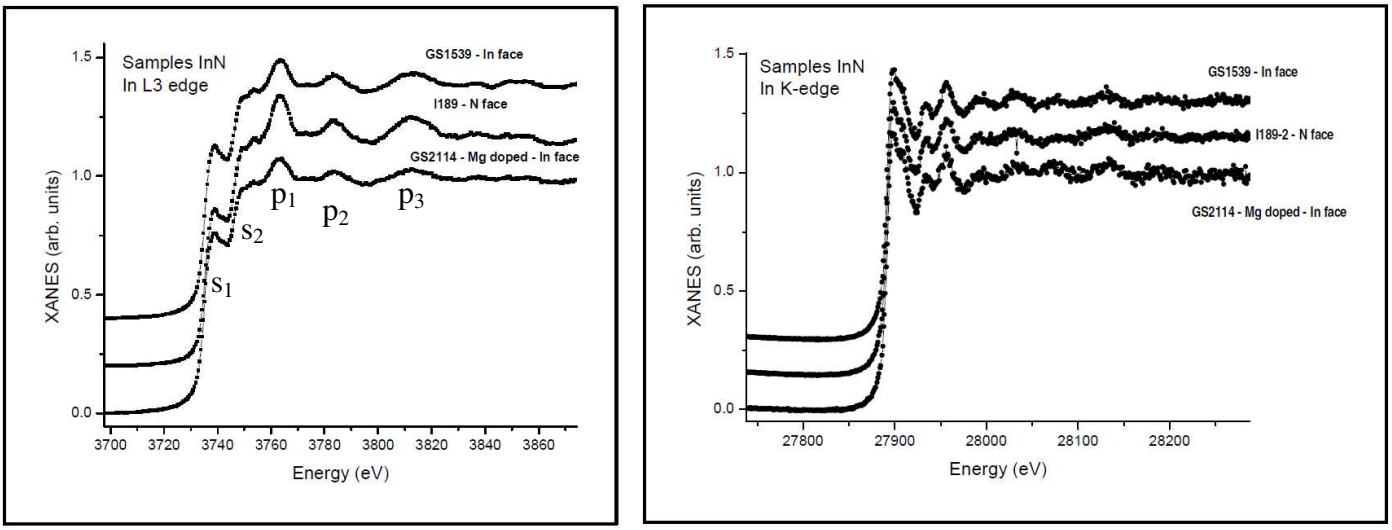

Fig. 2 XANES recorded at the In L3 and K edges from InN samples with In- and N-face polarities as well as from a Mg doped InN layer .

different atomic orbitals that are responsible for K and L3 edges. The K edge reflects mainly p-type orbitals, while L3 edge reflects mainly s- and d-type orbitals. The s orbital is spherical. Empty 4d and 5d orbitals may not contribute much to the covalent bonding in InN. They are therefore less asymmetric. In summary, there is no remarkable damping effect revealing a strong influence of the Mg dopant and/or residual impurities in any preferential crystallographic direction. Within the detection limit of the method, the presence of any secondary phases has not been revealed.

References:

1. J. T-Thienprasert, J. Nukeaw, A. Sungthong, S. Porntheeraphat, S. Singkarat, D. Onkaw,1 S. Rujirawat,and S. Limpijumnong, Appl. Phys. Lett. 93, 051903 (2008).
2. G. Martínez-Criado, R. Tucoulou, P. Cloetens, J. A. Sans, and J. Susini, Appl. Phys. Lett. 95, 151906 (2009).