ESRF	**Experiment title:** Study of Thermal Motion Induced resonant reflections in GaN	**Experiment number**: 28-01-821
Beamline:	**Date of experiment**: From: 11.06.2008 to: 17.06.2008	**Date of report**: 24 Sept. 2008
Shifts:	**Local contact(s)**: Simon D. Brown	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Guillaume Beutier*

Steve P. Collins*

Vladimir Dmitrienko
Elena Ovchinnikova

Report:

The aim of the proposal was to continue our investigations of Thermal Motion Induced (TMI) scattering. TMI is able to excite "forbidden" reflections of a crystal in Resonant X-ray Scattering (RXS), because the dynamic displacement of the resonant atoms from the highly symmetric sites causes an evolution of its tensor of scattering. TMI measures the differential of the tensor with the displacement. Prior to this experiment, it had only been observed in Ge and in ZnO (at XMaS).

During this run, we successfully investigated TMI in GaN at the Ga K edge (~10.367 keV). GaN crystallizes with the wurtzite structure (space group $P6_3mc$), like ZnO. In these crystals, TMI scattering contribute to forbidden reflections in competition with a temperature independent E1E2 contribution. Only their temperature dependence allows distinguishing between the two processes.

A large single crystal of GaN, in shape of a plate with the *c* crystallographic axis normal to the surface, was mounted in the Displex cryo-furnace of the diffractometer. The Vortex silicon drift detector was used to analyse the scattered intensity in energy and reject the fluorescence. We used the natural linear horizontal polarization of the beam delivered by the bending magnet. Most measurements were done without polarization analysis, but in some cases we used the (008) reflection of a graphite crystal to analyse the scattered beam.

The isotropic part of the absorption coefficient was extracted from powder measurements in transmission geometry during the run (Fig. 1), and the diffraction data were corrected for self-absorption, based on this determination. Since GaN is dichroic, more accurate spectra would be obtained if the dichroic part of the absorption was known, but the knowledge of the isotropic absorption is enough for the purpose of the study.

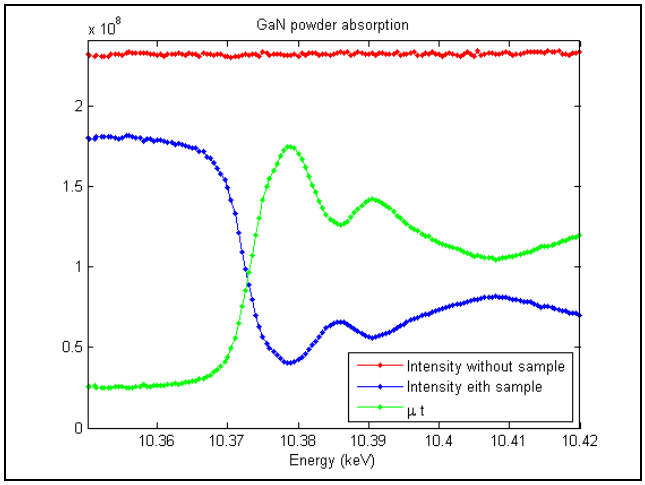

Figure 1: determination of the isotropic absorption coefficient

We measured the (1,1,3) and (1,1,5) forbidden reflections and the (3,0,3) weak reflection (a weak reflection is a reflexion that is not forbidden by the general conditions of the space group but by the particular conditions of the sites).

The (1,1,5) was found particularly strong, yielding several thousands of counts per second, and was measured extensively against energy, azimuth and temperature. Its energy-temperature map (Fig. 2) shows a similar behaviour to that of ZnO. As expected, the intensity globally increases with the temperature because of the TMI contribution, driven by higher thermal displacement of the atoms. At low temperature, the E1E2 dominates the TMI scattering and the intensity decreases while the temperature increases because of the Debye-Waller term. The temperature dependence is more complex around room temperature, because the TMI scattering and the E1E2 become of the same magnitude order with an energy dependent phase shift, and the map reveals their interferences. The experimental data can be nicely fitted with the same model proposed for ZnO, which gives us confidence about its validity.

(3,0,3) is a weak reflection, because its not allowed for the specific sites occupied by the Ga and N atoms, but it is not forbidden by the space group of the crystal. Thompson scattering occurs therefore because of the non-spherical electronic distribution around the sites. This process interferes at the Ga K edge with the E1E2 scattering and the TMI scattering, making the analysis more difficult.

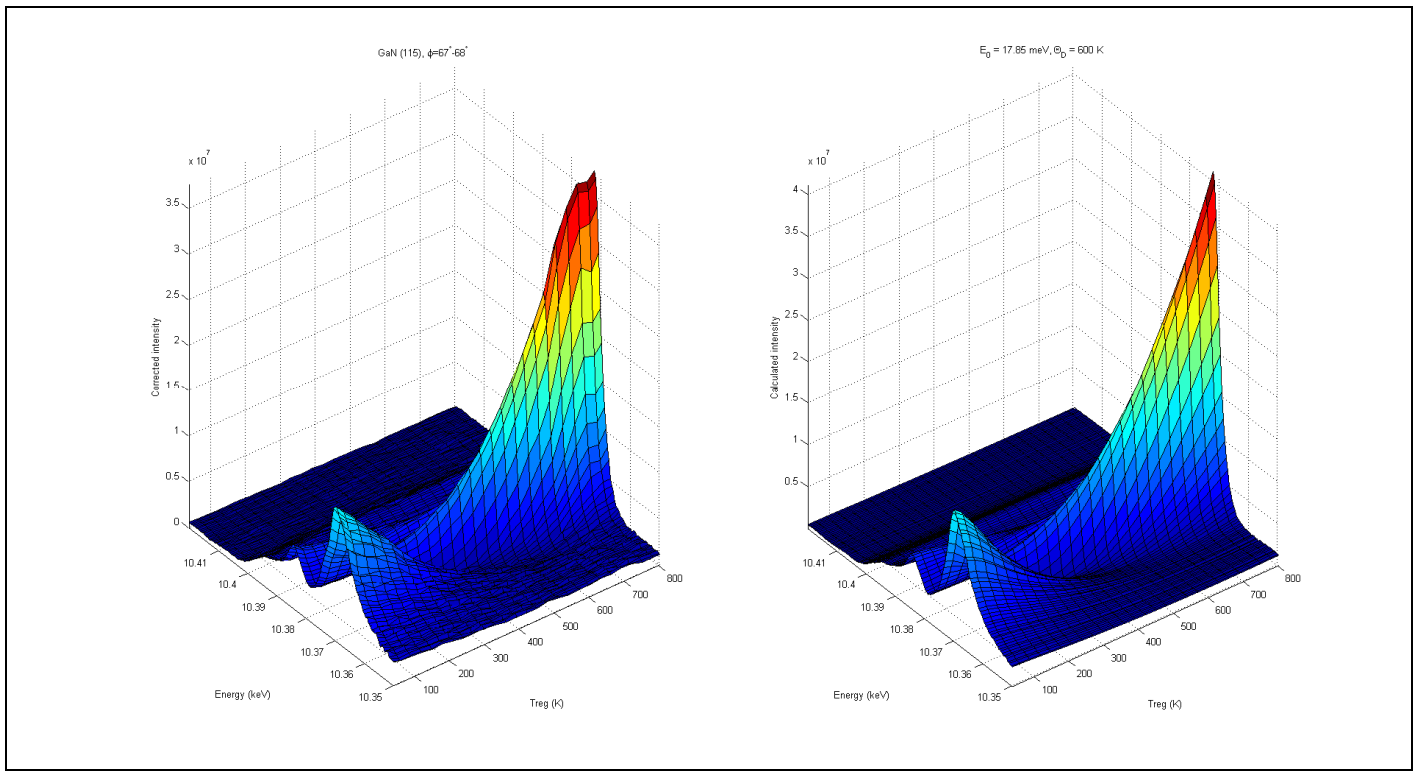

Figure 2: Temperature dependence of the energy spectra of the (1,1,5) forbidden reflection of GaN. Left: experimental data. Right: fit based on the model reported in Collins et al, Phys. Rev. B 68, 064110 (2003).

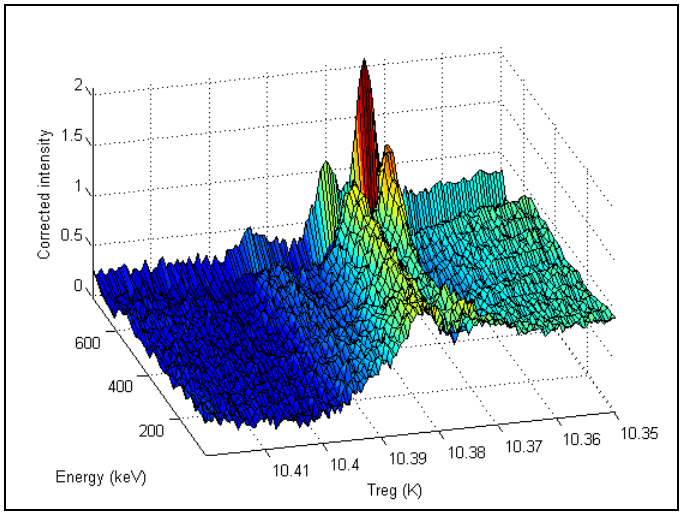

Figure 3: Temperature dependence of the energy spectra of the (303) weak reflection of GaN at the Ga K edge.

Azimuthal scans of the (115) forbidden reflection were performed at 3 different energies, with the polarization analyser at 0, 45 and 90 degrees. They show that the azimuthal dependence is independent of the energy, as was already notices in the case of ZnO. Due to geometrical limitations, we could not performe these scans over the full azimuthal range, and it seems difficult to assess whether the discrepancy between data and model for ZnO occurs for GaN as well.

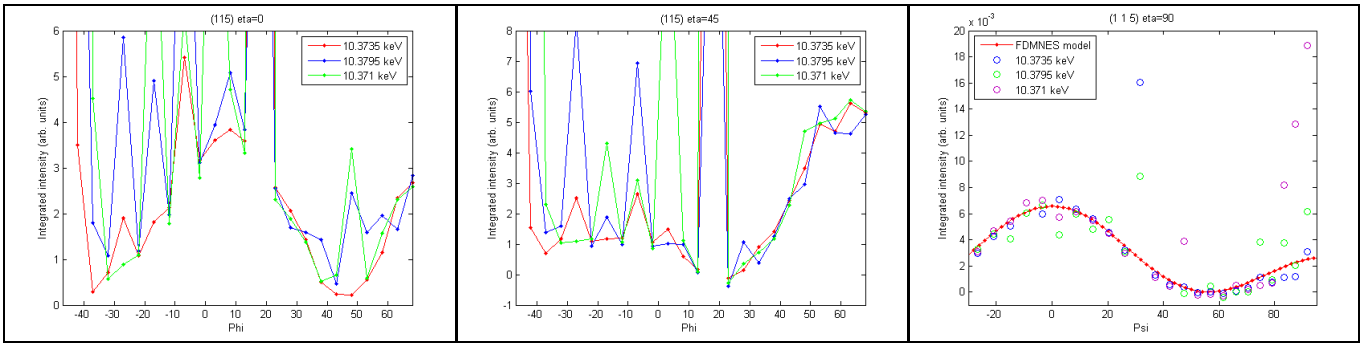

Figure 4: partial azimuthal scans of the (1,1,5) forbidden reflection at 3 different energies and 3 different angles of the polarization analyser. Multiple scattering occurs at many positions.