ESRF	**Experiment title:** Electron distribution and electron-electron correlations in NiO single crystals	**Experiment number**: HE-452
Beamline: ID 15B	**Date of experiment**: from: Sept.9th, 1998 7:00 to: Sept.14th, 1998 7:00	**Date of report**: Mar.1st, 1999
Shifts: 15	**Local contact(s)**: Abhay SHUKLA	*Received at ESRF:*

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Report:

NiO is a highly correlated material, and thus a good model for theoretical all-electron investigations. The Louie group in Berkeley has developed a new method for calculating multi-electron wave functions including electron-electron correlations, based on a variational quantum Monte Carlo approach (VQMC). This VQMC method is currently being applied to nickel oxide.

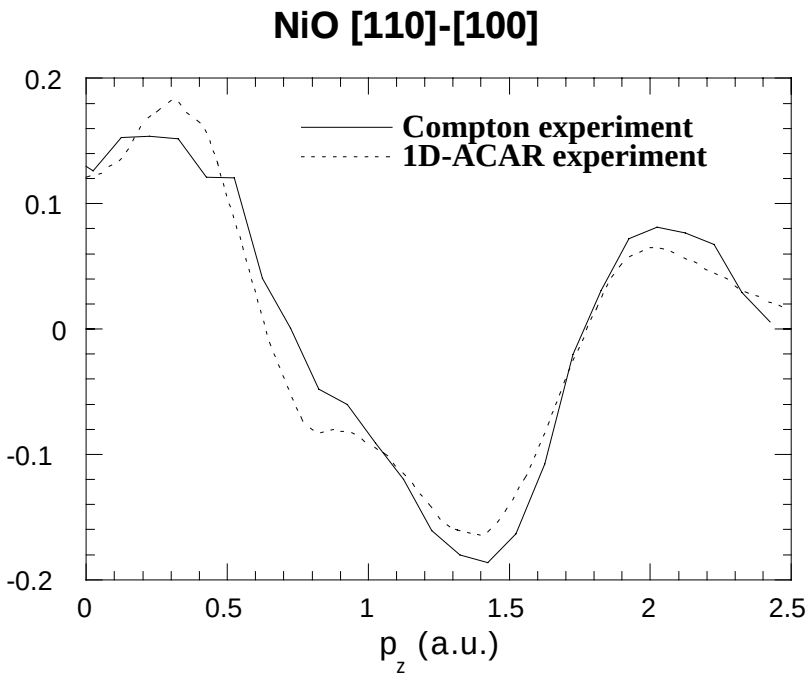
We performed three measurements on NiO single crystal, along directions [110], [100] and [211] : the experimental part of our study of electronic density in NiO is now achieved. During the experiment, the scattering angle was set at 173 degrees and the incoming photons were monochromatized at 56 keV. The data sets have been corrected for energy dependant effects such as photoelectric absorption in sample, analyzer and air (photon path between sample, analyzer and detector). Since the only electrons of interest are valence electrons, calculated core Compton profiles have been substracted from the total profiles using the QSCF approximation. The obtained valence profiles were normalized to the number of valence electrons.

Two main reasons led us to do these measurements :

1) An accurate estimation of the intensity of the multiple scattering contribution, which is an unwanted signal, had to be determined in order to get directional Compton profiles for comparison with theorical directional profiles; such a comparison gives access to the contribution of electron-electron correlations. By measuring direction [100] with samples of different thickness (1mm thick during HE-275 and 0.5mm thick during this experiment), we had the opportunity to check the pertinence of our results and of our calculation of the multiple scattering contribution. The agreement obtained between the two samples after data processing certifies the quality of our absolute directional Compton profiles and will permit direct comparison with theoretical results.

2) Positron annihilation measurements have been performed on NiO by T.Chiba (NIRIM, Japan) along the three principal directions and along [211].

In the figure below is shown the difference between two directional profiles ([110] minus [100]) obtained by Compton scattering from our measurements, and by positron annihilation.



The agreement between the two methods is very good :

positions of the three maxima are at the same values of p_z ;

a hole at $p_z = 0$ a.u. and a shoulder at $p_z = 0.9$ a.u. appear on both curves.

These good experimental results now await quantitave interpretations which will be provided by theoretical calculations.