

ESRF	Experiment title: Electron distribution and electron-electron correlations in NiO single crystal	Experiment number: HE-275
Beamline: IDISB	Date of experiment: from:26-August-97 to:02-Sep-97	Date of report: 26.02.98
Shifts: 15	Local contact(s): Thomas Buslaps	<i>Received at ESRF:</i> 02 MAR 1998

Names and affiliations of applicants (* indicates experimentalists):

Genevieve Loupiaz *, Universite Paris 6, LMCP

Samuel Chabaud*, Universite Paris 6, LMCP

Christophe Bellin*, Universite Paris 6, LMCP

Steve Louie, Berkeley

Report:

The aim of this project is to investigate the effects of electron-electron correlations in an electron system, NiO, which has d-electrons. Most of physical properties of such compounds originate from these d-electrons (magnetism, metal-insulator transition etc.) and their behavior may be strongly modified by the presence electron-electron correlations.

The experiment has been performed with the scattering angle settled at 160° and the synchrotron radiation has been monochromatized at 55.916 keV. We have measured 3 directional Compton profiles (DCPs) on single crystals.

The data sets have been corrected for energy dependent effects such as photoelectric absorption in sample, analyser and air (photon path between sample, analyser and detector) by using a local correction algorithm (P.Fajardo, T.Buslaps, ESRF).

Due to the flatness of core profile in momentum space, it is easy to subtract its contribution (calculated in QSCF approximation, collaboration with Arezki Issolah,

Universite de Tizi-Ouzou, Algerie) from the total measured DCP in order to get the valence DCP of interest alone. Experimental valence profiles are normalized to the number of valence electrons per unit cell.

This data-analysis is now in its last step : multiple scattering corrections. Such corrections, for absolute comparison with theoretical Compton profiles, is of highest importance (cf the continuation-proposal on NiO). It is under progress.

Together with comparison with all-electrons calculations (Prof. S. Louie, Berkeley), we will be able to compare with new positron annihilation (2D-ACAR) measurements performed by Toshinobu Chiba (NIRIM, Japan) on NiO single crystals. These 2D datas have been integrated along directions [100], [110], [111] and [211] in order to get 1D-ACAR for direct comparison with our Compton scattering results.

The preliminary results look promising.