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Experiment Report Form

The double page inside this form is to be filled in by all users or groups of users who have had access to beam time for measurements at the ESRF. Once completed, the original report should be sent, together with 5 reduced (A4) copies, to the User Office.

In addition, please send a copy of your file as an e-mail attachment to reports@esrf.fr**,** using the number of your experiment to name your file. This will enable us to process your report for the ESRF Annual Report.

Reports accompanying requests for additional beam time

If your report is to support **a new proposal**, the orginal report form should be sent with the new proposal form, and a copy of your report should be attached to each copy of your proposal. The Review Committees reserve the right to reject new proposals from groups who have not reported on the use of beam time allocated previously.

Reports on experiments relating to long term projects

Proposers awarded beam time for a long term project are required to submit an interim report at the end of each year, irrespective of the number of shifts of beam time they have used.

Published papers

All users must give proper credit to ESRF staff members and proper mention to ESRF facilities which were essential for the results described in any ensuing publication. Further, they are obliged to send to the Joint ESRF/ ILL library the complete reference and the abstract of all papers appearing in print, and resulting from the use of the ESRF.

Should you wish to make more general comments on the experiment, please note them on the User Evaluation Form, and send both the Report and the Evaluation Form to the User Office.

Deadlines for submission of Experimental Reports

- 1st March for experiments carried out up until June of the previous year;
- 1st September for experiments carried out up until January of the same year.

Instructions for preparing your Report

∑ fill in a separate form for each project or series of measurements.

∑ type your report, in English.

∑ include the reference number of the proposal to which the report refers.

∑ make sure that the text, tables and figures fit into the space available.

∑ if your work is published or is in press, you may prefer to paste in the abstract, and add full reference details. If the abstract is in a language other than English, please include an English translation.

∑ bear in mind that the report will be reduced to 71% of its original size. A type-face such as ìTimesî, 14 points, with a 1.5 line spacing between lines for the text, produces a report which can be read easily.

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ESRF	**Experiment title:** **Electronic density of Cu_2O in momentum space by Compton scattering**	**Experiment number**: HS 1292
Beamline: ID 15B	**Date of experiment**: from: 13.09.00 07:00 to: 19/09/00 7:00	**Date of report**: 27/08/2001
Shifts: 18	**Local contact(s)**: Marco DI MICHIEL	*Received at ESRF:*

Names and affiliations of applicants **(* indicates experimentalists)**

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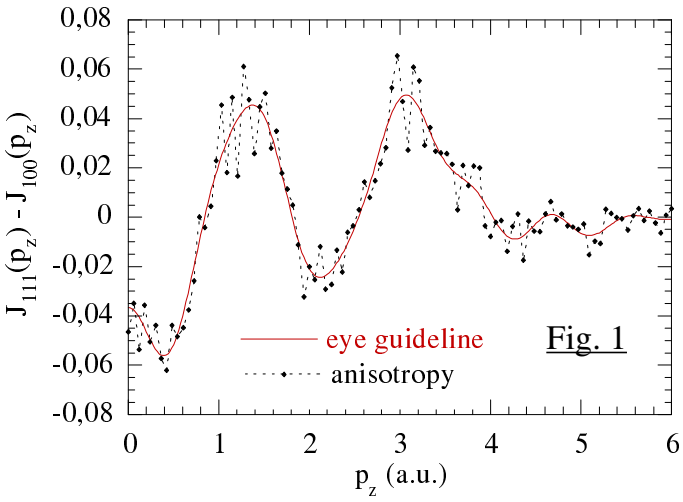
Report:

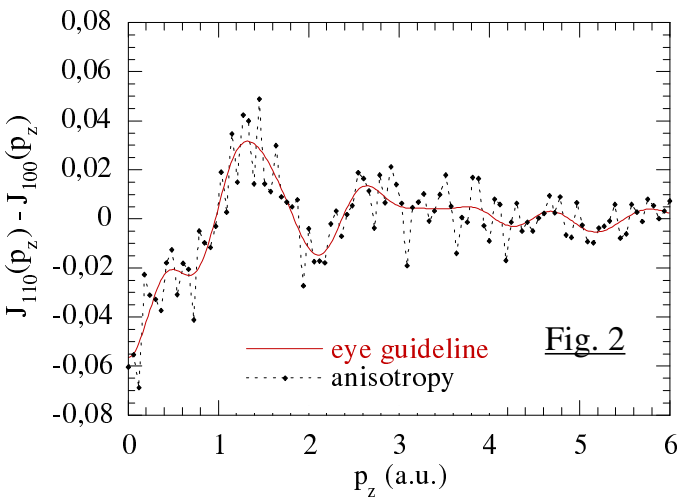
The aim of the experiment was to use Compton scattering in order to evidence the distorsion of the electronic density in Cu_2O, and more particularly to estimate the non-spherical distorsion of the ions, together with a tentative to clarify the question of hybridization of *d*-electrons with other electronic states. Until now, this question is not clearly answered ; the controversy was developped in a Nature article [1]. Let us recall the high sensitivity of the method to the spatially delocalized electrons, which are responsible of bonding. This sensitivity originates from the fact that Compton scattering delivers direct information on the ground state electronic momentum density. This method constitutes an excellent test of the quality of calculated wave functions.

The experiment has been performed with the scattering angle settled at 173 degrees and the synchrotron radiation has been monochromatized at 55.88 keV. We measured four Compton profiles with the scattering vector **K** aligned along four directions : [100], [110], [111] and [123].

The data sets have been corrected for energy dependant effects such as photoelectric absorption in sample, analyser and air (photon path between sample, analyser and detector). Since the only electrons of interest are valence electrons, calculated core Compton profile has been subtracted from the total profiles using QSCF approximation [2]. The resulting valence profile were then normalized to the number of valence electrons, and corrected from the multiple scattering contribution.

Discussion about Compton scattering results can be made by analysing the anisotropy between the directional measured profiles: the directional difference profiles $J_{hkl}(p_z) - J_{h'k'l'}(p_z)$ are virtually free from systematic errors, both theoretical and experimental ones. The figures below shows the anisotropy resulting from the difference between profiles measured along [111] and [100] crystallographic directions (Figure 1) and between [110] and [100] (Figure 2):





This anisotropy shown by Fig. 1 is dominated by a modulation with a large period in momentum space ; in particular, one can note the importance of the feature centered at $p_z = 3$ a.u.. The anisotropy obtained between both [100] and [110] directions (Fig. 2) is much lower at high momentum. The higher effect at high momentum, as one could foreseen, is given by the O-Cu-O bond which is aligned along the [111] direction, carrying *d*-type bonds.

A deep analysis of experimental measurements will receive help from *ab-initio* calculations. This Cu_2O study is part of the thesis of AmirAbbas Sabouri Dodaran : he his at present time performing a self consistent energy band calculation within the Kohn Sham density functional approximation theory and the local density approximation (LDA) using ab-initio pseudopotentials. The wave functions will be then expanded in plane waves for reconstructing Compton profiles and enable us a direct comparison between absolute directional profiles as well as anisotropies. This calculation is made within a collaboration in our laboratory with Prof. Francesco Mauri (LMCP, Univ. P6, Paris).

Both experimental results and theoretical modelization are the means for answering to questions raised for Cu_2O. Most of the outstanding results arise from real-space methods such as X-ray diffraction, whereas Compton scattering provides accurate information on delocalized electrons participating to bonding. These electrons are those of interest for our study, and thereby Compton scattering is a very adapted method for answering questions raised by Cu_2O : short-range Cu-Cu interaction (covalent bonding), charge distorsion around Cu, hybridization of d-electrons.

[1] J.M. Zuo, M. Kim, M.. O'Keeffe, J.C.H. Spence, Nature 401, 49 (1999)
[2] A. Issolah, Y. Garreau, B. Lévy, G. Loupias, Phys. Rev. B**44**, 11029 (1991)