

## 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 report should be submitted electronically to the User Office using the **Electronic Report Submission Application:**

<http://193.49.43.2:8080/smis/servlet/UserUtils?start>

### ***Reports supporting requests for additional beam time***

Reports can now be submitted independently of new proposals – it is necessary simply to indicate the number of the report(s) supporting a new proposal on the proposal form.

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.



# Experiment title:

Influence on the electronic structure of CoO from magnetic ordering

# Experiment number:

HE-1877

# Beamline:

ID08

# Date of experiment:

from: 2/3 - 2005 to: 8/3 - 2005

# Date of report:

# Shifts:

18

# Local contact(s):

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Received at ESRF:

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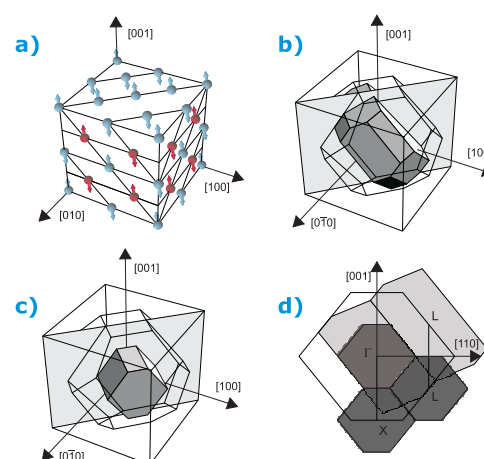
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# Report:

# INTRODUCTION / CoO STRUCTURE

CoO shows an antiferromagnetic transition at  $T_N = 289$  K. Above  $T_N$  it exhibits a paramagnetic phase where the magnetic ions compose an FCC lattice of the NaCl structure (lattice constant  $a = 4.26$  Å). On the other hand, below  $T_N$  CoO shows so-called type-II FCC antiferromagnetic (AF-II) order. Recent neutron and synchrotron X-ray diffraction studies\* reveal coexistence between the AF-II component and a different type of antiferromagnetic order, the type-I FCC (AF-I) order.

The magnetic structure of the resulting AF-I + AF-II ordering is shown in **Fig.1a**. Here the arrows indicate the direction of the magnetic moment of each ion according to the AF-II order, while colors are used to distinguish between the different orientations of the AF-I order. Moving along the face diagonal of the [010] face of this cubic cell every other magnetic moment is tilted a small angle in the negative or positive x-direction, as displayed by the alternating blue and red colors.



**Fig.1 a)** AF-I + AF-II ordering  
**b)** AF-II Brillouin Zone (BZ) inside FCC BZ  
**c)** AF-I + AF-II Brillouin Zone (BZ) inside FCC BZ  
**d)** BZ of the three different structures in the [110] plane containing the  $\Gamma$ -point.

\* Tomiyasu et al. Phys. Rev. B 70, 184411, (2004)

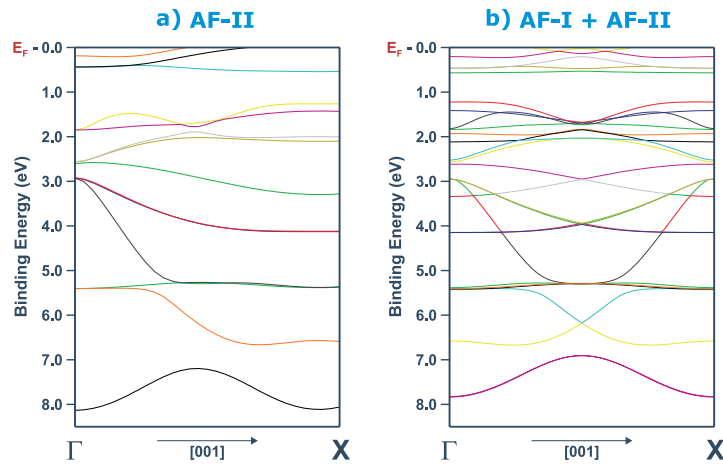
The paramagnetic phase has a unit cell with a single Co atom, while the unit cell of the AF-II phase is larger, containing two inequivalent Co atoms, one for each possible orientation of the magnetic moment. Since there are four possible orientations of magnetic moment in the AF-I + AF-II ordered phase, this unit cell has four inequivalent Co atoms and hence is even larger. The modification of the unit cell affects the symmetries in reciprocal space and the size of the Brilluoin zone (BZ). This is seen in **Fig.1b-c**, where the BZ of the paramagnetic phase is related to that of the AF-II and AF-I + AF-II phases, respectively. Distances in reciprocal space become rescaled. Directions that used to be inequivalent in the original structure will become equivalent and bands from one high symmetry direction will be folded into other high symmetry directions, as seen in **Fig.1d**.

## EXPERIMENTAL

Due to the insulating character of the compound it is not possible to perform photoemission measurements on bulk samples at low temperatures. Instead thin films are required in order to avoid electrostatic charge up effects. We have performed high photon energy angle-resolved photoemission spectroscopy (HARPES) measurements on thin CoO films grown on an Ag single crystal substrate. HARPES spectra from the film were acquired at a photon energy of 560 eV, using a Scienta SES-2002 electron analyzer. Measurements were performed at two different temperatures; above (325 K) and below (25 K) the Neel temperature of CoO (289 K). At this photon energy the experimental setup has a total energy resolution of  $\sim 150$  meV and a momentum resolution of  $\sim 0.05 \text{ \AA}^{-1}$ .

## THEORETICAL

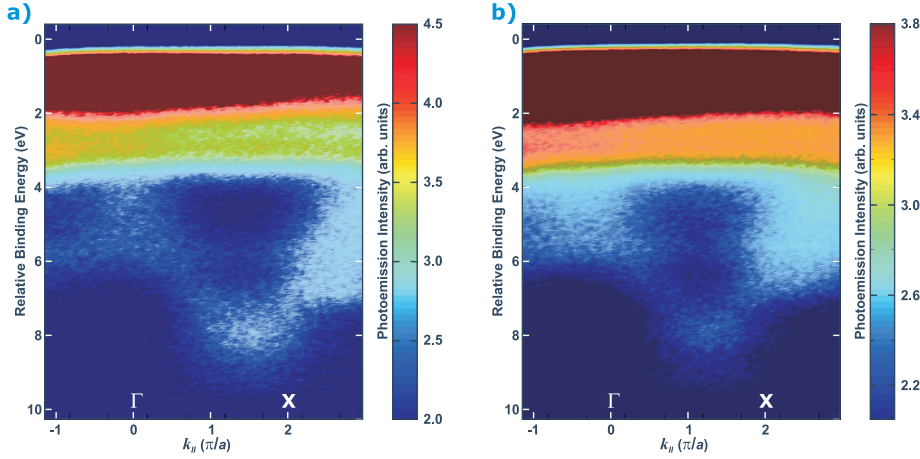
Band structure calculations have been performed on CoO in order to investigate the influence of different possible magnetic structures on the energy band structure. Calculations were performed with the WIEN2k program using a cubic cell with lattice parameter  $a = 4.26 \text{ \AA}$ . The result for CoO in the AF-II and AF-I + AF-II configurations, respectively, is presented in **Fig.2a-b**. The AF-I + AF-II structure shows an increased number of bands in the  $\Gamma$ -X direction as compared to the AF-II structure. It also shows a symmetric dispersion about the point half way between  $\Gamma$  and X.



**Fig.2** LSDA Energy band structure calculations in the  $\Gamma$ -X [001] direction for two different magnetic configurations. a) AF-II and b) AF-I + AF-II

## RESULTS

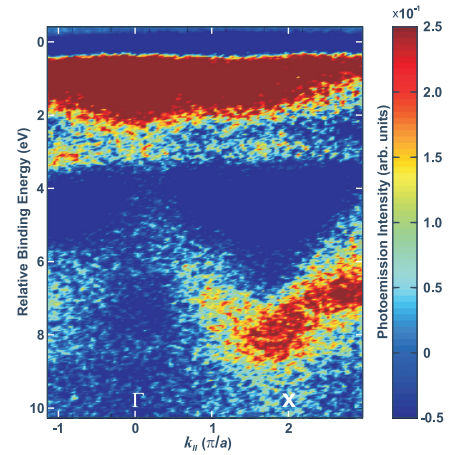
Angle resolved photoemission spectra of the valence band were recorded at a photon energy of 560 eV above ( $T = 325$  K) as well as below ( $T = 25$  K) the Neel temperature. **Fig.3** shows photoemission intensity as a function of  $k_{||}$  ( $\Gamma$ -X) and binding energy relative to the top of the valence band. The top-most part of the valence band is a  $\sim 3.5$  eV wide non-dispersive region. This area of strong spectral weight has its origin in Co 3d bands. The dispersive bands in the energy range  $\sim 4$ -8 eV are of O 2p character and show a lower intensity due to lower crosssection for photoemission at these energies.



**Fig.3** HARPES spectra for the  $\Gamma$ -X azimuth at two different temperatures: a) 25 K and b) 325 K. The dispersion of O 2p bands is clearly seen.

In **Fig.3** it is observed that the O 2p band show a clear upwards dispersion in the  $\pi/a$  to  $2\pi/a$  region. In comparison with **Fig.2**, this can be interpreted as a sign of the band symmetry induced by the AF-I + AF-II ordering. Hence, the present data indicates the influence on the electronic structure from the complex magnetic ordering.

In order to highlight the temperature dependence we show the difference between **Fig.3a** and **3b** in **Fig.4**. The O 2p bands display its most pronounced intensity difference in the region  $\pi/a < k_{||} < 2\pi/a$ . This is the region where the strongest differences in spectral weight is expected to show up, since a transfer of spectral weight from the paramagnetic band structure to the bands induced by magnetic structure should occur when the temperature is lowered through the transition temperature  $T_N$ . The intensity difference seen in the  $\pi/a$  to  $2\pi/a$  region is therefore further evidence of the magnetic structure effect on the electronic structure of CoO.



**Fig.4** Difference between Figs. 3a and 3b. The most significant discrepancy is located in the region  $\pi/a < k_{||} < 2\pi/a$ , indicating the presence of AF-I + AF-II ordering.

## CONCLUSIONS

The presented angle resolved photoemission data from thin films of CoO show clearly dispersive features along the  $\Gamma$ -X direction. The symmetry of this dispersion conforms to what is expected from an AF lattice with coexistence of two different magnetic structures (AF-I + AF-II). The same symmetry is found in band structure calculations performed on CoO in the assumed AF-I + AF-II structure. Further support for this idea comes from the transfer of spectral weight below  $T_N$ . It has its largest value in the region  $\pi/a < k_{||} < 2\pi/a$ , as expected from a lattice with the periodicity of the assumed AF-I + AF-II ordering.