ESRF	**Experiment title:** Study of magnetite by means of X-ray Anomalous Scattering: Relationship between magnetic, electronic and phonon scattering.	Experiment number: **HS-793**
Beamline:	**Date of experiment:** from: June 23-28 and March 25-30	**Date of report:**
Shifts:	**Local contact(s):** Hubert Renevier	*Received at ESRF:* - 2 MAR. 2000

Names and affiliations of applicants (* indicates experimentalists):

Joaquin García Ruiz, M. G. Proietti, G. Subías, J. Blasco and M.C. Sanchez,

Instituto de Ciencia de Materiales de Aragón. CSIC.-Universidad de Zaragoza.

Plaza San Francisco s/n., 50009 Zaragoza, Spain.

Hubert Renevier and Jean-Louis Hodeau.

C.N.R.S.-U.J.F., Laboratoire de Cristallographie, 38042 Grenoble Cedex, France.

Report:

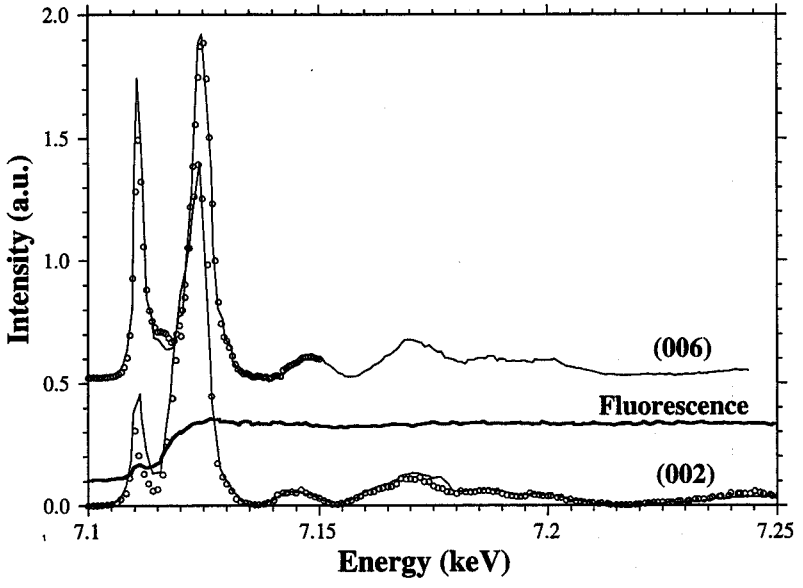
Mixed valence transition metal oxides exhibit many interesting properties such as superconductivity, colossal magnetoresistance and metal insulator phase transitions. Generally, the description of the electronic state of these compounds is made in basis of the ionic model and it implies the spatial or temporal charge localization in the transition metal atoms.

Magnetite is the archetypical mixed oxide. It was the first material in which a charge ordering transition was proposed to explain the metal insulator phase transition which occurs at 125 K. The classical mechanism to describe this transition states that the distribution of octahedral Fe3+ and Fe2+ ions changes from dynamic disorder to long range order by lowering the temperature. Nevertheless, this point has not yet been observed.

We measured the forbidden reflections (002) and (006) of the cubic cell by means of resonant scattering at the iron K-edge. Experiments were performed at the beamline D2AM at the ESRF in Grenoble. The evolution of the intensity of these reflections as a function of the incoming x-ray beam energy, the azimutal angle and the polarization dependence of the scattering process (components s-s and s – s+p) were studied. The analysis, of the diffraction peak intensities and the comparison between the (002) and (006) reflections show that they

are due to the anisotropy of the scattering factor produced by the splitting and ordering of the unoccupied density of states. Three energy regions can be distinguished: i) A resonance corresponding to the prepeak energy in the fluorescence spectrum which has some quadrupolar character. Ii) The main resonance at the edge, that is mainly of dipolar character and has its origin in the anisotropy of the dipolar scattering factor of the trigonal distorted octahedral iron atoms. Iii) The extended part, with a dipolar character,that shows an oscillatory behavior as a function of the energy.

The presence of the main resonance means that all the octahedra are identical on a time scale lower than 10^{-16} sec showing that no charge fluctuation occurs in magnetite at room temperature. Moreover, the experiments performed below the Verwey transition temperature, also show that no charge ordering occurs at the metal insulator phase transition. As a general conclusion we can say that octahedral iron atoms in magnetite can not be described as pure ionic Fe^{3+} or Fe^{2+} ions neither spatially or temporally. As a consequence, the Verwey transition should be due to the opening of a gap in the electronic band produced by the crystallographic distortion that takes place at the phase transition.



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-"Absence of charge ordering below the Verwey transition temperature in magnetite." J. García et at. Submitted Phys. Rev. Lett.

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