

**Experiment title:**

X-ray natural linear dichroism of paramagnetic ions in corundum

Experiment number:
HS-773**Beamline:**

ID26

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9

Local contact(s):

Christophe Gauthier

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01 MAR. 1999**Names and affiliations of applicants (* indicates experimentalists):**

Philippe SAINCTAVIT*, Bruno BOIZOT*, Aline RAMOS*, Delphine CABARET*

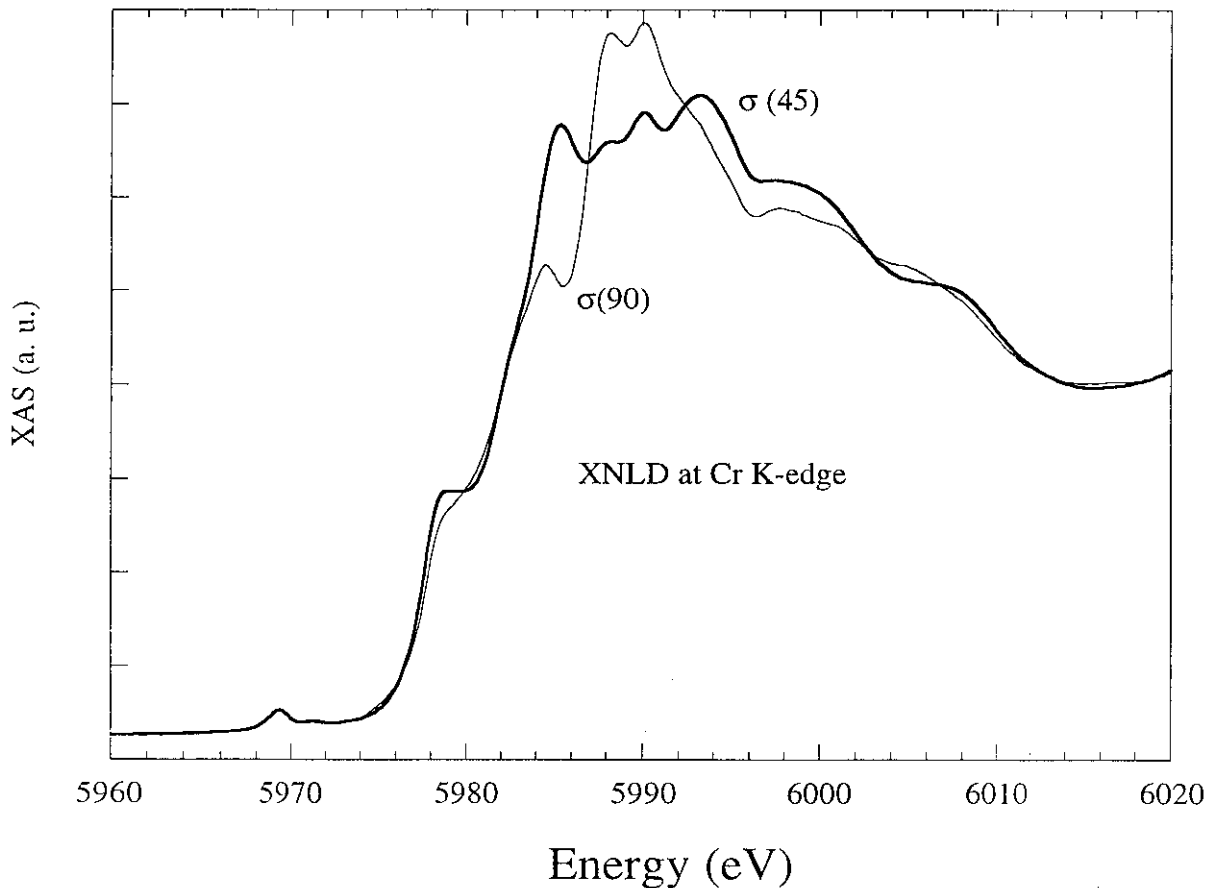
Laboratoire de minéralogie-cristallographie
UMR CNRS 7590, UPMC/UDD/IPGP
case 115, 4 place Jussieu,
75252 Paris cedex 05, France

Report:

The purpose of the experiment was the measurement of the natural linear dichroism in single crystals of ruby. Rubys are corundum single crystals doped with various amounts of chromium. The chromium ions are at the origin of the Ruby red colour. We have a whole series of rubys with chromium concentration varying from 60 ppm up to 1%. We have measured XANES and EXAFS spectra in three different rubys for different angles between the linear polarization vector and the crystal optical axis. The chromium concentration in the three samples studied are 60 ppm, 800 ppm and 1 %.

The XANES were recorded with the silicon diodes developed by Christophe Gautier and José Goulon. An excellent signal to noise ratio has been obtained, even for the lowest concentration. It has been possible to remove Bragg diffraction peaks in the first 150 eV in the three samples. A large dichroic signal has been measured (see figure below). The experimental isotropic and dichroic XANES signals are under way of interpretation: We are calculating the geometric relaxation around chromium in corundum using pseudo-potential band structure calculations. When these theoretical geometric parameters are known, we shall use the crystallographic coordinates of the relaxed structure and the self-consistent potentials to compute the dichroic theoretical XANES spectra in the framework of Full Multiple Scattering method.

The EXAFS spectra are more difficult to exploit. Due to Bragg diffraction it has been impossible to register an EXAFS spectrum without large spurious peaks. To cope with the problem we have registered several EXAFS spectra for various angles θ between the normal of the sample and the polarization vector. In the analysis of the data, we have tried to remove the Bragg peaks with linear combinations of several EXAFS measurements for slightly different angles θ . This method does not work, because some spurious linear dichroic oscillations superimpose to the EXAFS spectra. We are still working on this problem but think that the method developed by ID12A scientists to remove Bragg peaks in single crystals (see our new proposal) is certainly the best way to register good dichroic EXAFS spectra



XANES spectra at Cr K-edge for two different angles (thin line: $\theta=45^\circ$ and thick line: $\theta=90^\circ$) between the optical axis and the polarization vector. The chromium concentration is 800 ppm.