

Combined XAS and XMCD studies under pressure of iron and iron based compounds

MATHON O.¹, BAUDELET F.², DECREMPS F.³, ITIE J.-P.³, NATAF L.³,
PASCARELLI S.¹, POLIAN A.³

¹European Synchrotron Radiation Facility, B.P. 220, F-38043 Grenoble Cedex, France, ²Synchrotron SOLEIL, B.P. 48, F-91192 Gif-sur-Yvette Cedex, France, ³IMPMC, 140, rue de Lourmel, F-75015 Paris, France

X-ray Absorption Spectroscopy (XAS) and X-ray Magnetic circular dichroism (XMCD) performed simultaneously is a powerful technique to investigate condensed matter properties under high pressure. The high sensitivity of XMCD allows us to follow the magnetic transition and to correlate it to the local structure followed by XAS. Thus, we can obtain simultaneous information on the magnetic state and on the structural properties of the system (both determined under the same thermodynamic conditions) by probing the same volume of the sample.

These experiments have been performed on ID24, the energy dispersive beamline. The high flux, the beam stability, the highly focusing optics and the use of a quarter wave plate to produce circularly polarized X-rays, make this beamline particularly suited for combined XAS/XMCD high pressure measurements with a Diamond Anvil Cell (DAC) [1]. In particular, the small focal spot on the sample (about 5 by 5 μm^2 FWHM at the Fe-K edge) is an important factor to decrease the effect of pressure gradient inside the experimental volume of the DAC.

The Iron α - ε phase transition case is a good example to illustrate the possibility of combined XAS/XMCD on an energy dispersive beamline [2]. Under the application of an external pressure, Iron undergoes a transition around 13 GPa from the bcc α phase to the hcp ε structure, with the loss of its ferromagnetic long range order. Despite many experimental and theoretical investigations, the mechanism of this phase transition is still not clear. We took advantage of the combination of the two techniques to probe simultaneously the structure and the magnetic state. The magnetic and structural transitions are sharp, both are of first order and the pressure domain of the transition is about 2.4 GPa \pm 0.2 GPa. Our data seems to indicate that the magnetic transition slightly precedes the structural one, suggesting that the origin of the instability of the bcc phase in Iron with increasing pressure could be attributed to the effect of pressure on magnetism.

Investigation of the invar effect on Iron based alloys like Fe₃C [3], Fe₃Pt and Fe_{0.64}Ni_{0.36} will be also presented. These experiments confirm the 2 γ -state model in terms of gradual population of a low spin-small volume state at the expense of a high spin-large volume state under pressure. Only some results obtained on Fe_{0.64}Ni_{0.36} diverge curiously from this model, suggesting that the preparation and the magnetic history of the sample seems to be of crucial importance.

References

- [1] – O. Mathon, F. Baudelet, J.-P. Itié, S. Pasternak, A. Polian and S. Pascarelli, *J. Synchrotron Radiat.* 11, 423 (2004).
- [2] – O. Mathon, F. Baudelet, J.-P. Itié, A. Polian, M. d'Astuto, J.-C. Chervin and S. Pascarelli, *Phys Rev Lett* 93, 25503 (2004).
- [3] – E. Duman, M. Acet, E. F. Wassermann, J.-P. Itié, F. Baudelet, O. Mathon and S. Pascarelli, *Phys. Rev. Lett.* 94, 077502 (2005).