ESRF	Experiment title: The tailoring of magnetovolume instabilities and their observation in the pressure dependence of the K-edge circular dichroism of $(Fe_{3.68}Mn_{0.32})N$ alloys.	**Experiment number**: HE-1945
Beamline: ID24	**Date of experiment**: from: 27.04.2005 to: 03.05.2005	**Date of report**:
Shifts: 18	**Local contact(s)**: Olivier MATHON	*Received at ESRF:*

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Report:

The structure of Fe_4N, otherwise known as the mineral roaldite, is face centered cubic with a nitrogen atom located in the center octahedral interstitial position. It is ferromagnetic with a Curie temperature of about 760 K and carries an average magnetic moment of about 2.21 μB per Fe atom. N binds to the interstitial positions of *3d* metals essentially through the hybridization of the metalloid *2p* states and the states in the *3d* band of the host metal. This hybridization leads effectively to an increase of the metal's valence electron concentration *e/a* (electrons per atom). Substituting Mn [*(e/a)* = 7] in place of Fe in Fe_4N [*(e/a)* = 8.75] reduces the electron concentration to 8.67 in $(Fe_{3.68}Mn_{0.32})N$. This corresponds to a value where one finds the very interesting magnetic properties associated with strong magneto-volume instabilities in substitutional and interstitial *3d* systems, namely the Invar properties. The Invar behavior is generally explained by an effect called "moment-volume instability," which means that the volume of the unit cell and the magnetic moment of its atoms are correlated, and thermal lattice expansions can be compensated for or increased if at the same time the magnetic moment of the atoms change with temperature. $Fe_{0.65}Ni_{0.35}$ and Fe_3C are the archetypes of substitutional and interstitial alloys respectively.

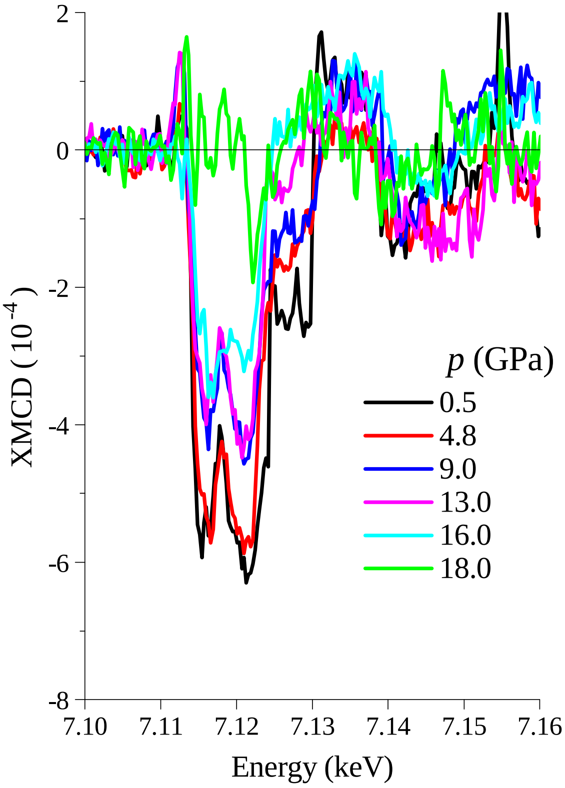

Figure 1. The XMCD spectra from ambient pressure up to 20 GPa at selected pressures

$(Fe_{3.68}Mn_{0.32})N$ was prepared by the nitrogenation of $Fe_{1-x}Mn_x$ powder in a flowing atmosphere of hydrogen/ammonia at 480 °C. We have investigated the XMCD at the *K*-edge of Fe in this material at room temperature and pressures up to 20 GPa on increasing and decreasing pressure. The measurements were made at the ESRF on the ID24 beam line installed on an undulator source. The circular polarization was attained using a quarter wave plate. Two sets of measurements at each pressure with both polarization elipticities and both magnetic field directions were taken in order to eliminate systematic errors arising from the quarter wave plate and the magnetic field. A magnetic field of

0.4 T was applied using an electromagnet, and a membrane type diamond anvil pressure cell was used in the experiments.

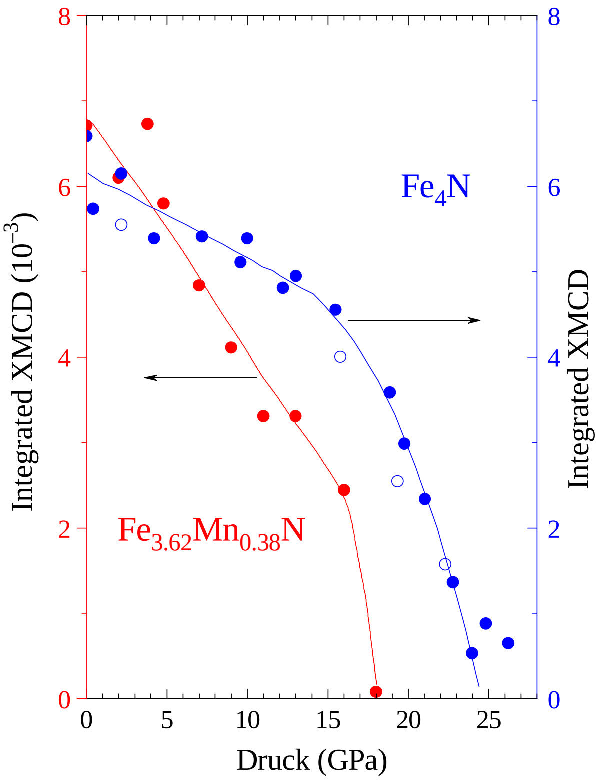

Figure 2. Integrated XMCD of $Fe_{3.62}Mn_{0.38}N$ and Fe_4N. The ordinate of the data of Fe_4N is scaled to the data of the present sample.

Fig. 1 shows the XMCD spectra from ambient pressure up to 20 GPa. The shape of the XMCD spectrum at 0.5 GPa is consistent with the spectrum of Fe_4N at same pressure obtained by Ishimatsu et al. [1]. We observe a systematic weakening of the signal with increasing pressure, especially in the range $7.11 \le E \le 7.13$ keV. The absolute value of the integrated XMCD obtained after subtracting the background intensity before and after the *K*-edge is plotted in Fig. 2. The intensity shows a gradual decrease with increasing pressure and, then, begins to decrease rapidly around 15 GPa. At about 20 GPa the intensity vanishes. The drop in the intensity is of similar character to that of Fe_4N [3] as seen in Figure 2.

The rapid decrease of the integrated XMCD indicates the possibility of the presence of a magnetovolume instability in $(Fe_{3.68}Mn_{0.32})N$. However, in order to be conclusive it is necessary to investigate the temperature dependence of the lattice constant of $(Fe_{3.68}Mn_{0.32})N$ as well as the equation of state.

Reference

N. Ishimatsu et al. *Nuclear Instruments and Methods in Physics Research A*, 467–468, (2001), 1061.