ESRF	**Experiment title:** High-pressure low-temperature x-ray diffraction of invar alloys : a way to understand the nature of the ferromagnetism of 3d metal and alloy	**Experiment number**: HS2735
Beamline: ID09	**Date of experiment**: from: 09 march 2005 to: 14 march 2005	**Date of report**: 10/07/05
Shifts: 15	**Local contact(s)**: Dr. Michael HANFLAND	*Received at ESRF:*

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Report:

The invar effect, almost no thermal expansion around the room temperature, is a subject of many experimental and theoretical studies since its discovery, more than one century ago [1]. It is clear and recognized that this unusual behaviour is related to magnetism, but the microscopic processes are still not fully understood. One of the most popular models proposed is the 2 γ-state model, in which iron can occupy two different states: a high spin (HS) – high volume state and a low spin (LS) – low volume state. When the temperature, or the pressure, is increased the LS state is populated at the expense of the HS one [2] and the usual thermal expansion due to the lattice vibrations is compensated. For Fe-Ni invar alloys, recent *ab-initio* calculations allow to propose a new microscopic explanation of invar effect [3]. According to this model, the invar effect is explained as a continuous transition from a ferromagnetic state at high volume to a disordered non-collinear configuration at low volume. In the latter model, no pressure transition is expected since the transition is continuous, whereas in the 2 γ-state model, the transition is expected to be a first order one.

Recently, x-rays diffraction experiments have been performed on Fe-Ni alloys (with different composition) up to 20 GPa [4], in order to obtain the volume and therefore the bulk modulus pressure dependence. In this work, the bulk modulus B is found to behave in very good agreement with what is expected from the non-collinear model. On the contrary, recent ultrasonic results show a linear dependence of B(P) with a discontinuity of the slope at 3 GPa [5].

At ambient conditions, the 2 γ-state model predicts that some LS states are thermally populated, so no kink in the pressure dependence of the volume can be observed. In order to distinguish the order of the transition, and thus the validity of one model to another, experiments have to be performed at low temperature, where no LS state can be thermally populated.

Our first objective was to perform high pressure x-ray diffraction experiment at low temperature on a polycristalline $Fe_{64}Ni_{36}$, the prototypical invar alloy. Moreover, even though Fe-Ni and Fe-Pt alloys have similar magnetovolumic properties, which lead to the invar effect, they have dissimilarities in their magnetic properties: iron-nickel is a weak ferromagnet, in contrast to iron-platinum which is a strong ferromagnet. So our second objective was to carry out the same experiment on a disordered $Fe_{72}Pt_{28}$. The comparison of the two equations of state gives a better understanding of the differences between those compounds and, then, of the nature of the ferromagnetism in 3d metals and alloys.

We have used membrane diamond anvil cells (MDAC) having a large x-ray conical aperture. The pressure medium was argon, gaskets were in stainless-steel and the pressure was measured with the luminescence of a ruby ball. The cell was placed into a cryostat equiped with windows. The temperature was determined with a thin thermocouple soldered on the brass diamond centring piece and thanks to the relative intensity of the luminescence peaks. Three different samples were compressed up to about 25 GPa at constant temperature (35 K). High pressure powder diffraction was performed on ID09 using the monochromatic (λ=0.4130 Å) angular dispersive method. Reflections were collected with a plane detector (MAR3450). During acquisition, the MDAC was rocked through ± 3° in order to improve the powder statistic.

Spectra collected for Fe-Ni and Fe-Pt are shown on figure 1, both at 2.5 GPa and 35 K. The hkl Bragg reflections 111, 200, 220, 311, 222 were observed up to highest pressure and give rise to an accurate determination (10^{-4}) of the cell parameter for both compounds as function of pressure. In the pressure range [3-5] GPa, we observe a kink in the evolution of the volume, similar to what is usually observed during a first order transition. However, in Fe-Ni, the magnetovolumic effect on the lattice parameter is less pronounced at low pressure, in good agreement with what can be expected from previous study [6]. The discussion of our results are in progress, especially in view of recent data that we have obtained using XMCD technic (cf report HE1946).

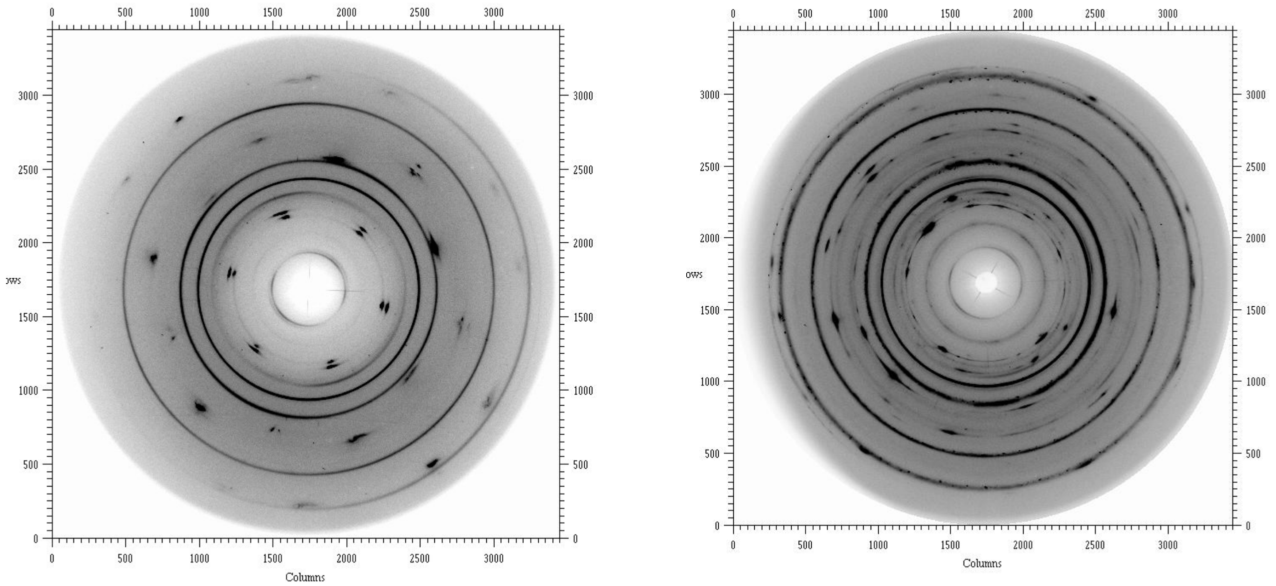

Figure 1: spectra collected at 2.5 GPa for $Fe_{64}Ni_{36}$ (on the left) and for $Fe_{72}Pt_{28}$ (on the right)

References

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