ESRF	**Experiment title:** **Spin polarized Momentum distributions in Ordered and disordered Fe_3Pt**	**Experiment number**:
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Report:

The $Fe_{(1-x)}Pt_x$ system exhibits the invar effect at concentrations around the stoichiometric ordered Fe_3Pt phase. The aim of our experiment was to investigate the spin polarised electron momentum distribution as a function of temperature between 15K and 550K, in the ordered (Cu_3Au) and disordered phases of the invar system Fe_3Pt, using the magnetic Compton scattering MCS technique. In order to investigate the momentum distribution of the spin moment and compare with LMTO, FLAPW and KKR electronic structure calculations, in order to determine if a Fe moment collapse occurs at high temperatures in the material as recently proposed by Srajer, from a discernible change in the MCS line shape at high temperature in Fe_3Pt [1].

Since the invar effect was discovered by Guillaume the mechanism producing near thermal expansion near room temperature has been widely debated. Weiss proposed a simple two state model, whereby thermal population of two nearly degenerate magnetic states exists in FCC Fe, a high spin ($2.8\mu_B$), high volume state and a low spin ($0.5\mu_B$) low volume state counteracts the thermal expansion of the lattice. However the existence of these spin states has not been observed at atmospheric pressure in any invar material. Our results do **not** support the earlier, less accurate, published ones [1].

MCS provides the only direct method of measuring the spin moment and has proved a useful technique in understanding the magnetism in both 3*d* and 4*f* materials. Furthermore since the Magnetic Compton Profile samples all spin polarised electrons in the system, regardless of wave-function symmetry it is a powerful check on spin polarised electron structure calculations. It is well known that structural order in this series strongly influences the magnetism, such that difference in T_c between ordered and disordered samples is ~100K being 350K and 490K for the disordered and ordered phases respectively.

In our experiment we measured ordered and disordered samples of Fe_3Pt along two of the major crystallographic axes namely 111 and 110, as a function of temperature. Measurements were made at low temperature 15K, below the BCT martensitic transition (100K), room temperature and at high temperature ~500K (10K above and 10K below T_c). *A total of 15 MCP's were collected during the 18 shifts of beam time awarded for this investigation*. The samples were characterised using a VSM to check they exhibited the required transition temperatures.

The results were analysed in the standard way and corrected for magnetic multiple scattering, the resulting MCP's were compared with LMTO and FLAPW electronic structure calculations for the ordered sample and single site Greens function KKR calculations for the disordered sample.

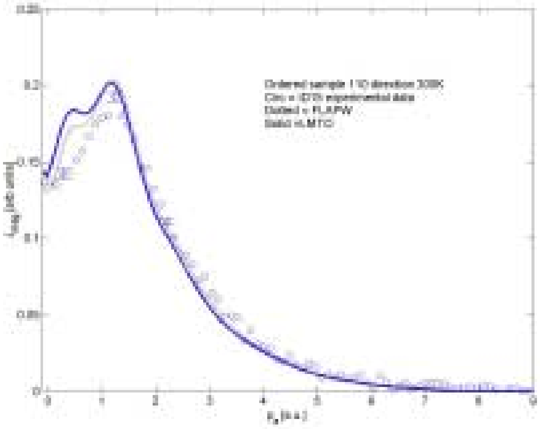


Fig.1. MCP for ordered Fe_3Pt resolved along 110 direction at 300K compared with LMTO and FLAPW calculations of equal integrated area.

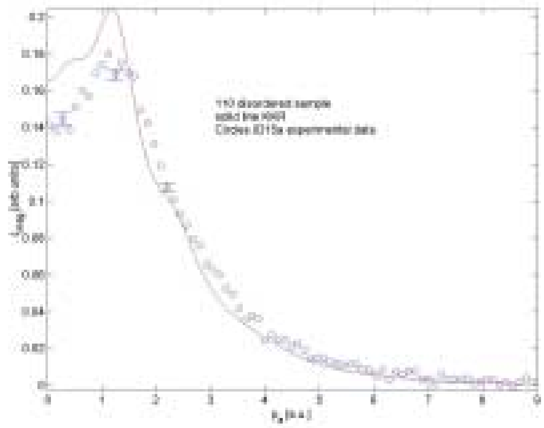
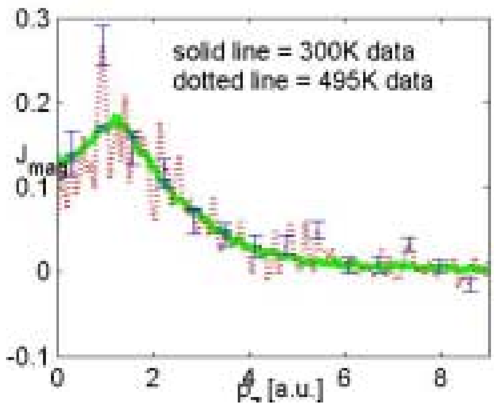


Fig.1. MCP for disordered Fe_3Pt resolved along 110 direction at 300K compared with KKR calculations of equal integrated area.

Fig 3. Comparison of high temeprature and room temperature MCP's for Fe_3Pt demonstrating that now change in the 3d Fe moment is observed in this material



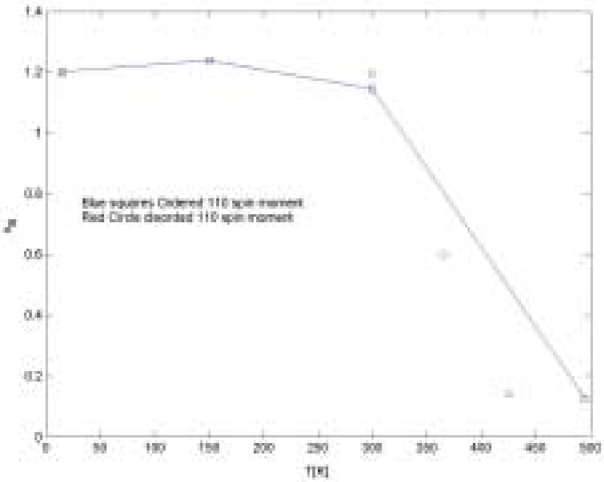


Fig. 4. Fe_3Pt spin moment as a function of temperature for 110 ordered sample.

In summary:

- Our results demonstrate that the spin polarised electron momentum distribution has the same characteristic shape as a Fe 3d type moment and does not exhibit any change in shape at high temperatures, in contradiction to a previous publication.
- The measured spin moments are in agreement with those expected for Fe_3Pt.
- The thermal evolution of the spin moment exhibits a maximum at ~100K, corresponding to the BCT(?) martensitic transition temperature in Fe_3Pt.
- Significant short range ordere exists above T_c in both samples.
- Comparison with electronic structure calculation shows that the Fe 3*d* band is modelled incorrectly in both the LMTO and KKR cases, the FLAPW code yields an improved lineshape for the ordered material.
- The result is now being submitted to Phys. Rev. B.
- Measurements at high pressure, where there is some evidence that a high spin/ low spin transition may occur, should now be made.

[1]. G. Srajer, *et al.*, J. Phys. Cond. Mat. L253 (1999)