ESRF	**Experiment title:** Spin moments in PdCo alloys and compounds studied by magnetic Compton scattering	**Experiment number:** HE- 160
Beamline: ID15a	**Date of experiment:** from: 9/5/97 to: 23/5/97	**Date of report:** 2/7/97
Shifts: *30*	**Local contact(s):** Thomas Tschentscher	*Received at ESRF:* 15 JUIL. 1997

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Report:

There were two main objectives of this experiment. First, to determine any differences in the magnetic Compton profiles (MCPs), and total moments of ordered and disordered polycrystalline Pd_3Co, which are predicted by theory'. In fact, we observed a small difference in the MCP at low momentum, which we attribute to a change in the magnetic contribution of the Pd 4d electrons. The second objective was to begin a series of measurements on ordered single crystal Pd_xCo_{1-x} alloys. In this *tranche* of beamtime, we made two successful measurements on Pd_3Co, along <110> and <111>, despite suffering a number of technical problems.

Magnetic Compton scattering is an established technique, useful for investigating the spin moments of magnetic materials. It measures the 1D projection of the electron momentum density, and in the magnetic case, by use of a reversible field and circularly polarised x-rays, only those electrons which contribute to the magnetic moment are measured. As such, it is a method for investigating spin-polarised band-structures.

Three shifts were lost due to beamline problems. During the single crystal measurements, we lost around 6 shifts due to an alignment problem. This took this length of time to discover because we were collecting apparently normal MCPs. In the polycrystal measurements, we had problems with sample movement as the permanent magnet rotated; the samples appeared to be mechanically soft. We were able to minimize this problem by lowering the scattering

angle from 170° to 160°. We are modifying the rotation mechanism to reduce the torque on the sample.

In figure 1, we present the MCPs of ordered and disordered Pd_3Co. At high momentum, where the contribution is attributed to the Co 3d electrons, no difference is observable. In the region $|p_z|<1$a.u., a difference, due to a change in the induced moment of the Pd 4d electrons is observed. We are analysing the data to obtain a quantitative comparison of the total moments. However, it appears that at low momentum, there is a slightly larger dip in the disordered case. The size of dip, compared to the rest of the profile, is due to a change in the contribution of the Pd 4d electrons, which is qualitatively in agreement with theory'. Further beamtime is necessary to investigate this in more detail. We would use powdered samples, which would ensure good directional averaging. Because of the heat treatments necessary to produce the ordered material, we cannot be sure that both samples have the same degree of polycrystallinity, even though they were cut from the same rod. We now have access to computer code (based on the KKR technique) which will enable us to calculate MCPs for both ordered and disordered materials,

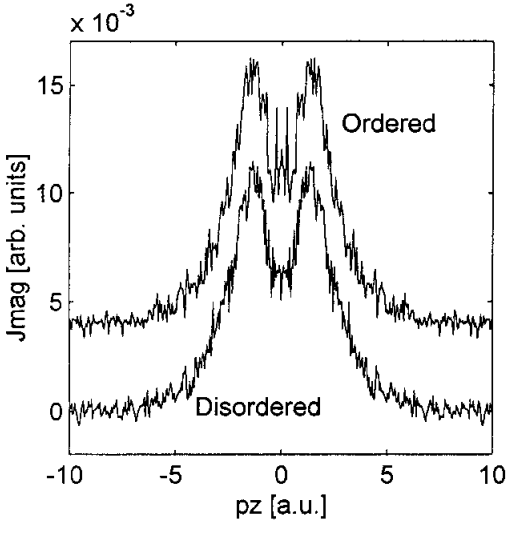

Figure 1

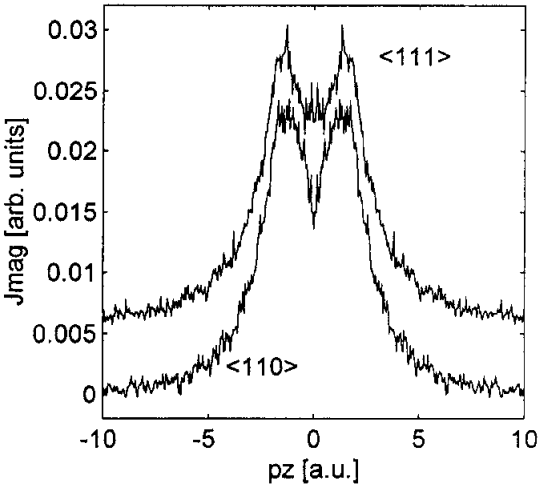

Figure 2

Figure 2 shows the MCPs for the single crystal material. These exhibit anisotropy at low momentum, where the <110> projection exhibits a deep narrow dip. This indicates that there is a negatively polarised contribution to the spin density. The Pd contribution is expected to be positive, and we hope to continue this study in a further beam time allocation in order to determine the origin of this feature. These data have interested T. Jarlborg (University of Geneva) such that he is planning to perform LMTO calculations of the band-structure and MCPs. We would also like to investigate the systemmatic changes involved when the Co is replaced by the other magnetic 3d transition metals, Fe and Ni.

[1] S. Kapryzk, et al., J. *Mag. Mag. Mat.* (1992) 104-107 2019.