ESRF	**Experiment title:** Study of the Sm spin density in $SmMn_2Ge_2$	**Experiment number**: HE780
Beamline: ID15A	**Date of experiment**: from: 07/06/00 to: 13/06/00	**Date of report**: 03/08/00
Shifts: 18	**Local contact(s)**: Joanne McCARTHY	*Received at ESRF:*

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Report:

The spin moments of the layered ternary compounds $SmMn_2Ge_2$, $GdMn_2Ge_2$ and $LaMn_2Ge_2$ were measured on the high energy beamline ID15A using the magnetic Compton scattering technique. Our earlier results of measurements made on $SmMn_2Ge_2$ using magnetic Compton scattering (ID15A - IHR time) showed large spin and orbital moments present in the low temperature ferromagnetic phase (<105K), whilst the existence of a Sm *4f* spin moment was observed for the first time in the high temperature ferromagnetic phase (155K to 345K). These earlier results will be published as a Rapid Communication in Phys. Rev. **B 62** (September 1st 2000). For the present experiment HE780, the aims were firstly to measure the magnetic Compton profiles (MCP) of $GdMn_2Ge_2$ (no *4f* orbital moment) in order to understand the effect on the moment of spin-orbit coupling, and $LaMn_2Ge_2$ (no *4f* moment at all) to determine the extent to which the Mn moment governs the magnetic behaviour. Secondly we aimed to make a systematic temperature study of the moments present in $SmMn_2Ge_2$. This compound is one example of naturally layered materials where the magnetic ordering depends critically on the Mn-Mn separation. For values above 2.87Å the compounds are ferromagnetic and below it they are antiferromagnetic. In $SmMn_2Ge_2$ the spacing is close to this borderline value and it is not surprising that it exhibits both re-entrant ferromagnetism and antiferromagnetism, the latter in the range 105-155K. It also shows GMR behaviour although with an opposite sign to the norm. Understanding its magnetic behaviour is of clear relevance to studies of artificial multi-layered GMR materials.

The MCPs of $GdMn_2Ge_2$ and $LaMn_2Ge_2$ were measured at 15K and the spin moments present on the Gd and Mn sites in $GdMn_2Ge_2$ and on the Mn sites in $LaMn_2Ge_2$ were determined. The MCPs are shown in Figs. 1 and 2. Unfortunately, due to an obscure error in the data collection program written for us at the ESRF the data for one of the magnetic field directions was repeatedly overwritten rather than summed in the raw datafile. This was not discovered until near the end of the experiment, the statistical errors were poor and

measuring times were subsequently much longer than would otherwise have been necessary. Consequently, only one temperature was measured for $SmMn_2Ge_2$ (it is planned to resubmit a proposal in order to complete the systematic temperature study). The MCP of $SmMn_2Ge_2$ measured at 230K along the *c*-axis (easy magnetic direction) is shown in Figure 3.

The data can be analysed in terms of Mn *3d* and Sm and Gd *4f* orbitals. At large momenta the spin resolved Compton profile must be well fitted by free atom modelling of the momentum density. This fact arises from the following energy considerations: the second moment of the Compton profile is proportional to the kinetic energy of the system and, via the virial theorem, the total energy. The small energy differences between free atom and solid that result in cohesion are necessarily associated with the low momentum region of the profile (p_z < 1.5 a.u.). This means that the high momentum region can be analysed confidently in terms of free atom Compton profiles. The Compton profile of a Sm *4f* electron is some 50% broader than that of a Mn *3d* electron and thus the MCP can be uniquely analysed at high momentum in terms of the *4f* and *3d* contributions. Fig. 3 shows the decomposition of the data by this method (the other figures show only the final fit, not the individual contributions). The total spin moments, as well as the individual *4f* and *3d* contributions for each of the three samples are given in the table. Combination of total spin moments measured here and bulk magnetisation measurements currently being made at Warwick University will allow us to determine the orbital moment present in each compound.

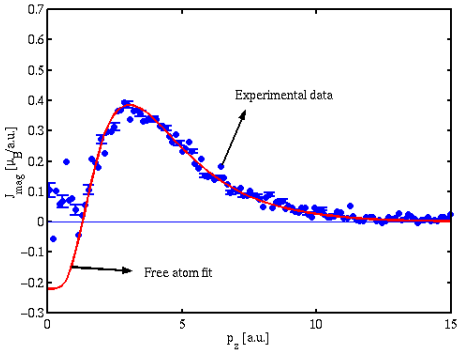

Fig. 1. $GdMn_2Ge_2$ at 15K

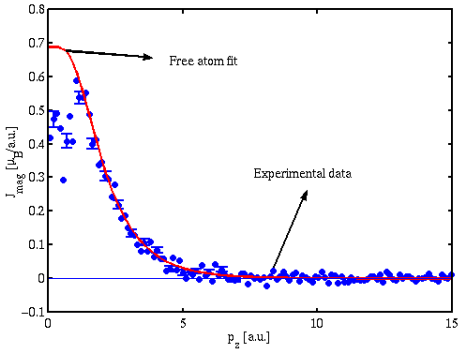

Fig. 2. $LaMn_2Ge_2$ at 15K

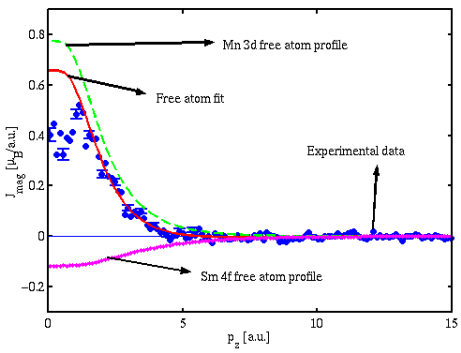

Fig. 3. $SmMn_2Ge_2$ at 230K

Magnetic moments [μ_B]	**$LaMn_2Ge_2$ at 15K**	**$GdMn_2Ge_2$ at 15K**	**$SmMn_2Ge_2$ at 230K**
Total spin	+2.7(1)	+3.6(1)	+2.2(1)
***4f* spin**	-	+8.3(1)	-0.9(1)
***3d* + delocalised spin**	+2.7(1)	-4.7(1)	+3.1(1)

Immediate conclusions are that firstly, we once again observe the presence of a Sm *4f* moment in the high temperature phase for $SmMn_2Ge_2$, confirming the findings of our earlier experiment. The fit at high momenta is only good if a Sm *4f* moment is included. This moment is of similar size at 230K when the external field is aligned both parallel (easy direction, -0.9μ_B) and perpendicular to the *c*-axis (-0.7μ_B). It is the Mn sublattice which hardens considerably (*3d* + delocalised moment decreases from 3.1μ_B to ~1μ_B). Secondly, in $GdMn_2Ge_2$, the Gd *4f* moment is aligned parallel to the total spin moment, and antiparallel to the Mn *3d* moment. The Mn *3d* moment is much larger in $GdMn_2Ge_2$ than for La or Sm. First analysis implies that this is due to the Mn spins being canted in $LaMn_2Ge_2$ and $SmMn_2Ge_2$, but aligning along the field direction in $GdMn_2Ge_2$. When canted, only their projections along the external magnetic field direction are measured. Lastly, the free atom fit to the $LaMn_2Ge_2$ data confirm that there is no *4f* moment present. Further analysis is now necessary to determine the effect of spin-orbit coupling, and to identify exactly the non-*4f* contribution using the $LaMn_2Ge_2$ data.