	Experiment title: X-ray absorption magnetic circular dichroism study of the magnetic properties of the newly discovered ferromagnet UBeGe	**Experiment number**: HC-2091
Beamline: ID12	**Date of experiment**: from: 09/09/2015 to: 14/09/2015	**Date of report**: 14/02/2017
Shifts: 9	**Local contact(s)**: WILHELM Fabrice	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Yuki Utsumi*, Stefano Agrestini*, Roman Gumeniuk*

Max-Planck Institut CPfS, Nöthnitzer Str. 40, 01187 Dresden - Germany

Report:

Uranium compounds are known to exhibit a wide range of physical properties including ferromagnetism, Pauli paramagnetism, heavy fermion behaviour and unconventional superconductivity. Particularly, the coexistence of superconductivity with ferromagnetism in uranium compounds [1, 2] has attracted great interest in the scientific community. Recently the new compound UBeGe with the ZrBeSi type of crystal structure was discovered in our group [3]. Magnetization study performed on polycrystalline samples revealed that UBeGe is ferromagnetic with Curie temperature T_C = 157 K, which is one of the highest T_C among known uranium compounds not containing ferromagnetic elements. The magnetic susceptibility obeys a Curie-Weiss law from 400 K down to 200 K. A Curie-Weiss fitting above 200 K indicates the large effective magnetic moment of μ_{eff} = 3.2 μ_B. The experimentally observed saturation moment is 2.4 μ_B. Band structure calculations have great difficulties to explain this number: LSDA+U with U = 0 eV finds M_{spin} = 1.8 μ_B and M_{orb} = -2.4 μ_B, with U = 2 eV: M_{spin} = 1.6 μ_B and M_{orb} = -1.9 μ_B and with U = 4 eV: M_{spin}= 2.1 μ_B and M_{orb} = -1.8 μ_B. The calculated values for M_{spin} and M_{orb} thus vary wildly depending on the choice of U.

In the proposal we planned a X-ray magnetic circular dichroism (XMCD) study at the U $M_{4,5}$ edges with the goal of a basic understanding of the electronic and local magnetic structure of Uranium in UBeGe. XMCD is a powerful method to obtain the orbital and spin magnetic moments of U 5f shell since $M_{4,5}$ edges involve the transition between 3d and 5f states. A large number of XMCD measurements at $M_{4,5}$ edge were performed on ferromagnetic uranium compounds demonstrating the capacity of this technique to provide reliable L_z and S_z values [4-6].

We have carried out x-ray magnetic circular dichroism (XMCD) experiments at the U-$M_{4,5}$ edge on polycrystalline sample of UBeGe at 2 K under a magnetic field of 3 T. The measured XAS and XMCD spectra are shown in Fig. 1. The XMCD signal at the M_4 edge possesses a single negative lobe as well as other reported uranium compounds [7], whereas a positive and a negative lobes are observed at the M_5 edge. Such double-lobe structure was also observed for UGe_{13}, UPt_3 and UPd_2Al_3 [7, 8] indicating that the hybridization, Coulomb and exchange, and crystal-field interactions cannot longer be treated as a perturbation with respect to the 5f spin-orbit interaction [7]. In Fig. 2 we report the hysteresis of the XMCD signal of the U M_4 edge measured at 2 K.

Information about the electronic configuration of the Uranium can be obtained by the branching ratio defined as $I_{5/2}/(I_{5/2} + I_{3/2})$ = 0.674 where $I_{5/2}$ and $I_{3/2}$ are the integrated areas under the white lines of the $3d_{5/2}$ (M_5 edge) and $3d_{3/2}$ (M_4 edge) peaks, respectively. The experimental value of the branching ratio is close to the value of 0.67 expected for a $5f^2$ configuration of Uranium (corresponding to an U^{4+} ion) [4].

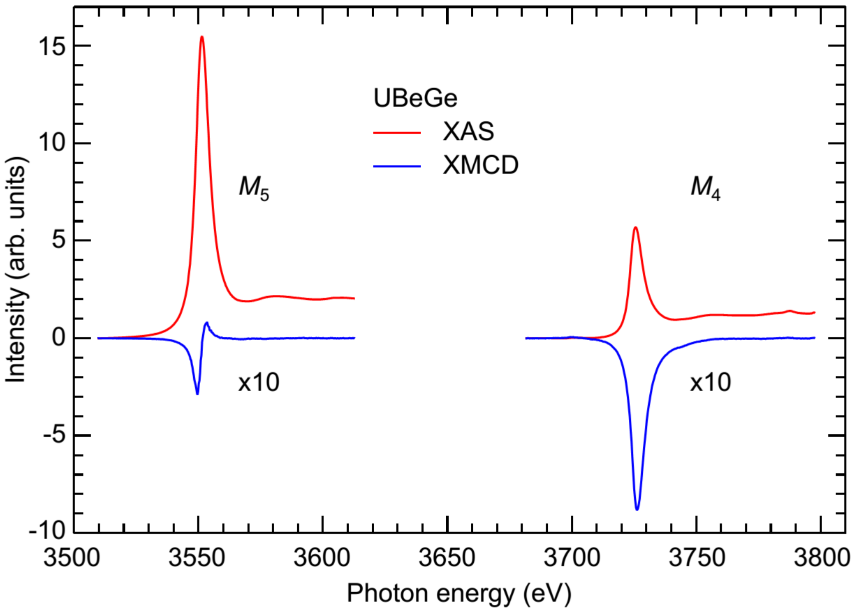

Fig. 1. U-M_5 and M_4 XAS (red) and XMCD (blue) spectra of UBeGe measured at T =2 K under an applied field of H = 3.0 T at the ID12 beamline of ESRF using circular polarized soft X-rays.

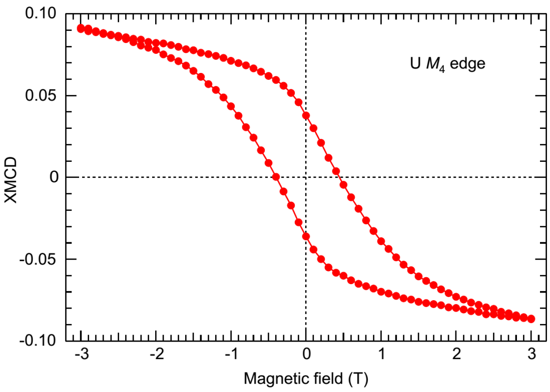

Fig. 2. Hysteresis of the XMCD signal of the U M_4 edge measured at 2 K.

By applying to our U-$M_{4,5}$ spectra the following sum rules developed by Thole et al. and by Carra et al.

$$Sz + 3Tz = \frac{n_h^{5f}}{2} \frac{2\int_{M5} \Delta\mu(E)dE - 3\int_{M4} \Delta\mu(E)dE}{\int_{M5+M4} [\mu^+(E) + \mu^-(E)]dE} \qquad Lz = \frac{3n_h^{5f} \int_{M5+M4} \Delta\mu(E)dE}{\int_{M5+M4} [\mu^+(E) + \mu^-(E)]dE}$$

we obtain an orbital moment of <Lz> = -1.66 μ_B and an effective spin moment <Sz> + 3<Tz> = 1.05 μ_B , where <Tz> is the magnetic dipole moment. We have considered n_h=12 according to a $5f^2$ configuration.

A comparison of the experimental value of the orbital moment and with that obtained by LSDA+U calculations suggests the need to consider a large value of the Coulomb repulsion for the UBeGe in order to reproduce the experimental values.

References

1. S. S. Saxena *et al.,* Nature 406 (2000) 587-592.D. Pesin and L. Balents, Nature Phys. **6**, 376 (2010).
2. D. Aoki *et al,* Nature **413** (2001) 613-616.
3. R. Gumeniuk *et al,*. Unpublished, MPI CPfS.
4. M. Finazzi *et al.,* Phys. Rev. B **55** (1997) 3010.
5. A. N. Yaresko *et al.,* J. Phys.: Condens. Matter **17** (2005) 2443-2452.
6. P. Dalmas de Réotier *et al.,* J. Alloys Comp. **271-273** (1998) 441-417.
7. P. Dalmas de Réotier *et al.,*Phys. Rev. B **60** (1998) 10606.
8. A. Yaouanc, et al., Phsy. Rev. B **58** (1998) 8793.