Experimental Report

31/03/2015

Proposal:	**5-41-772**	**Council:**	4/2014	
Title:	Magnetic structure study in CeCuAl3 single crystal			
This proposal is a new proposal				
Researh Area:	Physics			
Main proposer:	**KLICPERA Milan**			
Experimental Team:	KLICPERA Milan			
Local Contact:	OULADDIAF Bachir			
Samples:	CeCuAl3			

Instrument	Req. Days	All. Days	From	To
D10	7	6	22/09/2014	28/09/2014

Abstract:

CeCuAl3 crystallizes in the tetragonal BaNiSn3-type structure (space group I4mm, 107) and orders antiferromagnetically with Néel temperature 2.6 K. CeCuAl3 shows interesting magnetic behavior which is generally discussed as a result of interplay between the magnetic RKKY and Kondo interactions and the influence of the low lying excited CEF state. It is among a few cerium compounds where the strong magneto-elastic coupling resulting in new quasi-bound states, vibrons, was found. Despite numerous bulk studies, the unambiguous microscopic evidence of the magnetic ground state nature is still missing. Our previous test experiment on CYCLOPS and recent inelastic neutron scattering experiment (PANDA, MLZ) revealed the propagation vector (0.6, 0.4, 0) in CeCuAl3. The aim of proposed experiment is to determine all the details of the magnetic structure. The measurement will be performed on the same single crystal as all previous neutron scattering experiments.

Experimental report

Experimental title: **Magnetic structure study in $CeCuAl_3$ single crystal**

Proposal number: **5-41-772**

Instrument: **D10**

Date of experiment: 22. – 28.9. 2014

Local contact: Bachir Ouladdiaf

Experimental team: Milan Klicpera[1,2], Pavel Javorský[1]

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Abstract: $CeCuAl_3$ crystallizes in the tetragonal body-centered $BaNiSn_3$-type structure (space group I4mm, 107) and orders antiferromagnetically with Néel temperature of 2.7 K. $CeCuAl_3$ shows interesting magnetic behavior which is generally discussed as a result of interplay between the magnetic RKKY and Kondo interactions and the influence of the low lying excited CEF state. It is among a few cerium compounds where the strong magneto-elastic coupling resulting in new quasi-bound states, vibrons, was found. Despite numerous bulk studies, the unambiguous microscopic evidence of the magnetic ground state nature is still missing. Our previous test experiment on CYCLOPS and recent inelastic neutron scattering experiment (PANDA, MLZ) revealed the propagation vector (0.4, 0.6, 0) in $CeCuAl_3$. The aim of proposed experiment is to determine all the details of the magnetic structure. The measurement will be performed on the same single crystal as all previous neutron scattering experiments.

Scientific background:

$CeCuAl_3$ belongs to a relatively large group of RTX_3 compounds (R = rare earth, T = transition d-metal, X = p-metal) crystallizing in the tetragonal $BaNiSn_3$-type structure (space group I4mm, 107) [1]. This type of crystal structure is ordered non-centrosymetric derivate of $BaAl_4$-type structure. Among the Ce-based compounds, which naturally attract large attention because of often not fully localized 4f-electron, $CeTX_3$ compounds exhibit such interesting properties as heavy-fermion behavior, spin-density-wave-type magnetic ordering ($CeRhGe_3$ [2]) or pressure induced superconductivity ($CeRhSi_3$ [3] and $CeIrSi_3$ [4]). Another highly interesting phenomenon observed in $CeTX_3$ compounds is the presence of so called vibron states in $CeCuAl_3$, reported quite recently [5]. The vibron states are formed as a result of a strong interaction of crystal electric field (CEF) with phonon modes.

Beside the observation of exotic vibron states, $CeCuAl_3$ shows interesting magnetic behavior which is generally discussed as a result of interplay between the magnetic RKKY and Kondo interactions and the influence of the low lying excited CEF state (numerous studies, e.g. [6]). It orders antiferromagnetically with T_N = 2.7 K, but the unambiguous microscopic evidence of the magnetic ground state nature is still missing. We have performed thorough investigation of our single crystal by means of magnetization, specific heat and electrical resistivity measurements. From all performed measurements we can inter alia conclude that there is no other phase transition between T_N and 0.4 K.

Aim of the experiment:

The aim of the experiment on D10 instrument was to investigate the magnetic structure in $CeCuAl_3$.

We have performed a test Laue neutron diffraction experiment on CYCLOPS instrument. The high quality of our sample and a few (antiferro-) magnetic spots were observed leading to several possible propagation vectors which would describe all of them. Most recently, we have performed an inelastic neutron scattering experiment on our $CeCuAl_3$ single crystal on PANDA instrument in FRM II, Munich. In course of this experiment, we spent also some time to found the propagation vector (0.4, 0.6, 0) as well as the temperature development of magnetic moment.

Experimental details:

The orientation of $CeCuAl_3$ single crystal and the finding of UB matrix were done in the first step. Afterwards, we measured set of 24 nuclear reflections above and below T_N verifying so the crystal structure of our sample. Pure magnetic reflections described by the propagation vector (0.4, 0.6, 0) were investigated in the final step of the measurement. We obtained 25 independent magnetic reflections allowing us to reveal the magnetic structure of $CeCuAl_3$.

We also investigated two peaks at (½ ½ 0) and (-½ ½ 0) described by the propagation vector (½ ½ 0). The intensity of these peaks was much smaller than the one of magnetic peaks on reflections described by (0.4, 0.6, 0) propagation vector. Moreover, the temperature evolution (from 1.6 K to 200 K) of these peaks was investigated. No change in the intensity was observed by this measurement leading us to the assumption about the λ/2 contribution to the diffraction patterns.

Results:

The obtained intensity on measured magnetic peaks was fitted to the model magnetic structure employing the Rietveld analysis and Fullprof program. Far best agreement between the data and fit was obtained for magnetic structure with magnetic moments lying within the basal plane and described by basis vector (110). The amplitude modulated magnetic structure has two possible modifications leading to the identical agreement between the data and fit (R_F = 5.25%, R_{F2} = 9.1% and R_{wF2} = 9.9%, see Fullprof manual for details). The magnetic moments on Ce atoms at two crystallographic sites within the unit cell, (0, 0, z_{Ce}) and (½, ½, ½ + z_{Ce}), where $z_{Ce} \approx 0$, are oriented as depicted on Fig.1. The maximal ordered magnetic moment of 0.28 μ_B/Ce^{3+} was found in the compound. The results are well in agreement with previous neutron diffraction experiments as well as with bulk properties measured on $CeCuAl_3$.

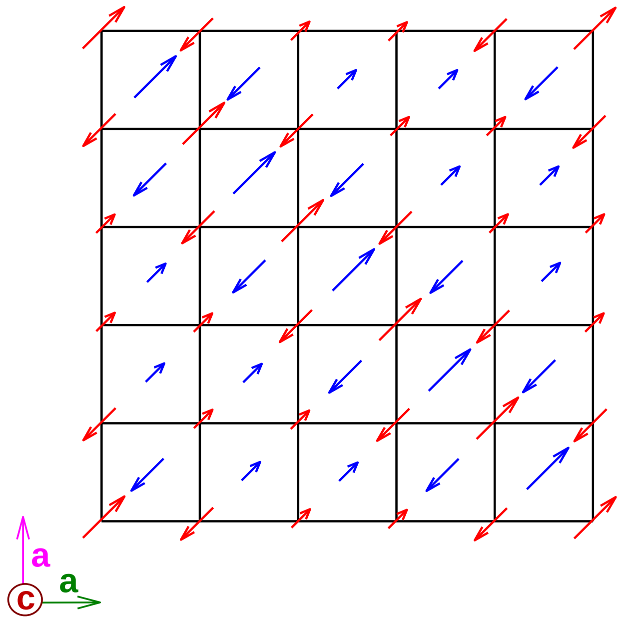

Fig.1 – The magnetic structure of $CeCuAl_3$. Magnetic moments within ab planes at z = 0 and z = ½ (red and blue arrow, respectively) are shown.

[1] M. Klicpera, P. Javorský, et al, *Intermetallics* **46**, 126-130 (2014)
[2] A. D. Hillier, D. T. Adroja, et al, *Phys. Rev. B* **85**, 134405 (2012).
[3] N. Kimura, K. Ito, et al, *Phys. Rev. Lett*. **95**, 247004 (2005).
[4] H. Mukuda, T. Fujii, et al, *Phys. Rev. Lett.* **100**, 107003 (2008).
[5] D. T. Adroja, A. del Moral, et al, *Phys. Rev. Lett*. **108**, 216402 (2012).
[6] M. Kontani, H. Ido, et al., *J. Phys. Soc. Jap*. **63**, 1652 (1994).