Experimental Report

Proposal: **5-31-2304** **Council:** 4/2014

Title: Magnetic structure investigation in CePd2Al2 compound

This proposal is a new proposal

Researh Area: Physics

Main proposer: **KLICPERA Milan**

Experimental Team: PASZTOROVA Jana
KLICPERA Milan

Local Contact: PUENTE ORENCH INES

Samples: CePd2Al2

Instrument	Req. Days	All. Days	From	To
D1B	1	1	24/11/2014	25/11/2014

Abstract:

Intermetallic CePd2Al2 compound crystallizes in the ordered non-centrosymmeric tetragonal structure of CaBe2Ge2-type (space group 129, P4/nmm). Although the ground state nature of CePd2Al2 has not been reported so far, other interesting features were found in this compound. The structural phase transition from tetragonal to orthorhombic structure (Cmma) was observed around 13.5 K. Such a structural transition is rather rare phenomenon among R2T2X2 compounds, which reveal stable crystal structure mostly. The highly interesting phenomenon in CePd2Al2 is the existence of quasi-bound states, vibrons, arising from strong magneto-elastic coupling and observed by inelastic neutron scattering as an additional peak in the energy spectra. CePd2Al2 thus naturally belongs to materials studied within our broader project focused on existence of vibron states and its influence on magnetic and structural properties. CePd2Al2 orders antiferromagnetically with Neel temperature 2.8(1) K. No other phase transition was observed down to 0.4 K. The aim of proposed experiment is to determine the magnetic structure of CePd2Al2.

Experimental report

Experimental title: **Magnetic structure investigation in $CePd_2Al_2$ compound**

Proposal number: **5-31-2304**

Instruments: **D1B**

Date of experiment: 24. – 25.11. 2014

Local contact: Inés Puente Orench

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

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Abstract: Intermetallic $CePd_2Al_2$ compound crystallizes in the ordered centrosymmeric tetragonal structure of $CaBe_2Ge_2$-type (space group 129, P4/nmm). Although the ground state nature of $CePd_2Al_2$ has not been reported so far, other interesting features were found in this compound. The structural phase transition from tetragonal to orthorhombic structure (Cmma) was observed around 13.5 K. The highly interesting phenomenon in $CePd_2Al_2$ is the existence of quasi-bound states, vibrons, arising from strong magneto-elastic coupling and observed by inelastic neutron scattering as an additional peak in the energy spectra. $CePd_2Al_2$ thus naturally belongs to materials studied within our broader project focused on existence of vibron states and its influence on magnetic and structural properties. $CePd_2Al_2$ orders antiferromagnetically with Néel temperature of 2.8(1) K. No other phase transition was observed down to 0.4 K. The aim of proposed experiment is to determine the magnetic structure of $CePd_2Al_2$.

Scientific background:

Intermetallic $CePd_2Al_2$ compound crystallizes at the room temperature in the ordered non-centrosymmeric tetragonal structure of $CaBe_2Ge_2$-type (space group 129, P4/nmm). $CePd_2Al_2$ belongs to a few cerium compounds where the inelastic neutron scattering revealed an additional peak in their spectra, which is ascribed to existence of vibron states arising from magneto-elastic coupling [1,2]. Furthermore, $CePd_2Al_2$ undergoes a structural phase transition from tetragonal to orthorhombic structure (Cmma) at around 13.5 K [1]. The same transition was observed also in $LaPd_2Al_2$ analog at much higher temperature of 91.5 K [1]. The thorough investigation of structural phase transitions in these compounds was reported in Ref. [1], see Fig.1. Such structural transition is rather rare phenomenon among $R_2T_2X_2$ compounds, which exhibit mostly stable crystal structure [3]. Moreover, the hypothesis about the stabilization of the high temperature tetragonal structure by this magneto-elastic coupling was discussed [1]. $CePd_2Al_2$ thus naturally belongs to materials studied within our broader project focused on existence of vibron states and its influence on magnetic and structural properties.

Our recent investigation of $CePd_2Al_2$ by means of magnetization, specific heat and electrical resistivity measurements revealed not only structural phase transition (as reported in [1]) but also the phase transition to antiferromagnetic state at the Nèel temperature of T_N = 2.8(1) K [4], see Fig.2. No other phase transition was observed down to 0.4 K, see Figs.3 and 4. Although the data in Ref. [1] are based on neutron diffraction, the work was focused on the structural transition at higher temperatures; the magnetic order was apparently not investigated.

Aim of the experiment:

The knowledge of the microscopic details of the magnetic order is essential for understanding magnetism in $CePd_2Al_2$. To determine the magnetic structure, we propose to perform powder neutron diffraction experiment on D1B instrument.

Results:

A comparison of diffraction patterns taken in paramagnetic and ordered state (at temperatures 5 K and 1.5 K, respectively) reveals several (about ten) clear peaks of magnetic origin, see Fig. 1. A small intensity on observed magnetic peaks documents a relatively small size of magnetic moment in the compound. The lattice parameters of orthorhombic structure determined at T = 5 K: a = 6.269(1) A, b = 6.130(1) A and c = 9.885(2) A are well in agreement with previous neutron diffraction study [1].

The number of magnetic peaks and mainly the intensity on them make the investigation of magnetic structure quite difficult. Nevertheless, the magnetic propagation vector can be determined unambiguously as incommensurate $\boldsymbol{k}$ = (0.06, 0.54, 0). Determined magnetic

propagation vector and known lattice parameters allowed to calculate possible magnetic structures by performing a thorough representation analysis. The fitting of model structures to the measured data lead to determination of magnetic structure, although the absolute direction of magnetic moments cannot be determined unambiguously. The incommensurate amplitude modulated magnetic structure with maximal value of magnetic moment about 2.05(4) μ_B/Ce^{3+}, still below value for free Ce^{3+} ion, was obtained. The magnetic moments point along the same direction, presumably along (or nearly along) orthorhombic [100] direction. The agreement factor R_m = 19.0% for pure a-axis direction of magnetic moments changes into R_m = 13.9% when considering 4 and 24 degrees deflection to the [010] and [001] directions, respectively.

The comparison of obtained magnetic structure to other representatives of $CePd_2X_2$ compounds leads to a good agreement as all the compounds exhibit similar propagation vector and magnetic moments are arranged along the same direction in space. Nevertheless, $CePd_2Al_2$ is a first representative of these compounds revealing incommensurate amplitude modulated magnetic structure. The determined magnetic structure will be a part of our broader paper on physical properties in $CePd_2(Al,Ga)_2$ compounds investigated by neutron scattering techniques.

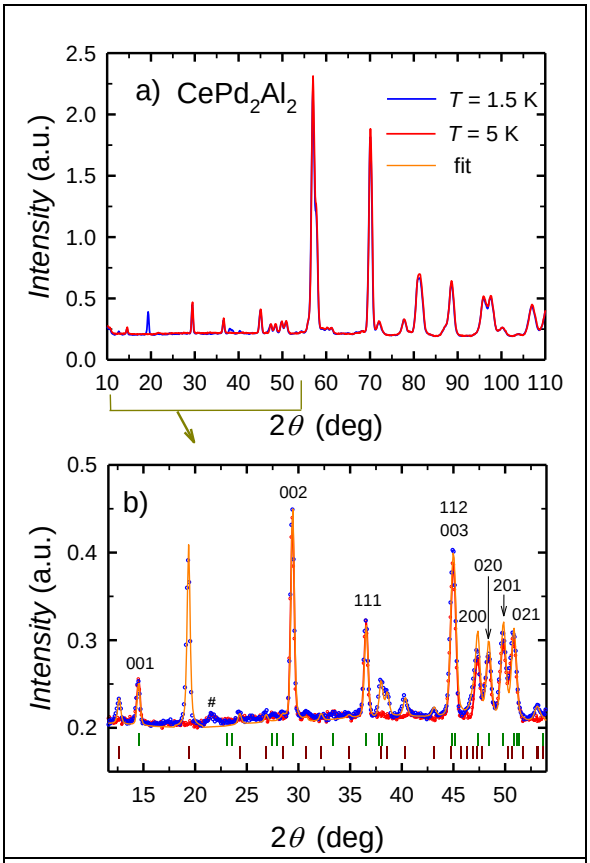

Fig.1 – Diffraction patterns taken using D1B diffractometer at 5 K and 1.5 K on $CePd_2Al_2$ powder.

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[2] P. Thalmeier, P. Fulde, *Phys. Rev. Lett.* **49**, 1588 (1982).
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[4] M. Klicpera, P. Javorský, A. Hoser, *J. Alloys Comp.* - accepted, in press.