Experimental report

27/11/2015

Proposal: 4-04-473 **Council:** 4/2015

Title: Crystal field excitations in NdPd5Al2

Research area: Physics

This proposal is a new proposal

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Samples: NdPd5Al2

Instrument	Requested days	Allocated days	From	To
IN4	3	3	09/11/2015	12/11/2015

Abstract:

Antiferromagnetic Nd5PdAl2 belongs to a family of tetragonal RPd5Al2 compounds (R is rare earth element or actinide) which are structurally related to RTX5 and R2TX8 (T is a transition metal, X is a p-metal) compounds. Several compounds from this broad family, based on Ce, Pu or Np, are considered as archetypal heavy-fermion superconductors. To investigate the role of the crystal field effects in the rich physical properties of these materials, we propose to study the crystal field excitations in NdPd5Al2. Based on the analysis of inelastic neutron scattering, magnetization measurements on single crystal and heat capacity data, we aim to determine the crystal field parameters in NdPd5Al2, which can be then compared to CePd5Al2 and compounds from the RTX5 series as well as to ab-initio calculations.

Experimental report: Crystal field excitations in $NdPd_5Al_2$

$NdPd_5Al_2$ belongs to a large family of tetragonal rare-earth based intermetallics which includes among others RPd_5Al_2, R_2TX_8 and RTX_5 compounds. Several of these compounds were intensively studied due to a connection between magnetic properties and heavy-fermion superconductivity. Crystal field (CF) generally lifts degeneracy of the ground state rare-earth ion multiplet and thus plays an important role in these compounds influencing fundamentally magnetocrystalline anisotropy. Unfortunately, CF in these compounds mostly cannot be studied directly by means of inelastic neutron scattering due to the limited size of samples grown by the flux method. The performed inelastic neutron experiment was focused on study of crystal field excitations in polycrystalline sample of $NdPd_5Al_2$ prepared by arc-melting. The compound crystallizes in the tetragonal $I4/mmm$ space group and $^4I_{9/2}$ ground state of Nd^{3+} ion is split by CF into 5 Kramers doublets here.

The powderized sample of $NdPd_5Al_2$ of total mass 12.3 g was wrapped into aluminium foil. The INS spectra were measured at incident energies 38.5, 28.9, 13.7 and 7.26 meV. Data for $E_i = 38.5$ meV were collected at the temperature of 2 K; data for $E_i = 28.9$ and 13.7 meV at temperatures 2, 5, 10, 20, 40, 80 and 150 K, respectively at 2, 10, 15, 20, 40 and 80 K to investigate the temperature development of the excitations. The spectra for $E_i = 7.26$ meV were measured at 2 and 40 K. Combining data for $E_i = 28.9$, 13.7 and 7.26 meV at the lowest measured temperature, i. e. 2 K, we clearly observed four peaks at energies approx. 3.0, 7.4, 8.6 and 17.1 meV corresponding to all excitations from the ground state as shown in the Fig. 1 and depicted by full lines in the CF energy level scheme (Fig. 2). The INS spectra for $E_i = 28.9$ (Fig. 3) and 13.7 meV (Fig. 4) at higher temperatures reveal another peaks at 14.1, 5.6 and 4.4 meV which can be interpreted as transitions from the first excited state to higher states (dashed lines in Fig. 2) and another broad peak around 9 meV which might presumably correspond to transition(s) from 7.4 meV and/or 8.6 meV to 17.1 meV CF level (dotted line in Fig. 2). It can be noticed that magnitude of the peaks corresponding to excitations from the ground state gradually decreases with increasing temperature, whereas magnitude of the peaks corresponding to transitions from excited states increases and changes substantially as the excited levels are significantly occupied which is in agreement with Boltzmann probability distribution.

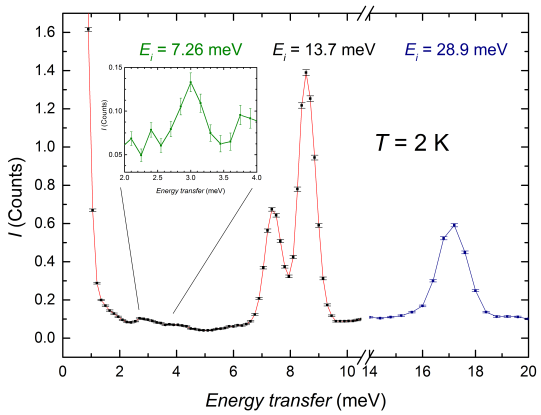

Fig. 1: INS spectra at $T = 2$ K: excitations from the ground state.

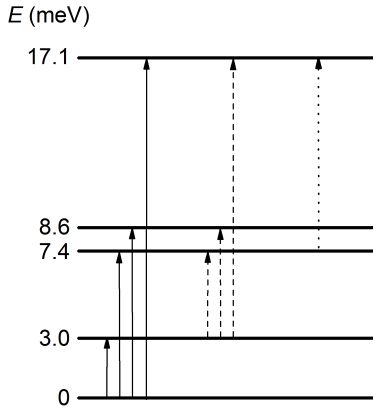

Fig. 2: Crystal field energy level scheme.

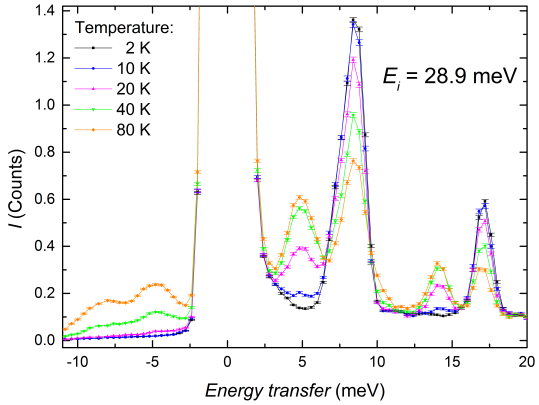

Fig. 3: INS spectra for $E_i = 28.9$ meV measured at various temperatures.

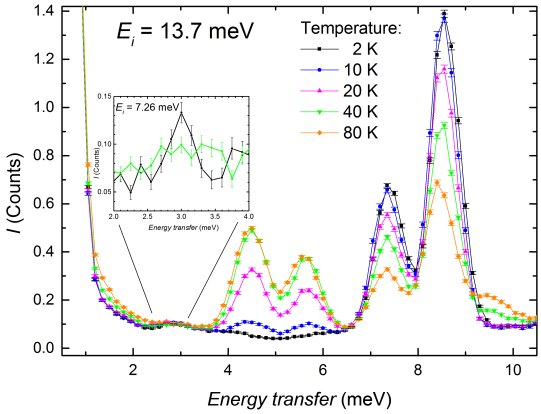

Fig. 4: INS spectra for $E_i = 13.7$ meV measured at various temperatures.