Experimental report

29/12/2017

Proposal: 5-31-2459 **Council:** 4/2016

Title: The magnetic structures of the newR3Pd5 compounds (R = Tb, Ho)

Research area: Materials

This proposal is a new proposal

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Experimental team:

Local contacts: Clemens RITTER

Samples: Terbium-palladium alloy/Tb3Pd5
Holmium-palladium alloy/Ho3Pd5

Instrument	Requested days	Allocated days	From	To
D1B	2	2	13/07/2016	15/07/2016

Abstract:

In our recent work we have investigated the “R2Pd3” phase (R = rare earth) and found that it actually corresponds to the stoichiometry R3Pd5. This compound is formed by R = Sc, Y, Gd-Lu, including Yb; all of them crystallizing in the Pu3Pd5 prototype [oS32, Cmcm]. Two Wyckoff sites are available in the unit cell for the R atoms, while three crystallographic positions are occupied by Pd atoms.
Antiferromagnetic behavior has been observed for Tb and Ho compounds with two subsequent transitions (TN1 = 13.5 K and TN2 = 6.5 K for Tb3Pd5, TN1 = 7.2 K and TN2 = 4.2 K for Ho3Pd5). Effective paramagnetic moments of 9.64 and 10.60 μB for Tb3Pd5 and Ho3Pd5, respectively, are obtained from the Curie-Weiss law, with negative values of paramagnetic Curie temperature (-11 K for Tb3Pd5 and -4 K Ho3Pd5) indicating antiferromagnetic interaction. The isothermal magnetization measurements confirm the antiferromagnetic ordering of the two compounds. From our data we cannot distinguish whether the two R sublattices distinctly order at the two different TN, or if both are simultaneously involved at the two transitions.
By neutron diffraction we plan to study the magnetic structures.

Report on Experiment 5-31-2459

Following the successful description of the new binary phases R_3Pd_5 as crystallizing in the Pu_3Pd_5 orthorhombic structure type with space group *Cmcm* [1], the aim of this neutron diffraction experiment was the determination of the magnetic structures of Tb_3Pd_5 and Ho_3Pd_5.

For both compounds the magnetic and specific heat data had indicated that the magnetic ground state should be antiferromagnetic with a supposed independent ordering of the two R-sublattices found by *R*1 on the Wyckoff site 4*c* and *R*2 on 8*e* [1].

The temperature dependence of the neutron diffraction patterns (thermodiffractograms) was measured on D1B taking spectra for 5 min every 0.5 K between 1.5 K and 20 K for Tb_3Pd_5 and every 0.1 K between 1.5 K and 15 K for Ho_3Pd_5. Longer scans of about 30 min were additionally taken at 1.5 K, 6 K, and 8 K for *R* = Tb and at 1.5 K, 3.5 K, 5 K and 15 K for *R* = Ho. Figure 1a shows the thermodiffractogram of Ho_3Pd_5 with figure 1b displaying the temperature dependence of two symptomatic reflections. The magnetic structure and its temperature evolution was determined using magnetic symmetry analysis. A unique magnetic propagation vector *k* = [1 0 0] is comprising both Ho-sublattices with, however, the Ho1-sublattice evolving strong magnetic order at T_N = 7 K, while the Ho2-sublattice orders much slower – apparently induced by the Ho1-sublattice – before it emerges as well strongly below 4 K. The magnetic structure sees ferromagnetic layers formed by Ho1 and Ho2 moments along the *a*-*c*-layers, coupled antiferromagnetically in *b*-direction

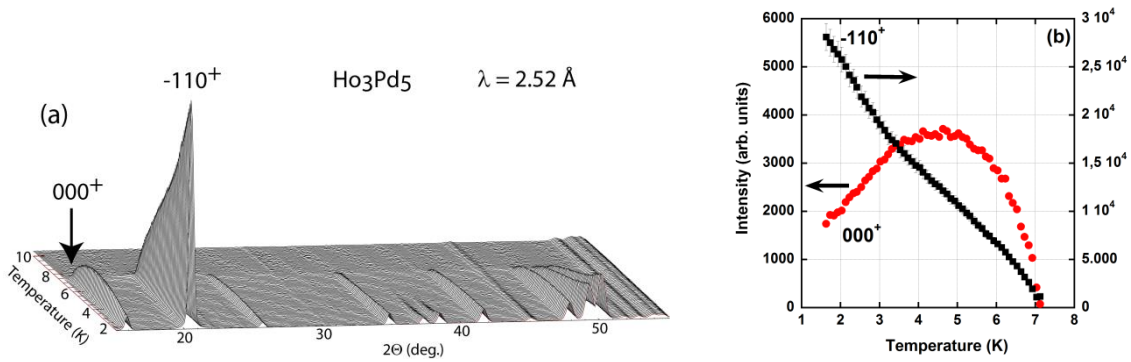

Figure 1. a) Thermodiffractogram of Ho_3Pd_5, b) T-dependence of two magnetic reflections.

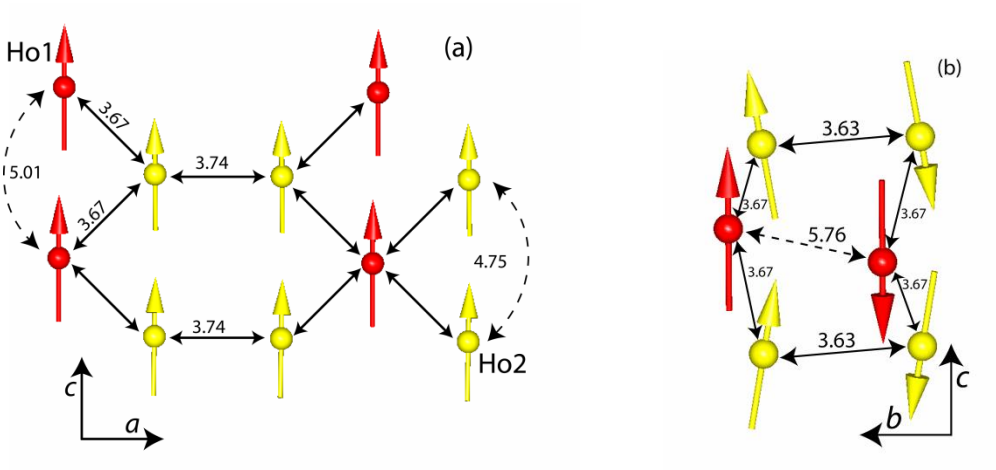

Figure 2. a) Magnetic couplings within the *a*-*c*-plane, b) *b*-*c*-plane of Ho_3Pd_5.

The thermodiffractogram of Tb_3Pd_5 shows a very different behaviour, magnetic peaks created through different magnetic propagation vectors appear at different temperatures: T_{N1} = 13 K sees k_1 = [1 0 ½], T_{N2} = 7 K sees k_2 = [0.76 0 0] and T_{N3} = 6K sees k_3 = [1 0 0]. Opposite to Ho_3Pd_5 it is the Ho2-sublattice which becomes first ordered in Tb_3Pd_5 following exclusively k_1 down to base temperature. The Ho1-sublattice adopts first an incommensurate magnetic structure with k_2 before it transforms over a coexistence region to k_3. Surprisingly the magnetic exchange interactions (Figure 4) acting in Tb_3Pd_5 are totally opposite to those found in Ho_3Pd_5 although the structural details of both compounds are nearly identical. Next nearest neighbour interactions being ferromagnetic in Ho_3Pd_5 become antiferromagnetic in Tb_3Pd_5 and vice versa. We are planning more detailed band structure calculations on these compounds and new additional neutron diffraction experiments on the Er_3Pd_5 compound having a different 4*f*-electronic charge distribution in order to tackle this strange anisotropy.

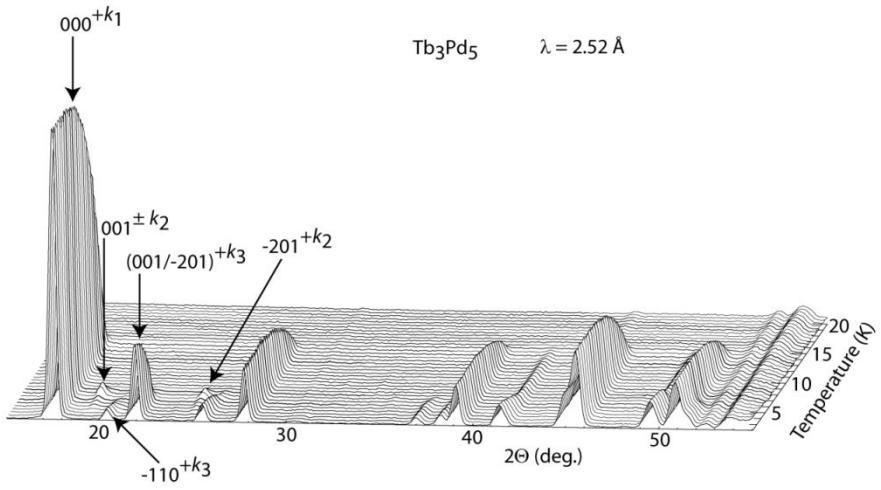

Figure 3. Thermodiffractogram of Tb_3Pd_5

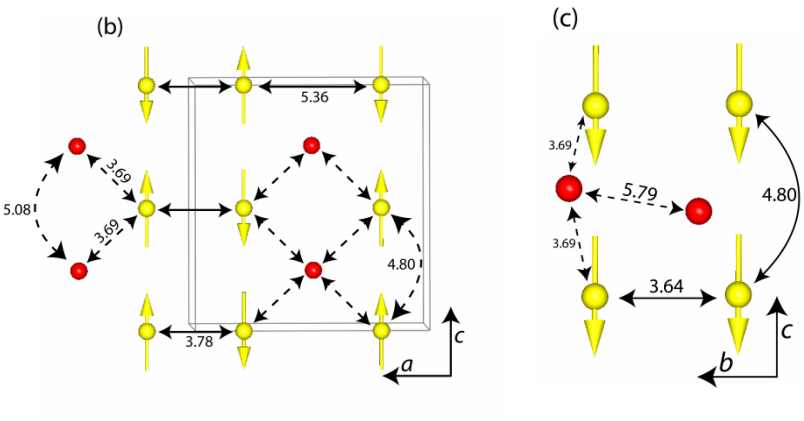

Figure 4. b) Magnetic couplings within the *a*-*c*-plane, c) *b*-*c*-plane of Tb_3Pd_5.

[1] A. Provino et al., Cryst. Growth Des. 2016, 16, 6001