Experimental report

07/08/2024

Proposal: **5-31-2955** **Council:** 4/2023

Title: Study of the magnetic structures of the novel room temperature magnetocaloric compounds R6 (Fe,Mn) Bi2 (R = Dy, Tb)

Research area: Physics

This proposal is a new proposal

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Samples: Dy_6MnBi_2
Tb_6FeBi_2
$Dy_6Fe_{0.5}Mn_{0.5}Bi_2$

Instrument	Requested days	Allocated days	From	To
D1B	1	3	15/09/2023	18/09/2023
D20	2	0		

Abstract:

Rare earth based intermetallic materials are among the novel magnetocaloric materials being studied in order to work at room temperature as well as in the gas liquefaction regions. We propose the study of 3 selected members of the family of magnetocaloric intermetallics R6(Fe,Mn)Bi2 (R=Dy, Tb). The goal is to determine the magnetic structure by using neutron diffraction, as a function of temperature, paying special attention to the low temperature phases which are expected to have a complex non-collinear arrangement of spins (incommensurate, canted AFM, etc.). The information will allow to check if, indeed, the rare earth ions are the sole responsible of the magnetic properties of the materials and to clarify the role of the transition metal ions. The full understanding of the magnetic structures in these series will help to design magnetocalorics with improved properties.

Study of the magnetic structures of the novel room temperature magnetocaloric compounds R_6 (Fe,Mn) Bi_2 (R = Dy, Tb)

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D1B instrument at ILL was used to resolve the crystal and magnetic structure of the polycrystalline Dy_6MnBi_2 and Tb_6FeBi_2 intermetallic compounds. Different regions of interest were measured in order to study the evolution of the magnetic phases, and to check the contribution to the magnetic moment of the rare earth and transition metals. Isotherms from 2 K to 450 K, using λ = 2.45 Å in high intensity mode clearly show the magnetic evolution of the compound.

The aim of these measurements is to determine the magnetic structure of magnetocaloric intermetallics Dy_6MnBi_2 and Tb_6FeBi_2 using neutron diffraction as a function of temperature, paying special attention to the low temperature phases which are expected to have a complex non-collinear arrangement of spins (incommensurate, canted AFM, etc.). The information may allow us check if, indeed, the rare earth ions are the sole responsible of the magnetic properties of the materials, which is commonly accepted in literature, and to clarify the role of the transition metal ions. The full understanding of the magnetic structures in these compounds help to design magnetocaloric materials with improved properties.

The magnetic measurements of these compounds show that in Tb_6FeBi_2 there are two phase transitions, a paramagnetic ferromagnetic transition at around 250 (depending on the sample) while there is a lower temperature spin rearrangement towards a more complex magnetic structure [1]. However, in Dy_6MnBi_2 there is just a transition around 300 K. In order to cover every region of interest several isotherms were obtained from 2 K to a temperature higher than the Curie temperature of each compound. An annular V sample holder, λ = 2.52 Å and high intensity mode were used to overcome the small quantity of compound and the high absorption of Dy.

The neutron measurements we were able to identify our main phases (Tb_6FeBi_2 and Dy_6MnBi_2). The nuclear crystallographic structures were resolved in the paramagnetic phase (450 K) and later adjusted at lower temperatures. In every case unit cell data agrees with the Fe_2P-type structure (space group P-62m, No. 189, hP9), as expected from previous X-Ray studies [1].

In addition, Figure 1 clearly shows the different magnetic transitions that take place in both samples with the temperature. In both cases, a magnetic phase with K=(0,0,0) appear bellow T_C, but in the case of Tb_6FeBi_2 new peaks appear bellow 150 K, corresponding to an incommensurate magnetic phase, which is still to be fully resolved (these peaks are signaled by red arrows in the left graph of Fig. 1).

Fig. 2 shows a preliminary analysis of 2 K diffactograms for both compositions. The incommensurate peaks can clearly be observed in Tb_6FeBi_2 (pointed by red arrows) while magnetic peaks appear only at the nuclear positions for Dy_6MnBi_2.

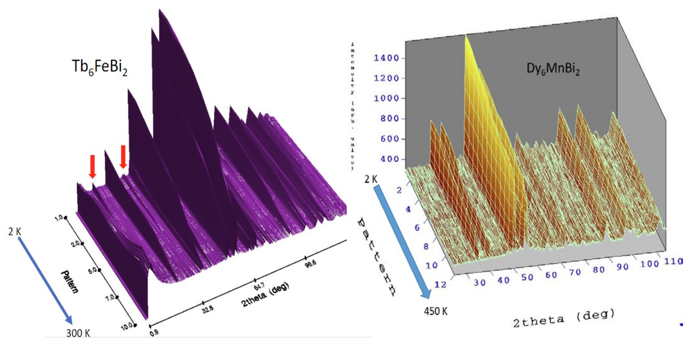

Figure 1: Tb_6FeBi_2 thermodiffractogram (left), Dy_6MnBi_2 thermodifractogram (right).

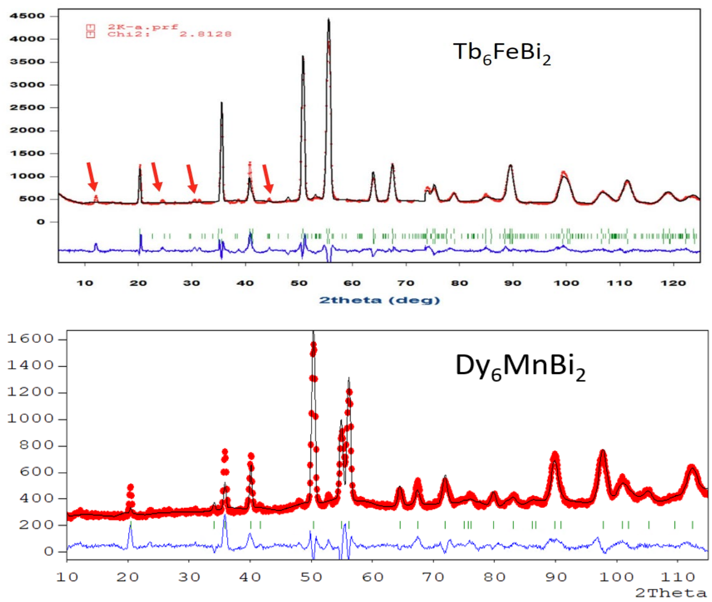

Figure 2: Tb_6FeBi_2 2 K diffractogram (top), Dy_6MnBi_2 2 K diffractogram (bottom).

[1] A. Oleaga, A. Herrero , A. Salazar, A.V. Garshev, V.O. Yapaskurt, A.V. MorozkinR. JAC 843, 155937 (2020).