Accepted Manuscript

Role of Ce substitution in the magneto-crystalline anisotropy of tetragonal $ZrFe_{10}Si_2$

D. Salazar, A. Martín-Cid, J.S. Garitaonandia, T.C. Hansen, J.M. Barandiaran, G.C. Hadjipanayis

PII: S0925-8388(18)32346-6

DOI: 10.1016/j.jallcom.2018.06.225

Reference: JALCOM 46561

To appear in: *Journal of Alloys and Compounds*

Received Date: 1 February 2018

Revised Date: 22 May 2018

Accepted Date: 19 June 2018

Please cite this article as: D. Salazar, A. Martín-Cid, J.S. Garitaonandia, T.C. Hansen, J.M. Barandiaran, G.C. Hadjipanayis, Role of Ce substitution in the magneto-crystalline anisotropy of tetragonal $ZrFe_{10}Si_2$, *Journal of Alloys and Compounds* (2018), doi: 10.1016/j.jallcom.2018.06.225.

Role of Ce substitution in the magneto-crystalline anisotropy of tetragonal $ZrFe_{10}Si_2$

D. Salazar[1,*], A. Martín-Cid[1], J.S. Garitaonandia[1,2], T.C. Hansen[3], J. M. Barandiaran[1,2], G. C. Hadjipanayis[4]

[1]*BCMaterials, Bizkaia Science & Technology Park, E-48160 Derio, Spain*
[2]*Faculty of Science and Technology, Univ. Basque Country (UPV/EHU) E-48080 Bilbao, Spain*
[3] *Institut Laue-Langevin, 71, avenue des Martyrs, 38042 Grenoble, France*
[4] *Dept. Physics & Astronomy, University of Delaware, Newark, DE, 19716, USA*

Abstract

We report the study of $Zr_{1-x}Ce_xFe_{10}Si_2$ (x = 0.0, 0.3 and 0.6) compounds, with tetragonal $ThMn_{12}$ structure, by means of neutron diffraction and Mössbauer spectroscopy to understand the role of Ce in the increasing magneto-crystalline anisotropy. Fitting of the ^{57}Fe Mössbauer spectra to the three Fe atomic positions, namely 8i, 8j and 8f, indicate that Ce displaces Fe from the 8i to the 8j positions and in parallel increases the quadrupole splitting (QS) in position 8f, correlating with the increase of the magneto-crystalline anisotropy. However, the hyperfine field B_{hf} remains constant for all Ce substitutions. The full occupancy of the 8j positions by Fe at Ce = 0.6 can explain the instability of the $ThMn_{12}$ structure for similar and higher Ce concentrations. Neutron diffraction experiments show the evolution of the magnetic moment and crystal structure as a function of temperature, showing Ce to cause an increase of the lattice parameters and tetragonal distortion. A large anomaly of the expansion coefficient, due to the spontaneous magnetostriction, is also disclosed. These results support a pure geometric influence of Ce on the magneto-crystalline anisotropy through a selective distortion of the lattice.

Keywords: $ThMn_{12}$-type structures, magnetocrystalline anisotropy, rare-earth-free magnets.

[*]Corresponding author: Daniel Salazar Jaramillo, email: daniel.salazar@bcmaterials.net