Available online at www.sciencedirect.com
Physica B 385–386 (2006) 317–319
www.elsevier.com/locate/physb

Magnetic ordering in $DyFe_6Sn_6$

J.M. Cadogan[a,*], O. Moze[b], D.H. Ryan[c], Suharyana[a], M. Hofmann[d]

[a] *School of Physics, The University of New South Wales, Sydney, NSW 2052, Australia*
[b] *INFM-CNR-S3, Dipartimento di Fisica, Università di Modena e Reggio-Emilia, Via G. Campi 213/A, Modena, 41100 Italy*
[c] *Centre for the Physics of Materials, Department of Physics, McGill University, 3600 University Street, Montreal, Que., Canada H3A 2T8*
[d] *Technische Universität München, FRM-II, 85748 Garching, Germany*

Abstract

We have determined the magnetic structure of the orthorhombic (Cmcm) intermetallic compound $DyFe_6Sn_6$ by neutron powder diffraction. The Fe sublattice orders antiferromagnetically at 559(5) K with moments along [1 0 0] and a propagation vector $\mathbf{k}_1 = [0\,1\,0]$. At 3.6 K, the Fe magnetic moment is $2.6(4)\mu_B$. The Dy sublattice orders at 19(2) K, quite independently of the Fe sublattice. The Dy order is canted and comprises ferromagnetic order along [0 0 1] and antiferromagnetic order along [0 1 0]; the respective propagation vectors are [0 0 0] and [0 1 0]. At 3.6 K, the Dy magnetic moment components are FM $5.0(3)\mu_B$ and AF $1.6(3)\mu_B$, leading to a net Dy moment of $5.2(4)\mu_B$ and a canting angle of 17(4)° away from the crystal *c*-axis towards the *b*-axis.

PACS: 75.25.+z; 75.50.Ee; 76.80.+y

Keywords: Rare-earth intermetallics; Magnetic ordering; Neutron diffraction

1. Introduction

The magnetic ordering processes of the R and Fe sublattices in the RFe_6Ge_6 and RFe_6Sn_6 (R = rare-earth) intermetallic compounds are independent of one another (e.g. Ref. [1]). The Fe sublattice orders antiferromagnetically and its Néel temperature remains essentially constant across a series at ~485 K for RFe_6Ge_6 or ~560 K for RFe_6Sn_6. The magnetic ordering of the R sublattice occurs two orders of magnitude lower in temperature than the Fe ordering. For R = Gd – Er, the rare-earth sublattice ordering temperatures range from 45 K for $GdFe_6Sn_6$ to 3 K for $ErFe_6Ge_6$, without affecting the Fe order.

Structurally, the RFe_6Ge_6 and RFe_6Sn_6 compounds are formed by placing R atoms between the hexagonal Fe planes of the parent FeGe or FeSn (B35) structure, resulting in orthorhombic or hexagonal structures. The orthorhombic structures are related to the underlying hexagonal cells: *a*(ortho) is parallel to *c*(hex) and *c*(ortho) is parallel to *a*(hex). The magnetic independence of the R and Fe sublattices is a direct consequence of this layered structure. The binary FeGe/FeSn structure comprises ferromagnetic Fe planes coupled antiferromagnetically to each other [2,3] and the local environment of the R atoms in the RFe_6Ge_6 and RFe_6Sn_6 structures leads to a net cancellation of the Fe–R exchange at the R sites, isolating them from the ordering of the Fe moments.

We have previously reported the results of our ^{57}Fe Mössbauer study of the entire RFe_6Ge_6 series [4]. The hyperfine field at the ^{57}Fe nuclei is virtually independent of the rare-earth present and our low-temperature Mössbauer studies show no evidence that the magnetic order of the Fe sublattice is affected by the ordering of the R sublattice, in agreement with neutron diffraction work. We have also carried out ^{119}Sn Mössbauer work on the RFe_6Sn_6 series [5–7]. The Sn atoms are non-magnetic but two-thirds of the ^{119}Sn nuclei experience transferred hyperfine fields of about 24 T from the magnetic Fe sublattice, in full agreement with our determinations of the magnetic structure of the Fe sublattice.

In this paper we determine the magnetic structures of the Dy and Fe sublattices in $DyFe_6Sn_6$ using high-resolution neutron powder diffraction.

---

*Corresponding author.
E-mail address: J.Cadogan@unsw.edu.au (J.M. Cadogan).

0921-4526/$ - see front matter © 2006 Elsevier B.V. All rights reserved.
doi:10.1016/j.physb.2006.05.029

2. Experimental methods

The $DyFe_6Sn_6$ sample was prepared by arc-melting stoichiometric amounts of the pure elements (Dy: 99.9%, Fe: 99.95%, Sn: 99.999%) under Ti-gettered argon. The arc-melted ingot was turned and re-melted four times to promote homogeneity. The sample was subsequently annealed at 900 °C for two weeks, sealed under vacuum in a quartz tube.

Powder X-ray diffraction was carried out using CuK_α radiation on an automated Nicolet–Stoe diffractometer. The Néel temperature of the Fe sublattice in $DyFe_6Sn_6$ was measured by differential scanning calorimetry on a Perkin–Elmer DSC-7, using the heat capacity peak at T_N as the signature of magnetic ordering. The ordering temperature of the Dy sublattice was determined by AC-susceptibility measurements made on a Quantum Design PPMS with an AC magnetic field of 700 A/m (rms) and a frequency of 137 Hz.

Neutron powder diffraction experiments were carried out on the E9 Fine Resolution Powder Diffractometer (FIREPOD) at the BER-II reactor, BENSC, Hahn-Meitner Institute, Berlin, Germany, and the DUALSPEC C2 high-resolution powder diffractometer located at the NRU reactor, Chalk River, Canada. The neutron wavelengths were 1.5831(1) Å on FIREPOD, and 2.3685(1) Å on DUALSPEC. The crystal structure was determined on DUALSPEC at 600 K with a wavelength of 1.3278(1) Å. Patterns were obtained over the temperature range 3–600 K and all diffraction patterns were analysed by the Rietveld method using FULLPROF [8]. All refinements included correction for the high neutron absorption by Dy.

3. Results and discussion

The annealed sample of $DyFe_6Sn_6$ was virtually single-phase, with a trace of $Dy_{11}Sn_{10}$ (tetragonal I4/mmm) present in the amount <3 wt%, as determined from the refinements of the X-ray and neutron diffraction patterns. The Néel temperature of the Fe sublattice in $DyFe_6Sn_6$ is 559(5) K. This value compares well with the value of 561 K determined by Rao [9]. Our previously determined Néel temperature of the Fe sublattice in YFe_6Sn_6 is 558(5) K [5], consistent with the fact that the R^{3+} ion has essentially no influence on the Fe ordering. AC-susceptibility measurements (Fig. 1) show that the Dy sublattice orders magnetically at 19(2) K.

In Fig. 2 we show neutron diffraction patterns of $DyFe_6Sn_6$ obtained on DUALSPEC. The crystal structure of $DyFe_6Sn_6$ is orthorhombic $TbFe_6Sn_6$-type, with the space group Cmcm (#63) [1,10]. The lattice parameters and atomic positions of $DyFe_6Sn_6$ were determined by refinement of the neutron powder diffraction pattern obtained at 600 K. The lattice parameters are: $a = 8.9384(4)$ Å, $b = 18.7625(9)$ Å and $c = 5.4368(3)$ Å. The conventional refinement R-factors (%) are: $R(\text{Bragg}) = 4.5$, $R(\text{F-struct.}) = 3.2$, $R(\text{wp}) = 6.9$ and $R(\text{exp}) = 2.1$. The refined atomic

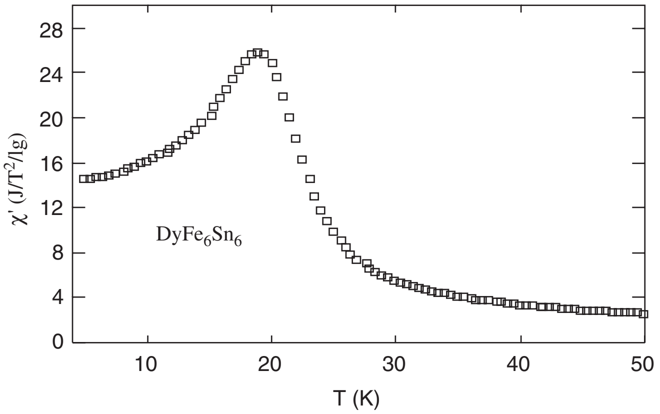

Fig. 1. AC-susceptibility trace of $DyFe_6Sn_6$ showing the magnetic ordering of the Dy sublattice at 19(2) K.

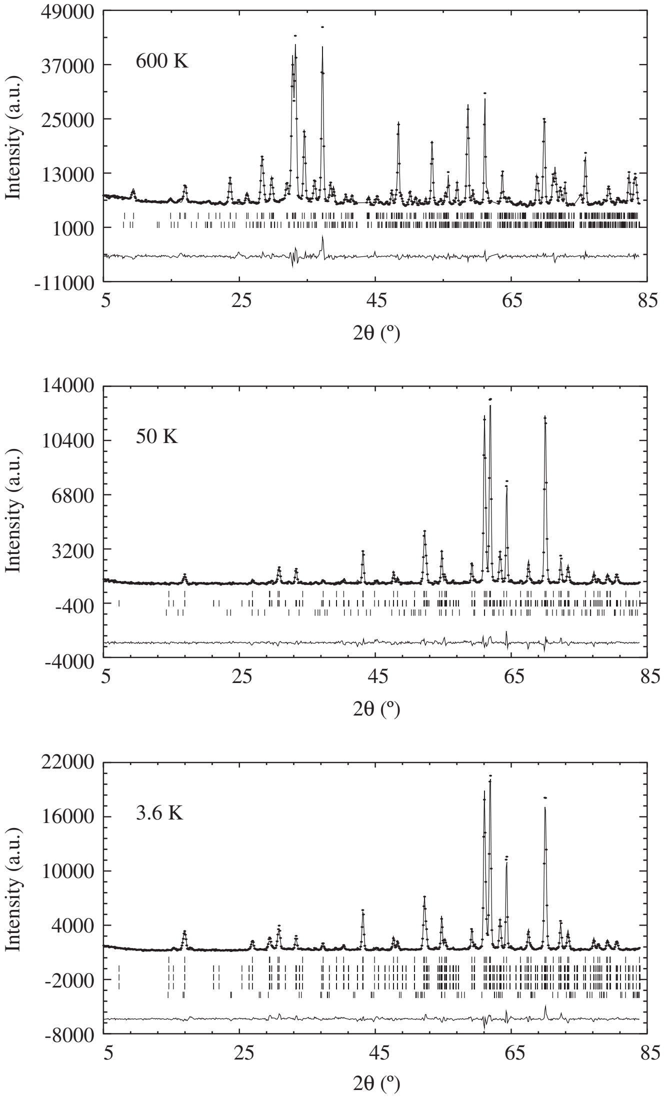

Fig. 2. Neutron powder diffraction patterns of $DyFe_6Sn_6$ obtained at (top to bottom) 600, 50 and 3.6 K. $\lambda = 2.3685(1)$ Å, except for the 600 K pattern where $\lambda = 1.3278(1)$ Å.

Table 1
Atomic positions in $DyFe_6Sn_6$ at 600 K

Atom	Site	x	y	z
Dy	4c	0	0.1297(5)	$\frac{1}{4}$
Fe	8d	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{2}$
Fe	8e	0.2464(9)	0	$\frac{1}{2}$
Fe	8g	0.2467(7)	0.1240(11)	$\frac{1}{4}$
Sn	4c	0	0.0435(15)	$\frac{1}{4}$
Sn	4c	$\frac{1}{2}$	0.0412(15)	$\frac{1}{4}$
Sn	4c	0	0.2102(16)	$\frac{1}{4}$
Sn	4c	$\frac{1}{2}$	0.2087(16)	$\frac{1}{4}$
Sn	8g	0.3301(7)	0.1230(7)	$\frac{1}{4}$

position parameters are given in Table 1. The refined values of B_{iso} at 600 K are 2.7(1), 1.8(1) and 1.8(1) $Å^2$ for Dy, Fe and Sn, respectively.

The neutron diffraction pattern of $DyFe_6Sn_6$ obtained at 50 K comprises nuclear scattering plus magnetic scattering from the Fe sublattice only. As in the case of YFe_6Ge_6 [11], which has the same crystal space group as $DyFe_6Sn_6$, the magnetic ordering of the Fe sublattice in $DyFe_6Sn_6$ results in the appearance of extra peaks with the condition $h + k = odd$ (nuclear scattering peaks obey $h + k = even$ for the Cmcm space group). Thus, we describe the Fe order as *anti-C* i.e. Fe moments related by the C-translation $+(\frac{1}{2}\frac{1}{2}0)$ are antiparallel. We have described the procedure for determining the magnetic ordering mode of the Fe sublattice in detail in our paper on YFe_6Ge_6 [11].

We obtained the best fit to the 50 K neutron diffraction pattern of $DyFe_6Sn_6$ with the Fe moments oriented along [1 0 0] with a propagation vector [0 1 0]. This ordering is a common feature of the RFe_6Ge_6 and RFe_6Sn_6 series ([1] and references therein). The refined Fe magnetic moment in $DyFe_6Sn_6$ at 50 K is 2.2(6)μ_B and the magnetic space group of the Fe sublattice is antiferromagnetic $C_P m'c'm'$. As described earlier, we confirmed the Fe sublattice magnetic ordering mode deduced from our neutron scattering experiments by ^{119}Sn Mössbauer spectroscopy.

The magnetization of a powder sample of $DyFe_6Sn_6$ was measured at 2 K in magnetic fields up to 9 T. The slow approach to saturation of the magnetization with applied field indicates that the Dy sublattice order involves both ferromagnetic and antiferromagnetic components. The magnetization at 2 K is far from saturated at 9 T and reaches 36.5 J/T/kg in 9 T which corresponds to a Dy moment of 7.9μ_B, significantly lower than the free-ion moment of 10μ_B. Clearly, the antiferromagnetic Dy component has not 'closed-up' by 9 T.

The neutron diffraction pattern at 3.6 K shown in Fig. 2 confirms the existence of FM and AF order in the Dy sublattice, as suggested by our magnetization data. At 3.6 K, the best fit to the diffraction pattern yielded Dy magnetic moment components of FM 5.0(3)μ_B along [0 0 1] and AF 1.6(3)μ_B along [0 1 0], leading to a net Dy moment of 5.2(4)μ_B and a canting angle of 17(4)° away from the crystal *c*-axis towards the *b*-axis. The Dy ordering mode is $F_Z A_Y$ using standard notation. The reduction in Dy moment from the 'free-ion' value is most likely due to crystal-field effects. The refinement *R*-factors (%) are: $R(\text{Bragg}) = 7.8$, $R(\text{F-struct.}) = 4.7$, $R(\text{mag-Fe}) = 12.8$ and $R(\text{mag-Dy}) = 12.5$.

Acknowledgments

This work was supported by the Australian Research Council, the Australian Nuclear Science and Technology Organisation (AMRF programme); the Natural Sciences and Engineering Research Council of Canada, Fonds pour la formation des chercheurs et l'aide à la recherche (Québec) and Istituto Nazionale per la Fisica della Materia (Italy). We are grateful to the staff at BENSC–Hahn-Meitner Institute and Chalk River Laboratories for assistance during the neutron diffraction experiments.

References

[1] J.M. Cadogan, D.H. Ryan, J. Alloys Compounds 326 (2001) 166.
[2] O. Beckman, K. Carrander, L. Lundgren, M. Richardson, Phys. Scripta 6 (1972) 151.
[3] L. Häggström, T. Ericsson, R. Wäppling, K. Chandra, Physica Scripta 11 (1975) 47.
[4] D.H. Ryan, J.M. Cadogan, J. Appl. Phys. 79 (1996) 6004.
[5] J.M. Cadogan, Suharyana, D.H. Ryan, O. Moze, W. Kockelmann, J. Appl. Phys. 87 (2000) 6046.
[6] J.M. Cadogan, Suharyana, D.H. Ryan, O. Moze, W. Kockelmann, IEEE Trans. Magn. 37 (2001) 2606.
[7] J.M. Cadogan, D.H. Ryan, O. Moze, Suharyana, M. Hofmann, J. Phys.: Condens. Matter 15 (2003) 1757.
[8] J. Rodríguez-Carvajal, Physica B 192 (1993) 55.
[9] X.-L. Rao, Ph.D Thesis, University of Dublin, unpublished, 1997.
[10] O.Ya. Oleksyn, H. Böhm, Z. Kristallogr. 213 (1998) 270.
[11] J.M. Cadogan, D.H. Ryan, I.P. Swainson, O. Moze, J. Phys.: Condens. Matter 10 (1998) 5383.