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Uniaxial antiferromagnetic ordering in $HoNiSi_2$. A neutron and magnetic study

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Abstract

The magnetic structure of the compound $HoNiSi_2$ has been studied by neutron diffraction and magnetic measurements. The paramagnetic neutron data confirmed the $CeNiSi_2$ type of structure reported earlier for this compound. The analysis of the data collected in the magnetically ordered regime (T_N=10 K) showed a collinear moment arrangement of the Ho moments along **c** invariant under the magnetic space group $C_pm'cm$ (Sh_{57}^{391}). The refined moment value at 1.5 K is $\mu_{Ho}=8.13(1)\mu_B$.

1. Introduction

Ternary rare earth (R) compounds of composition RMX_2 where M is a 3d element and X a metalloid (Si, Ge, Sn) with the $CeNiSi_2$ type of structure [1] (Cmcm space group) form a large family of compounds with interesting magnetic properties that are presently being investigated by several authors [2]. The present authors have undertaken a systematic study of the magnetic properties of the $RNiSi_2$ series. In previous investigations the light rare earths (R=Nd, Pr) [3] were found to order ferromagnetically with the easy magnetization direction along the shortest direction, i.e., the c direction. By contrast, the Tb compound [4] was found to display uniaxial antiferromagnetic ordering, with the easy magnetization direction also along **c**. As a continuation of this study, the present paper refers to the magnetic structure of the antiferromagnetic $HoNiSi_2$ [5] compound, which will be shown to display a different type of antiferromagnetic order.

2. Magnetic measurements

The temperature dependence of the magnetization was determined on a SQUID magnetometer in the temperature range 4.2–350 K. Results are shown in Fig. 1. As is shown in the inset of the figure, perfect Curie–Weiss behaviour is observed over almost the whole temperature range. The

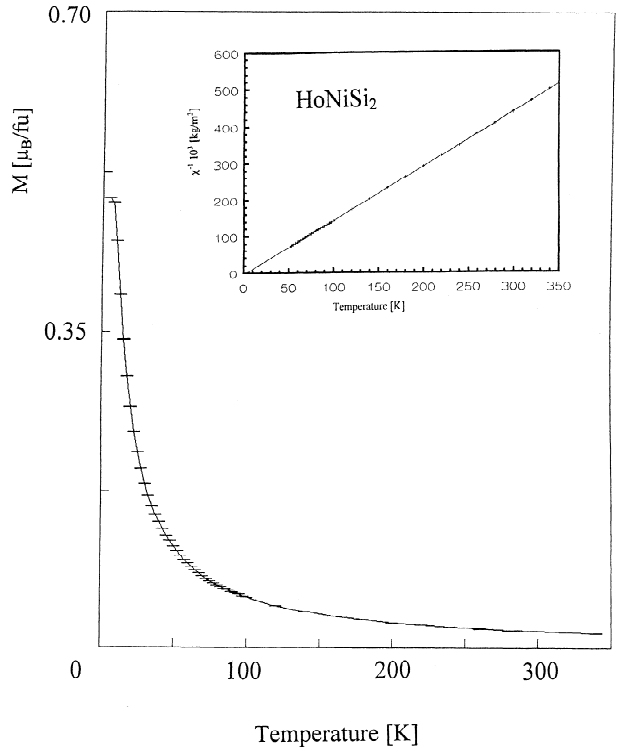

Fig. 1. Temperature dependence of the magnetization and reciprocal susceptibility (inset) of $HoNiSi_2$. Measurements were made in a field of 2 T.

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corresponding values of the effective moment and asymptotic Curie temperature are μ_{eff} =11.05μ_b and θ_p=3 K, respectively. The value of the effective moment is close to the free ion value (10.60μ_b) the temperature dependence of the magnetization is shown in the main part of the figure. No sharp magnetic transition is observed in the temperature range investigated although the shape of the curve shown suggests magnetic ordering to occur below about 10 K. The low value of the magnetic moment indicates that the ordering is of the antiferromagnetic type. Our data are in satisfactory agreement with those reported in [6].

3. Neutron diffraction

Neutron diffraction experiments were carried out on a powder sample of $HoNiSi_2$, in the temperature range 2–15 K. The data were collected with the D1A (double axis multicounter diffractometer) at the facilities of the ILL in Grenoble using a wavelength of 2.4783 Å. The step increment of the diffraction angle 2θ was 0.1°. The data were corrected for absorption and evaluated by the Fullprof Program [6].

3.1. Nuclear structure of $HoNiSi_2$

The neutron diffraction pattern collected in the paramagnetic state at 15 K, is shown in Fig. 2 (top part). The refined parameters given in Table 1 confirm the type of structure [1,2]. The R-factor values are satisfactory and

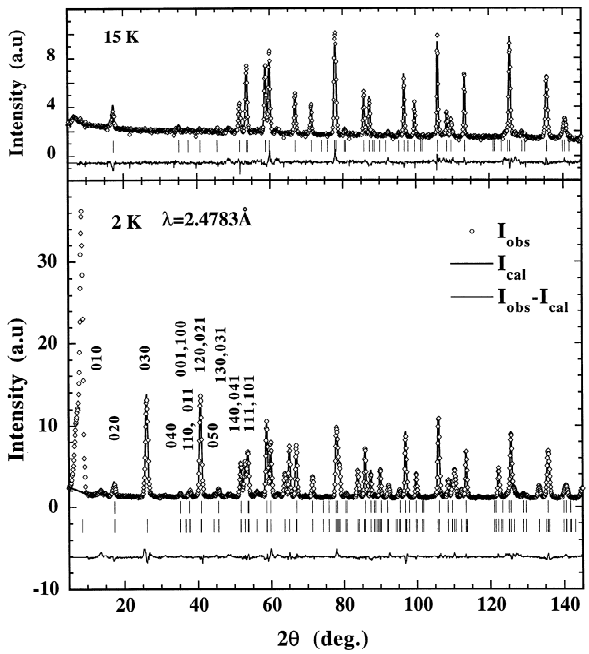

Fig. 2. Observed, calculated and difference neutron diagrams of $HoNiSi_2$: (a, top part) measured at 15 K (paramagnetic state); (b, bottom part) measured at 1.5 K (magnetically ordered state).

Table 1
Magnetic space groups of the Cmcm space group associated with the Cp lattice (**q**=(010)) and magnetic modes C(++−−) and A(+−−+) of the 4c site

Magnetic space group	x	y	z
$C_P\frac{222_1'}{m\,c\,m}i\,Sh_{51}^{301}$	-	-	-
$C_P\frac{222_1'}{m'\,c\,m}i'\,Sh_{57}^{391}$	-	-	A
$C_P\frac{222_1'}{m\,c'\,m}i'\,Sh_{59}^{414}$	-	-	-
$C_P\frac{222_1'}{m\,c\,m'}i'\,Sh_{62}^{453}$	A		
$C_P\frac{222_1'}{m'\,c'\,m}i\,Sh_{62}^{454}$	-	-	C
$C_P\frac{222_1'}{m\,c'\,m'}i\,Sh_{58}^{402}$	C	-	-
$C_P\frac{222_1'}{m'\,c\,m'}i\,Sh_{60}^{431}$	-	C	-
$C_P\frac{222_1'}{m'\,c'\,m'}i'\,Sh_{52}^{318}$	-	A	-

indicate no other significant deviation from the basic structure.

3.2. Magnetic ordering of $HoNiSi_2$

Magnetic ordering becomes visible below 10 K. The magnetic reflections over the whole magnetically ordered region do not obey the reflection conditions of the C-centered lattice. This means that the magnetic cell is primitive (C_P) and **q**=(010). The dominant intensities of the (0k0) k=2n+1 reflections indicate that the main axis of antiferromagnetism is along the a or c directions. Due to the special position (4c) of the Ho atoms, at the intersection of the m2m symmetry elements, the possible magnetic modes are restricted to a uniaxial arrangement with either the A(+−−+) or the C(++−−) type of mode (see Table 1). The sign change refers to the atoms (1) (0,−y,1/4); (2) (0,−y,3/4); (3) 1/2, 1/2+y,1/4); (4) (1/2, 1/2−y, 3/4). The refinement of the magnetic intensities has shown a collinear moment arrangement A(+−−+) of the Ho moments along **c** (Fig. 3, Table 2) which corresponds to the magnetic space group $C_pm'cm$ Sh_{57}^{391} [7–9]. The refined moment value at 1.5 K μ_{Ho}=8.13(1) [μ_B] is smaller than the free ion Ho^{3+} value gJ[μ_B]=10[μ_B] which is most probably due to crystal field effects. From the temperature dependence of the magnetic intensities and the ordered moment values shown in Fig. 4 one derives that the ordering temperature is T_N=10 K in good agreement with the magnetic measurements.

4. Concluding remarks

Both $HoNiSi_2$ and $TbNiSi_2$ have a uniaxial moment arrangement along the shortest axis, i.e., the **c** axis. For

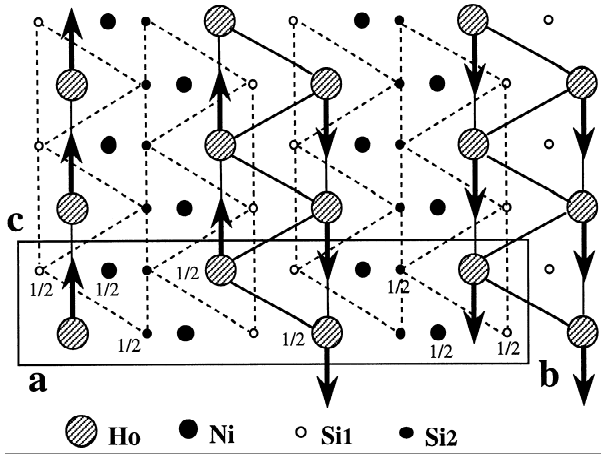

Fig. 3. Schematic representation of the collinear antiferromagnetic ordering of $HoNiSi_2$ when viewed along the [100] direction.

both compounds the exchange within the (010) layers (nearest neighbors) is ferromagnetic while the exchange between two successive layers separated by the Si_1–Si_1 double layers is antiferromagnetic (next near neighbors 3.98 Å). The results of the present investigation have shown, however, that the uniaxial magnetic structure of $HoNiSi_2$ differs from that of $TbNiSi_2$ by the fact that the moments of the rare earth atoms in two consecutive ferromagnetic (010) layers separated by a set of Ni–Si_2–Ni (010) triple layers are parallel in the Ho compound, while these ferromagnetic layers have a mutually antiparallel moment arrangement in the Tb compound.

These results show again that the exchange interactions in these $RNiSi_2$ compounds may vary quite substantially when proceeding through the lanthanide series, a property that leads to ferromagnetism for compounds formed with light lanthanides and to different types of antiferromagnetism for compounds formed with heavy lanthanides.

Table 2
Refined structural parameters of $HoNiSi_2$ in the paramagnetic state at 15 K and in the magnetically ordered state at 1.5 K. Space group Cmcm (No. 63). All atoms at 4c (0,y,1/4). B_{of} = overall temperature factor

Parameter/value	1.5 K	15 K
y_{Ho}	0.1054(4)	0.1059(2)
y_{Ni}	0.3238(5)	0.3236(1)
y_{Si1}	0.4593(15)	0.4599(5)
y_{Si2}	0.7506(14)	0.7497(4)
$\mu_{zHo}[\mu_B]$	8.13(4)	-
a (nm)	0.39464(4)	0.39479(2)
b (nm)	1.6424(2)	0.39309(5)
c (nm)	1.6428(1)	0.39276(2)
B_{of} (nm^2)	0.005(1)	0.004(1)
R_n(%), R_m(%)	6.15, 7.13	9.1, -
R_{wp}(%), R_{exp}(%)	20, 4.5	15, 8.2

References

[1] O.P. Bodak and E.I. Gladyshevskii, *Sov. Phys. Crystallogr., 14* (1970) 859.
[2] A. Szytula, in K.H.J. Buschow (ed), *Handbook of Magnetic Materials*, Vol. 6, 1991, p. 85.
[3] P. Schobinger-Papamantellos and K.H.J. Buschow, Uniaxial antiferromagnetic ordering in $TbNiSi_2$. *J. Less-Common Metals, 171* (1991) 321.
[4] P. Schobinger Papamantellos and K.H.J. Buschow, Ferromagnetic ordering of $NdNiSi_2$ and $PrNiSi_2$ studied by neutron diffraction and magnetic measurements. *J. Alloys Compnds., 185* (1992) 51.
[5] A. Gil, A. Szytula, Z. Tomkowicz, K. Wojciechowski and A. Zygmunt, *J. Mag. Magn. Mat., 129* (1994) 271.
[6] J. Rodríguez-Carvajal, *Physica B, 192* (1993) 55.
[7] (a) E.F. Bertaut, in G.T. Rado and H. Suhleds (eds), Magnetism, Vol. III, Academic Press, New York, 1963, Ch.4, p. 149. (b) E.F. Bertaut, *Ann. Phys., 9* (1975) 93.
[8] V.A. Koptzik, Shubnikov Groups (Moscow University Print 1966).
[9] W. Opechowski and R. Guccione, in G.T. Rado and H. Suhl (eds.), Magnetism IIA, Academic Press, London, 1965, Ch 3, p. 105.

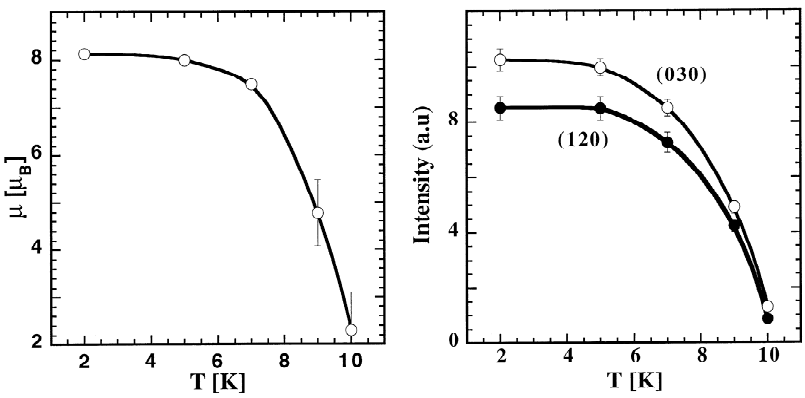

Fig. 4. (a) Temperature dependence of the Ho magnetic moment of $HoNiSi_2$. (b) Temperature dependence of the magnetic intensities [(030) and (120)] of $HoNiSi_2$.