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Magnetic properties of hp13 type $TFe_6Ge_6(T = Zr, Nb, Hf)$ alloys

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Abstract

We have made magnetization measurements, Mössbauer spectroscopy and neutron diffraction experiments on hexagonal hp13 type $TFe_6Ge_6(T = Zr, Hf, Nb)$ alloys; the 1a and 6i sites are entirely occupied by T(= Zr, Hf, Nb) and Fe, respectively. The alloys exhibit a simple antiferromagnetism with the magnetic moment of about $1\,\mu_B$/Fe atom at 295 K. The Néel temperature T_N, the paramagnetic Curie temperature θ_p and the internal field H_{in} are as follows: $T_N = 495\,K$, $\theta_p = 70\,K$ and $H_{in} = 227\,K$ for T = Zr; $T_N = 462\,K$, $\theta_p = 62\,K$ and $H_{in} = 198\,K$ for T = Hf; $T_N = 554\,K$, $\theta_p = 71\,K$ and $H_{in} = 198\,K$ for T = Nb. This is in contrast with complicated magnetic properties of the isotypic alloys such as $Fe_5Mn_2Ge_6$. © 2001 Elsevier Science B.V. All rights reserved.

Keywords: Antiferromagnetism; Neutron diffraction; Mössbauer spectra

Recently, we made magnetization measurements and neutron diffraction experiments on $M_{7-x}Mn_xGe_6$ (M = Co, Fe) alloys [1,2], which have a hexagonal layer structure (P6/mmm) of hp13 type (Pearson symbol), in which transition element layers consisting of 1a and 6i sites are well separated by Ge layers of 2c and 2e sites. The $Mn_4Fe_3Ge_6$ alloy is antiferromagnetic; the paramagnetic Curie temperature θ_P is positive and close to the Néel temperature T_N of 528 K. The high-field magnetization measurement for the $Fe_3Mn_4Ge_6$ alloy at 77 K reveals that the magnetization shows a steep increase around 110 kOe, suggesting the metamagnetic transition. More recently, we reported that the isotypic alloy $TiFe_6Ge_6$ exhibits simpler antiferromagnetic behaviors [3]; $\theta_P(= 70\,K)$ is much lower than $T_N(= 510\,K)$.

In the present work, we have made magnetization measurements, Mössbauer spectroscopy and neutron diffraction experiments for similar alloys TFe_6Ge_6 (T = Zr, Nb, Hf). The crystal structure of these alloys was already studied in 1981 [4]. Experimental methods were the same as these described in our earlier paper [3]. The prepared samples were $TFe_6Ge_{6+\delta}$ (T = Zr, Nb, Hf) since the alloys with $\delta = 0$ were found to have a ferromagnetic component with the Curie temperature of about 400 K arising from a small amount of an impurity phase. Therefore, we made the magnetization measurements on the alloys with $\delta = 0.2$.

Fig. 1 shows the magnetization σ in a field of 8.0 kOe versus temperature T curves for $TFe_6Ge_{6.2}$ (T = Zr, Nb, Hf). The magnetization below room temperature for T = Nb contains a weak ferromagnetic component which may be attributed to an impurity phase. The magnetization has a maximum at a temperature around 500 K which must be the Néel temperature T_N. The inverse susceptibility χ^{-1} versus temperature curves are also shown in Fig. 1. The susceptibility above T_N obeys the Curie–Weiss law, from which the paramagnetic Curie temperature θ_p and the effective Bohr magneton μ_{eff} are determined. These values are listed in Table 1. It is noted that the paramagnetic Curie temperatures are positive and much lower than the Néel temperatures.

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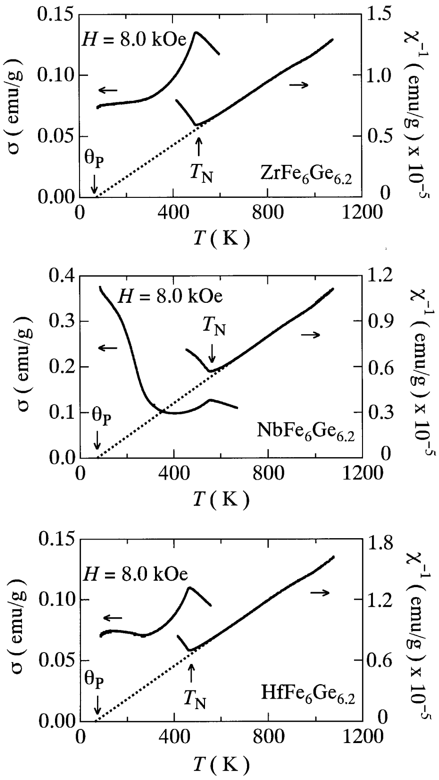

Fig. 1. Temperature dependence of magnetization σ in a field of 8.0 kOe and inverse susceptibility χ^{-1} for $TFe_6Ge_{6.2}$ (T = Zr, Hf, Nb).

Table 1
The Néel temperature T_N, the paramagnetic Curie temperature θ_p, the effective Bohr magneton μ_{eff} and the extrapolated internal field at 0 K H_{in0} for $TFe_6Ge_{6.2}$ (T = Zr, Hf, Nb)

	T_N(K)	θ_P(K)	$\mu_{eff}(\mu_B)$	H_{in0}(kOe)
$ZrFe_6Ge_{6.2}$	495	70	2.94	227
$HfFe_6Ge_{6.2}$	462	62	2.76	198
$NbFe_6Ge_{6.2}$	554	71	3.10	237

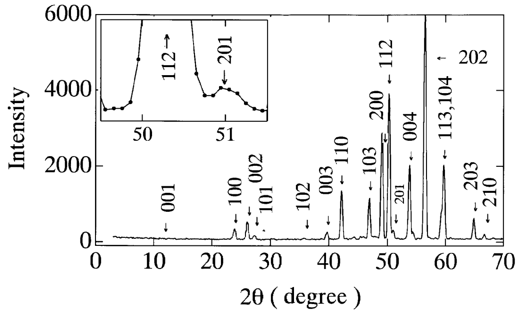

Fig. 2. Neutron diffraction pattern for $ZrFe_6Ge_{6.2}$ at 295 K.

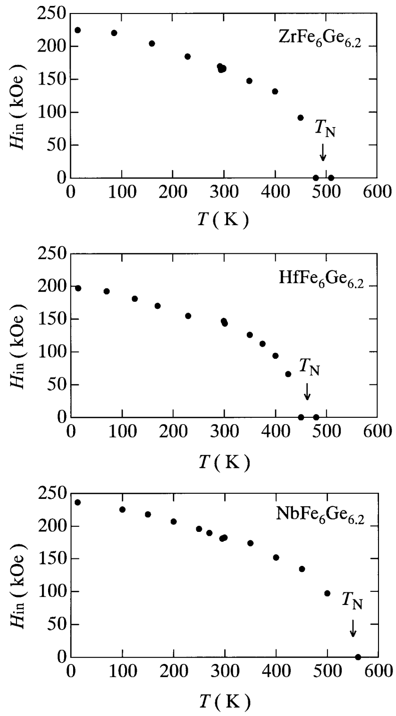

Fig. 3. Temperature dependence of internal field H_{in} for $TFe_6Ge_{6.2}$ (T = Zr, Hf, Nb).

We have made neutron diffraction experiments for $TFe_6Ge_{6.2}$ alloys at room temperature using the HERMES (wave length $\lambda = 1.817$ Å) of IMR installed in the JRR-3 M reactor at JAERI. For a typical example, Fig. 2 shows the neutron diffraction pattern of $ZrFe_6Ge_{6.2}$ in a lower Bragg angle range. The pattern is almost identical to that of $TiFe_6Ge_{6.1}$ [3]; the 0 0 1 line is absent. It is suggested that the magnetic structure of $TFe_6Ge_{6.2}$, (T = Zr, Nb and Hf) is similar to that of $TiFe_6Ge_{6.1}$, i.e., magnetic moments of Fe atom are ferromagnetically arrangement in the same c-plane and antiferromagnetically arranged between adjacent c-planes, and the direction of the magnetic moment is parallel to the c-axis. We determined the atomic site occupation from a Rietveld analysis [5] using the neutron diffraction intensities in which the data around the 1 0 1 and 2 0 1 reflections containing some magnetic contributions were removed. The results are as follows: Ge on 2c $(\frac{1}{3},\frac{2}{3},0)$, 2d $(\frac{1}{3},\frac{2}{3},\frac{1}{2})$ and 2e $(0, 0, z_1)$, T on 1a $(0, 0, \frac{1}{2})$ and Fe on 6i $(\frac{1}{2}, 0, z_2)$ with $z_1 = 0.158$ and $z_2 = 0.251$ for T = Zr; $z_1 = 0.159$ and $z_2 = 0.251$ for T = Hf; $z_1 = 0.164$ and $z_2 = 0.250$ for T = Nb. We also estimated the magnetic moment of about 1 μ_B/Fe atom from the 1 0 1 and 2 0 1 reflections.

Fig. 3 shows the internal field H_{in} versus temperature T curves for $TFe_6Ge_{6.2}$ (T = Zr, Hf, Nb) which are similar to the H_{in} versus T curves for $TiFe_6Ge_{6.1}$ [3]. The internal fields extrapolated to 0 K H_{in0} are also listed in Table 1.

We have also made the high-field magnetization measurements for $ZrFe_6Ge_{6.2}$ and $HfFe_6Ge_{6.2}$ at 77 K using a pulse magnet. The magnetization shows a continuous increase up to 200 kOe without the meta-magnetic behavior. This is also similar to that of $TiFe_6Ge_6$.

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