Magnetic properties of hp13 type TFe6Ge6(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 μ_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 $Fe_5Mn_2Ge_6$.

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.

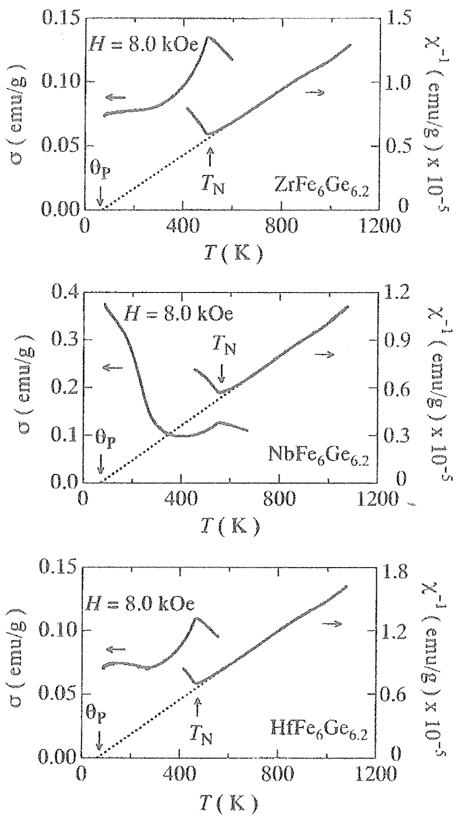

Fig. 1. Temperature dependence of magnetization σ in a field of 8.0 kOe and inverse susceptibility χ^{-1} for $TFe_6Ge_{6.2}$ (T = Zr, Hf, Nb).

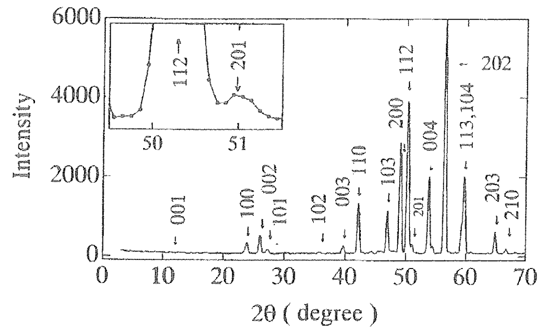

Fig. 2. Neutron diffraction pattern for $ZrFe_6Ge_{6.2}$ at 295 K.

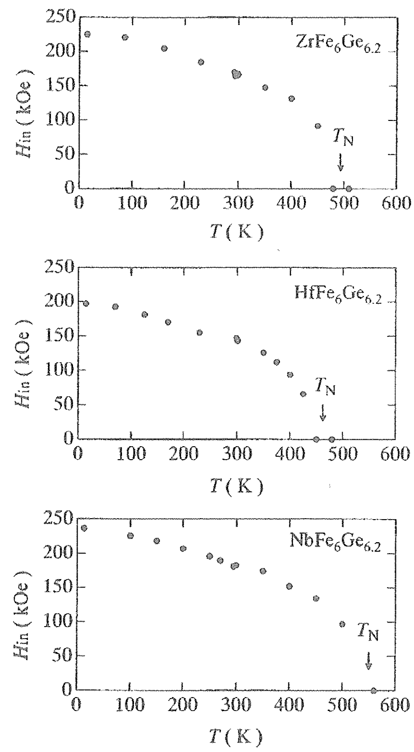

Fig. 3. Temperature dependence of internal field H_{in} for $TFe_6Ge_{6.2}$ (T = Zr, Hf, Nb).

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

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-3M 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 metamagnetic behavior. This is also similar to that of $TiFe_6Ge_6$.

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