Magnetic Structure of Fe₃Ga Studied by Neutron Diffraction*

By Nobuo Kawamiya** and Kengo Adachi**

The magnetic form factor and the magnetic moment per Fe atom (μ_{Fe}) are determined by neutron diffraction of single crystals. The Fe atoms on the B sublattice with 8 Fe nearest neighbors (NN) have the moment of $2.18 \mu_B$ and the e_g ratio (γ) of 0.60 at 290 K, where γ means the fraction of polarized electrons with the e_g symmetry and the remaining $(1-\gamma)$ have the t_{2g} symmetry. Those on the A and C sites with 4 Fe and 4 Ga NN have the moment of $1.50 \mu_B$ and γ of 0.48. The results are discussed with reference of the Mössbauer analysis and compared with the moments and internal fields of Fe₃Al and Fe₃Si.

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I. Introduction

The Fe–Ga alloy system resembles the Fe–Al system in that the Fe-rich primary solid solution has a large solubility^{(1)–(3)} and forms the Fe₃Al(D0₃) or the FeAl(B2) type superlattice structure⁽⁴⁾. The Fe–Ga system, however, differs from the Fe–Al system in that the low temperature phase of Fe₃Ga forms the Cu₃Au (L1₂) type structure instead of the Fe₃Al type. The magnetic properties and the hyperfine field for both the structures have been reported by the present authors and Nakamura⁽⁵⁾.

The Fe₃Al structure is characterized by four sublattices; A, B, C and D, where Fe atoms on A and C sites (Fe_I) have four Fe and four Al nearest neighbors (NN), and Fe atoms on B sites (Fe_{II}) have eight Fe NN's. The hyperfine field (H_{hf}) of Fe_I and Fe_{II} investigated in the previous work⁽⁵⁾ give a magnetic moment of $2.7 \mu_B$ per Fe_I and $1.7 \mu_B$ per Fe_{II} on the assumption of Wertheim's empirical formula⁽⁶⁾,

$$H_{hf}(\text{kOe}) = 120 \mu_{Fe} + 30 \bar{\mu},$$

where μ_{Fe} is a magnetic moment per "on-site" Fe atom and $\bar{\mu}$ is an average moment per atom forming the alloy. The atomic moments (μ) of Fe_I and Fe_{II} in the Fe₃Ga (D0₃) are considerably larger than those of isomorphous

Fe₃Al and Fe₃Si. Especially, $\mu(\text{Fe}_I)$ is about 20% larger than μ_{Fe} of pure iron.

To investigate the atomic moments and the magnetic form factors of Fe_I and Fe_{II} in the Fe₃Ga, the present work has made neutron diffraction of single crystals and compared the results with those of Fe₃Al and Fe₃Si.

Band calculations on Fe₃Al⁽⁷⁾ and Fe₃Si⁽⁸⁾ give a partial density of states (DOS) of Fe_I and Fe_{II} and can reproduce the atomic magnetic moments in a fair approximation^{(9)–(11)}, i.e., Fe_I has a density of states closely similar to that of pure Fe, however, Fe_{II} has a much modified DOS resulting in a reduction of the atomic moment. The partial DOS's of Fe_I and Fe_{II} in the Fe₃Ga seem, in general, to be similar to those of Fe₃Al: The magnetic form factors at room temperature are found to coincide with those of Fe₃Al at 0 K. However, the relationship between the H_{hf} and μ_{Fe} of the Fe₃Ga⁽⁵⁾ is different from that of Fe₃Al and Fe₃Si⁽¹²⁾: The former shows that

$$\frac{H_{hf}(\text{Fe}_I)}{H_{hf}(\text{Fe}_{II})} < \frac{\mu(\text{Fe}_I)}{\mu(\text{Fe}_{II})},$$

in contrast to Fe₃Al and Fe₃Si, where

$$\frac{H_{hf}(\text{Fe}_I)}{H_{hf}(\text{Fe}_{II})} > \frac{\mu(\text{Fe}_I)}{\mu(\text{Fe}_{II})}.$$

This difference cannot be interpreted by Wertheim-type assumptions⁽⁶⁾ but can be attributed to the effects of the second nearest or more distant neighbor interactions.

* The units used in this paper are converted to SI unit as follows: $1 \text{ \AA} = 10^{-10} \text{ m}$, $1 \text{ Oe} = 79.6 \text{ A/m}$ and $1 \mu_B = 1.1653 \times 10^{-29} \text{ Wb} \cdot \text{m}$.

** Faculty of Engineering, Nagoya University, Nagoya 464, Japan.

II. Neutron Diffraction by Unpolarized Neutrons

1. Sample preparation

Alloys of Fe₃Ga were prepared from Fe (99.99% pure) and Ga (99.999% pure) by a method described in the previous paper⁽⁵⁾. Single crystals were obtained by furnace-cooling of the molten Fe₃Ga in a strong temperature gradient. Successive water-quenching was required to prevent the crystal from transforming into the L1₂ phase during the cooling.

A spherical (4 mm in diameter) and a cylindrical (1 mm in diameter and 7 mm long) samples were made by using an electric discharge cutter and a grinder with a device to rotate samples. Then, they were polished electrochemically, annealed in evacuated quartz tubes at 1273 K (1000°C) for three days and quenched into water from 1073 K (800°C).

2. Unpolarized neutron experiments

The spherical samples was investigated in the first place with unpolarized neutrons at the Kyoto University Reactor (KUR). Diffraction intensities were measured with and without application of magnetic fields vertical and parallel to the scattering vector.

The superlattice reflections were extinction-free but required half λ correction in the case of all even (h, k, l) where λ is the wavelength (1.08 Å) of monochromatized neutrons. However, since the fundamental reflections suffered some secondary extinction, they were corrected

by Zachariasen's method to be discussed later.

Figure 1 shows a nuclear part I_o^N of the diffracted intensity divided by $(\Sigma b)^2/\sin 2\theta$ as a function of $(\sin \theta/\lambda)^2$, where θ is a Bragg angle, and Σb is a structure factor for nuclear scattering. The theoretical expressions of nuclear scattering for the fundamental and superlattice reflections are, respectively,

$$I_{c,f}^N = \{3b_{Fe} \exp(-B_{Fe} \sin^2 \theta/\lambda^2) + b_{Ga} \exp(-B_{Ga} \sin^2 \theta/\lambda^2)\}^2, \quad (1)$$

and

$$I_{c,s}^N = S^2 \{b_{Fe} \exp(-B_{Fe} \sin^2 \theta/\lambda^2) - b_{Ga} \exp(-B_{Ga} \sin^2 \theta/\lambda^2)\}^2, \quad (2)$$

where b , B and S denotes, respectively, the nuclear scattering amplitudes, the temperature factor and the degree of long range order; suffix c means "calculated".

The curve for the superlattice reflections in Fig. 1 will be concave toward the horizontal axis if B_{Ga} is substantially larger than B_{Fe} , and it will be convex, otherwise. The difference between B_{Ga} and B_{Fe} is estimated to be negligible within the experimental errors, and the common B factor is used throughout this investigation. Therefore, eqs. (1) and (2) are reduced to

$$I_{c,f}^N = (3b_{Fe} + b_{Ga})^2 \exp(-2B \sin^2 \theta/\lambda^2), \quad (3)$$

and

$$I_{c,s}^N = S^2 (b_{Fe} - b_{Ga})^2 \exp(-2B \sin^2 \theta/\lambda^2). \quad (4)$$

The extinction-corrected intensity of the fundamental reflections, I_o , is obtained by the use of Zachariasen's formula⁽¹³⁾:

$$I_{o,f}^* = I_{o,f} (1 + 2\eta I_{o,f})^{-1/2}, \quad (5)$$

where $I_{o,f}^*$ is an experimentally observed intensity reduced by the extinction and η represents the mosaic spread of crystal.

Figure 2 shows $I_{o,f}^*$ and theoretical curves utilized for correction. It has been found that the degree of extinction increases slightly when the domain walls are wiped out by applied fields. One can substitute $kI_{o,f}^*$ for $I_{o,f}$ in eq. (5) in a kinematical approximation and hence determine k and η . In this case, however, it is to be noted that this correction is affected

Fig. 1 Nuclear scattering versus $(\sin \theta/\lambda(\text{\AA}))^2$ for fundamental and superlattice reflections. The slope gives the Debye-Waller temperature factor.

Fig. 2 Calculated and observed intensities of fundamental lines. The curves represent the least-squares fitting by Zachariasen's formula described in the text.

by the value of B , and the latter, in return, can be affected by the former. Thus B in eqs. (3) and (4), and η in eq. (5) have been determined by iterative optimization by the use of the least-squares method.

The Debye temperature θ_D is estimated to be 302 ± 20 K, from the B value of $0.45 \pm 0.03 \text{ \AA}^{-2}$. The intensity ratio of the superlattice reflections to the fundamental ones gives a long range order parameter S of 0.96 ± 0.04 . That S is nearly equal to unity is consistent with the results of the Mössbauer analysis in the previous work⁽⁵⁾ which has shown a clear separation of the internal fields corresponding to the Fe_I (or B) and Fe_{II} (or A) sites in the D0_3 structure.

The magnetic part I^M of the fundamental and superlattice reflection intensities were derived from the intensity change according to applied fields parallel or perpendicular to the scattering vector. The applied field of 9.1 kOe was much larger than 4.8 kOe, the field required to obtain saturated magnetization.⁽⁵⁾

The expressions for I^M and I_s^M are;

$$I_{c,f}^M = (p_I + 2p_{II})^2 \exp \{-2B(\sin \theta/\lambda)^2\}, \quad (6)$$

$$I_{c,s}^M(\text{odd}) = S^2 p_I^2 \exp \{-2B(\sin \theta/\lambda)^2\}, \quad (7)$$

and

$$I_{c,s}^M(\text{even}) = S^2 (2p_{II} - p_I)^2 \exp \{-2B(\sin \theta/\lambda)^2\}, \quad (8)$$

where (odd) or (even) denotes that the diffraction indices h, k, l are all odd or all even, and p_I or p_{II} denotes the magnetic scattering amplitude (magnetic form factor multiplied by moment) of Fe_I or Fe_{II} , respectively. These p_I and p_{II} are given as

$$p_i = 0.27 \times 10^{-12} \mu_i(T) f_i(\sin \theta/\lambda),$$

where $\mu_i(T)$ and f_i denote, respectively, the atomic moment (μ_B) at a temperature, T , and the magnetic form factor of Fe_I ($i=I$) or Fe_{II} ($i=II$).

The half λ contamination was measured at the reciprocal lattice points of 110 and 211 corresponding to 220 and 422 reflections for $\lambda/2$, and it was estimated to be 0.14% of the regular (λ) neutron flux. Thus $\lambda/2$ reflections have a non-negligible effect on $I_{o,s}^N$ (even), i.e. the nuclear part of the superlattice lines with all even h, k and l .

Magnetic contribution I^M can be derived by two ways, i.e. (i) directly from I_o^M by the use of parameters B and S , (ii) relatively from the ratio of I^M/I^N by the use of η and/or $\lambda/2$ correction but without the use of B and S . The results from the two methods agree within the experimental errors for the least-squares fitted parameters. Nuclear (I^N) and magnetic (I^M) parts of a respective reflection are separated from measurements under magnetic fields; the observed intensity (I_o) is given as

$$I_o = I^N + I^M \quad \text{for } H//Q,$$

$$I_o = I^N \quad \text{for } H \perp Q,$$

and

$$I_o = I^N + \frac{2}{3} I^M \quad \text{for } H=0,$$

where H and Q denote the magnetic field and the scattering vector, respectively. The results are shown in Fig. 3, as compared with the calculated intensities. The fundamental lines are shown without extinction correction. Referring to eqs. (3)–(8), one can separate I^M from I^N for the fundamental and superlattice lines.

Thus the magnetic scattering amplitudes, p_i 's, are obtained from the square root of I^M by the use of eqs. (6), (7) and (8) as shown in Fig. 4. The extrapolation of p_i to $Q=0$ region is made by the use of the atomic moment from

Fig. 3 Calculated (I_c) and observed (I_o) reflection intensities under applied or zero magnetic fields: the subscripts m and n denote $\mathbf{H} \perp \mathbf{Q}$ and $\mathbf{H} \parallel \mathbf{Q}$, respectively, and no subscript means $\mathbf{H} = 0$.

Fig. 4 Magnetic scattering amplitudes versus $\sin \theta / \lambda (\text{\AA}^{-1})$ obtained by unpolarized neutron diffraction. The average amplitude, $\langle p_o \rangle$, means $(p_I + 2p_{II})/3$ at $\sin \theta / \lambda = 0$.

static measurements⁽⁵⁾, where the effects due to s-electron polarization and orbital moments are neglected. p_{II} is obtained from interpolation of p_I in eq. (7) and $(2p_{II} - p_I)$ in eq. (8).

III. Neutron Diffraction by Polarized Neutrons

Measurements with polarized neutrons were made by the use of a diffractometer in Japan Atomic Energy Institute at Tokai (JRR-2).

An intensity ratio of reflections with the polarization flipper off and on, meaning that the spin and the neutron moments are, respectively, parallel and antiparallel, is given by

$$R = \frac{(b+p)^2}{(b-p)^2}, \quad (9)$$

where b and p are, respectively, the nuclear and the magnetic scattering amplitudes.

In the case of incomplete polarization and/or flipping, the ratio R is expressed by Paoletti's equation⁽¹⁴⁾:

$$R = \frac{\pi(b+p)^2 + (1-\pi)(b^2 + p^2)}{\pi\phi(b-p)^2 + \pi(1-\pi)(b+p)^2 + (1-\pi)(b^2 + p^2)}, \quad (10)$$

where π is the polarization ratio, and ϕ the flipping ratio, which were calibrated experimentally to be 0.95 (π) and 0.93 (ϕ).

Factors affecting the analysis of the data were treated as follows: The secondary extinction was negligible in the case of superlattice reflections. On the other hand, it was not small in the case of fundamental reflections. Therefore, the superlattice lines alone were analyzed to give atomic form factors and anisotropy factors of the unpaired spin density.

No multiple scattering was ascertained to occur, by trial azimuthal rotations of the sample around the scattering vector. The Debye-Waller factor B is irrelevant in this ratio method, because B_{Fe} and B_{Ga} are considered to be equal within the experimental accuracy.

The magnetic scattering amplitudes, $p^{\text{exp}}(Q)$'s ($Q = \sin \theta / \lambda$) obtained relatively to the nuclear amplitudes are compared with the calculated ones:

$$p_i^{\text{cal}}(Q) = \mu_i f(Q) \times 0.27 \times 10^{-12} \\ = \mu_i \left\{ \langle j_0(Q) \rangle + A_{hkl} \left(\frac{5}{2} \gamma_i - 1 \right) \langle j_4(Q) \rangle \right\} \\ \times 0.27 \times 10^{-12}, \quad (11)$$

with

$$A_{hkl} = \frac{h^4 + k^4 + l^4 - 3(h^2 k^2 + k^2 l^2 + l^2 h^2)}{(h^2 + k^2 + l^2)^2}, \quad (12)$$

where i denotes the site I or II, and γ_i is the ratio of electrons with the e_g symmetry to the whole (e_g and t_{2g}) unpaired electrons of the site i . The spherical and not spherical form factor $\langle j_0(Q) \rangle$ and $\langle j_4(Q) \rangle$ have been taken from the calculation for a free ion atom by Weiss and Freeman⁽¹⁵⁾, which were reported to agree well with the experiments on metallic Fe and Fe₃Al. It is confirmed also in this work that Fe_I atoms with 8 Fe neighbors have a close resemblance to metallic Fe in the electronic structure, and therefore, in the magnetic scattering amplitudes.

In the case of Fe_{II} atoms, however, a more appropriate trial function for $p(Q)$ is given by:

$$p_{\text{II}}^{\text{cal}}(Q) \\ = \mu_{\text{II}} \left\{ \langle j_0(rQ) \rangle + A_{hkl} \left(\frac{5}{2} \gamma_{\text{II}} - 1 \right) \langle j_4(rQ) \rangle \right\} \\ \times 0.27 \times 10^{-12}, \quad (13)$$

where r represents a change in the radial (in Q space) distribution of $p_{\text{II}}(Q)$ compared with $p(Q)$ of metallic Fe.

Thus the parameters are determined to minimize the sum of the squared residual

$$Q_{\text{sp}} = \sum_{(hkl)} W_{hkl} (p_{hkl}^{\text{exp}} - p_{hkl}^{\text{cal}})^2, \quad (14)$$

where $p_{hkl}^{\text{cal}} = p_{\text{I}}^{\text{cal}}$ for all odd (h, k, l) and $p_{hkl}^{\text{cal}} = 2p_{\text{II}}^{\text{cal}} - p_{\text{I}}^{\text{cal}}$ for all even (h, k, l) and W_{hkl} is a statistical weight of the (h, k, l) reflections.

The parameters thus obtained are summarized in Table 1, as compared with Fe₃Al and Fe₃Si. The radial distribution of the unpaired spin density of Fe_{II} seems to be similar to Fe_I and Fe because the parameter r in eq. (13) falls upon 1.02 ± 0.03 (i.e., almost unity).

Results of magnetic scattering are shown in Fig. 5, for odd (h, k, l) , and in Fig. 6, for even (h, k, l) . The value of p_{I} and p_{II} at $Q=0$ is obtained on assumptions that s electron polarization and orbital magnetic moments are negligible, and that $\mu_{\text{I}} + 2\mu_{\text{II}}$ in eq. (11) is equal

Table 1 Magnetic moments, μ , internal fields, H , and γ 's in eq. (11).

	Fe ₃ Ga		Fe ₃ Al		Fe ₃ Si	
	0 K	290 K	0 K	0 K		
$\mu_{\text{I}}(\mu_{\text{B}})$	2.49	2.18	2.18	2.4		
$\mu_{\text{II}}(\mu_{\text{B}})$	1.71	1.50	1.50	1.2		
$\mu_{\text{I}}/\mu_{\text{II}}$	1.46	1.45	1.45	2.0		
$H_{\text{I}}(\text{kOe})$	360	318	334	320		
$H_{\text{II}}(\text{kOe})$	230	204	234	204		
$H_{\text{I}}/H_{\text{II}}$	1.56 _s	1.55 ₉	1.42 ₇	1.56 ₉		
$\gamma(\text{Fe}_{\text{I}})$	0.60	0.60	0.60	—		
$\gamma(\text{Fe}_{\text{II}})$	0.48	0.48	0.49	—

Fig. 5 Magnetic scattering amplitude for all odd (h, k, l) . The curve denotes the semi-empirical form factor described in the text.

Fig. 6 Magnetic scattering amplitude for all even (h, k, l) . The curve denotes the semi-empirical form factor described in the text.

to the saturation magnetic moments per unit formula (Fe₃Ga). The ratio of the e_g vs the total unpaired electrons at site i , γ_i , is obtained from eqs. (11) and (13). These figures and Table 1 show that Fe₃Ga resembles closely Fe₃Al in

the distribution and the non-sphericity of the unpaired electrons. It is to be noted that μ_i 's of Fe₃Al at 0 K coincide with those of Fe₃Ga at room temperature. The μ_i 's of Fe₃Ga at 0 K in Table 1 are obtained from the extrapolation by the use of the temperature dependence of the saturation magnetization.

IV. Summary and Discussion

The unpaired electron population of e_g and t_{2g} symmetry at Fe_I and Fe_{II} sites are estimated from the μ_i (0 K) and γ_i values in Table 1. The results are shown in Table 2. It is to be noted that μ_I is 13% larger than the atomic moment of pure Fe. Thus the μ_I of Fe₃Ga is like that of Fe₃Si rather than of Fe₃Al. The μ_{II} , however, is much larger than those of Fe₃Al and Fe₃Si.

It is shown that Fe_I and Fe_{II} have similar t_{2g} electrons and that the difference between μ_I and μ_{II} is mainly due to that in the e_g electron population. This difference has been interpreted by Pickart and Nathans⁽⁹⁾⁻⁽¹¹⁾ as a decrease of e_g electrons in the down-spin (majority spin) bands of the partial DOS of Fe_{II}. However, the band calculations for Fe₃Al⁽⁷⁾ and Fe₃Si⁽⁸⁾ show that Fe_{II} is more electronegative and has more up-spin electrons than Fe_I. Therefore, the difference $\Delta\mu$ ($=\mu_I - \mu_{II}$) should be attributed to the increase in up-spin electrons with e_g symmetry in the partial DOS of Fe_{II}. In the case of Fe₃Ga, the $\Delta\mu$ (0.78 μ_B) is considered to be due to filling of 0.68 up-spin electrons in the e_g subbands of Fe_{II}.

It is interesting to compare the atomic moments μ_i 's with the internal fields H_i 's in these D0₃ compounds. Fe₃Ga is characteristic in that

$$H_I/H_{II} = 1.56 > \mu_I/\mu_{II} = 1.45.$$

This implies that the second nearest neighbor

Table 2 Unpaired electrons of e_g and t_{2g} symmetry at Fe_I and Fe_{II} sites.

	e_g	t_{2g}	total
Fe _I	1.50	0.99	2.49
Fe _{II}	0.82	0.89	1.71
difference	0.68	0.11	0.78

(2NN) interactions must be taken into account for the analysis of the internal fields (H_i) in terms of the atomic magnetic moments, μ_i 's. Thus one can presume that

$$H_I = \alpha\mu_I + 8\beta\mu_{II} \quad (15)$$

and

$$H_{II} = \alpha\mu_{II} + 4\beta\mu_I + 6\gamma\mu_{II}, \quad (16)$$

where α , β and γ represent the effects of the on-site, NN and 2NN atomic moments, respectively, and numerical factors of the second and third terms represent the coordination number of NN or 2NN magnetic atoms.

It has been known that any analysis of H_i as a function of μ_i gives α in the range of 105 ± 15 kOe/ μ_B ⁽⁵⁾⁽⁶⁾⁽¹²⁾⁽¹⁶⁾⁻⁽¹⁸⁾. This range of α determines that of β from eq. (15) and that of γ from eq. (16). Thus, a probable assignment of α , β and γ is given in Table 3. The values of β are consistent with those obtained in Fe-rich solid solutions where "simple dilution" holds⁽¹⁹⁾. However, the values of γ are characteristic of alloying elements, i.e., γ is positive and nearly half of β in Fe₃Al; almost null in Fe₃Si; and distinctly negative in Fe₃Ga.

In summary, Fe₃Ga has magnetic form factors closely resembling those of Fe₃Al, in their symmetry and radial distribution. Fe₃Ga has a larger magnetic moment per formula unit than those of Fe₃Al and Fe₃Si with D0₃ structures, however, it has relatively small internal fields (H_{II}) due to the negative γ representing the 2NN interaction.

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Table 3 Possible assignments of α , β and γ in eqs. (15) and (16). The signs, $\pm$, are put in order. The values of β are in good agreement with those assigned in the primary solid solutions of iron⁽¹⁴⁾.

	Fe ₃ Ga	Fe ₃ Al	Fe ₃ Si
α (kOe/ μ_B)	105 $\pm$ 15	105 $\pm$ 15	105 $\pm$ 15
β (kOe/ μ_B)	7.4 $\mp$ 2.6	8.9 $\mp$ 2.6	7.1 $\mp$ 3.8
γ (kOe/ μ_B)	-2.0 $\mp$ 0.0 ₁	3.9 $\mp$ 0.8	1.5 $\pm$ 2.5

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