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Strong pressure dependences of the magnetization and Curie temperature for CrTe and MnAs with NiAs-type structure

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Abstract

To study the strong magneto-volume effects observed in CrTe and MnAs with NiAs-type crystal structure, first-principle band calculations are carried out by a self-consistent linear muffin-tin orbital method within the atomic sphere approximation. The equilibrium volume of the unit cell is obtained as a function of the magnetization M , which gives the volume magnetostriction. The dependence on M of the bulk modulus is also estimated. The coefficients a_0 and b_0 in the Landau expansion, $\Delta E(M) = a_0 M^2/2 + b_0 M^4/4$, are estimated by the fixed-spin-moment method. The calculated results for CrTe and MnAs are compared with those for bcc Fe. It is shown that the values of $|a_0|$ and b_0 for CrTe and MnAs are so small that the correction term from the magneto-volume coupling constants becomes significant. This fact gives a strong pressure dependence of the spontaneous magnetization. The pressure dependence of the Curie temperature is also discussed by making use of the magneto-volume coupling constants estimated in the present paper. The large volume magnetostriction observed in CrTe and MnAs is explained by the present calculations.

1. Introduction

Transition-metal monochalcogenides CrTe and MnAs with the NiAs-type crystal structure have recently attracted much attention because their magnetic properties are very sensitive to the atomic distance. These compounds are known to be metallic ferromagnets. The pressure dependences of the saturation moment M_s and the Curie temperature T_C are very strong. For CrTe the ferromagnetic state was found to disappear at 3–3.5 GPa [1, 2]. Recently, Ishizuka *et al* [3] found that the pressure-induced magnetic phase transition takes place at about 7 GPa in $\text{Cr}_{0.48}\text{Te}_{0.52}$. On the other hand, MnAs shows a first-order transition at T_C , accompanied by a structural transformation from the NiAs-type to the MnP-type structure [4]. Such a crystallographic transformation can be prevented when As atoms in MnAs

are partially replaced with Sb atoms [5]. The observed values of $\partial \ln M_s / \partial P$ and $\partial \ln T_C / \partial P$ are -0.12 and -0.16 to -0.20 GPa^{-1} for $\text{Cr}_{0.923}\text{Te}$ [6] and -0.040 and -0.35 GPa^{-1} for $\text{MnAs}_{0.7}\text{Sb}_{0.3}$ [7] respectively. These P dependences are very strong compared with the values of $\partial \ln M_s / \partial P = -0.0030 \text{ GPa}^{-1}$ and $\partial \ln T_C / \partial P \sim 0$ observed for bcc Fe metal [8]. Recently, Kanomata [9] observed the pressure dependence of M_s for Fe to be $\partial \ln M_s / \partial P = -0.0036$. These strong P dependences for CrTe and MnAs have been considered to come from a strong dependence of the exchange integral on the interatomic distances [10].

Many band calculations for CrTe and MnAs with the NiAs-type structure have already been carried out [11, 12]. Takagaki *et al* [13] studied theoretically the pressure effect on the electronic band structure of CrTe. They showed that the ferromagnetic state is stable at the observed lattice constant, while the antiferromagnetic state is stabilized at smaller volumes. Goto *et al* [7] showed by band calculations that the magnetic moment for MnAs is very sensitive to the lattice parameters.

It is possible to estimate by band calculations the volume magnetostriction when the unit cell volume with minimum energy is obtained as a function of the magnetic moment. It is also possible to obtain the bulk modulus when the total energy is calculated as a function of the unit cell volume. For such calculations, a fixed-spin-moment (FSM) method [14, 15] is available for the band calculation, as the total energy is obtained as a function of the unit cell volume and the magnetic moment without any adjustable parameters, as introduced by Lang and Ehrenreich [16] for example. This theory is extended to the case at finite temperature by taking into account the effect of spin fluctuations [17].

In this paper, the strong pressure dependences of the magnetization and the Curie temperature for CrTe and MnAs are discussed by calculating the total energies as a function of the unit cell volume and the magnetic moment in the FSM method. In section 2, a formal theory for the magneto-volume effect is given. The FSM band calculations for CrTe and MnAs are carried out in section 3. The pressure dependence of the Curie temperature is discussed in section 4 by using the spin fluctuation theory. Our conclusion and discussion are given in section 5.

2. Magneto-volume effect

The total energy for the system with magnetic moment M at volume V is written as

$$E(M, \omega) = \omega^2 / 2\kappa_0 + \Delta E(M, \omega), \quad (1)$$

where the volume fraction $\omega = (V - V_0) / V_0$, V_0 is the equilibrium volume at $M = 0$ and κ_0 the compressibility at $M = 0$. $\Delta E(M, \omega)$ in equation (1) is expanded with respect to ω as

$$\Delta E(M, \omega) = \Delta E_0(M) + \omega \left(\frac{\partial \Delta E(M, \omega)}{\partial \omega} \right)_0 + \frac{1}{2} \omega^2 \left(\frac{\partial^2 \Delta E(M, \omega)}{\partial \omega^2} \right)_0. \quad (2)$$

The coefficients in equation (2) are expanded with respect to M^2 as

$$\begin{aligned} \Delta E_0(M) &= \frac{1}{2} a_0 M^2 + \frac{1}{4} b_0 M^4, \\ (\partial \Delta E(M, \omega) / \partial \omega)_0 &= -C_1 M^2 - C_2 M^4, \\ (\partial^2 \Delta E(M, \omega) / \partial \omega^2)_0 &= -G_1 M^2 - G_2 M^4. \end{aligned} \quad (3)$$

The equations of state for the pressure P and magnetic field B are given by

$$P = -(\partial E(M, \omega) / \partial \omega)_M, \quad (4)$$

$$B = (\partial E(M, \omega) / \partial M)_\omega. \quad (5)$$

From equation (4) one gets

$$\omega = -\kappa_M\{P - C_1M^2 - C_2M^4\}, \quad (6)$$

where

$$\kappa_M^{-1} = \kappa_0^{-1} - G_1M^2 - G_2M^4. \quad (7)$$

Equations (6) and (7) give the volume magnetostriction and the M dependence of the bulk modulus. From equations (5) and (6), the magnetic equation of state is given by

$$B = a_0(P)M + b_0(P)M^3, \quad (8)$$

where

$$a_0(P) = a_0 + 2\kappa_0C_1P, \quad (9)$$

$$b_0(P) = b_0 - 2\kappa_0C_1^2 + 4\kappa_0(C_2 + \kappa_0C_1G_1)P. \quad (10)$$

Similar discussions were also given by Belov [18], Wohlfarth [8] and Shimizu [19].

When $a_0(P) < 0$ and $b_0(P) > 0$, the spontaneous magnetic moment M_s is given by

$$M_s(P)^2 = |a_0(P)|/b_0(P). \quad (11)$$

Then the pressure dependence of M_s is written as

$$\frac{\partial \ln M_s}{\partial P} = -\kappa_0\{C_1/|a_0| + 2(C_2 + \kappa_0C_1G_1)/(b_0 - 2\kappa_0C_1^2)\}, \quad (12)$$

at $P = 0$.

3. FSM calculations

The electronic structures of CrTe and MnAs are calculated by the self-consistent linear muffin-tin orbital (LMTO) method within the atomic sphere approximation (ASA) with the exchange-correlation potential by von Barth and Hedin [20]. A hexagonal unit cell of the NiAs-type structure contains two transition-metal atoms (Cr or Mn) and two anions (Te or As). The observed ratios c/a of the lattice parameters are used in the present calculations. In order to get a larger packing fraction of atoms we introduce two empty atoms with $Z = 0$ in the unit cell, where Z is the atomic number. The positions of each atom in the unit cell are given in [7]. Self-consistent calculations are carried out at 216 k points in the irreducible $1/24$ Brillouin zone. The basis set with angular momenta up to $l = 2$ is adapted for all atoms including empty atoms.

The FSM calculations are carried out for CrTe and MnAs. Figures 1 and 2 show the calculated results of the total energy for CrTe and MnAs as a function of the unit cell volume V , for various values of M . The minimum energies at $M = 0$ are obtained at $V_0 = 35.5$ and 26.7 \AA^3 for CrTe and MnAs respectively. These values for the theoretical unit cell volume at $M = 0$ are a little smaller than the observed ones above T_C . The theoretical unit cell volume is estimated as a function of M . The relative volume changes ω are shown in figure 3. In order to compare these results for CrTe and MnAs with the results for bcc Fe, we have carried out the same numerical calculations for Fe. The equilibrium unit cell volume at $M = 0$ is obtained as $V_0 = 9.95 \text{ \AA}^3$, which is also a little smaller than the observed value above T_C . The result obtained for ω in Fe is shown in figure 3.

The bulk modulus κ_M^{-1} is obtained by the curvature of the total energy at the minimum. In figure 4 the estimated bulk moduli for CrTe, MnAs and bcc Fe are shown as a function of M^2 . When the calculated κ_M^{-1} is fitted in the form of equation (7), the values of κ_0 , G_1 and G_2 are estimated. Using κ_M thus estimated we can also evaluate the values of C_1 and C_2 from

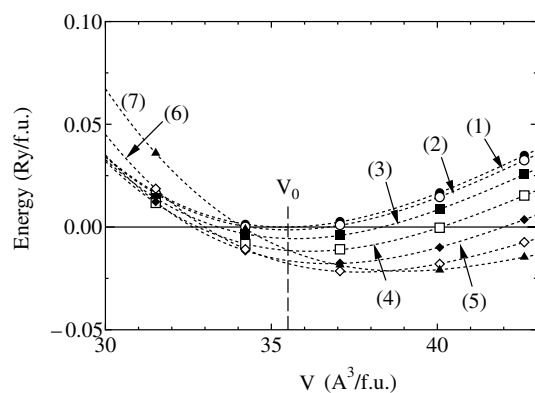


Figure 1. Calculated total energies for CrTe as a function of the unit cell volume V . Curves (1)–(7) are for $M = 0.0, 0.5, 1.0, 1.5, 2.0, 2.5$ and $3.0 \mu_B/\text{fu}$ respectively.

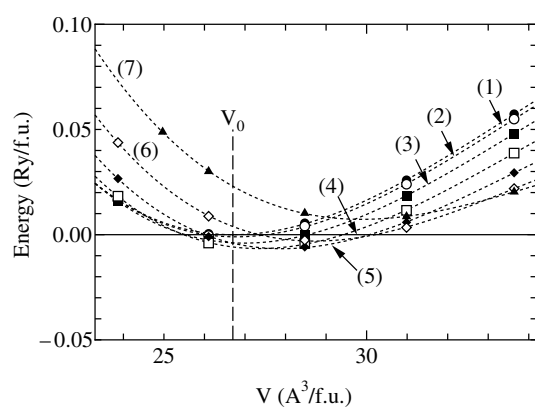


Figure 2. Calculated total energies for MnAs as a function of the unit cell volume V . Curves (1)–(7) are for $M = 0.0, 0.5, 1.0, 1.5, 2.0, 2.5$ and $3.0 \mu_B/\text{fu}$ respectively.

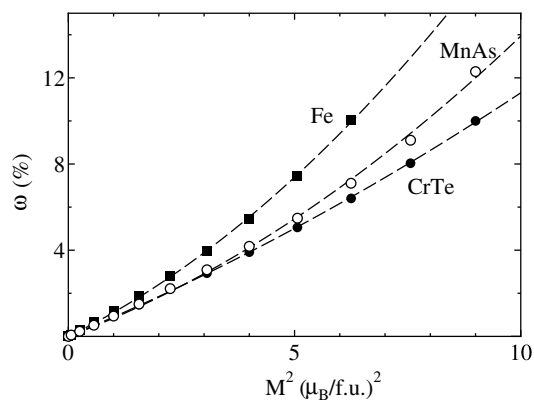


Figure 3. Calculated results of ω . Closed and open circles and closed squares are for CrTe, MnAs and bcc Fe respectively. The broken curves are those fitted to the form of equation (6) in the text.

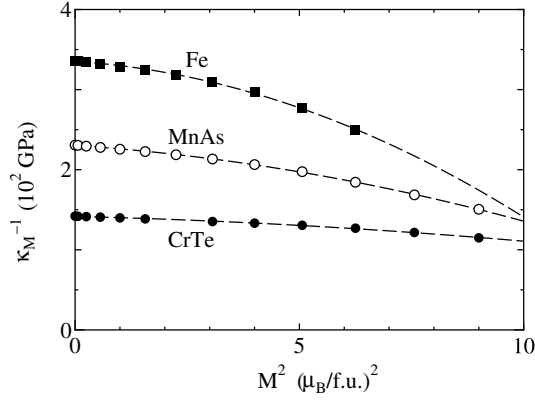


Figure 4. Calculated results of κ_M^{-1} . Closed and open circles and closed squares are for CrTe, MnAs and bcc Fe respectively. The broken curves are fitted to the form of equation (7) in the text.

Table 1. Calculated values of V_0 , κ_0 , $\kappa_0 C_1$, $\kappa_0 C_2$, G_1 , G_2 , a_0 , b_0 , $2\kappa_0 C_1^2$, M_V and $M_s(0)$, $\partial \ln M_s / \partial P$ and $\partial \ln T_C / \partial P$ for CrTe, MnAs and bcc Fe, together with the observed values for M_s , $\partial \ln M_s / \partial P$ and $\partial \ln T_C / \partial P$.

	CrTe	MnAs	Fe
V_0 ($\text{\AA}^3/\text{f.u.}$)	35.5	26.7	9.95
κ_0 (GPa^{-1})	0.706×10^{-2}	0.434×10^{-2}	0.298×10^{-2}
$\kappa_0 C_1$ ($(\mu_B/\text{f.u.})^{-2}$)	0.874×10^{-2}	0.788×10^{-2}	1.02×10^{-2}
$\kappa_0 C_2$ ($(\mu_B/\text{f.u.})^{-4}$)	0.170×10^{-3}	0.477×10^{-3}	0.798×10^{-3}
G_1 ($\text{GPa}/(\mu_B/\text{f.u.})^2$)	1.41	3.78	3.73
G_2 ($\text{GPa}/(\mu_B/\text{f.u.})^4$)	0.168	0.568	1.57
a_0 ($\text{T}/(\mu_B/\text{f.u.})$)	-7.20×10^2	-3.85×10^2	-5.23×10^3
b_0 ($\text{T}/(\mu_B/\text{f.u.})^3$)	1.27×10^2	1.58×10^2	1.33×10^3
$2\kappa_0 C_1^2$ ($\text{T}/(\mu_B/\text{f.u.})^3$)	0.83×10^2	0.82×10^2	0.75×10^2
M_V ($\mu_B/\text{f.u.}$) (Cal.)	2.38	1.56	1.98
$M_s(0)$ ($\mu_B/\text{f.u.}$) (Cal.)	4.04	2.25	2.04
M_s ($\mu_B/\text{f.u.}$) (Obs.)	2.5 [6]	3.2 [7]	2.2 [8]
$\partial \ln M_s / \partial P$ (GPa^{-1}) (Cal.)	-0.091	-0.105	-0.37×10^{-2}
$\partial \ln M_s / \partial P$ (GPa^{-1}) (Obs.)	-0.12 [6]	-0.04 [7]	-0.30×10^{-2} [8] -0.36×10^{-2} [9]
$\partial \ln T_C / \partial P$ (GPa^{-1}) (Cal.)	-0.103	-0.132	-0.5×10^{-2}
$\partial \ln T_C / \partial P$ (GPa^{-1}) (Obs.)	-0.26 [6]	-0.35 [7]	~ 0 [8]

the calculated results of ω fitted in the form of equation (6) at $P = 0$. The estimated values of these coefficients are listed in table 1. It was found that the values of the magneto-volume coupling constants C_1 and C_2 for CrTe and MnAs are smaller than those for Fe.

Now we are going to estimate the Landau coefficients a_0 and b_0 in equation (3) at the equilibrium unit cell volume V_0 . The number of electrons with majority and minority spins, N_+ and N_- , are given by $(N + M)/2$ and $(N - M)/2$, where N and M are the total number of electrons and the spin moment divided by μ_B . Under the constraint of fixed values of N_+ and N_- , the electron density $n_+(r)$, $n_-(r)$ and the potentials for electrons can be calculated by using the usual Kohn–Sham self-consistent equations, which give two Fermi levels μ_+ and μ_- in the majority and minority spin bands respectively [14, 15]. For an arbitrary M , the system is not in the equilibrium state, so $\mu_+ \neq \mu_-$. However, the constrained state becomes

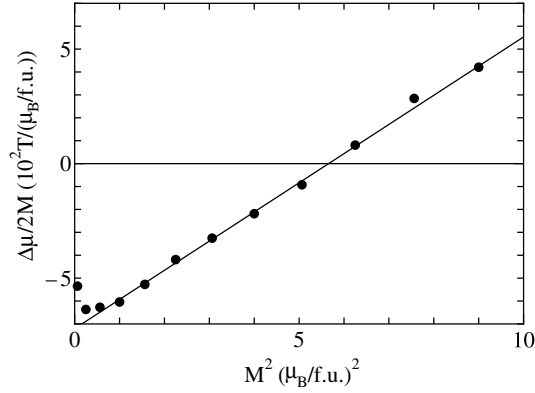


Figure 5. Calculated result of $\Delta\mu/2M$ for CrTe at V_0 . The straight line is fitted by $\Delta\mu/2M = a_0 + b_0M^2$.

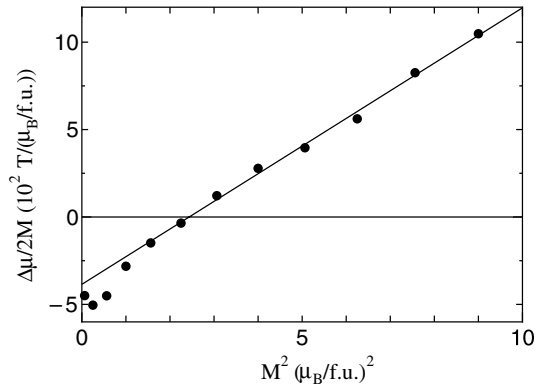


Figure 6. Calculated result of $\Delta\mu/2M$ for MnAs at V_0 . The straight line is fitted by $\Delta\mu/2M = a_0 + b_0M^2$.

an equilibrium state at the magnetic field $B = (\mu_+ - \mu_-)/2\mu_B$, as $\partial\Delta E(M)/\partial M = B$ and $\partial\Delta E(M)/\partial N_{\pm} = \mu_{\pm}$. This means that the state with the given M is stabilized at this B .

By making use of equation (8) at $P = 0$, one gets

$$\Delta\mu/2\mu_B = a_0M + b_0M^3, \quad (13)$$

where $\Delta\mu = \mu_+ - \mu_-$. We can fit the calculated results for $\Delta\mu$ in the form of equation (13), as shown in figures 5–7 for CrTe, MnAs and Fe respectively. The estimated values of a_0 and b_0 are shown in table 1. The moments M_V and $M_s(0)$ at a constant $V (=V_0)$ and at a constant $P (=0)$ are given by

$$M_V = \sqrt{|a_0|/b_0}, \quad M_s(0) = \sqrt{|a_0|/\{b_0 - 2\kappa_0 C_1^2\}} \quad (14)$$

respectively. The calculated results for M_V and $M_s(0)$ are shown in table 1, together with the observed values. The agreement between the calculated and observed values of $M_s(0)$ for CrTe and MnAs is not so good, but our calculated values are rather close to the results obtained using spin polarized band calculations [11, 13]. It is pointed out here that the difference between M_V and $M_s(0)$ is rather large for CrTe and MnAs, compared with that for Fe. This is because the values of $|a_0|$ and b_0 for CrTe and MnAs are one order of magnitude smaller than those for Fe, while the values for $2\kappa_0 C_1^2$ are almost the same as each other.

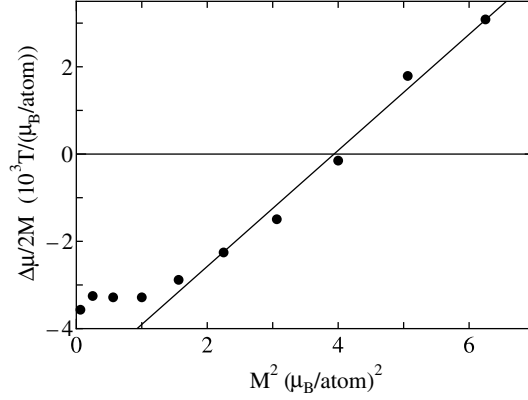


Figure 7. Calculated result for $\Delta\mu/2M$ of bcc Fe at V_0 . The straight line is fitted by $\Delta\mu/2M = a_0 + b_0M^2$.

From equation (12), together with the coefficients listed in table 1, we can estimate the pressure dependence of M_s . The estimated values of $\partial \ln M_s / \partial P$ together with the observed ones are shown in table 1. The value of the second term in the curly bracket in equation (12) is almost the same as that of the first term. This means that the higher-order coupling constants C_2 and G_1 of the magneto-elastic energy play an important role. The agreement between the calculated and observed values is satisfactory. It was shown that the values of $\partial \ln M_s / \partial P$ for CrTe and MnAs are very large compared with the value for Fe. This is because the pressure dependence of b_0 is rather strong for CrTe and MnAs. The coefficients of P in $a_0(P)$ and $b_0(P)$ given by equations (9) and (10) for CrTe and MnAs are not so different from those for Fe. However, the values of $|a_0|$ and $b_0 - 2\kappa_0 C_1^2$ for CrTe and MnAs are one order of magnitude smaller than those for Fe, as shown above. Therefore, the pressure dependence of M_s for CrTe and MnAs becomes much stronger than that for Fe.

4. Pressure dependence of T_C

In order to discuss the pressure dependence of T_C , the model developed in section 2 is extended to the case at finite temperature, by taking into account the effect of spin fluctuations on the Landau–Ginzburg model. The magnetic free energy density is given by

$$\Delta f_m(\mathbf{r}) = \frac{1}{2}a_0|\mathbf{m}(\mathbf{r})|^2 + \frac{1}{4}b_0|\mathbf{m}(\mathbf{r})|^4 + \frac{1}{2}D|\nabla \cdot \mathbf{m}(\mathbf{r})|^2, \quad (15)$$

where $\mathbf{m}(\mathbf{r})$ is the magnetization density. The magneto-elastic energy is introduced by

$$\Delta f_{mv}(\mathbf{r}) = -\omega\{C_1|\mathbf{m}(\mathbf{r})|^2 + C_2|\mathbf{m}(\mathbf{r})|^4\} - \frac{1}{2}\omega^2\{G_1|\mathbf{m}(\mathbf{r})|^2 + G_2|\mathbf{m}(\mathbf{r})|^4\}. \quad (16)$$

The free energy $F(M, \omega)$ is given by a sum of the elastic energy $\omega^2/2\kappa_0$, magnetic and magneto-elastic terms as

$$F(M, \omega) = \frac{\omega^2}{2\kappa_0} + \frac{1}{V} \int d^3r \{\Delta f_m(\mathbf{r}) + \Delta f_{mv}(\mathbf{r})\}. \quad (17)$$

The equations of state for the pressure P and magnetic field B are given by

$$P = -\langle (\partial F(M, \omega) / \partial \omega)_M \rangle, \quad (18)$$

$$B = \langle (\partial F(M, \omega) / \partial M)_\omega \rangle, \quad (19)$$

where $\langle \dots \rangle$ denotes a thermal average. One gets from equation (18)

$$\omega = -\kappa_M P + \kappa_M C_1 \{M^2 + \xi(T)^2\}, \quad (20)$$

where

$$\kappa_M^{-1} = \kappa_0^{-1} - G_1 \{M^2 + \xi(T)^2\}, \quad (21)$$

Here, $\xi(T)^2$ is a mean square amplitude of spin fluctuations [21] given by

$$\xi(T)^2 = \frac{1}{V} \sum_q \langle |\mathbf{m}(\mathbf{q})|^2 \rangle, \quad (22)$$

and $\mathbf{m}(\mathbf{q})$ is the Fourier component of $|\mathbf{m}(\mathbf{r})|$. In equation (20) we neglect the higher-order terms with respect to M^2 and $\xi(T)^2$. Similar discussions have also been given by Entel and Schröter [17].

Equation (19) is rewritten with the use of equation (20) as

$$B = a(T, P)M + b(T, P)M^3, \quad (23)$$

where

$$a(T, P) = a_0 + 2\kappa_0 C_1 P + \left\{ \frac{5}{3}b_0 - 2\kappa_0 C_1^2 + 4\kappa_0 C_1 G_1 P + \frac{20}{3}\kappa_0 C_2 P \right\} \xi(T)^2, \quad (24)$$

$$b(T, P) = b_0 - 2\kappa_0 C_1^2 + 4\kappa_0 \{C_2 + \kappa_0 C_1 G_1\} P. \quad (25)$$

The Curie temperature T_C at $P = 0$ is given by $a(T_C, 0) = 0$ and one gets

$$\xi(T_C)^2 = \frac{3}{5} |a_0| / \{b_0 - \frac{6}{5}\kappa_0 C_1^2\}. \quad (26)$$

Moriya and Usami [22] discussed the magneto-volume effect in a weak ferromagnet. They have obtained

$$\xi(T_C)^2 = \frac{3}{5} |a_0| / b_0, \quad (27)$$

which is a little different from our equation (26). The value of $|a_0|/b_0$ in equation (27) is M_V^2 at a constant volume as given by equation (14).

The temperature dependence of the volume magnetostriction is determined by the ratio $\eta(T)$ of the magnitude of the mean square of the local moment at T to its value at $T = 0$ as

$$\omega = \kappa_0 C_1 M_s(0)^2 \eta(T), \quad (28)$$

where $M_s(0)$ is given in equation (14). In our theory, $\eta(T_C)$ is written with the use of equations (14) and (26) by

$$\eta(T_C) = \frac{3}{5} \{b_0 - 2\kappa_0 C_1^2\} / \{b_0 - \frac{6}{5}\kappa_0 C_1^2\}, \quad (29)$$

while $\eta(T_C) = 3/5$ in Moriya and Usami's theory [22]. The estimated values of $\eta(T_C)$ are shown in table 1. The values of $\eta(T_C)$ for CrTe and MnAs are rather smaller than 0.6 in Moriya and Usami's theory. This means that the magneto-volume effect in these compounds is very strong, as observed in [6, 7].

Moriya [23] and Lonzarich and Taillefer [24] have discussed spin fluctuations in a weak ferromagnet. By making use of the fact that $\xi(T_C)^2$ is proportional to $T_C^{4/3}$ [23], we get, with the use of equations (24) and (25),

$$\frac{\partial \ln T_C}{\partial P} = -\frac{3}{2} \kappa_0 \{C_1 / |a_0| + (10C_2 + 6\kappa_0 C_1 G_1) / (5b_0 - 6\kappa_0 C_1^2)\}, \quad (30)$$

where we neglect the pressure dependence of the coefficient of $T_C^{4/3}$ in $\xi(T_C)^2$. The calculated values are given in table 1, together with the observed ones. The value of the second term in the curly bracket in equation (30) is almost the same as that of the first term. This means

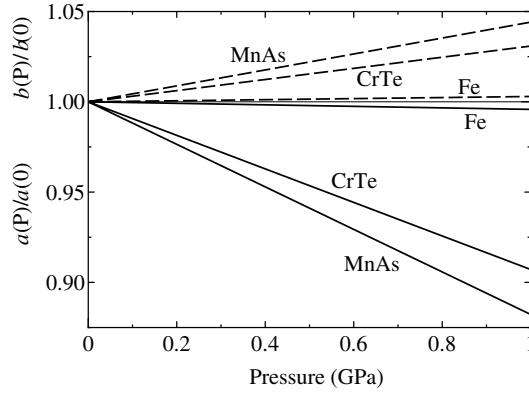


Figure 8. Pressure dependences of $a(P)/a(0)$ (solid line) and $b(P)/b(0)$ (broken line) for CrTe, MnAs and Fe.

that the higher-order coupling constants play an important role. The difference between the calculated and observed results is attributed to the pressure dependence of the coefficient of $T_C^{4/3}$ in $\xi(T_C)^2$, that is, to the pressure dependence of the characteristic temperature T_0 of spin fluctuations. Takahashi [25] obtained the pressure dependence of T_C , by assuming that the local spin fluctuation amplitude is almost constant, as

$$\frac{\partial \ln T_C}{\partial P} = \frac{3}{2} \frac{\partial \ln M_s}{\partial P}. \quad (31)$$

When the higher-order terms in the magneto-elastic energy, C_2 and G_1 , are neglected, our result for equation (30) coincides with equation (31), as $\partial \ln M_s / \partial P = -\kappa_0 C_1 / |a_0|$. However, it should be noted that equation (31) is derived from the zero-point spin fluctuations, while equation (30) is derived from the thermal ones.

5. Conclusion and discussion

In this paper, the magneto-volume effects for CrTe and MnAs with a hexagonal NiAs structure have been discussed using the first-principles calculation of the FSM method based on the LMTO method within the ASA. The strong pressure dependences of the magnetization and the Curie temperature observed for CrTe and MnAs were considered to come from a strong dependence of the exchange integral on the interatomic distances [10]. However, it has been shown by band calculation that these strong P dependences come from the fact that the values of the Landau coefficients $|a_0|$ and b_0 for these compounds are one order of magnitude smaller than those for bcc Fe, while the magneto-volume coupling constant is almost the same. This fact means that the relative value $b_0(P)/b_0(0)$ depends strongly on P as does $a_0(P)/a_0(0)$. Figure 8 denotes the P dependences of $a_0(P)/a_0(0)$ and $b_0(P)/b_0(0)$ for CrTe, MnAs and Fe, calculated by equations (9) and (10). As seen in figure 8, the pressure dependences of $a(P)$ and $b(P)$ for CrTe and MnAs are much stronger than those for Fe.

The strong temperature dependence of the volume magnetostrictions observed for CrTe and MnAs is due to the fact that $\eta(T_C)$ in equation (29) is small. This is because the value of b_0 itself is small and its correction terms from the magneto-volume coupling $\kappa_0 C_1$ are relatively large. The large difference between the magnetizations M_V and $M_s(0)$ at constant volume and constant pressure is also due to this fact. It is concluded that CrTe and MnAs are weak ferromagnets with small values of $|a_0|$ and b_0 , although the magneto-volume couplings are

almost the same as those for bcc Fe. The Stoner factor $S = 1 - ID_0$ can be estimated from the calculated value of a_0 , where I and D_0 are the exchange integral and density-of-states at the Fermi level. The values of S for CrTe and MnAs calculated at the theoretical lattice constants are -0.124 and -0.066 respectively, while the value of S for bcc Fe is -0.493 . As the absolute values of S for CrTe and MnAs are very small compared with that for Fe, it can be concluded that these compounds are very weak ferromagnets. The calculations for other weak ferromagnets, e.g. Ni₃Al and ZrZn₂, will be carried out in the near future.

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