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P–T–B magnetic phase diagram of itinerant-electron metamagnets

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Abstract

Temperature and pressure dependencies of a metamagnetic transition (MT) in an isotropic itinerant-electron system are discussed in terms of a spin fluctuation model based on the Ginzburg–Landau theory, including magnetoelastic energy. It has been shown that the critical magnetic field B_C of the MT increases as temperature T and pressure P increase. Both first- and second-order transitions of the magnetization at the Curie temperature T_C are derived, depending on the characteristic quantity $q(0)$ of the MT given by Landau parameters. It has been obtained that the T_C of the first-order transition is proportional to $(P_C - P)^{1/2}$ near the critical pressure P_C, as has been observed in MnSi and $La(Fe,Si)_{13}$. By the numerical calculations, a three-dimensional (P, T, B) magnetic phase diagram is obtained.

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1. Introduction

Two peculiar phenomena in itinerant-electron metamagnetism, i.e., a field-induced first-order phase transition from the paramagnetic state to the ferromagnetic one at low temperature and a maximum in the temperature dependence of susceptibility at high temperature, are the consequence of a special feature of the density-of-states near the Fermi level. These phenomena have been observed in many transition-metal compounds YCo_2, $Co(S,Se)_2$, and also 5f-electron system UCoAl [1]. Moreover, some ferromagnetic materials, e.g., MnFe(P,As) [2] and $La(Fe,Si)_{13}$ [3], show a first-order transition at the Curie temperature T_C. It has been observed in these compounds that a field-induced metamagnetic transition (MT) takes place just above T_C around room temperature. Such magnetic properties have attracted much attention for applications to magnetostrictive and magnetocaloric materials as a large magnetization jump takes place at T_C [4].

The effect of pressure on the MT has also been observed in MnSi [5–9], $Co(S,Se)_2$ [10], $Hf(Fe,Co)_2$ [11], U(Co,Fe)Al [12] and others. Under hydrostatic pressures, these compounds show a first-order transition at T_C. A P–T–B magnetic phase diagram was schematically illustrated for MnSi [13]. Moreover, Fujita et al. [14] have recently discussed the pressure-induced anomalies around the critical end point in $La(Fe,Si)_{13}$. Therefore, it is important to discuss the temperature- and field-induced magnetic transitions, together with the pressure effect, in itinerant-electron ferromagnets.

In this paper, the dependencies on temperature and pressure of the critical field of MT are discussed in terms of a spin fluctuation model based on the Ginzburg–Landau theory including the magnetoelastic energy, where temperature dependence of the Landau coefficients a, b and c is neglected. In Section 2, the magnetic equation of state is derived by the spin fluctuation model based on the Ginzburg–Landau theory, including the magnetoelastic energy. In Section 3, a strong pressure dependence of T_C of the first-order transition is obtained. In Section 4, the P–T–B magnetic phase diagram is numerically obtained for itinerant-electron metamagnets. Our conclusions and discussion are given in Section 5.

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2. Magnetic equation of state

The magnetic part of the free energy density $\Delta f_{\mathrm{m}}(r)$ is written by the Ginzburg–Landau theory as

$$\Delta f_{\mathrm{m}}(r) = \tfrac{1}{2}a|m(r)|^2 + \tfrac{1}{4}b|m(r)|^4 + \tfrac{1}{6}c|m(r)|^6 + \tfrac{1}{2}D|\nabla m(r)|^2, \quad (1)$$

where $m(r)$ is the magnetization density at location r. A magnetoelastic energy is introduced as [15]

$$\Delta f_{\mathrm{me}}(r) = -C_{\mathrm{mv}}\omega|m(r)|^2, \quad (2)$$

where ω is the volume fraction $(V - V_0)/V_0$, V_0 the equilibrium volume at $m(r) = 0$, and C_{mv} a magnetovolume coupling constant. The total free energy per unit volume ΔF is given by the sum of Eqs. (1) and (2) and the elastic energy $\omega^2/2\kappa$ as [16]

$$\Delta F = \omega^2/2\kappa + \frac{1}{V}\int\{\Delta f_{\mathrm{m}}(r) + \Delta f_{\mathrm{mv}}(r)\}\,\mathrm{d}^3r. \quad (3)$$

Here, κ is the compressibility. The ΔF is given by a functional of M, ω and the Fourier components $m(q)$ of $m(r)$ [17,18].

Takahashi and Nakano [19] have recently discussed the magnetovolume effect of itinerant-electron ferromagnets, taking into account the effect of the volume on the spin fluctuation spectrum. They have found a new thermal expansion term, showing T^2-like temperature dependence. In the present paper, however, such a new term is not included and only the magnetoelastic energy equation (2) is taken into account.

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

$$P = -\left\langle\left(\frac{\partial}{\partial\omega}\Delta F[M,\omega,\{|m(q)|^2\}]\right)_M\right\rangle, \quad (4)$$

$$B = \left\langle\left(\frac{\partial}{\partial M}\Delta F[M,\omega,\{|m(q)|^2\}]\right)_\omega\right\rangle, \quad (5)$$

where $\langle\cdots\rangle$ denotes a thermal average. From Eqs. (4) and (5), one gets a magnetic equation of state as [16]

$$B = a(T,P)M + b(T)M^3 + c(T)M^5, \quad (6)$$

where

$$a(T,P) = a(0) + 2\kappa C_{\mathrm{mv}}P + \left\{\tfrac{5}{3}b(0) + \tfrac{4}{3}\kappa C_{\mathrm{mv}}^2\right\}\xi_{\mathrm{T}}(T)^2 + \tfrac{35}{9}c(0)\xi_{\mathrm{T}}(T)^4,$$

$$b(T) = b(0) + \tfrac{14}{3}c(0)\xi_{\mathrm{T}}(T)^2,$$

$$c(T) = c(0), \quad (7)$$

and

$$a(0) = a - 2\kappa C_{\mathrm{mv}}^2\xi_0^2,$$

$$b(0) = b - 2\kappa C_{\mathrm{mv}}^2,$$

$$c(0) = c. \quad (8)$$

Here, $\xi_{\mathrm{T}}(T)^2$ and ξ_0^2 are mean square amplitudes of thermal and zero point spin fluctuations and a, b and c are renormalized by the zero point spin fluctuations [20]. It should be noted that the Landau coefficients $a(0)$, $b(0)$ and $c(0)$ in Eq. (8) are observable quantities say by Arrott plots at low temperature, and that the effect of the magnetovolume interaction is taken into account in these coefficients.

Among the Landau coefficients in Eq. (6), only $a(T,P)$ is influenced by P. This is because we assumed a simple form of the magnetoelastic energy given by Eq. (2). When we add higher order terms of $m(r)$ to Eq. (2), the Landau coefficients $b(T)$ and $c(T)$ in Eq. (6) are also influenced by P. A priori band structure calculation gives the volume dependencies of the Landau coefficients a, b and c. Yamada et al. [21] have actually estimated the volume dependencies for CrTe and MnAs. They have found that the volume dependence of a is large and the dependencies of b and c are small. In this paper, we neglect these higher order terms of the volume magnetostriction.

3. *P*-dependence of T_C

An MT occurs [22] when

$$a(T,P)>0, \quad b(T)<0, \quad c(T)>0,$$

$$\tfrac{3}{16}<a(T,P)c(T)/b(T)^2<\tfrac{9}{20}. \quad (9)$$

A first-order transition takes place when

$$\tfrac{5}{28}<a(T,P)c(T)/b(T)^2<\tfrac{3}{16}. \quad (10)$$

A second-order transition takes place when

$$a(T,P)c(T)/b(T)^2<\tfrac{5}{28}. \quad (11)$$

From Eqs. (9)–(11), the magnetic phase diagram can be estimated. Before doing so, B and M, in Eq. (6), are scaled as $\tilde{B} = B/B_0$ and $M = \tilde{M}/M_0$, respectively, where

$$B_0 = \tfrac{4}{5}|b(0)|M_0^3,$$

$$M_0 = \sqrt{3|b(0)|/10c(0)}. \quad (12)$$

Here, B_0 and M_0 are the values at $a(0)c(0)/b(0)^2 = \frac{9}{20}$, i.e., at the critical end point of the existence region of the MT [23]. In this case the paramagnetic susceptibility $(\chi(T) = a(T,P)^{-1})$ shows a maximum in its temperature dependence. The temperature $T_{\max}$, where $\chi(T)$ reaches a maximum, is given by

$$\xi_{\mathrm{T}}(T_{\max})^2 = \frac{3}{14}\frac{|b(0)|}{c(0)}\left(1 - \frac{14}{5}\eta\right), \quad (13)$$

where

$$\eta = \frac{2}{7}\kappa C_{\mathrm{mv}}^2/|b(0)|. \quad (14)$$

The value of η has been estimated for $Lu(Co,Al)_2$ as 0.01 from the detailed magnetization measurements [24].