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## LETTER TO THE EDITOR

# Effects of inhomogeneity on the magnetism of $Fe_{1-x}Co_xSi$

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### Abstract

Considering the magnetic ordering observed in  $Fe_{1-x}Co_xSi$  compounds, the inhomogeneity effect on the Curie temperature of the inhomogeneous system is studied by using the coherent potential approximation. In the model system introduced in the present study, the magnetically ordered state can be realized in a finite concentration range between the insulating spin gap state corresponding to FeSi and the metallic paramagnetic state corresponding to CoSi. The concentration dependences of the density of states and Curie temperature are the main focuses of investigation. The density of states at the Fermi level is strongly suppressed by the inhomogeneity effect. The suppression of the density of states also leads to suppression of the transition temperature. Although the electron correlation effect generally suppresses the Curie temperature similarly, the inhomogeneity effect on the suppression of the transition temperature cannot be replaced with the correlation effect of the effective Coulomb interactions.

Fe<sub>1-x</sub>Co<sub>x</sub>Si compounds show interesting magnetism and they have been studied for a few decades [1–3]. FeSi has attracted interest as one of the Kondo insulators among 3d transitionmetal compounds [4, 5], and the ground state of the compound is non-magnetic. On the other hand, the ground state of CoSi is diamagnetic. Neither of these compounds has any magnetic ordering. However, Fe<sub>1-x</sub>Co<sub>x</sub>Si (0.1  $\leq x \leq 0.7$ ) compounds are magnetically ordered. By using the spin fluctuation theory [6], this interesting magnetism of Fe<sub>1-x</sub>Co<sub>x</sub>Si was studied in [7]. In that study, the authors calculated the temperature dependence of the spin fluctuation, they succeeded in obtaining a value of the Curie temperature that was more realistic than that obtained by using the random phase approximation.

However, they treated the density of states using the rigid-band approximation; they did not take account of the inhomogeneity effect accurately. In the present letter, in order to investigate the inhomogeneity effect on the magnetism of compounds more effectively, we apply the coherent potential approximation (CPA) to a system corresponding to  $Fe_{1-x}Co_xSi$  compounds.

Since we concentrate on the inhomogeneity effect, we do not take the spin fluctuation into account; we apply the Hartree-Fock approximation to treat the many-body interaction.

In a practical calculation, one needs to assume a band structure for the system. According to the study via a band calculation [8], the form of the DOS of FeSi is very similar to that of the DOS of CoSi, and there seems to be a difference only as regards the position of the Fermi level in the density of states of each compound; in the DOS of FeSi the Fermi level sits in the gap, and the DOS at the Fermi level is finite in the case of CoSi. Therefore, in the present study, we assume that the form of the DOS for x = 0 corresponding to FeSi is the same as that for x = 1 corresponding to CoSi, and the difference in DOS between two systems for x = 0and 1 appears only in the energy level of each DOS.

The Hamiltonian that we treat in the present study is as follows:

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\text{site}},$$

where

$$\mathcal{H}_0 \equiv \sum_{k,\sigma} (\varepsilon_k - \mu_\sigma) c_{k\sigma}^{\dagger} c_{k\sigma}, \tag{1}$$

$$\mathcal{H}_{\text{site}} \equiv \sum_{i,\sigma} \{\xi_i \varepsilon_A + (1 - \xi_i) \varepsilon_B\} c_{i\sigma}^{\dagger} c_{i\sigma} + \sum_i \{\xi_i U_A + (1 - \xi_i) U_B\} c_{i\uparrow}^{\dagger} c_{i\uparrow} c_{i\downarrow}^{\dagger} c_{i\downarrow}, \tag{2}$$

where  $\xi_i$  denotes a random variable defined as  $\xi_i = 1$  ( $i \in A$ ) and 0 ( $i \in B$ ), and the concentration x is defined as  $x \equiv \sum_i \xi_i / N$ ; N denotes the number of lattice sites. The Zeeman energy is included in  $\mu_{\sigma}$  as  $\mu_{\sigma} \equiv \mu + g\mu_{\rm B}H\sigma/2 \equiv \mu + h\sigma$  ( $\sigma = \pm 1$ ). Since we assume that the form of the DOS for x = 0 is same as that for x = 1 as mentioned above, the dispersion  $\varepsilon_k$  is assumed not to depend on x and the difference of A and B sites appears in the energy level difference of  $\varepsilon_A$  and  $\varepsilon_B$ . It is also assumed that  $U_{A(B)}$  is independent of the concentration x. These assumption and the model Hamiltonian were also used in [9] to study ferromagnetic alloys. Following [9], we apply the Hartree–Fock approximation to the Coulomb interaction term in the Hamiltonian (2), and then the Hartree-Fock Hamiltonian is obtained as follows:

$$\mathcal{H}_{\text{site}}^{\text{HF}} = \sum_{i,\sigma} \{ \xi_i \varepsilon_{\text{A}\sigma}^{\text{HF}} + (1 - \xi_i) \varepsilon_{\text{B}\sigma}^{\text{HF}} \} c_{i\sigma}^{\dagger} c_{i\sigma} - \sum_i \{ \xi_i U_{\text{A}} n_{\text{A}\uparrow} n_{\text{A}\downarrow} + (1 - \xi_i) U_{\text{B}} n_{\text{B}\uparrow} n_{\text{B}\downarrow} \}, \tag{3}$$

where  $n_{A(B)\sigma}$  denotes the expectation value of the electron density with  $\sigma$  at the A (B) site. The Hartree term is included in  $\varepsilon_{A(B)\sigma}^{HF}$  as  $\varepsilon_{A(B)\sigma}^{HF} \equiv \varepsilon_{A(B)} + U_{A(B)}n_{A(B)-\sigma}$ . Applying the CPA to the present system by introducing the coherent potential  $S_{\sigma}(i\varepsilon_n)$ , the

CPA condition is expressed as the following equation [9]:

$$x \frac{\varepsilon_{A\sigma}^{HF} - S_{\sigma}(i\varepsilon_n)}{1 - G_{\sigma}^{CPA}(i\varepsilon_n)(\varepsilon_{A\sigma}^{HF} - S_{\sigma}(i\varepsilon_n))} + (1 - x) \frac{\varepsilon_{B\sigma}^{HF} - S_{\sigma}(i\varepsilon_n)}{1 - G_{\sigma}^{CPA}(i\varepsilon_n)(\varepsilon_{B\sigma}^{HF} - S_{\sigma}(i\varepsilon_n))} = 0,$$
(4)

where  $\varepsilon_n$  denotes the Matsubara energy  $\varepsilon_n = (2n + 1)\pi T$  at temperature T. The CPA Green function  $G_{\sigma}^{\text{CPA}}(i\varepsilon_n)$  and the total DOS  $\rho_{\sigma}(\varepsilon)$  of the system are expressed as

$$G_{\sigma}^{\text{CPA}}(i\varepsilon_n) = \int d\nu \frac{\rho_0(\nu)}{i\varepsilon_n + \mu_{\sigma} - \nu - S_{\sigma}(i\varepsilon_n)},$$
(5)

$$\rho_{\sigma}(\varepsilon) = -\frac{1}{\pi} \operatorname{Im} G_{\sigma}^{\operatorname{CPA}}(\varepsilon + \mathrm{i}\delta), \tag{6}$$

where  $\rho_0(\nu)$  is the non-interacting DOS. We assume the form of the DOS for the non-interacting homogeneous system instead of the band structure itself in the present study. Considering the band structure obtained in the band calculation study [8], we assume an artificial form of the

non-interacting DOS that has a gap and a sharp peak near the gap as follows:

$$\rho_0(\nu) = \frac{1}{2} \frac{V^2 + (\nu - \varepsilon_f)^2}{(\nu - \varepsilon_f)^2} g\left(\nu - \frac{V^2}{\nu - \varepsilon_f}\right),\tag{7}$$

$$g(x) = \frac{1}{\sqrt{2\pi W^2}} \exp\left(-\frac{x^2}{2W^2}\right),$$
(8)

where  $\nu \neq \varepsilon_f$  and  $\rho_0(\nu) = 0$  in the case  $\nu = \varepsilon_f$ . The above form of the non-interacting DOS comes from the DOS with the hybridization gap in the periodic Anderson model which has the hybridization V between conduction electrons and f electrons with the energy level  $\varepsilon_f$ . Note that we introduce the above artificial form (7) in order to realize the structure which has a gap and a sharp peak near the gap, and also note that the values V and  $\varepsilon_f$  themselves have no physical meaning in the present model. We use the Gaussian form (8) in the non-interacting DOS (7) for convenience as regards the numerical integral. In the practical calculation, we take the width of the Gaussian as the energy unit (W = 1), and set V = 0.8 and  $\varepsilon_f = 1$ . For simplicity, we assume the values of  $U_A$  and  $U_B$  to be the same, and this same value is denoted by  $U: U = U_A = U_B$ .

Here let us comment on the determination of the values  $\varepsilon_A$  and  $\varepsilon_B$ . Obviously, the absolute values of  $\varepsilon_A$  and  $\varepsilon_B$  are not important, but the relative value  $\varepsilon_A - \varepsilon_B$  is crucial. Thus, for simplicity, we set  $\varepsilon_B \equiv 0$ . Assuming that the pure B system (x = 0) corresponds to FeSi which has a gap at the Fermi level, we determine the electron density at B sites for x = 0 such that the Fermi level  $\varepsilon_{\rm F}^0(x=0)$  sits in the gap for the non-interacting case; for the present model, we obtain  $n_{\rm B}(x=0) \equiv \sum_{\sigma} n_{\rm B\sigma}(x=0) = 1$  from the non-interacting DOS (7). In the case x = 1, which corresponds to CoSi, the electron density at A sites for x = 1 should be more than  $n_{\rm B}(x=0)$ ; we assume  $n_{\rm A}(x=1) \equiv \sum_{\sigma} n_{{\rm A}\sigma}(x=1) = 1.8$  in the practical calculation. We determine the value of  $\varepsilon_A$  such that the Fermi level  $\varepsilon_F^0(x=1)$  for x=1 is equal to  $\varepsilon_F^0(x=0)$ for x = 0; the value of  $\varepsilon_A$  is obtained as  $\varepsilon_A \simeq -0.725$  for the present model. Finally, the model parameters  $\varepsilon_A$ ,  $\varepsilon_B$ ,  $n_A(x = 1)$ , and  $n_B(x = 0)$  are determined. In the practical calculation, for given values of U and x, we calculate the HF-CPA condition (4) and obtain the value of the Fermi level  $\varepsilon_{\rm F}(x)$  (or the chemical potential  $\mu(x)$ ) at temperature T such that the total density  $n_{\text{tot}}(x) \equiv xn_A(x) + (1-x)n_B(x)$  is equal to  $xn_A(x=1) + (1-x)n_B(x=0)$ , which is expressed as 1.8x + (1 - x) = 0.8x + 1 in the present model. The electron density  $n_{A(B)\sigma}$ at each site A (or B) is obtained from the site-dependent Green function:

$$G_{A(B)\sigma}(i\varepsilon_n) = \frac{G_{\sigma}^{CPA}(i\varepsilon_n)}{1 - G_{\sigma}^{CPA}(i\varepsilon_n)(\varepsilon_{A(B)\sigma}^{HF} - S_{\sigma}(i\varepsilon_n))},$$
(9)

$$n_{\mathcal{A}(\mathcal{B})\sigma} = \int d\varepsilon \,\rho_{\mathcal{A}(\mathcal{B})\sigma}(\varepsilon) f(\varepsilon) \tag{10}$$

$$\equiv \int \mathrm{d}\varepsilon \left( -\frac{1}{\pi} \operatorname{Im} G_{\mathcal{A}(\mathcal{B})\sigma}(\varepsilon + \mathrm{i}\delta) \right) f(\varepsilon), \tag{11}$$

$$f(\varepsilon) = \frac{1}{e^{\beta\varepsilon} + 1},\tag{12}$$

where  $\beta = 1/T$ . The coherent potential  $S_{\sigma}(i\varepsilon_n)$  can be expressed by using the CPA condition (4) and the definition of the site-dependent Green function (9) as

$$S_{\sigma}(i\varepsilon_n) = \frac{xG_{A\sigma}(i\varepsilon_n)\varepsilon_{A\sigma}^{HF} + (1-x)G_{B\sigma}(i\varepsilon_n)\varepsilon_{B\sigma}^{HF}}{xG_{A\sigma}(i\varepsilon_n) + (1-x)G_{B\sigma}(i\varepsilon_n)}.$$
(13)

Here we summarize the self-consistent procedure used to calculate the CPA Green function and the site-dependent Green function. First, we introduce some adequate input for the sitedependent Green function. We denote the input Green function as an 'OLD' one:  $G_{A(B)\sigma}^{OLD}$ . Next we calculate the electron density  $n_{A(B)\sigma}$  at A (B) sites from  $G_{A(B)\sigma}^{OLD}$  using (10). Then, using the electron density  $n_{A(B)\sigma}$ , we determine the value of  $\varepsilon_{A(B)\sigma}^{HF}$  including the Hartree term. The coherent potential  $S_{\sigma}$  is obtained by using (13), and the CPA Green function  $G_{\sigma}^{CPA}$ is calculated from (5). Finally, we obtain the output of the site-dependent Green function denoted as a 'NEW' one:  $G_{A(B)\sigma}^{NEW}$ , using the relation (9). The OLD  $G_{A(B)\sigma}^{OLD}$  and the NEW  $G_{A(B)\sigma}^{NEW}$  are compared with each other, and the self-consistent calculation is repeated until they converge. After the convergence, we obtain self-consistent solutions for the Green functions and the coherent potential. Hereafter, we omit the spin indices of the quantities obtained from paramagnetic solutions. In the scheme with the Hartree–Fock approximation, we can obtain the magnetic susceptibility from paramagnetic solutions by expanding all quantities in the first order of h [9]. The total magnetic susceptibility  $\chi_s(T)$  is expressed in terms of the partial magnetic susceptibility  $\chi_{A(B)}(T)$  as

$$\chi_{\rm s}(T) = x \chi_{\rm A}(T) + (1 - x) \chi_{\rm B}(T). \tag{14}$$

The partial magnetic susceptibilities are expressed as follows:

$$\begin{pmatrix} \chi_{\rm A} \\ \chi_{\rm B} \end{pmatrix} = \frac{1}{D} \begin{pmatrix} 1 - U\chi_{\rm B}^0 + UY_{\rm A} & UY_{\rm B} \\ UY_{\rm A} & 1 - U\chi_{\rm A}^0 + UY_{\rm B} \end{pmatrix} \begin{pmatrix} \chi_{\rm A}^0 \\ \chi_{\rm B}^0 \end{pmatrix}, \tag{15}$$

$$D \equiv \begin{vmatrix} 1 - U\chi_{\rm A}^{0} + UY_{\rm B} & -UY_{\rm B} \\ -UY_{\rm A} & 1 - U\chi_{\rm B}^{0} + UY_{\rm A} \end{vmatrix},$$
(16)

$$Y_{A(B)} \equiv -\frac{1}{\pi} \int d\varepsilon \operatorname{Im} \left[ \frac{\{ (G^{CPA}(\varepsilon + i\delta))^2 - H(\varepsilon + i\delta) \} K_{A(B)}(\varepsilon + i\delta) }{\{ 1 - (\varepsilon_{B(A)}^{HF} - S(\varepsilon + i\delta)) G^{CPA}(\varepsilon + i\delta) \}^2} \right] f(\varepsilon),$$
(17)

$$H(i\varepsilon_n) \equiv \int d\nu \frac{\rho_0(\nu)}{(i\varepsilon_n + \mu - \nu - S(i\varepsilon_n))^2} = -\int d\nu \frac{1}{i\varepsilon_n + \mu - \nu - S(i\varepsilon_n)} \frac{d\rho_0(\nu)}{d\nu}, \quad (18)$$

$$K_{\rm A}(i\varepsilon_n) \equiv \frac{\pi - (\varepsilon_{\rm B}^{\rm HF} - \varepsilon_{\rm B}^{\rm HF}) - (\varepsilon_n)}{1 - (\varepsilon_{\rm A}^{\rm HF} + \varepsilon_{\rm B}^{\rm HF} - 2S(i\varepsilon_n))G^{\rm CPA}(i\varepsilon_n) + (\varepsilon_{\rm A}^{\rm HF} - S(i\varepsilon_n))(\varepsilon_{\rm B}^{\rm HF} - S(i\varepsilon_n))H(i\varepsilon_n)},$$
(19)

$$K_{\rm B}(i\varepsilon_n) \equiv \frac{1 - x - (\varepsilon_{\rm A}^{\rm H} - S(i\varepsilon_n))G^{\rm CPA}(i\varepsilon_n)}{1 - (\varepsilon_{\rm A}^{\rm HF} + \varepsilon_{\rm B}^{\rm HF} - 2S(i\varepsilon_n))G^{\rm CPA}(i\varepsilon_n) + (\varepsilon_{\rm A}^{\rm HF} - S(i\varepsilon_n))(\varepsilon_{\rm B}^{\rm HF} - S(i\varepsilon_n))H(i\varepsilon_n)}.$$
(20)

The above relations, equations (14)–(20), were first derived in [9]. We follow these relations and calculate the magnetic susceptibility and determine the Curie temperature  $T_{\rm C}$ .

Let us show the numerical results. Figure 1 shows the dependence on the concentration (x) of the total DOS  $\rho(\varepsilon)$ . In the case x = 0, the Fermi level sits in the gap of the DOS and the system become insulating; this corresponds to the FeSi case. We can obviously see that the form of the DOS changes drastically with changing x and does not simply shift. Of course, the total electron density  $n_{tot}(x)$  increases linearly with increasing x, since the Fermi level is determined such that  $n_{tot}(x)$  is equal to  $xn_A(x = 1) + (1 - x)n_B(x = 0)$  (which is equal to 0.8x + 1 in the present calculation). However, one can see that the concentration dependence of the partial electron density at A or B sites,  $n_{A(B)}(x)$ , is not simple (see the inset of figure 1(a)). For  $x \simeq 0.5$ , the DOS loses the peak structure, and the DOS at the Fermi level is strongly suppressed compared to that obtained by the rigid-band approximation (figure 2). This strong suppression is caused by inhomogeneity of the system. Let us see the concentration dependence of the coherent potential, indicating inhomogeneity. Figures 3(a) and (b) show the concentration dependence of the imaginary part Im  $S(\varepsilon + i\delta)$  of the coherent potential. With x increasing from x = 0 to 0.5 or with x decreasing from x = 1 to 0.5, the absolute value of



**Figure 1.** (a) The concentration dependence of the total DOS  $\rho(\varepsilon)$  from x = 0 to 1 in intervals of 0.1 (U = 2 and T = 0). The inset shows the concentration dependence of the electron density  $n_{A(B)}(x)$  at A (B) sites. The lower panel (b) shows an enlargement around the Fermi level ( $\varepsilon = 0$ ).

Im  $S(\varepsilon + i\delta)$  increases overall, as expected. In particular, one can see that the suppression of the DOS at the Fermi level is the strongest, since the imaginary part of the coherent potential around  $\varepsilon = 0$  is the most enhanced. It is also confirmed that the real part Re  $S(\varepsilon + i\delta)$  of the coherent potential approaches  $\varepsilon_A^{\text{HF}}$  and  $\varepsilon_B^{\text{HF}}$  for x = 1 and 0, respectively, in figure 3(c).

Next we turn to the magnetic susceptibility. Figure 4 shows the temperature dependence of the magnetic susceptibility for several values of x ( $0 \le x \le 1$ ). For x = 0, the system has a gap and the magnetic susceptibility decreases exponentially as temperature decreases. For low concentration, the magnetic susceptibility has an upturn at lower temperature. This upturn becomes a divergence for  $x \ge 0.09$ ; the ground state of the system becomes ferromagnetic. At the other end of the concentration range, x = 1, the divergence of the susceptibility disappears and the susceptibility at the lowest temperature has a finite value. Needless to say, this finite value corresponds to Pauli paramagnetism enhanced by the Stoner factor  $1/(1 - U\rho_A(0; x = 1)) = 1/(1 - U\rho(0; x = 1))$ ; one can confirm that the value of the susceptibility  $\chi_s(T = 0)$  at absolute zero for x = 1 (all sites are A sites) is consistent with  $\rho(0; x = 1)/(1 - U\rho(0; x = 1))$ . The inverse  $1/\chi_s(T)$  of the susceptibility is also shown



Figure 2. Comparison of the concentration dependence of the total DOS  $\rho(0)$  at the Fermi level calculated by using the CPA and that calculated by using the rigid-band approximation (U = 2 and T = 0).

in the inset of figure 4. The temperature dependence of  $1/\chi_s(T)$  at higher temperature seems to be linear in T. In fact, the temperature dependence of  $1/\chi_s(T)$  obtained by using the Hartree–Fock approximation is not linear, but rather proportional to  $T^2 - T_c^2$ . However, if  $T - T_C \ll T_C$  ( $T > T_C$ ), the inverse of the susceptibility is proportional to  $2T_C(T - T_C)$ ; the apparent linearity of  $1/\chi_s(T)$  is seen only at  $T \simeq T_C$ .

The concentration dependence of the Curie temperature is shown in figure 5. For comparison, we also show some results obtained using the rigid-band approximation for several values of U. As might be expected, the inhomogeneity suppresses the Curie temperature; values of the Curie temperature calculated using the present CPA scheme are lower than those obtained using the rigid-band calculation for all x. The suppression of the Curie temperature is related to the suppression of the DOS and the enhancement of the imaginary part of the coherent potential.

This situation is similar to that for the suppression of Curie temperature by the electron correlation effect; it is well known that the correlation effect generally suppresses the Curie temperature<sup>1</sup>. In order to see the relation between the inhomogeneity effect and the correlation effect on the suppression of the transition temperature, we compare the present result calculated using the CPA with that obtained by using the rigid-band approximation. In the results obtained by using the rigid-band approximation, one can see a systematic enhancement of the Curie temperature with increasing U for all x. The electron correlation effect on the Curie temperature can be described in terms of the renormalized effective Coulomb interaction [10]. Thus, if the inhomogeneity effect on the suppression of the transition temperature is replaceable with the correlation effect, the concentration dependence of the transition temperature calculated by using the CPA should be consistent with that obtained by using the rigid-band approximation for some effective Coulomb interaction U. In other words, denoting the transition temperature calculated by using the CPA in the system for U and xas  $T_{\rm C}^{\rm CPA}(U; x)$  and that calculated by using the rigid-band approximation as  $T_{\rm C}^{\rm RBA}(U; x)$ , an effective value  $\tilde{U}$  of the Coulomb interaction such that  $T_{\rm C}^{\rm CPA}(U; x) = T_{\rm C}^{\rm RBA}(\tilde{U}; x)$  for all x should exist. We can see that the concentration dependence cannot be described by a rigidband approximation with an appropriate effective Coulomb interaction  $\tilde{U}$ : we can see that the relation  $T_{\rm C}^{\rm RBA}(U = 1.5; x) < T_{\rm C}^{\rm CPA}(U = 2.0; x) < T_{\rm C}^{\rm RBA}(U = 2.0; x)$  does not hold for lower concentrations.

<sup>1</sup> The Hartree–Fock approximation without account taken of the correlation effect generally gives an unrealistically high Curie temperature.



**Figure 3.** (a) The concentration dependence of the imaginary part Im  $S(\varepsilon + i\delta)$  of the coherent potential from x = 0.1 to 0.5 in intervals of 0.1 (U = 2 and T = 0). (b) Im  $S(\varepsilon + i\delta)$  from x = 0.5 to 0.9 in intervals of 0.1 (U = 2 and T = 0). (c) The concentration dependence of the real part Re  $S(\varepsilon + i\delta)$  of the coherent potential from x = 0.1 to 0.9 in intervals of 0.1 (U = 2 and T = 0). Thin solid curves indicate  $\varepsilon_{\rm A}^{\rm HF}$  (upper) and  $\varepsilon_{\rm B}^{\rm HF}$  (lower) for U = 2, respectively.

In summary, considering  $Fe_{1-x}Co_xSi$ , we have mainly concentrated on calculating the concentration dependence of the Curie temperature and the DOS of the inhomogeneous system in which there are two kinds of site with different energy levels, by using the CPA, and have investigated the inhomogeneity effect on the transition temperature.

- (1) The form of the DOS changes drastically as the concentration changes. In particular, the DOS at the Fermi level is strongly suppressed by the inhomogeneity.
- (2) The transition temperature is also suppressed. There are two points that should be emphasized. The first is that the effect of the inhomogeneity on the suppression of the transition temperature cannot be described in terms of an effective Coulomb interaction. The second is that the simple Stoner criterion cannot be applied to the inhomogeneous system. The DOS at the Fermi level, which is used in the simple Stoner criterion, is suppressed by the inhomogeneity. Also, the extended Stoner criterion derived from equations (14), (15), and (16) should be applied to the inhomogeneous system.



**Figure 4.** The temperature dependence of the magnetic susceptibility  $\chi_{S}(T)$  for several values of x from x = 0 to 1 in intervals of 0.1 (U = 2). The inset shows the inverse  $1/\chi_{S}(T)$  of the magnetic susceptibility.



Figure 5. The concentration dependence of the Curie temperature calculated by using the CPA (U = 2). For comparison, results obtained by using the rigid-band approximation for several values of U (U = 1, 1.5, and 2) are also shown.

Concerning the intermediate concentrations of  $Fe_{1-x}Co_xSi$  compounds, if the rigid-band approximation is assumed, the DOS at the Fermi level is high enough for the appearance of ferromagnetism in the Stoner criterion. In the inhomogeneous system, however, it should be noted that the DOS is suppressed by the inhomogeneity effect, and the apparent height of the DOS at the Fermi level cannot be used even in the simple Stoner criterion. This inhomogeneity effect on the magnetism should also be important in investigating magnetic properties of other compounds. In a recent study of the magnetic transition observed in  $FeSi_{1-x}Ge_x$ , for example, it was expected that the transition temperature would be more suppressed by the inhomogeneity effect if the CPA-type treatment was applied to the system, although in fact the rigid-band approximation was assumed in the study [11].

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