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First-principles calculation of the Curie temperature Slater–Pauling curve

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Abstract

It is well known that the magnetizations as a function of the valence electron number per atom of 3d transition metal substitutional alloys form the so-called Slater–Pauling curve. Similarly, the Curie temperatures of these alloys also show systematic behaviour against the valence electron number. Though this fact has long been known, no attempt has been made so far to explain this behaviour from first principles. In this paper we calculate T_C of 3d transition metal alloys in the framework of first-principles electronic structure calculation based on the local density approximation.

1. Introduction

It is well known that the magnetizations as a function of the valence electron number per atom of 3d transition metal substitutional alloys form the so-called Slater–Pauling curve. Similarly, the Curie temperatures of these alloy systems also show systematic Slater–Pauling-like behaviour against the valence electron number. Though the whole shape of the Slater–Pauling curve for the Curie temperature resembles that of the magnetization, details of their behaviours are different. While the magnetizations fall roughly on a common curve as a function of the electron number, the Curie temperatures behave differently depending on the system. This fact implies that Curie temperatures depend not only on the magnetization but also on the magnetic exchange interaction coefficients that differ from system to system. Though the behaviour of the magnetization of 3d transition metal alloys is well explained from first principles [1–3], no similar attempt has been made so far to explain the behaviour of the Curie temperature.

Recently, calculation of the magnetic transition temperature using the exchange coupling constants obtained from first-principles calculation in the framework of the local density functional approximation (LDA) of the density functional method was applied to various metallic systems [4, 5]. In many cases the results seem to be fairly consistent with experimentally observed Curie or Néel temperatures. In this study, we apply a similar

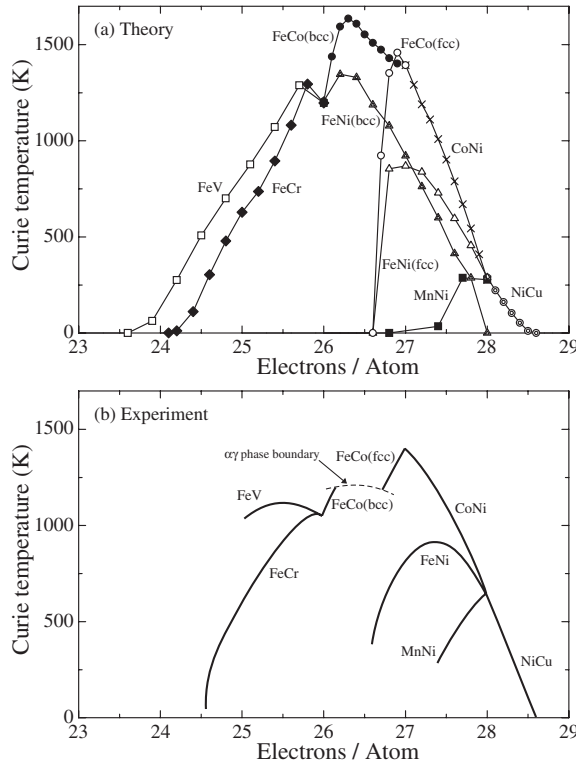


Figure 1. Theoretical and experimental [8] Curie temperatures.

approach to 3d transition metal alloys in order to explain the systematic behaviour of the Curie temperature.

2. Calculation

We calculated the electronic structure of 3d transition metal alloys using the Korringa–Kohn–Rostoker method combined with the coherent potential approximation and the local density approximation (KKR-CPA-LDA method) [1, 3]. From the obtained spin density distributions, the exchange coupling constants J_{ij} were calculated with the method proposed by Liechtenstein [4]. The J_{ij} s thus obtained were used as inputs to calculate the Curie temperature T_C in the framework of the cluster-like approximation (CA) proposed by Mano [6, 7].

While the original work by Mano supposed systems composed of Ising spins, we consider classical spins. This needs a small modification of the formalism. In addition, we have to treat two kinds of magnetic ions while the original work treated a single kind of magnetic ion in diluted systems. In the following, we explain the CA in the case that only the nearest neighbour interactions are taken into account for simplicity since the extension to a general case is straightforward. When two kinds of magnetic ion, A and B, coexist and only the nearest neighbour interactions are considered, the magnetization X_A and X_B can be written in the one-site approximation of the CA as

$$\begin{aligned}
 X_A &= \sum_{n_A=0}^z Q_{n_A}^z \sum_{k_A=0}^{n_A} D_{k_A}^{n_A}(X_A) \sum_{k_B=0}^{n_B=z-n_A} D_{k_B}^{n_B}(X_B) P(2\beta\{J^{A-A}(n_A - 2k_A) + J^{A-B}(n_B - k_B)\}) \\
 &= f_A(X_A, X_B)
 \end{aligned}$$

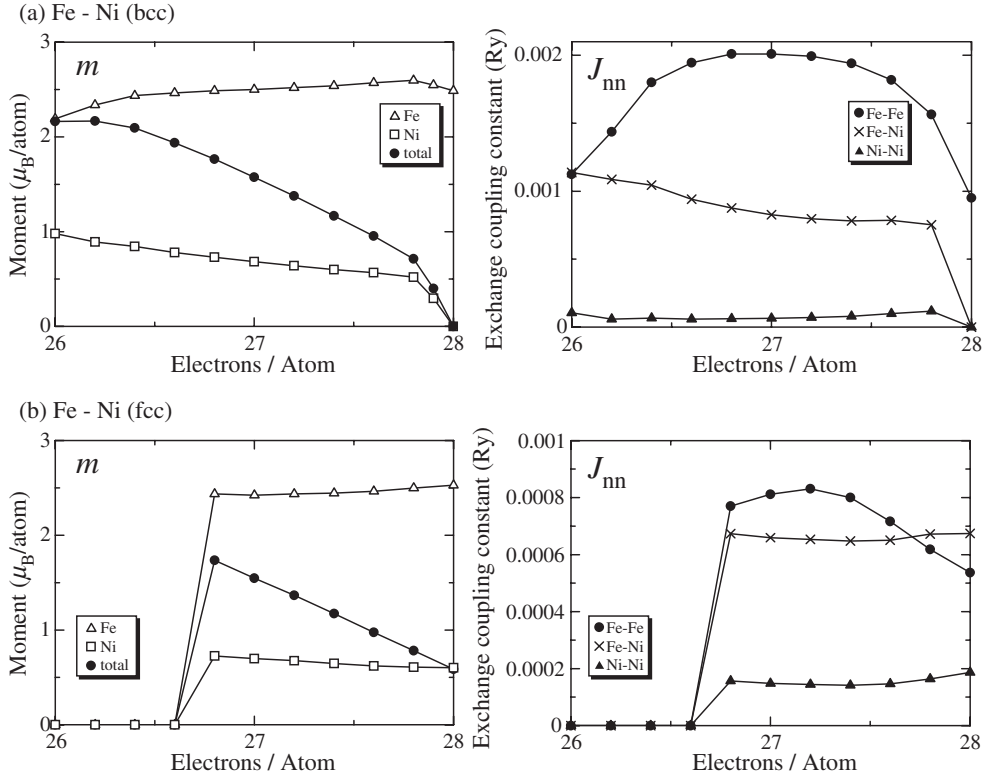


Figure 2. Magnetic moments m and the coupling constants between the nearest neighbours J_{nn} of Fe-Ni alloys.

and

$$X_B = \sum_{n_A=0}^z Q_{n_A}^z \sum_{k_A=0}^{n_A} D_{k_A}^{n_A}(X_A) \sum_{k_B=0}^{n_B=z-n_A} D_{k_B}^{n_B}(X_B) P(2\beta\{J^{B-A}(n_A - 2k_A) + J^{B-B}(n_B - k_B)\})$$

$$= f_B(X_A, X_B),$$

where z is the number of neighbours, $P(x)$ is the Langevin function, $P(x) = \coth(x) - 1/x$ and J^{A-B} is the exchange coupling constant between A and B,

$$H_A = -2J^{A-A} \sum_{(i,j)} S_i^A \cdot S_j^A - 2J^{A-B} \sum_{(i,j)} S_i^A \cdot S_j^B.$$

The definitions of Q_n^z and D_k^n are the same as in the original work [6]:

$$Q_n^z = \binom{z}{n} p^n (1-p)^{z-n}$$

and

$$D_k^n(X) = \binom{n}{k} \left(\frac{1+X}{2}\right)^{n-k} \left(\frac{1-X}{2}\right)^k,$$

where p is the concentration of A. Expanding f_A and f_B to the first order of X_A and X_B , we obtain coupled equations about X_A and X_B . From the condition that the coupled equations have a solution other than $X_A = X_B = 0$, the magnetic transition temperature of the system can be

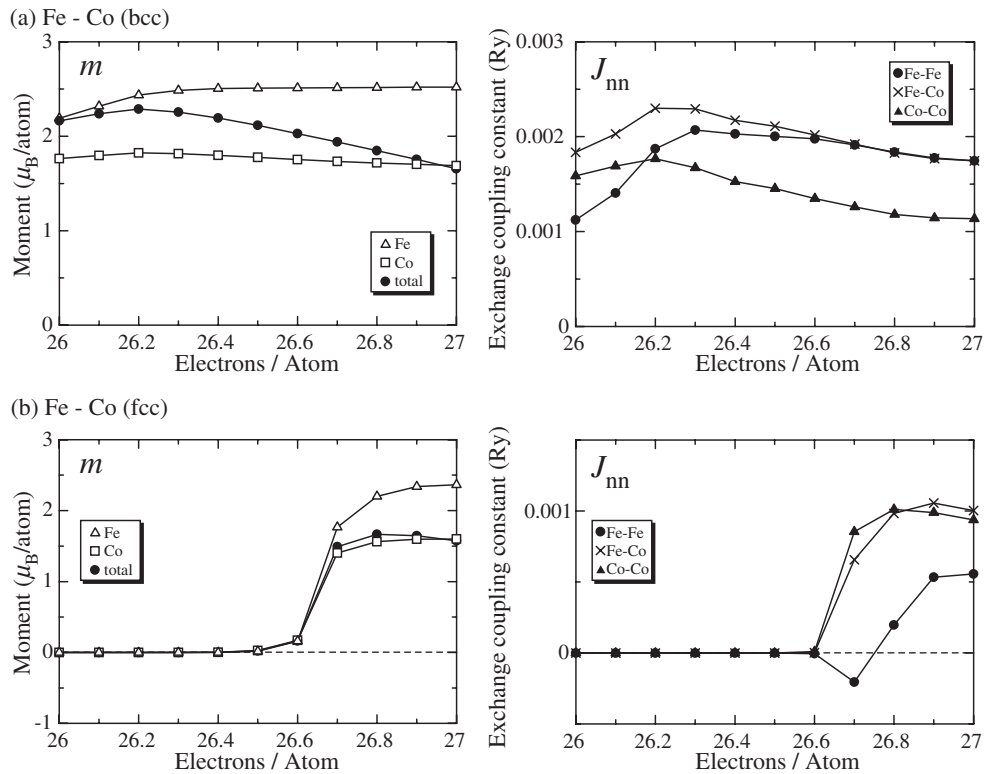


Figure 3. Magnetic moments m and the coupling constants between the nearest neighbours J_{nn} of Fe-Co alloys.

obtained. Other neighbours are also taken into account in the same way as the original CA [7]. In the present calculations, we took three different types of neighbours that have relatively large components of J_{ij} for the calculation of T_C .

3. Results and discussions

The calculated T_C are summarized in figure 1. The overall Slater–Pauling-like behaviour of T_C is well reproduced by the present calculation although it underestimates T_C in the cases of weak ferromagnets. This is mainly due to the fact that, for weak ferromagnets, the localized magnetic moments are not well developed and longitudinal magnetic fluctuation, which is not considered in the present calculation, plays a role.

The Curie temperature depends on both the magnetization and on J_{ij} . In figures 2–4, the changes in the total and local magnetic moments and the coupling constant between the nearest neighbours, J_{nn} , for each alloy are shown. Since the coupling constants between the nearest neighbours J_{nn} are much larger than those between other neighbours, it might be of primary importance in determining T_C . Thus, for Fe–Ni alloy (bcc), the behaviour of T_C is similar to that of the magnetic moment. For Fe–Ni alloy (fcc), however, the situation is a little different from the bcc case. From $Z = 28.0$ down to $Z = 26.8$, the magnetic moment increases monotonically while T_C has a maximum at $Z = 27.0$ and then decreases. This behaviour cannot be explained just by the behaviour of the magnetization. It is clear that this behaviour originates from the

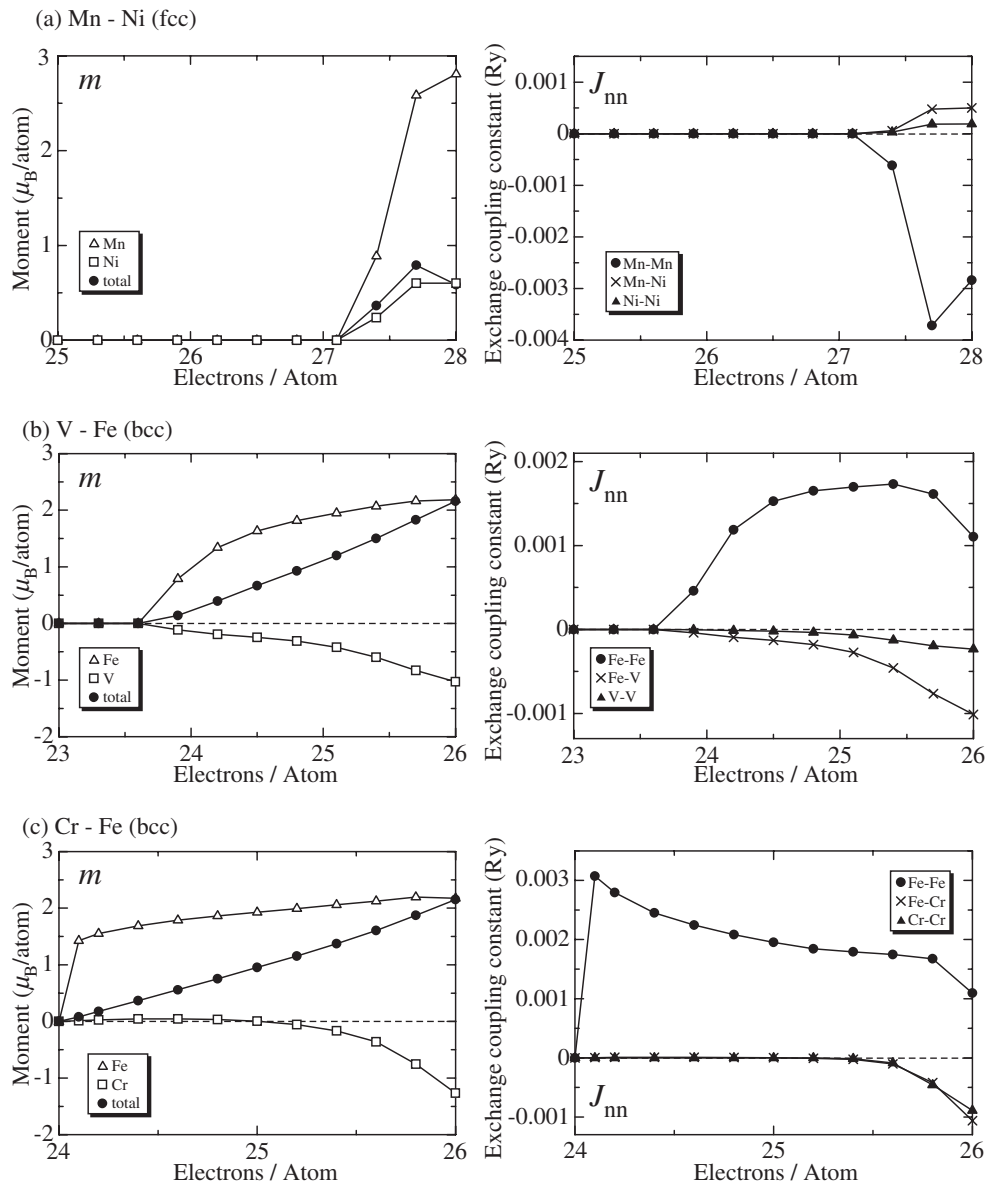


Figure 4. Magnetic moments m and the coupling constants between the nearest neighbours J_{nn} of Mn-Ni, V-Fe and Cr-V alloys.

change in J_{nn} : J_{nn} between Fe atoms shows a similar behaviour. Though the maximum of J_{nn} is located at $Z = 27.2$, the Fe concentration is still low and hence the maximum value of T_C occurs in the region of higher concentration where the magnetization further increases.

For Fe-Co alloy (bcc), T_C is a maximum at $Z = 26.3$ while the magnetic moment is a maximum at $Z = 26.2$. The behaviour of T_C reflects the fact that J_{nn} between Fe atoms takes a maximum at $Z = 26.3$ and J_{nn} between Fe and Co is also large there. For the fcc Fe-Co alloy we can see an interesting behaviour of J_{nn} : as the Fe concentration increases (as Z decreases),

the magnetic moment increases initially, but suddenly decreases at $Z = 26.6$ and then vanishes. This is explained as follows: below $Z = 26.7$, J_{nn} between Fe atoms is negative and hence the system is frustrated. In this situation, the magnetization can no longer be stable.

Behaviours similar to fcc Fe–Co can also be seen for other alloys. In the Mn–Ni alloy, J_{nn} between Mn atoms is negative. It is considered that the Ni sites are ferromagnetic while the Mn sites are local moment disorder states (spin-glass-like state) in the Mn–Ni alloy. The calculated J_{nn} reproduces such a character and this is taken into account for the present T_C calculation.

V–Fe and Cr–Fe alloys also have negative J_{nn} s. In this case, not only J_{nn} between V atoms (Cr atoms) but also that of V (Cr) and Fe atoms is negative. As a result, Fe and V (Cr) couple antiparallel to each other. In other words, the sign of the magnetic moment of Fe and V (Cr) is opposite in the low concentration region of V (Cr), as shown in figure 4. Contrary to the fcc cases, however, the negative J_{nn} s do not cause any frustration in these bcc systems. Both V–Fe and Cr–Fe alloys have a maximum of T_C at $Z \sim 25.8$ while such a behaviour cannot be seen in the behaviour of magnetic moments. This comes from the fact that J_{nn} between Fe atoms increases whereas that of Fe and V (Cr) decreases as the V (Cr) concentration increases.

In summary, we applied the KKR-CPA-LDA method to 3d transition metal alloys and calculated their Curie temperature. The results show that the overall Slater–Pauling-like behaviour of T_C is well reproduced by first-principles calculation.

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