

Electronic structure and magnetism of $\text{Fe}_{3-x}\text{Cr}_x\text{Si}$ alloys

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Abstract

The study of the electronic structure and magnetic properties of the $\text{Fe}_{3-x}\text{Cr}_x\text{Si}$ compound is motivated by the Mössbauer and neutron spectroscopy measurements showing unusual behaviour of Cr in such alloys. The site preferences of Cr in Fe_3Si and the effect of local environment on formation of local magnetic moments are examined using self-consistent spin-polarised TB-LMTO method. The results of calculations essentially confirm the values and orientations of magnetic moments of iron and chromium atoms. However, they do not explain an experimental observation of almost equal occupation of A, B and C sites by chromium. © 2002 Elsevier Science B.V. All rights reserved.

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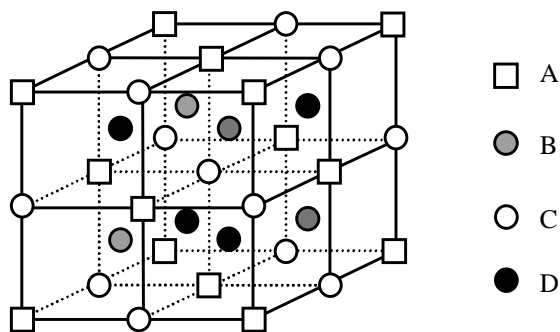
1. Introduction

The crystal structure of the ordered Fe_3Si alloy is of DO_3 -type (see Fig. 1). The crystal lattice can be described as four interpenetrating face-centred cubic Bravais lattices originated at $(0, 0, 0)$, $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$, $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ and $(\frac{3}{4}, \frac{3}{4}, \frac{3}{4})$ positions and abbreviated as A, B, C, and D, respectively. In ordered Fe_3Si , Fe atoms occupy A, B and C sites whereas Si atoms are located at D sites. There are two iron sites that are not equivalent. Two of them, (A, C-sites), are surrounded by four Fe and four Si atoms in the first coordination sphere and have tetrahedral site symmetry; the second one, B-site, is surrounded by eight Fe atoms and has cubic site symmetry. The

different nearest atom configurations at these sites cause the electronic structure as well as magnetic properties connected with these positions to be different. The occupation of D sites exclusively by silicon is well confirmed by neutron experiments also for chromium doped alloys $\text{Fe}_{3-x}\text{Cr}_x\text{Si}$ [1]. The observed scattering length for the D sites is very close to the scattering length of pure silicon. Some Mossbauer experiments [2] suggest a minor disorder between B sublattice and silicon D sublattice. The relative abundance of the additional observed sextet assigned to iron atom in D position is, however, only about 3%.

Burch et al. [3] showed that transition metal impurities reveal a noticeable preference of occupation of one type of Fe site depending on the number of 3d electrons. Transition metal

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Fig. 1. The DO_3 -type structure.

impurities on the left-hand side of Fe in the Periodic Table of Elements (e.g. Mn or V) demonstrate strong preference for B site occupation whereas atoms to the right of Fe (e.g. Co) prefer (A, C) sites. These results were confirmed by NMR spin-echo experiments on $Fe_{3-x}T_xSi$ (T—transition metal) ternary compounds [4,5]. The selectivity of occupation was also supported by band structure calculations of Fe_3Si alloy [6–8]. KKR-type calculations of the site selectivity and local magnetic moments have recently been carried out by Kaprzyk et al. [8]. Unfortunately, the case of Fe_3Si with iron substituted by chromium was not considered in this paper. This case seems particularly interesting because the aforementioned rules of the site selective occupation are violated as shown in the series of experiments [1,9–10]. Two phases were identified in the studied samples of the $Fe_{3-x}Cr_xSi$ system. In the range $0 < x < 0.4$ the alloys crystallise in the DO_3 -type structure. According to these experiments chromium can be found in a DO_3 -type structure at (A, C) and B positions with only a weak preference for the B site [9]. For a higher concentration of chromium (x larger than about 0.4, see [10]) an additional A15 phase appears, whose relative volume increases with an increase of the chromium concentration. It is known [11] that the influence of Cr on the ordering in Fe–Cr–Si alloys is visible mainly in a decrease of the rapidity of the well-ordered domain creation process due to the lower mobility of Si in the presence of Cr. The slow cooling is therefore required to produce the well-ordered samples. The details of the heat treatment have been described in [10].

Fe_3Si is ferromagnet with a Curie temperature of 840 K [10] and measured mean magnetic moment per atom of $1.17 \pm 0.02 \mu_B$ at room temperature [9]. The Curie temperature decreases linearly with the increase of chromium concentration reaching $T_C = 712$ K for $x = 0.4$ [10]. The magnetic moment of iron on the B site was found [10] to be $2.44 \mu_B$, and about $1.18 \mu_B$ for (A, C) sites. The magnetic moments of chromium were determined to be $(2.03 \pm 1.3) \mu_B$ for Cr at a B site and $(0.41 \pm 0.63) \mu_B$ for (A, C) sites [10] with orientation antiparallel to magnetic moments of iron. The magnetic moments of chromium as well as the magnetic moments of iron decrease linearly with the concentration of Cr. Silicon has small negative moment due to the induced polarisation of conduction electrons. In light of these findings, the chromium atoms should substantially modify the electronic structure of Fe_3Si . Both, the antiparallel orientation of Cr magnetic moments and the effects of the local environment are of great interest for this family of alloys.

The purpose of this paper is to present the electronic and magnetic properties of the $Fe_{3-x}Cr_xSi$ system obtained by band structure calculations in the range $0 \leq x \leq 0.5$.

One-electron band energies for different distributions of atomic site occupancies were calculated and the site preferences of Cr atoms which follow from the differences between these band energies were studied. The magnetic moments on Fe and Cr atoms were also calculated for different crystallographic positions. The calculations show an influence of the local environment on the magnetic moments of Fe and Cr. Local densities of states at various sites as well as for various spin orientations were analysed. A simple interpretation of the result is presented.

2. Method of calculations

The electronic band structures and the magnetic moments for ordered $Fe_{3-x}Cr_xSi$ alloys with DO_3 type structure were carried out within the framework of the local spin density approximation (LSD), using the self-consistent spin-polarised TB-LMTO method in the atomic sphere approxima-

tion (ASA) [12]. The exchange correlation potential was taken in the form of von Barth and Hedin [13].

The band structure and the magnetic moments were computed for the experimental values of the lattice parameter [10]. The latter increases linearly with chromium content in the considered range of Cr concentration. The initial atomic configurations for each atom were taken to be the same as for pure elements. The self-consistent band calculations were performed for at least 250 k -points in the irreducible wedge of the Brillouin zone.

The electronic properties of the $\text{Fe}_{3-x}\text{Cr}_x\text{Si}$ compound have been calculated for the supercell structure and for the four values of the parameter x : 0; 0.125; 0.25; 0.375; 0.5. The supercell structure with 32 atoms in the cell can be divided into 32 simple cubic sublattices. Eight of them are occupied by Si atoms (D positions), whereas Fe and Cr randomly occupy the remaining sublattices (A, B, C positions).

3. Results and discussion

In order to study the site preference of Cr atom in Fe_3Si (in DO_3 structure—Fig. 1) we substitute some of Fe atoms in the supercell of the parent Fe_3Si compound by Cr atoms with a probability which in general might be different for different sublattices. There are one, two, three and four chromium atoms in the supercell consisting of 32 atoms for the aforementioned values of concentration $x = 0.125, 0.25, 0.375$ and 0.5 , respectively. Two kinds of inequivalent sites for Cr atom, (A, C) and B positions, in the DO_3 -type structure are taken into consideration.

Our *ab-initio* total energy calculations strongly suggest the site preference of Cr atoms, which prefer to occupy the B sublattice. Due to the small size of the supercell, the possible configurations for the low concentration ($x = 0.125$), are restricted to one Cr atom per supercell, occupying either the B sublattice or one of the (A, C) sites. The energy of the former configurations is about 40 mRy/atom lower. For $x = 0.25$ the configurations with Cr atoms occupying only B sites (two sites per unit cell in this case) has the lowest energy. The

configuration with an equal occupation of B and (A, C) sites is about 60 mRy/atom higher in energy and for the configuration with Cr atoms occupying only (A, C) sites it is about 140 mRy/atom higher than that for the former configuration. For higher concentrations the B site preference is maintained, but energetically more favourable are configurations with a partial occupation of A sites. The lowest energy configurations are obtained for one Cr atom per supercell occupying (A, C) site and two ($x = 0.375$) or three ($x = 0.5$) atoms occupying the B sites. All other configurations examined lie at least 25 mRy/atom higher. In contrast, experiments [1,10] indicated only a weak preference for the B-site [1]. Essentially, chromium enters both B and (A, C) sublattices with almost equal probability.

In Fig. 2 the spin-projected total densities of states of $\text{Fe}_{3-x}\text{Cr}_x\text{Si}$ are presented. Hereafter the

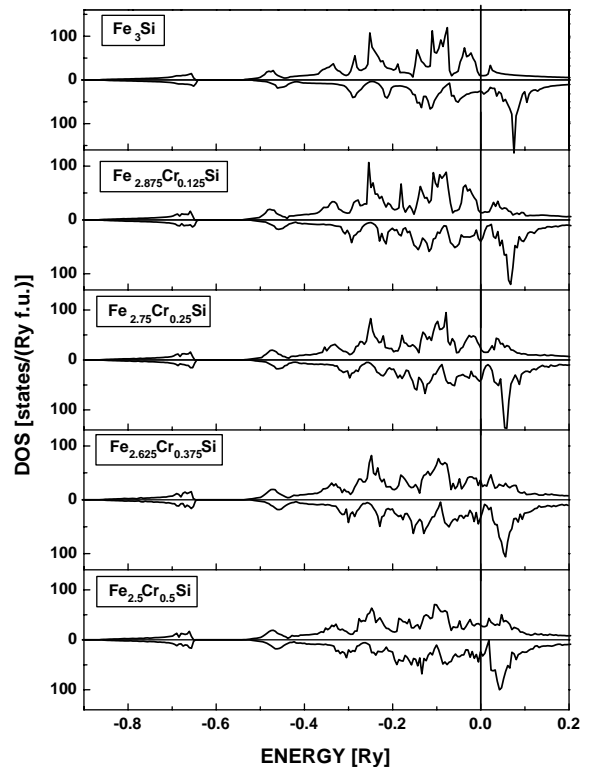


Fig. 2. The spin-projected total density of states for $\text{Fe}_{3-x}\text{Cr}_x\text{Si}$ alloys: Fe_3Si , $\text{Fe}_{2.875}\text{Cr}_{0.125}\text{Si}$, $\text{Fe}_{2.75}\text{Cr}_{0.25}\text{Si}$, $\text{Fe}_{2.625}\text{Cr}_{0.375}\text{Si}$ and $\text{Fe}_{2.5}\text{Cr}_{0.5}\text{Si}$. The vertical lines mark the Fermi level.

DOS presented on the upper half plane of each figure corresponds to the spin-up orientation and the lower to the spin-down. The vertical lines indicate the position of the Fermi level. The total DOS for $\text{Fe}_{3-x}\text{Cr}_x\text{Si}$ ($0 \leq x \leq 0.5$) consists of the lower part (below -0.69 Ry), which contains mainly s-states of Si, and the higher part (above -0.5 Ry), where mainly d-states of Fe and Cr atoms and p-states of Si atom contribute. The gap $-0.64 < E < -0.53$ Ry reflects the large separation of atomic 3s and 3p levels of silicon and 3s silicon and 3d levels of iron or chromium in comparison with the corresponding band widths. The 3s band does not overlap on this energy scale with 3p and 3d bands. In general, an influence of the fluctuations of environment on the deep subband is mainly driven by a change of symmetry. For the silicon s-subband which is mainly formed by spherical 3s states this effect is negligible. The impact of the deep subband on the thermodynamic properties is not essential, and therefore in the following we concentrate on the changes induced by chromium doping in the upper subband. This band is mainly governed by d-states of Fe or Cr, but the role of p-electrons of Si is also important. As chromium is added the reconstruction of this band is mainly driven by hybridisation. The smearing of some peaks in the total DOS and partial filling of some of the valleys in DOS with an increase of Cr concentration is observed (Fig. 2). The shape of the density of states strongly depends on the atomic configuration of the nearest neighbour shell. For B sites, both for iron and chromium (Figs. 3 and 5), the structure is sharp. For the parent Fe_3Si compound the nearest neighbours are atoms of only one type (iron) and they also dominate for higher concentrations of chromium in the whole range examined. The nearest neighbour shell of (A, C) sites is formed by two types of atoms: iron and silicon ($x = 0$). For higher concentrations also chromium can be found in the surrounding. The fact that more types of atoms occur in the nearest neighbour shell (richer distribution of atomic levels) and the fact that extended 3p-states are involved in the mixture with 3d-states cause the traces of atomic d-levels in the DOS being less visible for (A, C) sites than for B sites (Figs. 4 and 6).

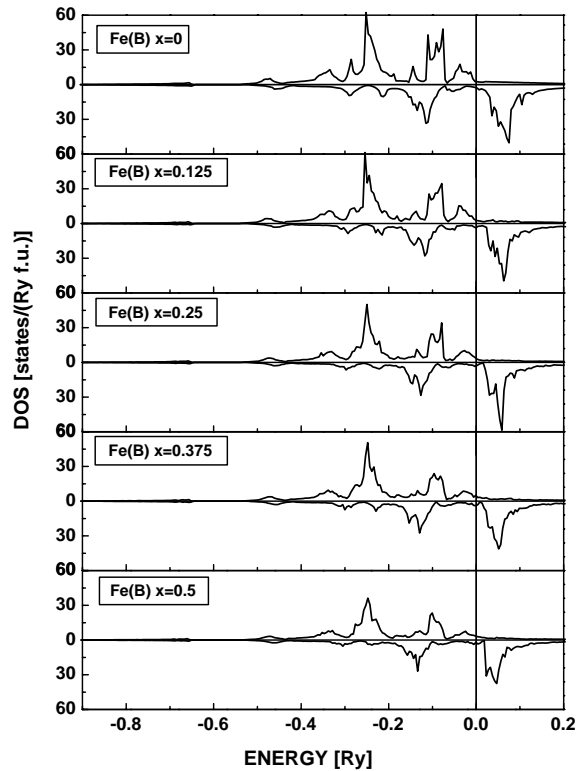


Fig. 3. The spin-projected density of states for Fe in B position for Fe_3Si , $\text{Fe}_{2.875}\text{Cr}_{0.125}\text{Si}$, $\text{Fe}_{1.75}\text{Cr}_{0.25}\text{Si}$, $\text{Fe}_{2.625}\text{Cr}_{0.375}\text{Si}$ and $\text{Fe}_{2.5}\text{Cr}_{0.5}\text{Si}$. The vertical lines mark the Fermi level.

Comparing the corresponding local densities of states of chromium and iron (Figs. 3 and 5 or Figs. 4 and 6) it is seen that the dominant chromium peaks are shifted with respect to the iron peaks. In a consistent way, the chromium “impurity” subbands build up with doping inside the total densities of states between the iron-dominated peaks. This explains the observed partial filling of the valleys between them (Fig. 2).

The densities of states for different spin orientations are shifted on the energy scale (nonvanishing magnetisation). The atomic energy position of impurities are also spin dependent. The reconstruction of the spin dependent bands with doping depends on the relative position of impurity energy levels with respect to the pure bands of the same spin orientation. In particular one can expect a significant change of magnetisation with doping if the impurity subbands prefer unoccupied region of

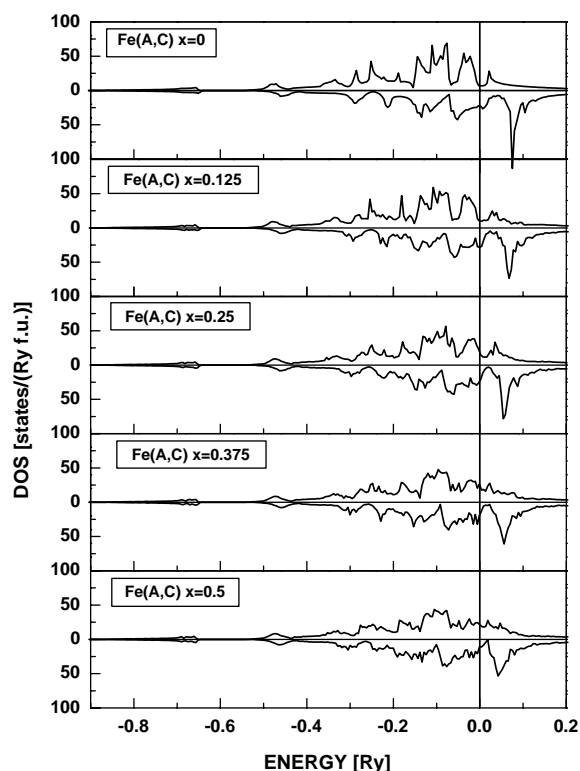


Fig. 4. The spin-projected density of states for Fe in (A, C) position for $\text{Fe}_{3-x}\text{Cr}_x\text{Si}$ alloys: Fe_3Si , $\text{Fe}_{2.875}\text{Cr}_{0.125}\text{Si}$, $\text{Fe}_{1.75}\text{Cr}_{0.25}\text{Si}$, $\text{Fe}_{2.625}\text{Cr}_{0.375}\text{Si}$ and $\text{Fe}_{2.5}\text{Cr}_{0.5}\text{Si}$. The vertical lines mark the Fermi level.

DOS for one spin direction and occupied region for other. It is the case for the system discussed.

The higher chromium peak in the total majority DOS (Fig. 5) is fully located above the Fermi energy, E_F . This introduces new states in this region in the total DOS (Fig. 2). This results in the relative increase of the number of d-holes in the majority subband with respect to the minority band, i.e. a decrease of the iron moment. Similar changes in the minority band occupation are less drastic because the chromium peak is partially located above and partially below the Fermi level and this influences both the number of electrons and the number of holes. Note that the spin orientations of majority and minority subbands of iron and chromium (see e.g. Figs. 3 and 5) are reversed which means that the magnetic moments of both atoms are antiparallel. This fully agrees with the experimental results of [1,10].

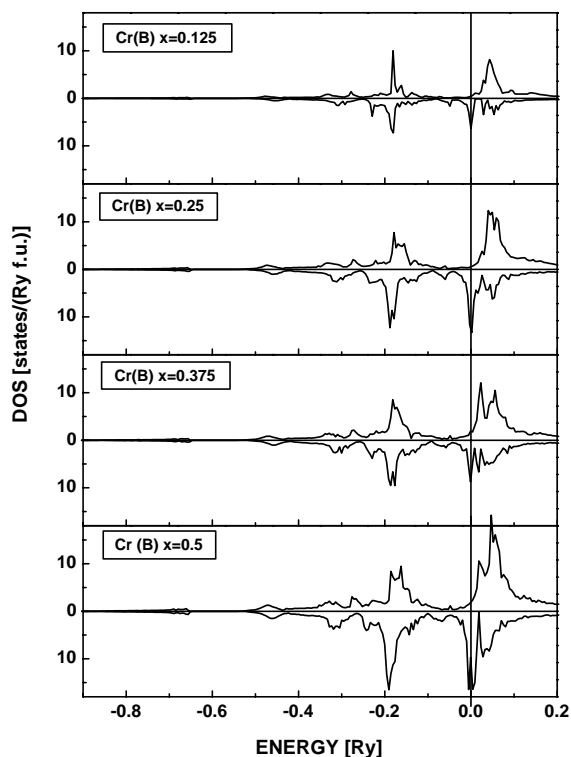


Fig. 5. The spin-projected density of states for Cr in B position for $\text{Fe}_{2.875}\text{Cr}_{0.125}\text{Si}$, $\text{Fe}_{1.75}\text{Cr}_{0.25}\text{Si}$, $\text{Fe}_{2.625}\text{Cr}_{0.375}\text{Si}$ and $\text{Fe}_{2.5}\text{Cr}_{0.5}\text{Si}$.

The magnetic moments on Cr and Fe atoms depend on the position of the atom in the unit cell and on the atomic configuration of its environment (Fig. 7). To visualise the latter effect we put on the figure two points for the same atomic position and for the same concentration, which correspond to configurations of the largest and the smallest values of magnetic moment. For small concentrations these data flow together. The iron moment for the B site is close to its BCC value and depends only weakly on concentration. The reason is that for this position the nearest neighbour surrounding is dominated by iron atoms in the whole concentration range. The slight spread of Fe (B) magnetic moments for a given concentration increases with doping. The spread of moments reflects the changes in the occupation of nearest neighbour shells. The magnetic moment of Fe (B) ranges from $2.40 \mu_B$ for the case with one Cr atom in the nearest neighbour shell to $2.67 \mu_B$ if no Cr

atoms occupy two nearest neighbour shells. The relatively weak magnetic perturbation of iron on a B site induced by nearest neighbour chromium atoms, which in this case are located on (A, C) positions, means that the chromium induced changes of local DOS of Fe (B) equally affect both spin directions. The symmetric spin perturbation is a reflection of what happens with concentration on Cr atoms on (A, C) sites (Fig. 6). The corresponding local DOS has the higher “chromium-like” peaks located fully in the unoccupied energy band region. The occupied

region of the discussed DOS changes almost equally for both spin subbands.

The magnetic moment of iron on (A, C) positions significantly changes with concentration. The number of magnetic nearest neighbours (Fe and Cr) is two times smaller than for B sites. The magnetic moment of iron strongly depends on the number of Cr atoms located in the first and the second neighbour shells. Its value is reduced in comparison with the magnetic moment of iron in the parent compound ($1.35 \mu_B$). For $x = 0.5$ and for iron atoms not surrounded by other chromium atoms, the value of the magnetic moment of iron equals $0.96 \mu_B$, in essential agreement with the results of [10]. In another extreme case, when 3 Cr atoms are located in the nearest- and one chromium in the next-nearest neighbour shells, the magnetic moment of iron drops down to $0.22 \mu_B$. The significant decrease of the iron moment with concentration arises from the reconstruction of the majority band above the Fermi level (Fig. 4). To understand the decrease of the moment with substitution of Cr it is instructive to invoke the local densities of states of neighbouring Cr atoms, which in this case are located on B positions. An asymmetry of the location of higher “chromium-like” peaks with respect to the Fermi level for different spin orientations is observed (Fig. 5). The magnetic moments of Cr are anti-parallel to iron moments. For low concentration

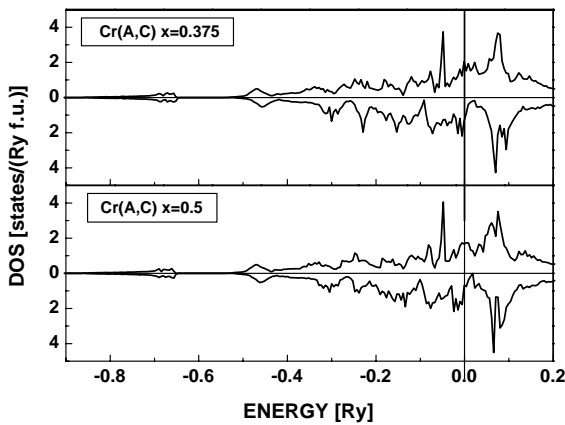


Fig. 6. The spin-projected density of states for Cr in (A, C) position for $\text{Fe}_{2.625}\text{Cr}_{0.375}\text{Si}$ and $\text{Fe}_{2.5}\text{Cr}_{0.5}\text{Si}$.

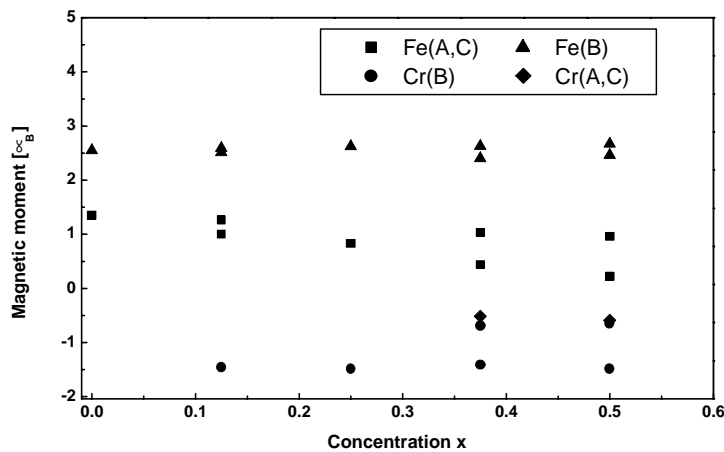


Fig. 7. The dependence of the local magnetic moment on the concentration x for $\text{Fe}_{3-x}\text{Cr}_x\text{Si}$ alloys.

($x < 0.375$) only the occupation of B positions by Cr is nonvanishing. In this region, the corresponding magnetic moment is $\mu_{\text{Cr}} \approx -1.49 \mu_{\text{B}}$, which is a very reasonable value in the light of the experimental data [10]. For $x \geq 0.375$ there is a nonvanishing probability of finding Cr atoms in the nearest neighbour shell. This fact is reflected in an increase of the spread of the points for a given concentration for all types of atoms and for all sites. The largest effect is observed for Cr (B). For a configuration with no Cr atom in the nearest surrounding the magnetic moment of Cr in a B position remains almost the same as for lower concentrations. If at least one Cr atom occupies the nearest neighbour shell than the magnetic moment of chromium drops to $-0.51 \mu_{\text{B}}$. The magnetic moment of Cr on (A, C) positions, corresponding to the lowest energy configuration, equals $-0.69 \mu_{\text{B}}$ for a chromium concentration of $x = 0.375$ and decreases to $-0.59 \mu_{\text{B}}$ for $x = 0.5$ (in these two cases differences in the local environments are only in the 4th neighbour shell). These results essentially support the experimental findings of [1,10]. Moreover, in accordance with [10], the existence of the chromium moment on (A, C) sites was quite uncertain in the light of the experimental data. Our calculations confirm that the estimated moments in [10], together with their orientations, were correct.

A negligible small negative moment is also induced on silicon atoms with the values ranging from -0.098 to $-0.023 \mu_{\text{B}}$. The larger values correspond to the larger average magnetic moment of the nearest neighbour surrounding i.e. to configurations with no chromium atoms in the nearest neighbour shell. Similarly, the average silicon polarisation decreases with an increase of the concentration of chromium. Small negative polarisation of silicon atoms was postulated also by Moss and Brown [14] and by Dobrzyński [15].

All theoretical values of magnetic moments concern the lowest energy configurations only. In this case, the moments of Cr and Fe are antiparallel in full agreement with experiment [10]. For some higher energy configurations, where a larger number of Cr atoms are present in the nearest neighbour shell, a parallel alignment of Fe and Cr moments can occur as well. Such a

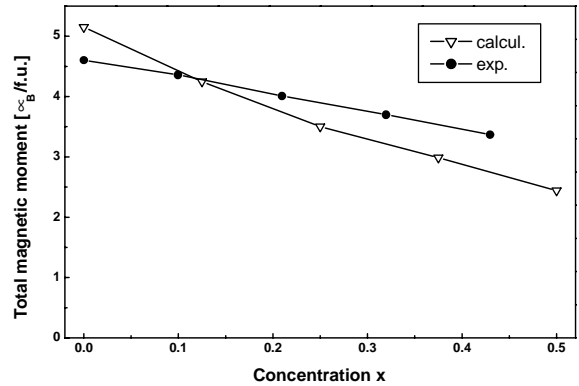


Fig. 8. The dependence of the magnetic moment on the concentration x for $\text{Fe}_{3-x}\text{Cr}_x\text{Si}$ alloys. The calculated values are denoted as triangles for configurations of the lowest total energies. The experimental ones [10] are marked as circles.

configuration has been found by us for $x = 0.5$, in which the Fe atom has four Cr atoms as first nearest neighbours. This situation is well known for chromium rich alloys. Moroni and Jarlborg found parallel iron and chromium moments in their spin-polarised self-consistent LMTO calculations for FeCr_3 [16]. In their case, however, the configurations found are low energy ones whereas in the system considered by us they correspond to high energy (> 40 mRy) and therefore they should play no role at ambient temperatures.

Fig. 8 presents the concentration dependence of the total magnetic moment obtained by averaging over different low energy configurations. The calculated decrease of the moment is more pronounced than the experimentally measured one. The change of the magnetic moment with concentration is mainly determined by the decrease of the magnetic moment on iron atoms in (A, C) positions. The changes of the magnetic moment of chromium are of lesser importance due to their small weight in the total magnetisation.

4. Conclusions

The self-consistent band structure calculations presented in this paper indicate the existence of a strong preference of the B-site occupation by chromium while the experiments [1,10] show that

this preference is rather weak. The restrictions caused by the small size of the supercell do not allow one to analyse the concentration dependence of the magnetic moments in finer steps. In the low concentration region they only enable the consideration of configurations with extreme opposite sublattice occupations. One can nevertheless conclude that B sites are preferred by chromium. In an oversimplified 32 atom supercell picture, the chromium atoms occupy solely B sites for $x = 0.125$ and $x = 0.25$. For $x > 0.25$ also (A, C) sites can be occupied by Cr, but the B positions remain preferred. For $x > 0.25$ the probability of finding a chromium atom on a B position is twice as large as for A or C positions. This situation is in apparent disagreement with the results of experiments [1,9,10], where practically no preferential occupation of iron sites by chromium was observed. A slight preference towards B-sites is much smaller than the calculations would indicate. At present, we have no explanation for this fact.

The influence of the local environment on the local magnetic moment in $\text{Fe}_{3-x}\text{Cr}_x\text{Si}$ was also studied. We have found that the magnetic moments on Fe and Cr atoms strongly depend on the crystallographic position and on the type of atoms in the nearest neighbour shell. The values of magnetic moments on Fe and Cr atoms significantly decrease if some chromium atoms are in the first or second nearest neighbour shells. It is mainly a consequence of the chromium doping induced changes in the majority subband above the Fermi level, which increases the number of holes in this band. The magnetisation of the chromium subsystem is antiparallel to the iron one and both magnetisations change linearly with concentration.

The obtained linear dependence of the total magnetic moment on concentration is in reasonable agreement with experiment [9], but is slightly more rapid. However, the fact that the magnetic moments obtained for pure Fe_3Si are larger than experimentally observed shows that not all features of the electronic structure were caught and

some refinement of the theoretical approach is required to improve the agreement of theoretical and experimental values. The experiments were done at room temperature and our calculations are strictly valid at absolute zero, what should explain some of the observed differences. The discrepancy, however, is too large to be attributed to only the temperature effect ($T/T_C \sim 0.4$).

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