Magnetic and structural properties of Fe\textsubscript{3-x}Cr\textsubscript{x}Al\textsubscript{0.5}Si\textsubscript{0.5}

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Abstract. Results of X-ray, neutron, magnetization and Mössbauer measurements on polycrystalline samples of Fe\textsubscript{3-x}Cr\textsubscript{x}Al\textsubscript{0.5}Si\textsubscript{0.5} (x = 0, 0.125, 0.250, 0.375 and 0.5) alloys are presented. The alloys crystallize in the structure of DO\textsubscript{3} type, and their unit cell volumes are practically independent of the chromium concentration. X-ray and neutron diffraction confirmed the phase homogeneity of all the samples. Neutron and Mössbauer measurements disclosed that Cr atoms occupy preferentially B-sites, while D sites are almost entirely occupied by Al and Si. The total magnetisation as well as the site and individual magnetic moments \( \mu_{\text{Fe}(A,C)} \), \( \mu_{\text{Fe}(B)} \) and \( \mu_{\text{Cr}(B,D)} \) have been found to be linearly dependent on the chromium concentration.

1. Introduction

Fe\textsubscript{3}Al and Fe\textsubscript{3}Si alloys crystallize in DO\textsubscript{3}-type of structure, see Fig.1. Its unit cell within space group F-43m (no. 216) can be described in terms of four interpenetrating fcc lattices: (A,C) - sites originating from (0,0,0) and (½, ½, ½), respectively, B-site originating from (¼, ¼, ¼), and D-site originating from (¾, ¾, ¾). A, B and C-sites in fully ordered structure are occupied by iron atoms, whereas the D-site is occupied by aluminium or silicon.

When chromium is substituted for iron a number of interesting properties occur. The lattice parameter of alloys based on Fe\textsubscript{3}Si increases linearly with chromium content, while it decreases linearly with same (absolute) slope in Fe\textsubscript{3-x}Cr\textsubscript{x}Al alloys \cite{1, 2}. Thus the composition of Fe\textsubscript{3-x}Cr\textsubscript{x}(Al\textsubscript{0.5}Si\textsubscript{0.5}) should exhibit lattice parameter independent of the concentration of chromium. The locations of Cr impurities, as well as their magnetic moments are also different \cite{1, 2}. From the crystal structure point of view, one should note that the nearest-neighbour configurations \cite{1} make the B-sites inequivalent with respect to the symmetry-equivalent A and C ones. This results in the diffraction pattern characterized by three types of structure factors:

\[
F_{hkl}^{(1)} = \sqrt{(f_A - f_C)^2 + (f_B - f_D)^2}
\]

corresponding to the superstructure lines with \( h,k,l \) - all odd and

\[
F_{hkl}^{(2)} = (f_A + f_C) - (f_B + f_D)
\]

corresponding to the \( h+k+l = 4n + 2 \), where \( n \) is integer, and

\[
F_{hkl}^{(3)} = f_A + f_C + f_B + f_D
\]

corresponding to the fundamental reflections with \( h+k+l = 4n \), where the \( f_i \) is the effective scattering amplitude of the \( i-th \) site. The symmetry non-equivalence of B and (A,C) iron sites is reflected in different on-site magnetic moments. The experiments \cite{2-5} and calculations \cite{6, 7} show that the 3d impurities tend to occupy preferentially one or another of iron sites, (A,C) or B. The element placed to the left of Fe in the Periodic Table of Elements should locate preferentially in B sites, while the elements to the right of Fe enter preferentially the (A,C) sites \cite{7-9}. Accepting such...
rules, and assuming the same form-factors \( f_A = f_C = f_{A,C} \), the appropriate formulas for magnetic structure factors can be written in the simple form:

\[
F_{hkl}^{(1)} = i (f_B - f_D),
\]

\[
F_{hkl}^{(2)} = 2f_{A,C} - f_B - f_D, \tag{5}
\]

\[
F_{hkl}^{(3)} = 2f_{A,C} + f_B + f_D. \tag{6}
\]

The studies of Fe\(_3\)(Al\(_x\)Si\(_{1-x}\)) alloys \([8, 9]\) showed that the magnetic moments depend on the relative concentration of Al and Si. In contrast to the weak moments found at D-sites, the values of magnetic moments at (A,C) and B positions turned out not to vary systematically with Cr content \([8]\). The analysis of the spin-density distributions, carried out by the Maximum Entropy Method analysis \([10]\) showed that magnetic moments of \( \mu_{Fe(B)} \) vary linearly with silicon content.

Figure 1. The unit cell of the DO\(_3\)-type structure.

Ab-initio total energy calculations of Fe\(_{3-x}\)Cr\(_x\)Al \([11]\) strongly suggested the B-site preference of Cr atoms. Similarly, the self-consistent band structure calculations \([12]\) as well as recently published self-consistent TB-LMTO calculations disclosed the existence of a strong preference of the B-site occupation by chromium \([13]\). On the other hand, CPA calculation of Fe\(_{3-x}\)Cr\(_x\)Al \([14]\) did not show definite preference of Cr to the B-sites, especially at larger Cr content. According to ab-initio calculations, chromium in Fe\(_3\)Si perturbs the neighbouring iron atoms and this perturbation seems to be local and most efficient when Cr atoms are n.n. to iron atoms at both (A,C) - and B-positions \([15]\). In light of the experimental observation, chromium in Fe\(_3\),Cr,Si alloys enters both (A,C) and B sites \([1, 2, 16-18]\) while certain preference to the occupation of B-site in Fe\(_3\)Al was observed \([1, 2, 14]\). One should note that in the case of Fe\(_3\)Al it is very difficult to achieve full DO\(_3\)-type ordering, and B–D disorder is usually observed. This little B–D disorder, included in the calculations \([19]\), appeared to be not responsible for the lack of preferential occupation of sites in the case of chromium in Fe\(_3\)Si. Our recent measurements were carried out on Fe\(_{3-x}\)Cr\(_x\)Al\(_{0.5}\)Si\(_{0.5}\) \([20]\) with the aim to have same volume per atom, which should permit to study in better way the effects of local surroundings.

2. Sample preparation

The sample preparation has been described in \([20]\). The sample annealing procedure, however, was slightly modified. Because the losses of mass came from the evaporation of chromium and aluminium due to their high vapour pressure, the composition of the alloys was checked by X-ray and Mössbauer measurements after each stage of thermal history. The experience of previous experiments \([1, 2, 16-18]\) taught that special care should be dedicated to the sample annealing procedures.
3. X-ray diffraction

X-ray diffraction measurements were performed using conventional Bragg-Brentano powder diffractometer (HZG-4, University of Bialystok, Poland) with CoK\(\alpha\) radiation, \(\lambda = 1.78893\) Å. These measurements have revealed the homogeneity of all Cr-doped samples at room temperature. With an increase of the chromium content, the intensities of the superstructure reflections decrease. It is well-known that certain B-D disorder appears systematically in Cr-doped Fe\(_3\)Al [21]. The superstructure lines with \(h, k, l\) - all odd are directly sensitive to the difference of amplitudes at B and D positions (see eq. 4). Our Mössbauer spectroscopy results exclude the presence of iron in these positions, especially for alloys with higher concentration of chromium. Thus, this type of disorder may concern the partial occupation of D-sites by chromium only. Unfortunately, the intensities of (200) lines are not sensitive to this kind of disorder (see eq. 5). This is due to the fact that the atomic scattering factors of iron and chromium as well as aluminum and silicon are hardly distinguishable in X-ray diffraction experiment.

According to the results presented in Table 1, in Fe\(_{3-x}\)Cr\(_x\)Al\(_{0.5}\)Si\(_{0.5}\) alloys the effective scattering amplitude of the (A,C) - sites were found to be close to iron atomic scattering factors, which means that Al and Si atoms do not enter (A,C) positions. However, from the occupancies of D – sites it follows that the samples are not exactly stoichiometric and contain both Al and Si in the ratio slightly deviating from the nominal 1:1 proportion. Such situation was discussed in detail in ref. [20]. Alternative explanation for the increase of the scattering amplitude at D sublattice seems to be B-D disorder, caused by Cr atoms occupying partly D site. Therefore, the model with the B-D disorder and untouched (A,C) sites had also to be considered. The latter conclusions are supported by Mössbauer experiments (see section below).

In the light of previous results [20] where the AgK\(\alpha\) radiation, \(\lambda = 0.55926\) Å, was used, the obtained isotropic Debye-Waller factors versus increasing chromium concentration were as follows: 0.376(12) - for undoped alloy and 0.353(19), 0.357(14), 0.380(14) and 0.344(18) \(\text{[Å]}^2\) for the consecutive chromium-containing alloys. Therefore in order to reduce the free parameters during the refinements presented below the weighed average value \(B = 0.366\) \(\text{[Å]}^2\) was fixed for all alloys. Moreover, according to results reported in [20] it was assumed that (A,C) positions are fully occupied by iron atoms and the chromium atoms enter predominantly (in the range of error bars) B sublattice. The diffraction patterns were analysed by Rietveld – type profile refinement method using FullProf program [22]. For better readability the goodness-of-fit parameters defined in ref. [22] are also quoted.

![Table 1: Structural parameters for Fe\(_{3-x}\)Cr\(_x\)Al\(_{0.5}\)Si\(_{0.5}\) alloys, i.e. lattice parameter – a, site occupancies - and agreements factors [22] obtained from X-ray measurements at room temperature.](https://example.com/table1.png)

The analysis of the occupations of the B and D – sites allow to compare the estimated compositions of the powder samples with the nominal ones according to the equations:

\[
\xi_{Fe(B)} \cdot f_{Fe} = (1 - x_{Cr(B)}) f_{Fe} + x_{Cr(B)} \cdot f_{Cr}
\]  

(7)
and

\[
\zeta_{Si(D)} \cdot f_{Si} = \left(1 - \gamma_{Cr(D)}\right) \cdot \left(\frac{f_{Si} + f_{Al}}{2}\right) + \gamma_{Cr(D)} \cdot f_{Cr}
\]  

(8)

where \( \zeta \) - site occupancy. In the later equation the ratio aluminium to silicon equal to 1:1 was fixed.

Results obtained by X-ray diffraction powder technique show that the samples are single DO\(_3\) phase. This conclusion means that for the heat treatment applied here the estimated sample compositions do not differ from the nominal ones.

Another important finding is observed independence of the lattice parameter (see 2\(^{\text{nd}}\) row of Table 1) of the Cr concentration. Let's recall that experiments previously carried out on Fe\(_{3-x}\)Cr\(_x\)Si [1, 16, 17] showed a contraction of the unit cell volume against chromium concentration in the range up to \( x = 0.4 \), while the opposite trend was observed in Fe\(_{3-x}\)Cr\(_x\)Al system [18] up to \( x = 0.6 \). For better insight into the nature of magnetic moments it is important to be sure that the parameters of the unit cell as well as interatomic distances remain independent of chromium content.

4. Neutron scattering

In order to determine magnetic structure, the neutron powder data were collected at the reactor MARIA (IEA, Swierk) at 10 K (see Fig. 2) and at room temperature using 2-axis diffractometer and an unpolarized incoming-neutron wavelength of \( \lambda = 0.985 \) Å. The measurements were carried out in the range of 10\(^{0}\) – 110\(^{0}\) scattering angles \( 2\theta \) with the 0.1\(^{\circ}\) step size.

![Figure 2](image)

**Figure 2.** RT neutron powder diagrams experimental, calculated and the residual ones obtained for nominal Fe\(_{2.875}\)Cr\(_{0.125}\)Al\(_{0.5}\)Si\(_{0.5}\) alloy, with marked N-nuclear and M- magnetic Bragg peaks. All peaks can be indexed within DO\(_3\)-type of structure. However, for better readability of the figure, some of the peaks shown have been left without indices.

Analysis of the neutron intensities cannot distinguish aluminium and chromium due to similar values of their neutron scattering lengths. Fortunately, in the light of X-ray results, rather small B-D disorder is present in measured samples. The neutron data confirm again the expectation that the lattice parameter of the alloys should be practically independent of the chromium concentration [20]. They show unambiguously that the chromium atoms locate predominantly at B-sites. As a result, (A, C) are treated as containing iron atoms only, while B – sites are occupied by iron and chromium ions. In order to reduce the number of free parameters, the chemical compositions at D positions were set to the ones given by the X-ray data (see Table 2). The distribution of atoms among the (A, C) and B...
crystallographic sites obtained by the use of X-ray and neutron scattering as well as the on-site occupancies remain in very good agreement. Moreover, judging from the temperature dependence of the magnetic moments measured for Fe$_{2.875}$Cr$_{0.125}$Al$_{0.5}$Si$_{0.5}$ at 10 K and at RT (the only sample for which the measurements have been carried out at RT—see Fig. 2), Curie temperature must be well above RT. The magnetic structure is commensurate with the nuclear one, thus all observed intensities disclose both nuclear and magnetic contributions of scattering amplitudes, i.e.:

$$I_{hhk} \propto |F_{hhk}|^2 = |F_N|^2 + \frac{2}{3}|F_M|^2$$

(9)

where the appropriate structure factor components are equal to

$$F_{hhk} = \sum_j b_j e^{-i \vec{G}_{hhk}} = \sum_j b_j \exp \left( -i \cdot \left( \frac{2\pi}{a} h, \frac{2\pi}{a} k, \frac{2\pi}{a} l \right) \cdot \left( x_j, y_j, z_j \right) \right)$$

(10)

and

$$F_{hhk}^M = \vec{\chi} \sum_j \tilde{p}(\vec{K}) e^{i \vec{K} \cdot \vec{r}_j}$$

(11)

with

$$\tilde{p}(\vec{K}) = 0.2695 \cdot \mu_j \cdot f_j(\vec{K})$$

(12)

$$\vec{\chi} = \left[ \vec{m} - (\vec{K} \cdot \vec{m}) \cdot \vec{K} \right]$$

(13)

where $b_j$ - is the neutron scattering amplitude of the $j$-th atom, $f_j$ - magnetic form factor of the $j$-th atom and $\mu_j$ - magnetic moment of the $j$-th atom.

Table 2. Structural and magnetic parameters for Fe$_{3-x}$Cr$_x$Al$_{0.5}$Si$_{0.5}$ alloys as well as GOF (goodness of fit) parameters obtained from neutron measurements collected at 10 K and at room temperature.

| Site occupancy | Chromium nominal concentration $-x$ | 0.125RT | 0.12510K | 0.2510K | 0.37510K | 0.510K |
|----------------|-------------------------------------|---------|---------|---------|---------|-------|
| Fe(A,C)        | Fixed to 1                          | Fixed to 1 | Fixed to 1 | Fixed to 1 | Fixed to 1 |
| Fe(B)          | 0.91(4)                             | 0.91(3) | 0.78(5) | 0.66(6) | 0.57(4) |
| Cr(B)          | 0.09(3)                             | 0.09(3) | 0.22(5) | 0.34(6) | 0.43(4) |
| Al/Si(D)$^1$   | 0.984                               | 0.984 | 0.989 | 0.956 | 0.949 |
| Cr(D)          | 0.016                               | 0.016 | 0.011 | 0.044 | 0.051 |
| Individual magnetic moments [$\mu_0$/atom] | | | | | |
| $\mu_{Fe(A,C)}$ | 1.49(13)                           | 1.51(12) | 1.45(18) | 1.36(15) | 1.29(17) |
| $\mu_{Fe(B)}$  | 2.38(17)                           | 2.44(14) | 2.34(15) | 2.20(17) | 2.06(19) |
| $\mu_{Cr(B,D)}$ | 1.44(14)                           | 1.44(11) | 1.52(17) | 1.62(20) | 1.69(21) |
| On-site magnetic moments [$\mu_0$] | | | | | |
| $\mu_{(A,C)}$  | 1.49(13)                           | 1.54(12) | 1.45(18) | 1.36(15) | 1.29(17) |
| $\mu_{(B)}$    | 2.04(32)                           | 2.09(25) | 1.49(35) | 0.90(41) | 0.45(35) |
| $\mu_{(D)}$    | -0.023                             | -0.023 | -0.017 | -0.071 | -0.086 |

$^1$ The ratio aluminum to silicon was fixed to 1:1 during whole of the series refinement.
The best description of the magnetic part of the neutron powder diagram is obtained for antiferromagnetically coupled Cr and Fe. All magnetic moments of iron are oriented parallel to each other. According to [20] the concentrations of iron at (A,C) sites were equal to: 0.98(1) for x = 0.125 at RT, and 0.99(3), 0.94(6), 0.97(5), 0.95(3) at 10K for x = 0.125, 0.25, 0.375 and 0.5, respectively. Therefore in order to reduce the number of free parameters during data refinements for all measured alloys the Fe(A,C) occupancy was assumed to be equal to one. The most likely distribution of atoms in the samples as well as their magnetic moments arrangement are presented in Table 2. The individual magnetic moments and the magnetisation per formula unit, $\mu_{\text{tot}}$ versus chromium concentration diminish linearly with Cr concentration, see Table 2. The behaviour of the moments at A and C sites can be easily understood in terms of Cr atoms appearing at neighbouring B-sites. The decrease of the moment at B-site is clearly connected with negative contribution coming from chromium moments. Magnetic moments per formula units are in good agreement with the ones measured in magnetisation studies at 10 K, see Table 3. Such measurements were carried out using vibrating sample magnetometer (VSM Lake Shore model 7300) under magnetic fields up to 1.2 T in the temperature 10 K and 300 K.

| Cr content | x = 0 | x = 0.125 | x = 0.25 | x = 0.375 | x = 0.5 |
|------------|------|--------|--------|---------|-------|
| 10K        | 5.5(3) | 4.8(4) | 4.2(3) | 3.6(2) | 3.1(2) |
| 300K       | 4.7(3) | 4.2(3) | 3.6(2) | 3.1(2) | 2.7(3) |

6. Mössbauer spectroscopy

The $^{57}$Fe Mössbauer measurements have been carried out in the constant acceleration mode at room temperature using $^{57}$Co source in Cr matrix. The spectrometer was calibrated before and after measurements. The measured spectra were fitted using superposition of elementary sextets broadened by Gaussian distribution of hyperfine magnetic field. The values of hyperfine fields obtained from the measurements are presented in Table 4. The values with stars in this Table denote those ones, which were fixed ones during fitting procedure.

For perfect ordering of the alloy the spectrum should contain only two sextets connected with iron atoms Fe(A,C) surrounded by 4Fe(B), 4Si/Al(D) (Fe(4)) and Fe(B) surrounded by 8Fe(A,C) (Fe(8)). The intensity ratios of those sextets are equal to 2. For better description of the spectrum of Fe$_3$(Si/Al) one needs to use an additional broad sextet Fe(7) with the hyperfine magnetic field between values obtained for Fe(8) and Fe(4). It means that there exists a small disorder in the studied alloy. The value of isomer shift of Fe(7) is equal within the error bars to the value observed for Fe(8). It means that observed disordering are probably between (A,C) and (D) sites. Small part of Fe(A,C) atoms occupies the Al/Si(D) sites.
Table 4. The hyperfine fields parameters obtained from the best fits of the Mössbauer spectra of the Fe$_{3-x}$Cr$_x$Al$_{0.5}$Si$_{0.5}$ alloys. B denotes the magnetic hyperfine field, $\sigma_B$ - standard deviation of Gaussian distribution, IS - the isomer shift relative to $\alpha$-Fe and A means the intensity of the local components.

| Chromium content -x | sextet | B[T]      | $\sigma_B$ [T] | IS [mm/s] | A [%]    |
|---------------------|--------|-----------|----------------|-----------|----------|
| 0                   | S(8)   | 29.87 ± 0.04 | 0.41 ± 0.11 | 0.06 ± 0.01 | 31.5 ± 2.9 |
|                     | S(7)   | 25.74 ± 0.79 | 2.2 ± 1.2    | 0.05 ± 0.03 | 10.8 ± 4.4 |
|                     | S(4)   | 20.73 ± 0.03 | 1.01 ± 0.06  | 0.21 ± 0.01 | 58.1 ± 2.9 |
|                     | S(8)   | 29.29 ± 0.09 | 0.91 ± 0.07  | 0.061 ± 0.005 | 24.4 ± 1.3 |
|                     | S(7)   | 25.2 ± 0.6   | 2.11 ± 0.36  | 0.048 ± 0.011 | 16.4 ± 2.3 |
|                     | S(4)   | 20.32 ± 0.04 | 1.26 ± 0.05  | 0.205 ± 0.005 | 43.7 ± 1.3 |
| 0.125               | S(3)   | 14.95 ± 0.09 | 1.2 (*)      | 0.178 ± 0.009 | 15.5 ± 0.5 |
|                     | S(8)   | 28.06 ± 0.15 | 1.47 ± 0.13  | 0.053 ± 0.007 | 21.4 ± 1.9 |
|                     | S(7)   | 24.35 ± 0.28 | 1 (*)        | 0.041 (*)     | 14.1 ± 1.5 |
| 0.25                | S(4)   | 20.19 ± 0.11 | 1 (*)        | 0.201 ± 0.006 | 28.7 ± 1.6 |
|                     | S(3)   | 14.87 ± 0.15 | 2.26 ± 0.19  | 0.17 (*)      | 30.3 ± 1.9 |
|                     | S(2)   | 8.31 ± 0.23  | 1 (*)        | 0.151 ± 0.024 | 5.4 ± 0.7 |
|                     | S(8)   | 26.96 ± 0.17 | 1.5 (*)      | 0.053 ± 0.011 | 16.1 ± 1.5 |
|                     | S(7)   | 23.13 ± 0.37 | 1.8 (*)      | 0.023 ± 0.018 | 15.5 ± 1.7 |
| 0.375               | S(4)   | 19.69 ± 0.17 | 1.24 ± 0.25  | 0.199 ± 0.014 | 18.7 ± 4.5 |
|                     | S(3)   | 14.48 ± 0.33 | 2.42 ± 0.51  | 0.16 (*)      | 39.8 ± 7.4 |
|                     | S(2)   | 7.9 ± 1.1    | 3.0 ± 0.49   | 0.14 (*)      | 9.9 ± 3.8 |
|                     | S(8)   | 25.31 ± 0.48 | 1.79 ± 0.33  | 0.046 ± 0.013 | 14.8 ± 3.7 |
|                     | S(7)   | 21.62 ± 0.51 | 1.8 (*)      | 0.026 ± 0.031 | 13.3 ± 4.2 |
| 0.5                 | S(4)   | 18.94 ± 0.28 | 1.67 ± 0.34  | 0.18 (*)      | 18.6 ± 4.7 |
|                     | S(3)   | 14.05 ± 0.25 | 1.94 ± 0.21  | 0.14 (*)      | 28.6 ± 3.2 |
|                     | S(2)   | 7.5 (*)      | 2.6 (*)      | 0.13 (*)      | 24.5 ± 0.5 |

For quantitative description of the site preference of Cr atoms in the studied alloys let us assume that the relative intensities of given sextets are proportional to the probability of finding of the iron atom with given chemical environments. Assuming random distribution of iron atoms at given sublattices one can calculate probabilities of finding iron atoms surrounded by n other Fe atoms in the n.n. shell for given x.

Full analysis of these data and their comparison with ab-initio calculations will be presented in a separate paper.

7. Conclusions
The studies have confirmed that the lattice parameter of the alloys is independent of chromium content, so the results obtained for the magnetic moments of iron and chromium reflect mainly an influence of local surroundings. The linear variation of magnetic moments with chromium makes it tempting to assume an influence of the nearest-neighbour shells only. This, however, needs to be confirmed by calculations that are underway. One should point out that the data obtained may be qualified as high-quality ones as rather negligible disorder could be claimed. Apparently, the chromium magnetic moment orients antiparallel to iron, and it is relatively large, about 1.5 Bohr magneton.

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