Mössbauer effect study and Monte Carlo simulation of $Fe_{3-x}Ti_xAl$ (x=0…1) alloys

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Ternary alloys $Fe_{3-x}M_xAl$ with M = Ti, V, Cr, Mn and Mo, based on iron aluminides Fe_3Al are considered to be potential high-temperature structural materials because of their high strength combined with excellent oxidation and corrosion resistance [1-6]. The basic Fe_3Al alloy undergoes a continuous transformation from highly ordered DO_3 structure to an imperfectly ordered B2 structure at critical temperature $T_C^{DO3-B2} \approx 820$ K. Ternary 3d element like Ti, V, Cr, Mn and Mo improves the high temperature strength of Fe_3Al by stabilization of the DO_3 ordered structure up to temperatures well above 820K. The Ti additions leads to some extreme change in Fe_3Al properties than others elements. The investigations performed by Ohnuma [9] indicate that the partial replacement of Fe atoms by Ti atoms in the Fe-rich binary Fe-Al alloys results in stabilization of the B2 (FeAl) and DO_3 (Fe_3Al) phases and in increase of the A2-B2-DO_3 successive order-disorder transition temperature.

In this presentation, we show that the combined Mössbauer spectroscopy and Monte Carlo (MC) computer simulation results very well explain the structural and magnetic properties of alloys system $Fe_{3-x}Ti_xAl$ in the range of titanium concentration from x = 0.0 to x = 1.0. With special attention the formation of the Heusler phase Fe_2TiSn with $L2_1$ structure was investigated [7,8].

The investigated compounds $F_{3-x}Ti_xAl$ (x = 0, 0.2, 0.45, 0.55, 0.65, 0.75, 1) were prepared by arc melting in high purity argon atmosphere. After melting the samples were mechanically crashed and next annealed for 1h at 900°C and next for 4h at 400°C. The ^{57}Fe Mössbauer spectra were recorded at room temperature using a conventional constant acceleration spectrometer with a ^{57}Co(Rh) source with an activity of about 50mCi. All the spectra were analyzed by MOSMOD computer program which is a direct implementation of Voigt-based fitting method of Rancourt and Ping [10].

In the simulation procedure the modeling *bcc* crystal of 54000 atoms with the periodic boundary conditions was used. In each steps of the (MC) simulation the two different atoms from modeling crystal were randomly chosen and exchanged if it leads to the decrease in energy of system. The energy of the system was calculated in the terms of pair interaction:

$$E = -\sum_{s}^{2} \sum_{i \neq j} N_{ij}^{s} \cdot w_{ij}^{s}$$

where N^s_{ij} is the number of (i-j) pairs, w_{ij} are pair energies between atoms (i-j) where (i,j = Fe, Ti, Al); s denote the number of shell. The positive values of w_{ij}^{s} leads to ordering process whereas negative values to the clasterization.

The values of the interchange pair energies were taken from paper of Ohnuma [9] and are collected in Table nr 1.

Table 1. The pair energies for Fe-Al-Ti system from [9].

i-j	w_{ij}^1 [meV]	w_{ij}^2 [meV]
Fe-Al	144	64
Fe-Ti	136	-90
Al-Ti	208	104

In the modeling crystal of the disordered ternary $Fe_{3-x}Ti_xAl$ system is about thirty local configurations of Fe atoms. From (MC) simulation was established that within ($L2_1$) ordered domains, independently of titanium concentration in the alloy, the loading configurations of Fe atoms can be constructed on the base of only the six *nn bcc* clusters. These clusters are shown in Fig 1.

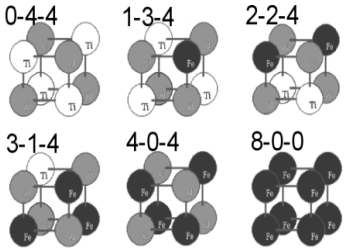

Fig. 1. The six loading *nn bcc* cluster of Fe atoms. The index (X-Y-Z) describes number of Fe, Ti and Al atoms surrounding the Fe atom in the central position, respectively.

The specified six Fe atoms configurations (Fig 1) were used in analysis of Mössbauer spectra.

Figure 2 shows the Mössbauer spectra for investigated $Fe_{3-x}Ti_xAl$ alloys with x = 0.0, 0.2, 0.45, 0.55, 0.65, 0.75 and 1.00.

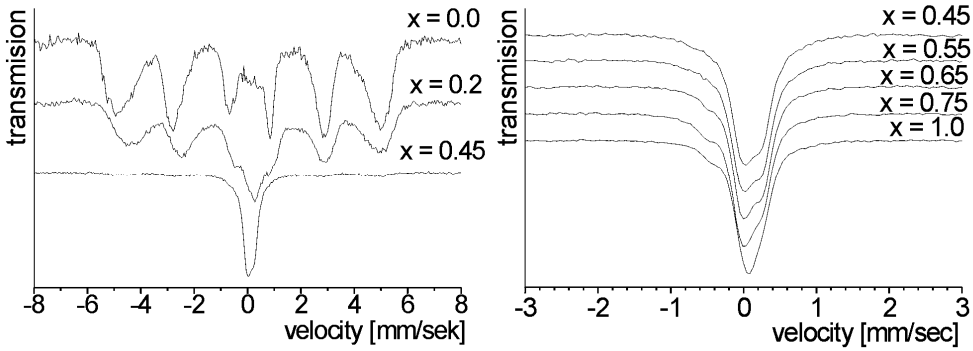

Fig. 2. The Mössbauer spectra of $Fe_{3-x}Ti_xAl$ alloys.

The measured in the room temperature Mössbauer spectra of $Fe_{3-x}Ti_xAl$ alloys exhibit ferromagnetic splitting for x <0.45 and show existence of a paramagnetic state for x>0.45.

However it was find that there are clusters of Fe atoms having high magnetic moment in the all range of titanium concentration.

The analysis of Mössbauer spectra , basing on MC results, has given not only good fitting of spectra but also very reasonable description of changes in contribution of specific components. In Fig. 3-(a) are shown contributions of spectral components connected with *nn bcc* configurations: (0-4-4), (1-3-4), (2-2-4), (3-1-4), (4-0-4) and (8-0-0). In Fig. 3-(b), for comparison, are shown contributions of *nn bcc* configurations resulting from MC simulation.

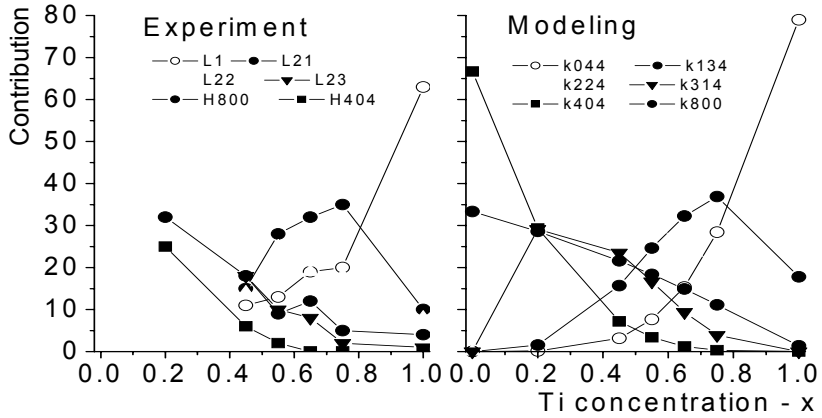

Fig. 3. The comparison of contribution of *nn bcc* configurations received from Mössbauer spectra analysis and Monte Carlo simulation. The L1, L21, L22, L23, H800, H400 components are connected with (0-4-4), (1-3-4), (2-2-4), (3-1-4), (8-0-0) and (4-0-4) configurations, respectively.

As it should be expected a good compatibility is obtained. The results of investigations can be summarized as follows.

1. The strong preference of Ti atoms to occupy Fe sites in the $Fe_{3-x}Ti_xAl$ system is observed.
2. The Heusler phase with $L2_1$ structure is formed for Ti concentration $x>0.45$.
3. In the range of Ti concentration $x<0.45$ a ferromagnetic components are observed in Mossbauer spectra, connected with clusters of Fe atoms having high magnetic moment.

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