STRUCTURAL AND MAGNETIC PROPERTIES OF Fe-Cr-Al ALLOYS WITH DO3-TYPE STRUCTURE

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The results reported here were published in [1]. Fe_3Si and Fe_3Al alloys are very interesting intermetallic compounds for number of reasons. They crystallize in DO_3 - type structure (Fig.1), in which iron occupies two inequivalent positions. One of these is surrounded in the nearest-neighbour shell by eight iron atoms in bcc iron and possesses a high magnetic moment of the order of 2.2-2.5 μ_B.

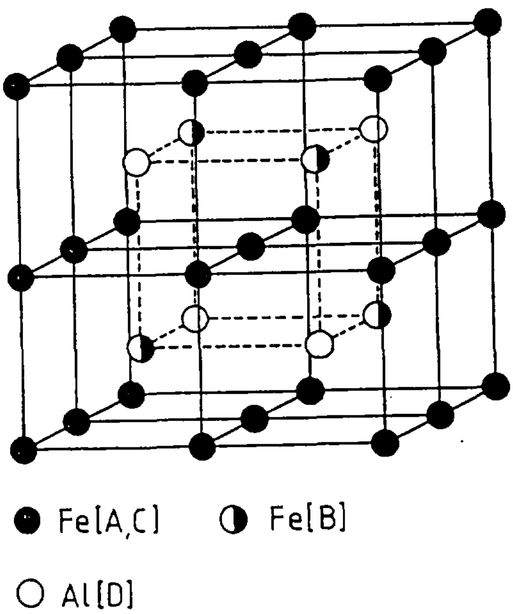

Fig. 1. DO_3-type strukture

This site is usually abbreviated by B, whereas the letters A and C stand for other sublattices in which iron is surrounded by four iron and four Si or Al atoms.The magnetic moment found at these sites is much lower and equals about 1.1 μ_B in Fe_3Si and 1.4 μ_B in Fe_3Al. The fourth position D is occupied uniquely when perfect order is achieved, by silicon or aluminium atoms. The presence of the two inequivalent positions in the lattice make the alloys almost ideally suited for studies of the magnetic moment dependence on the local environment. In addition, the structure itself changes to B2 and A2 under disordering so the physical origins of the order-disorder process can be studied as well. The two isomorphous alloys, according to the band structure calculations, should show very similar properties but this is not the case. The most striking differences can also be seen in their mechanical properties: Fe_3Si is brittle, whereas Fe_3Al is ductile. It is also interesting to note that the DO_3 ordering is rather easily achieved in the Fe_3Si alloy, whereas it is extremely difficult to order Fe_3Al alloy fully. A rather small difference in the lattice constants (5.655 A for Fe_3Si compared to 5.793 A for Fe_3Al) results nonetheless in a great decrease of the effective exchange interaction from about 22 meV in Fe_3Si to about 9 meV in Fe_3Al, yet the magnetic moments per formula unit (4.86 and 5.08 μ_B at room temperature, respectively) as well as the Curie temperatures (830 and 760 K) do not differ significantly.

Actually the property which raised the most of interest in these alloys is the preferential occupation of sites by the transition metal impurities substituted for iron. In the number of papers it has been shown that in the Fe_3Si alloy, the elements to the left of iron in the periodic table of elements occupy preferentially B-sites, whereas those to the right of iron locate at (A,C)-sites. Observed changes of the local hyperfine fields have been explained in the frame-work of the local-environment model implying that - at least as far as the hyperfine fields are concerned - configuration of the nearest-neighbour shell is the only important factor in these alloys. The spin wave studies [2] indicated, however, that the exchange forces are of much longer range, calling in fact for the band structure approach. Such an approach was used to explain the mechanism of preferential site occupation in Ref. [3]. Although this explanation for Fe_3Si-based alloys should apply seemingly well to the Fe_3Al-based alloys, it has been noticed that the preferential occupation of sites in the latter alloy is not so clear if Mn is substituted for iron [4].

In the recent studies of Fe_3Si alloy with Cr substitution [5], [6], it was found, to the authors' surprise, that chromium does not locate preferentially at the B-sites but rather spreads evenly between A-, B- and C-sites. It was also found that chromium may assume magnetic moments comparable to the iron ones at both sites. However, in contrast to the behaviour of Mn impurity, the chromium moments are oriented antiparallel to the direction of the iron moments. Therefore it became interesting to study the behaviour of chromium in Fe_3Al alloy.

Magnetization studies using the magnetic balance were performed at the Institute of Physics in Białystok. Also X-ray powder diffraction diagrams were obtained in Białystok on the X-ray diffractometer with Fe Kα radiation (λ=1.93597 A). Powder neutron diffraction experi-ments were conducted on the D20 diffractometer at the Institute Laue-Langevin in Grenoble, while polarized neutron research was carried out on POLAR 2 diffractometer at the Studsvik Neutron Research Laboratory.

The powder sample compositions have been checked by means of X-ray microanalysis. The composition of the bulk samples dedicated to polarized neutron studies have been estimated from the difference of masses measured before and after arc-melting.

The analysis of the neutron intensities cannot discriminate between aluminium and chromium because the neutron scattering lengths of these two elements are not much different (3.45 and 3.64 fm, respectively). Because it is apparent that in our samples rather strong A-D disorder is present, the analysis of neutron data themselves can show anambigously the occupation of sites by iron only. Happily, one can combine neutron and Mössbauer data [7]. Inspection of both leaves no doubt that chromium enters predominantly B-sites, and it is reasonable to expect that the only other position which can be occupied by chromium will be the D-site which has the same nearest neighbourhood as the neigh bourhood of the B-sites. This conclusion is fully confirmed by the observed [7] dependence of the isomer shift on the chromium concentration.

X-ray, neutron, magnetization and Mössbauer effect studies carried out on $Fe_{3-x}Cr_xAl$ alloys with x<0.6 showed that chromium atoms occupy preferentially B-sites and enter also D-positions [1]. Their magnetic moments are small, if any, and they diminish the value of the neighbouring iron atoms by roughly 0.1 μ_B per chromium atom. This value agrees well with the one found in Ref. [8]. In spite of high counting statistics in neutron diffraction patterns, the determination of magnetic moments for various crystallographic sites did not allow either detection of the nonzero magnetic moment of chromium or a difference between the iron moments at the B- and D-sites.

Therefore, the final data analysis has been carried out under an assumption of zero magnetic moments of chromium atoms, and identical iron moments of iron at the B- and D-sites. The undisturbed magnetic moments of iron at (A,C)- and B- (or D)-sites were estimated to be 1.54 (22) and 2.58 (22) μ_B, respectively, at T=10 K, 1.51 (27) and 2.32 (14) μ_B, respectively, at T= 300 K. These values agree well with the ones obtained in Ref. [9] for Fe_3Al. It is also shown that the iron moments decrease if an extra aluminium atom is found in the nearest surrounding, and this decrease is 0.37 (10) and 0.26 (6) μ_B at T=10 K and 300 K, respectively. A markedly different behaviour of chromium in Fe_3Si and in Fe_3Al concerns the occupation of atomic sites by chromium, the value of its magnetic moment, as well as a change of lattice constant with the chromium content. On the grounds of known differences in exchange interactions in both parent alloys [2], [10], it is suggested that different behaviour of chromium is due to a subtle interplay of magnetic and nonmagnetic interactions.

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