Conference Paper

Investigation of Changes of Short-range Ordering and Electron Density in Simulating Alloys Based on Iron

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Abstract

Short-range ordering and electron density in simulation alloys, containing Cr, Mo, W and V as a doping addition, were studied by Mossbauer spectroscopy and positron annihilation methods. A number of peculiarities was observed in alloys with vanadium as a doping.

1. Introduction

Improvement of radiation stability of construction materials is a problem of great importance in modern nuclear engineering for developers, metal scientists and operators. Results of investigations [1.2] showed, that short-range ordering nanodomains generation with period ≤ 5 nm in iron and nickel maintained non-interruptive accelerated recombination of vacancies and interstitial atoms and minimized formation of vacancy voids and dislocation saving the crystal structure of the alloy.

Acceleration of vacancies and interstitial atoms recombination in the alloys crystalline structure takes place during aging of the non-stoichiometric metastable structure at the expense of appearance crystalline lattice static distortions generated because of density oscillations. Lattice static distortions are drains and traps for vacancies and interstitial atoms.

.Study of recombination effectiveness at distortions of different sorts is of the essential interest and is explained by size factors difference. Difference of volumes and in

electron sub-system create ordered static distortions (stresses). because of size effect, their influence being determined by their concentration to a significant part. The factors mentioned may change not only the interstitial atoms and vacancies mobility, but the mechanism of their annihilation [2] within a defined range of content and temperature. A new state may be created. That's a dissipative structure. This process is called self-organization.., which takes place as a two-way process including destruction of crystalline structure in offset cascades and formation of nano-domains of short-range ordering. Thus determination of generated phases parameters [s of great importance for nuclear material science. One of the most sensitive methods of determination of the short range ordering is Mossbauer spectroscopy. It must be accompanied by positron annihilation to determine defects and changes of electron density.

2. Experimental results

Experiments were carried out using sets NGRS in NRNU MEPhI 30 hours and ORTEC (ITEP) The samples were cylindrical plates Ø15x0.5 mm^3. They were annealed at 1200-1300°C during 30 hours. The samples were rolled till 40 mcm before carrying out NGR experiments. Samples containing 2,4,6 и 8%. of Cr and V. Results are shown in fig.1 and in table1. The most important characteristics is the difference of the real probability of surrounding the iron atom from the statistical one. That.i called the short-range-ordering parameter.

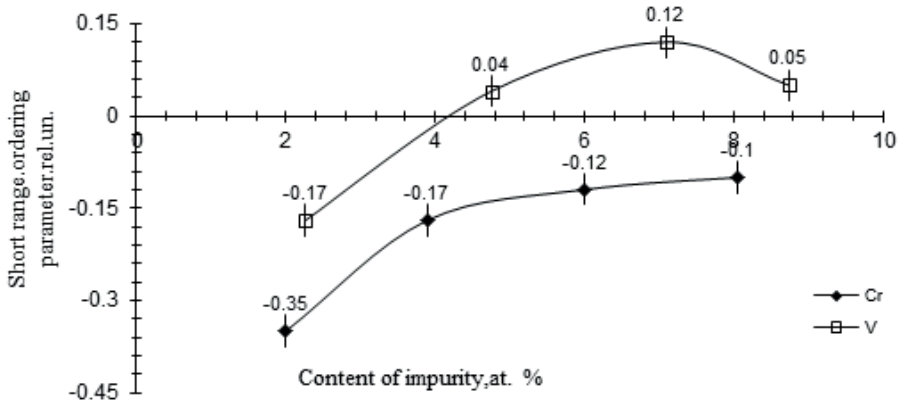

Figure 1: Dependence of short-range ordering parameter on impurity content.

Here τ_1,τ_2,τ_3- positron lifetimes in the non-defective volume, a vacancy and a cluster. I_1,I_2,I_3 are parts of detected fluxes of annihilation photons with lifetimes τ_1,τ_2,τ_3. lav. –lavsan (the source lay).

Table 1: Results of investigations.

Spectra	τ_1, пс	I_1 %	τ_2, пс	I_2 %	τ_3, пс	I_3 %	χ^2	Lav%
o-armco	136±1	69±0,9	314±4	31±0,9	нет	нет	1,1	27
1-Cr 2%	145±4	44±0,5	309±9	47±0,6	1010±50	9±0,3	1,06	27
2-Cr4%	153±4	49±0,5	310±10	42±0,6	1030±70	9±0,5	1,04	27
3-Cr 6%	150±4	48±0,6	310±10	44±0,7	1150±60	8±0,2	1,15	27
4-Cr 8%	146±5	46±0,6	310±10	45±0,8	1060±50	9±0,2	1,03	27
5-V 2%	130±8	29±0,7	260±7	58±0,8	850±50	13±0,3	0,84	27
6-V 4%	153±5	40±0,6	315±9	49±0,7	1180±50	11±0,2	1,05	27
7-V 6%	149±4	48±0,5	320±10	43±0.7	1180±60	9±0,2	0,99	27
8- V 8%	157±4	50±0,6	320±10	41±0,8	1060±50	9±0,3	1,00	27

It may be concluded using the obtained results that doping by chromium and vanadium give different results determined by different inter-atom bonds, so the electron density must change in different ways. It may be seen that the minimal electron density is achieved in the alloy containing 2% of vanadium and not less than 8% in chromium alloys. That must lead to different neighborhood of the nearest vicinity atoms resulting in different bonds and electron densities. Ternary alloys containing 9% of chromium as well as binary alloys doped by tungsten and molybdenum were studied in order for clearing the optimal content of the alloy.

The dependence of the positron average lifetime on the size factor is the most interesting and is shown in fig.2.

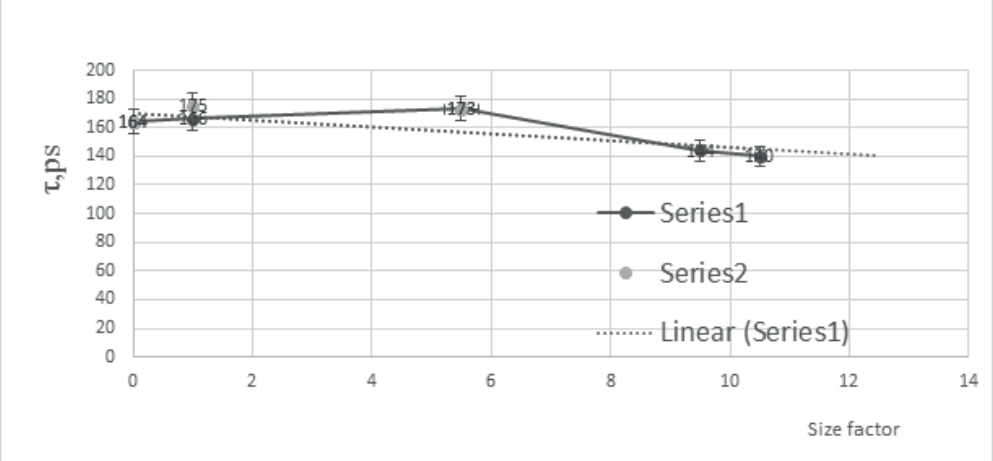

Figure 2: Dependence of the average positrons' lifetime on the size factor.

3. Discussion of results

Investigations of short-range ordering and changes of electron density in binary and ternary iron alloys. It was obtained that the average chromium concentration in the iron atom generalized coordination sphere in Fe-Cr alloys was higher than chromium content in the alloy independently on its concentration. That situation gives the possibility to declare the set of short range ordering (SRO) of short-range order (SR) in iron- chromium solid solutions with 2-8 at.% chromium content. It may be calculated that $\alpha < 0$, the module of α being increased with concentration reduction and tending to zero when chromium concentration increases. That means the appearance of disordered distribution in the solid solution (see fig.1).

The probability of detecting one chromium atom nearby iron atoms is higher for impurity concentrations of 2-8 at% of Cr than that determined by statistics, but the probability of finding no atoms in the vicinity of iron is less than statistical. That shows that the maximal number of Fe-Cr links and the minimal number of Cr-Cr links are formed, the last being typical for SRO – SR. (α <0). The number of surrounding by two atoms is reduced at increasing chromium concentration, but the probability of surrounding by three and four atoms within the generalized coordination sphere increases. It should be marked that at chromium concentration 8 at. % the gap between statistically calculated and experimental probabilities of one and two atoms in the generalized coordination sphere is reduced and the number of surroundings with three and four atoms is increased, this means the tendency of solid solution stratification

Another picture is observed for Fe-V system. The probability of finding one atom in the vicinity of iron is higher and probability of finding no atoms is lower than statistical provided 2.26 at.% of V. So we observe SRO of SR type like that in iron (the SRO parameter is -0.17). The character of atoms distribution in the nearest coordination sphere is changed and the number of iron atoms without vanadium atoms in the nearest coordination sphere is increased provided increasing the vanadium concentration up to 4,75 at.%. Thus the number of Fe-V links is reduced and the number of V-V links increases, the last being typical for SS ($\alpha > 0$). It is resulted in changing the short-range ordering parameter sign at high concentrations of V and tting the SRO SS type, the parameter changing being heterogenic. It is nearby zero for 8% at. of V and is nearly homogeneous and disordered.

The positron annihilation experiments show the most significant changes provided doping by 2% of V. In 9% Cr ternary alloys with Mo and W this impurity is the most significant, V being the main in the ternary alloy Fe-Cr-V.

4. Conclusions

1. Model Fe-Cr and Fe-V (2-8%) alloys were studied by methods of Mossbauer spectroscopy and positron annihilation. Regions of short-range ordering and short-range stratification were determined. It was shown that only short-range ordering exists in alloys containing chromium.
2. It was shown that in ternary alloys with chromium content 9% this doping is the most significant.

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