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MODELLING AND EXPERIMENTAL MOSSBAUER SPECTRA OF SOLID SOLUTION FE(SN)

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The Fe-Sn binary system is characterized by the solubility of Tin in γFe and αFe, as well as the presence of regions of existence of various intermetallic compounds on the state diagram with an increase in temperature [1]. The solubility of Sn in α-Fe is maximal (9.2% at.) at 900°C and decreases to 3.2% at. Sn (at 600°C).

In a solid solution of α-Fe(Sn), there are 8 neighboring atoms in the nearest environment of the Fe atom. If we assume that Sn atoms are equally likely to replace the positions of Fe atoms from the nearest environment, then we can calculate the probability of the appearance of *m* Sn atoms in the nearest environment of the Fe atom using the binomial distribution

$$P(m; C_{Sn}) = \frac{8!}{m!(8-m)!} C_{Sn}^{m} (1 - C_{Sn})^{8-m}, \quad (1)$$

At the same time, each configuration of the nearest environment corresponds to its own partial spectrum. The substitution of an Iron atom for a Tin atom leads to a decrease in the hyperfine field. In [2], the changes in the hyperfine magnetic field and isomeric shift were determined when one Fe atom was mixed with an Sn atom in the first coordination sphere of an Iron atom in a solid solution at different impurity concentrations in the solution. There is a average decrease in the hyperfine field by 22.15 ±0.14 kOe.

Using the MSTools software package [3], the Mossbauer spectra of Fe nuclei were modeled according to the method [4] when the atoms of Iron atoms were replaced by impurity atoms. At the same time, the change ΔH=22 kOe is accepted. The relative intensities I(*m*) of all partial spectra were calculated for solid solutions of Fe-2.1% at Sn, Fe-2.5% at Sn, Fe-5% at Sn, Fe-7.8% at Sn. Using the technique [5], the Mossbauer spectra of a solution of α-Fe(Sn) with different concentrations of Sn atoms were modeled (Fig.1).

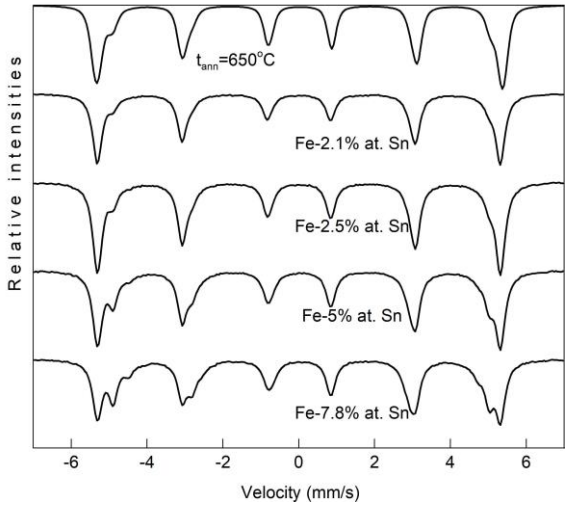

Fig.1. Comparison of the partial spectrum of a solid solution α-Fe(Sn) and the simulated spectra

Figure 1 shows the partial spectrum of the solid solution α-Fe(Sn) separated from the experimental spectrum of the layered system Sn(4 μm)-Fe(10 μm) after annealing at 650°C for 5 hours. Comparison of experimental spectra with simulated spectra shows a good correlation.

REFERENCES

[1] N.P. Lyakishev, Diagrams of the State of Double Metal Systems. Moscow: Mashinostroenie, 1997.
[2] I. Vincze, and A.T. Aldred, Phys. Rev. B, vol.9. no 9. p.3845, 1974.
[3] V.S. Rusakov, Mossbauer spectroscopy of locally inhomogeneous systems. Almaty, 2000.
[4] A.K. Zhubaev, T.S. Mukhanbetzhan and S.K. Yerezhepova, IOP Conf. Series: Journal of Physics: Conf. Series, 1281, 012097, 2019.
[5] A.K. Zhubaev, and B.Zh. Suleimanov, Izvesia vuzov. Fizika, vol.61, no 8/2, pp.151-154, 2018.