

SHORT-RANGE ORDER IN Fe-5 at.% Re ALLOY

V. M. Silonov and L. Enkhtor

The method of diffuse scattering of X-rays was used to establish the existence of a short-range order in the Fe-5 at.% Re alloy and to determine its parameters.

The short-range order in the arrangement of atoms of the components of a solid solution is a fundamental phenomenon. It has been established more than in 60 systems [1], among which, however, iron-based solid solutions are few in number despite the fact that they have found wide practical application. For example, the short-range order has been studied only in bcc Fe-Al, Fe-Mo and Fe-W alloys and in fcc Fe-Pt, Fe-Pd and Fe-Ni alloys. Since the data on the short-range order are used in the production of new precision alloys and in the analysis of anomalous changes in their physical properties, the extension of the range of bcc iron-based alloys becomes important. The goal of the present work is to establish the fact of the existence of a short-range order in the iron-rhenium system.

A sample of the Fe-5 at.% Re alloy was smelted from pure charge materials in the atmosphere of pure argon and subjected to remelting upon mixing by a magnetic field. The specimen was ground on emery paper with a gradual decrease of the grain size and polished on diamond powder paste to produce a mirrorlike surface.

The intensity of X-ray diffuse scattering of (XDS) was measured on an X-ray diffractometer (Fe K_{α} -radiation, a plane monochromator—a silicon single (111) crystal). Recording was made by means of a scintillation counter BDS-6 (3-4% accuracy).

The radiation intensity scattered by the specimen was converted to electron units by normalizing them to the intensity scattered by molten quartz. Then, from the XDS intensity, we subtracted the intensity of scattering by air and the intensities of Compton and double Bragg scattering according to the procedure described in the literature [2]. The XDS intensity minus the secondary components was written in the form

$$J_i(x_j) = nC_A C_B (f_A - f_B)^2 \sum_{i=0}^{i_{\max}} \alpha_i \left[C_i \frac{\sin q_j r_i}{q_j r_i} + E_i(x_j) + F_i(x_j) \right], \quad (1)$$

where n is the number of atoms in the unit cell; C_A and C_B are the concentrations of the alloy components; f_A and f_B are the form factors of atoms of the components with account taken of the corrections $\Delta f'$ and $\Delta f''$ for the anomalous dispersion; $x_j = a q_j / (2\pi)$; $q_j = 4\pi \sin \theta_j / \lambda$; a is the crystal lattice parameter; λ is the wavelength of X-radiation; θ_j is the Wulf-Bragg angle for a j th experimental point; α_i and C_i are, respectively, the short-range order parameter and the coordination number on the i th coordination sphere; $E_i(x_j)$ and $F_i(x_j)$ are, respectively, the modulating functions of the linear and quadratic size effects. In the Born-Bagbie model the functions $E_i(x_j)$ and $F_i(x_j)$ depend on the ratio of the moduli of elasticity C_{12}/C_{11} and C_{44}/C_{11} and on the concentration derivative $\beta = \frac{1}{V} \frac{\partial V}{\partial C_B}$ in the following way:

$$E_i(x_j) = -2[f_A(x_j) - f_B(x_j)] < f(x_j) > nC_A C_B \beta I_1(i, x_j), \quad (2)$$

©1998 by Allerton Press, Inc.

Authorization to photocopy items or personal use, or the internal or personal use of specific clients, is granted by Allerton Press, Inc. for libraries and other users registered with the Copyright Clearance Center (CCC) Transactional Reporting Service, provided that the base fee of \$50.00 per copy is paid directly to CCC, 222 Rosewood Drive, Danvers, MA 01923.

$$F_i(x_j) = \langle f(x_j) \rangle^2 n C_A C_B \beta^2 I_2(j, x_j), \quad (3)$$

where V is the volume of the unit cell; $\langle f(x_j) \rangle = C_A f_A + C_B f_B$ is the average atomic factor of the alloy components.

Katsnelson et al. [3] have tabulated the functions $I_1(i, x_j)$ and $I_2(i, x_j)$ for various sets of the ratios C_{12}/C_{11} and C_{44}/C_{11} . The values of the elastic constants of the Fe-5 at.% Re alloy calculated through the use of a model potential [4] according to Leibfried [5] are $C_{11} = 24.9 \times 10^{10}$, $C_{12} = 14.7 \times 10^{10}$ and $C_{44} = 12.2 \times 10^{10}$ N/m².

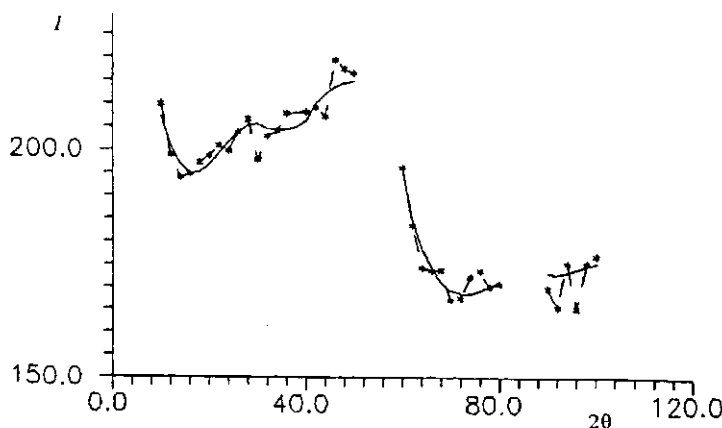


Fig. 1

Experimental (stars) and synthesized (solid line) XDS curves for Fe-5 at.% Re alloy (the intensity I is in electron units, the slip angle 2θ is in degrees).

From the results of measurements of the XDS intensity of a solid solution of Fe-5 at.% Re (see Fig. 1) we can see that the curve of the dependence of XDS on the slip angle 2θ of the specimen has no diffusion maximum characteristic of concentrated solutions. In order to verify the fact of the existence of a short-range order, it is necessary to perform qualitative and quantitative analyses of these data.

Numerical calculations of the short-range order parameters were performed by means of the least-squares method. It is known that these parameters determined from the XDS may depend on the concentrations of the components C , the Debye temperature T_D and on the parameter of static displacements β . Therefore, we first refined the values of C , T_D and β and then calculated the short-range order parameters which were then used to construct the synthesized curve of the XDS intensity and to calculate the sum of the rms deviations. The minimum value of the sum of the rms deviations found by varying the values of C , T_D and β appeared to correspond to the following values: $C = 5$ at.% Re, $T_D = 595$ K, $\beta = 0.05$. The 5 at.% Re concentration found by the XDS method coincides with the concentration in the weighed sample. The value of the Debye characteristic temperature of the alloy significantly exceeds the Debye temperature of iron (445 K). An analogous rise of T_D that occurs upon alloying iron with tungsten has been reported by Katsnelson et al. [6] and by Il'ina et al. [7]. It should be noted that the rise of T_D reported by Il'ina et al. [7] was found from temperature measurements of the intensity of structural reflexes. The value of the parameter of static displacement β was found to be substantially lower than that calculated from the dependence of the crystal lattice parameter on the concentration.

The calculated short-range order parameters on the first four coordination spheres of the Fe-5 at.% Re alloy are equal to -0.02 , 0.03 , -0.005 and 0.01 . The alternation of the signs revealed is characteristic of solid solutions with a short-range order.

In order to estimate the reliability of the values of concentration of the components C , the Debye temperature T_D , the displacement parameter β and of the short-range order parameters α_i , we calculated the synthesized XDS intensity curve $I_{\text{syn}}(2\theta)$ (see Fig. 1) which was then compared with the experimental $I_{\text{exp}}(2\theta)$ curve. The values of $I_{\text{syn}}(2\theta)$, apart from the contributions of the Laue, thermal, Compton and double Bragg scatterings (which depend on the concentrations of the components and the Debye

temperature), also include the contribution due to the effects of static displacements and short-range order. From Fig. 1 we see that the experimental and synthesized XDS intensity curves obtained for the Fe-5 at.% Re alloy are close to each other.

Thus, we have established the existence of a weak short-range order in the Fe-5 at.% Re alloy.

REFERENCES

1. V.I. Iveronova and A.A. Katsnelson, *Short-Range Order in Solid Solutions* (in Russian), Moscow, 1977.
2. V.M. Silonov and L. Enkhtor, *Fiz. Met. Metalloved.*, vol. 80, no. 5, p. 79, 1995.
3. A.A. Katsnelson, O.V. Kris'ko, V.M. Silonov, and T.V. Skorobogatova, *Dep. VINITI*, no. 4751, Moscow, 1983.
4. A.O.E. Animalu, *Phys. Rev.*, vol. B8, no. 8, p. 3542, 1973.
5. G. Leibfried, "Gittertheorie der mechanischen und thermischen Eigenschaften der Kristalle", in: *Handbuch der Physik*, vol. 7, part 2, Springer-Verlag, Berlin, Heidelberg, New York, 1955.
6. A.A. Katsnelson, V.M. Silonov, and Abu Al' Shamlat Salama, *Vestn. Mosk. Univ. Fiz. Astron.*, no. 5, p. 66, 1994.
7. V.A. Il'ina, V.K. Kritskaya, G.V. Kurdyumov, et al., *Fiz. Met. Metalloved.*, vol. 4, no. 3, p. 417, 1957.

11 October 1996

Department of Solid-State Physics