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Abstract

Full Text

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FEATURES OF DIFFUSE X-RAY SCATTERING AT THE ZONE STAGE OF AGING OF THE AlAg ALLOY

(Presented by Academician G. V. Kurdyumov on 29 IV 1969)

Experimental data are presented on diffuse scattering (d.s.) of X-rays by AlAg single crystals in the vicinities of all reciprocal-lattice nodes accessible for Cu K_{α} radiation at the zone stage of aging of this alloy.

Fig. 2. Projections of sections of the d.s. region by the Ewald sphere onto the $X^{*}OY^{*}$ plane of the reciprocal lattice. The X^{*} axis is parallel to the nodal line $[H, K, L]$; the Z^{*} axis is parallel to the axis of rotation of the crystal, and the Y^{*} axis is perpendicular to it; $a, ,$—AlAg 40%; —AlAg 20%; φ—the angle between $[H, K, L]$ and the direction to the given point of the d.s. region.

AlAg single crystals (20 and 40 wt.% silver) were grown by the deformation-annealing method. The specimens were annealed at 550° for 6 h, quenched in ice water, and then, in order to enhance the intensity of the d.s. effects, tempered for 10 min at 150°.

The d.s. was studied by the crystal-rotation method (^{1}). From series of X-ray diffraction photographs (Fig. 1), taken in the vicinities of the nodes under investigation, the regions of diffuse scattering (d.s.r.) were constructed (Fig. 2) by the method described in (^{2}).

Let us consider the principal features of the O.D.S.

1. In the vicinity of all investigated reciprocal-lattice nodes of the O.D.S., alongside the trivial isodiffuse surface (i.s.) of zero intensity O_2, there are

two more i.s. of reduced intensity—O_1 and O_3. Between them the intensity of the D.S. does not differ appreciably from the background.

2. These i.s. divide the O.D.S. into two subregions: I and II. Subregion I has a shape that does not differ from spherical; its center is close to the corresponding reciprocal-lattice node of the matrix, and its diameter does not exceed 0.015 $\mathring{A}^{-1}$. The scattering intensity in subregion I is considerably higher than in subregion II and increases sharply on approaching the node.
3. The i.s. O_2 and O_3 in the vicinity of the nodes (111) and (200) have a symmetry that does not differ appreciably from spherical. In the vicinity of distant nodes the symmetry of these surfaces (and of the O.D.S. themselves) is axial; the axis of symmetry is the nodal line $[H, K, L]$. The shape of these surfaces is close to elliptical. Table 1 gives the dimensions of their semiaxes.

Table 1

Nodes (H, K, L)		(111)	(200)	(220)	(222)	(311)	(400)	(331)	(420)	(422)
Dimensions of the semi-axes of i.s. O_2 ($\mathring{A}^{-1}$)	a	0.021	0.0222	0.021	0.021	0.021	0.022	0.018	0.023	0.021
Dimensions of the semi-axes of i.s. O_2 ($\mathring{A}^{-1}$)	c	0.021	0.022	0.021	0.021	0.021	0.028	0.021	0.027	0.030

Note. The mean diameter of the zones, calculated from the values of the semiaxis a, is 70 Å.

4. The distribution of D.S. intensity in subregion II at distant nodes depends on the angle φ (Fig. 2a). At $\varphi = 0$ and 180° (and values close to them) it is practically equal to zero, while at $\varphi = 90°$ it is maximal. At the

Series of X-ray diffraction patterns. Vicinities of nodes: a –(111), b –(220), c –(422). The appearance of the extraspots is reproduced schematically. The arrows indicate the direction toward the primary beam (p.b.); $\Delta\alpha$ is the angle of rotation of the crystallite from the position at which the Ewald sphere passes exactly through the node of the reciprocal lattice.

Figure 2: Series of X-ray diffraction patterns. Vicinities of nodes: a –(111), b –(220), c –(422). The appearance of the extraspots is reproduced schematically. The arrows indicate the direction toward the primary beam (p.b.); $\Delta\alpha$ is the angle of rotation of the crystallite from the position at which the Ewald sphere passes exactly through the node of the reciprocal lattice.

node (220) the zero value of the intensity is observed only near $\varphi = 0°$, whereas near $\varphi = 180°$ the intensity differs appreciably from zero. In this connection it is expedient to consider two further D.S. subregions (III and IV), in which the intensity is appreciably reduced.

5. Alloys with 20 and 40 wt.% silver have practically identical O.D.S. (Fig. 2c, d); the difference between them consists only in the fact that the D.S. intensity in the second case is somewhat higher.

Let us discuss possible explanations of the features of the D.S. A comparison of electron-microscopic (^{3}, ^{4}) and x-ray ($^{5-7}$) data makes it possible to draw the unambiguous conclusion that the principal contribution to the D.S. is made by zones, or, more precisely, subregion II of the D.S. represents a shape effect and the finite dimensions of these zones. The spherical symmetry of the outer i.s. O_2 in the vicinity of near nodes indicates the spherical shape of the zones. Thus, the elongation of the O.D.S. at distant nodes noted above cannot be explained by the shape of the zones.

There is no single opinion regarding the origin of the i.s. O_3. In (^{8}) a three-phase model of this alloy was proposed (unprecipitated solid solution, zones, and a transition layer depleted in the alloying component). A zone together with the transition layer surrounding it will constitute a disturbance ("hole" (^{9})) in the matrix. The D.S. produced by such an alloy will be composed of scattering by zones and by holes (^{9}, ^{10}). Since the radii of the zones and holes are not the same, and the signs of their scattering amplitudes are opposite, interference of these two types of scattering will produce an i.s. of reduced intensity O_3.

However, analysis of the integral D.S. intensity in the vicinity of the zero node (^{7}) shows that the AlAg alloy at the zone stage of decomposition is not three-phase but two-phase: it consists of zones and an almost equilibrium phase purified of the alloying component. Such a model of the alloy, without additional refinements, encounters difficulties in explaining the origin of the i.s.

Fig. 1. Series of X-ray diffraction patterns. Vicinities of nodes: **a** –(111), **b** –(220), **c** –(422). The appearance of the extraspots is reproduced schematically. The arrows indicate the direction toward the primary beam (p.b.); $\Delta\alpha$ is the

angle of rotation of the crystallite from the position at which the Ewald sphere passes exactly through the node of the reciprocal lattice.

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O_3. In fact, if its origin is explained only by the correlation of scattering by zones, then it is natural to expect that the correlation function should depend substantially on the initial concentration of the alloy, and consequently alloys of different composition should have noticeable differences in the diffuse-scattering regions, which is not observed experimentally.

The difficulties in interpreting the diffuse-scattering region O_3 can be overcome if one assumes that the AlAg alloy at the zone stage is two-phase, but that each zone is surrounded by a transition layer in which the vacancy concentration is substantially higher than the equilibrium value ($\sim 7\%$). The possibility of vacancy retention by zones was pointed out in (11–14). Physically such a situation is quite understandable if one takes into account: a) after transfer from the region of the homogeneous state to a lower temperature, the alloy is supersaturated with vacancies, which are subsequently removed from the solution; b) the formation and growth of zones are associated with a vacancy mechanism of diffusion (15, 16); c) the zones themselves may be effective vacancy sinks. Owing to the supersaturation with vacancies, the transition layer will be physically distinct; its structure factor will differ from the structure factor of the matrix, and, as a consequence of this, the diffuse-scattering region O_3 will appear.

Let us turn to consideration of the possible nature of the regions of reduced intensity III and IV. The fact that at the node (220) only one of them is observed indicates the different nature of regions III and IV.

A natural explanation of the origin of region III is the following. Suppose that the lattice parameters of the matrix and of the zone differ by an amount Δa^*; then the centers of the interference maxima of the diffuse scattering by the zones and by the holes will be displaced relative to one another. As a consequence, the symmetry of the diffuse-scattering region will become axial, the extent of the diffuse-scattering region along the nodal straight line will increase with increasing indices of the node, and, because of the superposition of the interference maxima considered above, displaced relative to one another, a region of reduced intensity will appear.

The interpretation of diffuse-scattering region O_1 and of regions I and IV is somewhat more complicated. They are associated with the superposition, on the diffuse scattering considered above, of scattering on defects in the matrix arising from its coherent bonding with the zones (10), and also on defects of the transition layer created by vacancies. This is indicated by the sharp increase in diffuse-scattering intensity in region I as the reciprocal-lattice node is approached, and by the dependence of the distribution of diffuse-scattering intensity on the angle φ.

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* An exact determination of Δa is difficult because of the position of the diffuse-scattering regions considered above. An estimate of Δa from the difference in the lengths of the semi-axes gives a value of ~ 0.04 Å.

Note: Figure translations are in progress. See original paper for figures.

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