New Approach to Short-Range Ordering in GP(2) Zones in Al-3.82wt.%Cu Alloy

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Synopsis

X-ray diffuse scattering intensity measurement has been carried out for the Al-3.82%Cu single crystal in which GP(2) zones are found. The two dimensional equi-intensity contour maps in h1 h2 0 plane are obtained from surveying around several reflections. The diffuse intensity around 2 1 0 reflection, which shows a cross like streak, is carefully examined. Warren-Cowley short-range order parameters, a1, are estimated from the diffuse intensities around 2 1 0 reflection. The component of the intensities coming from atomic displacements was subtracted from the total diffuse intensity. It is found that the equi-intensity contours after the correction of the atomic displacements shows an anisotropic distribution and the GP(2) zone is an ellipsoid with a modified layer structure.

1. Introduction

There have been many investigations on GP(2) zones in Al-Cu alloy. The first investigation was carried out by Guinier [1], and he has proposed the model of the zones which are constructed of the ordered four layers' structure made of aluminium atomic layer and three copper rich layers[one of them seems to be 100at.%Cu, the others 20 to 25at.%Cu]. Gerold[2] and Baur[3] have reported another model consisting of

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pure aluminium and pure copper layers to explain the X-ray diffuse intensity. By the observation of the diffraction contrast in electron micrographs of thin foil of Al-Cu alloy, Nicholson and Nutting [4] showed that the matrix lattice surrounding GP(2) zone is deformed. The layer structures of GP(2) zones has been also investigated using the two-beam lattice fringe technique [5, 6] and the weak-beam technique [7] of electron microscopy.

In this paper, the precise measurements of the x-ray diffuse scattering from GP(2) zones are presented to elucidate the short-range ordering of copper atoms in the zones. For this purpose, an atomic size effect in the X-ray diffuse intensity distribution around some symmetrical points in the reciprocal space has been considered by employing the same formula as those in Sparks [8] and Borie's [8,9] method of calculating short-range order parameters, $a_1$.

2. Short-range Ordering and X-ray Diffuse Scattering

The coherently scattered intensity from a binary alloy can be written as the sum of the intensity associated with the fundamental Bragg peaks, $I_F$, and the total diffuse intensity, $I_D$, where $I_D$ can be written as the sum of three terms

$$ I_D = N x_A x_B (f_A - f_B)^2 (I_{SRO} + I_{SE} + I_{TDS,H}). \quad \text{(1)} $$

Where $I_{SRO}$ is the scattering due to local order, $I_{SE}$ is the so-called size-effect term and $I_{TDS,H}$ is due to first order thermal diffuse and Huang scattering. $N$ is the number of atoms in X-ray irradiation, $x_A$ and $x_B$ the atomic fractions of components A and B, respectively, and $f_A$ and $f_B$ their atomic scattering factors. Each term can be expanded to a trigonometric series in electron unit.

$$ I_{SRO} = \sum_{1mn} \alpha_{1mn} \cos 2\pi (h_1 l + h_2 m + h_3 n). \quad \text{(2)} $$

$$ I_{SE} = \sum_{1mn} (h_1 x y_{1mn} + h_2 y y_{1mn} + h_3 z z_{1mn}) \sin 2\pi (h_1 l + h_2 m) $$

$$ + h_3 n) \quad \text{(3)} $$
The integers $l, m, n$ define a particular lattice site according to the relation in f.c.c. lattice

$$
\gamma_{lmn} = \frac{1a_1}{2} + \frac{ma_2}{2} + \frac{na_3}{2}
$$

where $a_1, a_2, a_3$ are the translational vectors of the cubic unit cell, and $h_1, h_2, h_3$ are the continuous coordinates in reciprocal space. The $\alpha_{lmn}$ (or $\alpha_i$) are the short-range order parameters defined by

$$
\alpha_{lmn} = 1 - \frac{p_{AB}}{p_{1mn}}
$$

where $p_{1mn}$ (or $p_{1i}$) is the probability of finding a B atom at the end of a vector $\gamma_{lmn}$ (or $r_i$, radius ith shell) when the origin is occupied by an A atom. Other Fourier coefficients are given by

$$
\begin{align*}
\gamma^X_{lmn} &= 2\pi [F_{AA}\langle X^A_{lmn} \rangle + F_{AB}\langle X^{AB}_{lmn} \rangle + F_{BB}\langle X^{BB}_{lmn} \rangle] \\
\delta^X_{lmn} &= -2\pi^2 [F_{AA}\langle (X^A_{lmn})^2 \rangle + F_{AB}\langle (X^{AB}_{lmn})^2 \rangle + F_{BB}\langle (X^{BB}_{lmn})^2 \rangle] \\
\epsilon^{XY}_{lmn} &= -4\pi^2 [F_{AA}\langle X^A_{lmn} Y^B_{lmn} \rangle + F_{AB}\langle X^{AB}_{lmn} Y^{AB}_{lmn} \rangle + F_{BB}\langle X^{BB}_{lmn} Y^{BB}_{lmn} \rangle]
\end{align*}
$$

where

$$
\begin{align*}
F_{AA} &= f_A^2 \left( \frac{x_A}{x_B} + \alpha_{lmn} \right) / (f_A - f_B)^2 \\
F_{AB} &= 2f_A f_B (1 - \alpha_{lmn}) / (f_A - f_B)^2 \\
F_{BB} &= f_B^2 \left( \frac{x_B}{x_A} + \alpha_{lmn} \right) / (f_A - f_B)^2
\end{align*}
$$

The definition of $\gamma_{lmn}^X, \gamma_{lmn}^Z, \delta_{lmn}^X, \delta_{lmn}^Z, \epsilon_{lmn}^{YZ}$ and $\epsilon_{lmn}^{ZY}$ are also analogous to the above mentioned Fourier coefficients. $X_{lmn}^{ij}$, $Y_{lmn}^{ij}$ and $Z_{lmn}^{ij}$ are the deviations of an i atom and j atom from their average positions. The averages $\langle X_{lmn}^{AA} \rangle$, etc. are taken for all i-j pairs separated by constant distance $(r_{lmn}^i - r_{lmn}^j)$.

It has been considered by Sparks [9] et al. that the term (4) has
little effects on $\alpha_{1mn}$ at the reciprocal points far away from the Bragg reflections.

3. Experimental Procedure

A conventional double axes X-ray spectrometer was used during this work. As the X-ray source MoKα₁ radiation monochromatized by a flat plate of LiF single crystal was employed. MoKα₂ component in MoKα radiation was cut off by knife edges of a divergent slit with 0.15 mm in width and 4 mm in height placed at a distance 50 mm from the monochromator. Scattered beam from a sample impinges into a scintillation counter through two slits with 0.3 mm and 1 mm in width respectively. The horizontal and vertical angular resolutions were estimated as 0.09° and 2.5° respectively. The received X-ray was counted through a single channel pulse height analyser to eliminate the components of $\lambda/2$ and $\lambda/3$. The intensity due to the harmonics could not be observed in the intensity profile around 1 0 0 reflection of Al-3.82wt.%Cu solid solution single crystal. The intensity measurement was carried out at 295 K. The stability of the X-ray source and of the counting electronics was checked many times by detecting the 1 0 0 diffuse scattering intensity during the measurement process.

99.996% purity aluminium and 99.996% copper were melted in a high purity Alumina crucible in atmosphere. After the ingot of 15 mm X 80 mm was hot-forged to 2 mm in thickness, the strip was cold-rolled to 0.6 mm in thickness. The single crystals were produced by the same strain annealing method as that of Hida et al [10]. The dimensions of the single crystal used for X-ray scattering intensity measurement were 5 mm in width, 0.6 mm in thickness and 12 mm in length. This crystal was homogenized at 775K and then quenched into iced water. After ageing of an hour at 353K and 24 hours at 433K, GP(2) zones were nucleated. The resistivity changes (see fig.1, curve A) are recognized as the formation of GP(2) zones [10, 11].

4. Results and Analyses

Figure 2 shows the observed equi-intensity contour map of diffuse scattering around 2 1 0 reciprocal point. The vectors $q// \ v$ and $q\perp \ v$ in the figure are the wave vector parallel and perpendicular to the re-
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Fig. 1 Changes of electrical resistivity during ageing at 433K in Al-3.82wt.%Cu alloy quenched from 775K. The intermediate heat treatment is 353K x 60 min. and 475K x 5 min. for curve A and B respectively.

Fig. 2 The diffuse scattering distribution from GP(2) zones, looking around (210) reflection in the h1 h2 0 plane. The black dots in the figure present the measurement points.
ciprocal lattice vector $\mathbf{G} = 2\mathbf{a}_1^* + \mathbf{a}_2^*$.  

The each black dot in the figure means the point, where the intensity was measured for 5 minutes at 295K. Two diffuse streaks belonging to [1 0 0] and [0 1 0] directions were detected. The asymmetric feature can be considered to depend on the size effect of the equation (3) in section 2. The diffuse intensities, caused by GP(2), around 1/2 0 0, 1 0 0, 1 1 0, 2 0 0 and 2 2 0 reflections were also measured. The equi-intensity contours of 100 counts per 5 minutes are shown in fig.3.

![Diagram of equi-intensity contours](image)

**Fig. 3** The equi-intensity (100 counts per 5 minutes) countors in $h_1 h_2 0$ plane.

The equation of diffuse intensity for f.c.c. crystal was written, provided $I_{TDS.H}$ is neglected as mentioned in section 2, as follows.

$$I_D = I_{SRO} + I_{SE} = \sum_{1mn} \sum_{1mn} \cos2\pi(h_1 l + h_2 m + h_3 n)$$

$$-\sum_{1mn} (h_1 y_1 + h_2 y_2 + h_3 y_3) \sin2\pi(h_1 l + h_2 m + h_3 n).$$

As it can be considered that all of $\alpha_{1mn}$ which belong to the ith nearest neighbour atoms are equivalent, that is to say, $\alpha_{1mn} = \alpha_{mnl} = \alpha_{nml}$
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\[ I_{SRO} = \sum_{i=1}^{\infty} a_i C_i (h_1 h_2 h_3) \]

where \( z_i \) is the coordinate number of the ith shell, for example, \( z_1 = 12 \) for the f.c.c. lattice. \( C_i \) is the sum of cosine terms. The measurement of intensity have been carried out in the reciprocal \( h_1 h_2 0 \) plane, and then the term \( I_{SRO} \) is consequently expressed as follows.

\[
I_{SRO} = a_0 + 12a_1 [(\cos \pi h_1 \cos \pi h_2 + \cos \pi h_1 + \cos \pi h_2)/3]
+ 6a_2 [(\cos 2\pi h_1 + \cos 2\pi h_2 + 1)/3]
+ 24a_3 [(\cos 2\pi h_1 \cos \pi h_2 + \cos \pi h_1 \cos \pi h_2 + \cos \pi h_1 \cos \pi h_2)/3]
+ 12a_4 [(\cos 2\pi h_1 \cos \pi h_2 + \cos \pi h_1 + \cos \pi h_2)/3]
+ 24a_5 [(\cos 3\pi h_1 \cos \pi h_2 + \cos \pi h_1 \cos 3\pi h_2 + \cos 3\pi h_1
+ \cos 3\pi h_2 + \cos \pi h_1 + \cos \pi h_2)/6]
+ 8a_6 [\cos 2\pi h_1 \cos 2\pi h_2]
+ 48a_7 [(\cos 3\pi h_1 \cos 2\pi h_2 + \cos \pi h_1 \cos 3\pi h_2 + \cos 2\pi h_1 \cos \pi h_2 + \cos 3\pi h_1 \cos \pi h_2 + \cos 2\pi h_1 \cos 3\pi h_2 + \cos \pi h_1 \cos 2\pi h_2)/6]
+ 6a_8 [(\cos 4\pi h_1 \cos 4\pi h_2 + 1)/3]
+ \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots 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On calculating the parameters by using the least squares method, the intensity contour around 210 reflection is used, because the Bragg scattering is absent at 210 point and also the effect of thermal diffuse intensity is considered to be enough small at the comparatively low indices h1 h2 0 [12]. It is also assumed that Compton modified scattering is almost constant in the region where the measurement is carried out. The contribution of the diffuse scattering from the matrix was subtracted as a flat background around 210 reflection. It is assumed that there is almost no contribution of the matrix to the diffuse intensity used on calculating ai.

The region where the intensity was measured around 210 reflection, h1 = 1.89 - 2.22 and h2 = 0.87 - 1.16, was divided into grids of Δh1 = Δh2 = 0.01 in width, and the region of h1 = 1.50 - 1.70 and h2 = 0.30 - 0.70 was divided into Δh1 = Δh2 = 0.02 in width. The intensities observed at 1420 points around 210 reflection employed as the I0 values, in equations (Sa) and (Sb).

The optimum α1 to α8 and γ1mn are calculating by the least squares method with the computer FACOM 230-38. The α0 must be determined experimentally by measuring the absolute intensity of diffuse scattering from zones as it had been obtained by Moss [13] for Cu3Au alloy. But α0 was normalized to be unity in the present work. The results obtained are tabulated in Table 1. It was found that there had been the stability of the solution in putting one to eight to the suffix i of ai. Figure 4 shows the short-range order parameters for α1mn on distance γ1mn.

In order to synthesize the diffuse intensity in two-dimensional reciprocal space, the α1mn α0 to α8, obtained from the above mentioned method were put into the equation (Sa). Figure 5 shows the diffuse intensity, where the size effects have been excluded. It is found that the equi-intensity contour has an anisotropy elongated to [100] direction around 100 reflection and to [010] direction around 210 reflection.
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Table 1

The optimum $\alpha_{1mn}$ and $\gamma_{1mn}$ calculated by the least squares method

<table>
<thead>
<tr>
<th>neighbour</th>
<th>l m n</th>
<th>$\alpha_{1mn}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1 1 0</td>
<td>0.023</td>
</tr>
<tr>
<td>2</td>
<td>2 0 0</td>
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</tr>
<tr>
<td>3</td>
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<td>7</td>
<td>3 2 1</td>
<td>0.014</td>
</tr>
<tr>
<td>8</td>
<td>4 0 0</td>
<td>-0.048</td>
</tr>
</tbody>
</table>

$\gamma_{110}^x = -0.229$ 
$\gamma_{110}^y = 0.077$ 
$\gamma_{011}^y = 0.403$ 

$\gamma_{020}^y = 0.117$

Fig. 4 The short-range order parameters $\alpha_{1mn}$ as a function of $r_{1mn}$. $\alpha_0$ is normalized to unity.
5. Discussion

The determination of the short-range order parameters is an interesting point of view in GP(2) zones. It is particularly important to estimate the reasonable lattice distortion in GP(2) zone for obtaining the short-range order parameters. In the first approximation, we took the size effect up to the second nearest neighbours. And then we preferred the tetragonal symmetry as the size effect of GP(2) zone to the cubic symmetry, because the standard deviation of the least squares method become small by adopting the tetragonal symmetry. The suitability of this approximation must be reflected in the diffuse intensity contour of fig. 5. It is important matter that the equi-intensity contour for which the size effects have been excluded has an anisotropy elongated to [0 1 0] direction around 2 1 0 reflection. After all, the problem lies in the application of $a_t$ which should be used for some sort of spherical zone [14]. In the case which we, however, make bold to apply the $a_t$ to even disk shaped GP(2) zones, characteristic of fluctuation of solute concentration in GP(2) zone will be reflected in atomic interaction or the correlation length which will be mentioned later.
It is reasonable that a given fluctuation of copper concentration in GP(2) zones exists in the direction not only of parallel but also of perpendicular to the disk shaped zone, considering the dumping oscillation of \(a_{1mn}\) versus \(r_{1mn}\) as in figure 4. That is to say, the GP(2) zone's layer structure constructed of layers of copper and of aluminium atoms would not be always an appropriate model. If the correlation function is simply assumed as

\[
\psi(\gamma, \gamma') + (A \exp(-|\gamma - \gamma'|/\Lambda))/|\gamma - \gamma'|
\]

where \(\Lambda\) is the correlation length, its Fourier transform gives the diffuse intensity as follows.

\[
I_{SRO} = \psi(q) = A / (\Lambda^{-2} + q^2)
\]

This shows that the diffuse profile is regarded as Lorentzian. The correlation lengths of the solute concentration obtained graphically from the relation, the inverse of the synthesized intensity versus the scattering wave vector \(q\) squared, are nearly 4.8 nm in length and 10 nm in diameter respectively as shown in figure 6.

![Diagram](image)

**Fig. 6** The inverse of the synthesized diffuse intensity \(I_{syn}\) as a function of wave vector \(q\) squared. The correlation length of a given fluctuation of Cu solutes in GP(2) zones are obtained from this function.
The diffuse scattering intensity synthesized from the values of $\alpha_{1mn}$ shows an anisotropy which satisfies the f.c.c. symmetry (see figure 5). This implies that the short-range order interaction in the system is anisotropic and GP(2) zone is an ellipsoids, which is somewhat different from the layer structure. If $\alpha_1$ is connected to a given elastically atomic interaction not to the probability function, it seems to be reasonable that GP(2) zone has the f.c.c. symmetry and a given anisotropy of the ellipsoid. Such a quality has been found for a dielectric, NiCr$_2$O$_4$ as an example [15].

Linear embryos of GP(2) zones may be formed in the matrix at the early stage of the phase transition. As the atomic interaction, however, occurs among the embryos, some of them have a chance to nucleate an ellipsoid of GP(2) zone by the attractive force among the embryos. The ellipsoidal nucleus may be related to the correlation length, $\Lambda$ corresponded to the phase of each zone. The stability of the nucleus of GP(2) zone will be discussed in terms of a phase motion partially reported by Frenkel et al [16] and Horovitz et al [17].

6. Conclusion

The optimum short-range parameter $\alpha_1$ and the symmetry of the tetragonality of GP(2) zones are calculated by the least squares method from the equi-intensity contour around 2 1 0 reflection of GP(2) zones. This implies that the short-range interaction in the system shows an anisotropy with the f.c.c. symmetry and the GP(2) zone is an ellipsoid, which has the modulated structure characterized by fluctuation of solute concentration. The GP(2) zone is different from the simple layer structure proposed before. The correlation lengths of solute concentration obtained from the diffuse scattering intensity synthesized from the value of $\alpha_1$ are nearly 4.8 nm in length and 10 nm in diameter respectively.

References

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