

Acta Cryst. (1960). **13**, 60

A note on the structure of Guinier–Preston zones in Al–Cu alloys. By KAREL TOMAN, *The Institute of Technical Physics, Prague 5, Cukrovarnická 10, Czechoslovakia*

(Received 3 September 1959)

In recent years several authors have attempted to refine the model of G.P. zones in Al–Cu alloys. Gerold (1954) calculated the displacements of atomic planes (001) in the G.P. zone on the assumption that the zone contains one copper-rich (001) plane only. In a later paper Toman (1957) tried to calculate not only the displacements but also the concentrations of copper in different (001) planes of the G.P. zone. His calculation, based on the least-squares treatment of the *relative* diffuse-intensity distribution in streak [00 l], did not contain any assumptions about the distribution of copper in the zone. The result was rather different from the Gerold's. The copper atoms were found not to be concentrated in the central atomic plane only, but a distribution of copper among several (001) planes was found. The displacements of (001) planes of the zone were found to be much less important than in Gerold's model.

In a recent paper Gerold (1958) expresses doubt about Toman's model, especially the distribution of copper atoms. This arrangement of copper atoms would lead, according to Gerold, to stresses sufficient to break the coherency of the zone with the matrix.

The basis for Toman's calculation was the *relative* diffuse intensity on which the intensity of the direct beam and matrix Bragg reflections (000), (002), (004) was superposed. This makes the determination of diffuse intensity in these ranges of streak rather uncertain and it is possible that errors in extrapolation and interpolation might influence the result unfavourably. It was therefore desirable to make use of another method to ascertain which model is correct.

A suitable method can be based upon the *absolute* measurement of the diffuse intensity in the streak not too close to the diffuse maxima on the reldrod [00 l]. In order to obtain the same diffuse intensity at this relp, more copper atoms in zones are necessary according to Toman's model than according to the Gerold's, where the atomic plane displacements are more important.

For a symmetrical Bragg arrangement with the main plane—the plane containing the primary and reflected beams—horizontal, the power P diffracted on the G.P. zones and entering the G.M. counter (whose entrance slit has the width $\Delta \ll 2\lambda R/(Na \sin \theta)$ and the height $\eta > 2\lambda R/Na$) is

$$P = P_0 K \frac{1}{2} n N F^2(l) \sin^2 \pi N k / \sin^2 \pi k .$$

R is the crystal-to-slit distance, N is the dimension of a zone (supposed square) measured in a of the matrix (4.05 Å) as a unit, and n is the number of zones in 1 cm.³ of the alloy. The constant $K = B(e^2/mc^2)^2 \Delta \lambda / (2\mu Ra)$, where B is the polarisation factor and μ is the linear absorption coefficient. The function $F(l)$ contains the structure parameters of the zone

$$F(l) = 2f_{ai} [m_0 + 2 \sum_1^{\infty} ((1 + m_i) \cos \pi \alpha_i l - \cos \pi m_i l) ;$$

here m_i is the atom fraction of copper in the i th plane (001) of the zone, α_i is the distance of the i th plane

of the zone from the center of the zone (0th plane) and n_i is the distance of the i th (001) plane in the undisturbed lattice from the center of the zone. (Both, α_i and n_i are measured in $a/2$ as a unit of the distance.)

The power $P_{\max.}$ corresponding to the maximum setting of crystal for constant l is

$$P_{\max.} = P_0 K \frac{\mathcal{N}}{6} \mathcal{F}^2(l) N \quad (1)$$

where \mathcal{N} is the number of Cu atoms segregated in zones in 1 cm.³ and

$$\mathcal{F}^2(l) = F^2(l) \left/ \sum_{-\infty}^{\infty} m_i . \right.$$

In the experimental part of this work the cross-profile of the diffuse streak [00 l] for constant $l = 2.5$ was measured. The crystal used (4 wt.% Cu) was aged at room temperature for 3000 min. The measured $P_{\max.}$ was 459 ± 13 imp./min. and N was 6.3. The incident power P_0 was determined by making use of the measurement of the radiation diffracted from a plate made of amorphous selenium. $P_0 = 1.17 \cdot 10^8$ imp./min. was found. The constant K involving the geometrical constants of diffractometer is $3.02 \cdot 10^{-30}$. $\mathcal{N} \mathcal{F}^2$ calculated according to (1) is $1.24 \cdot 10^{24}$.

In the Table 1 we show \mathcal{F}^2 calculated for different models of the G.P. zone.

Table 1

Model	\mathcal{F}^2	\mathcal{N}
Gerold type $\alpha_1 = 0.900$	781	$1.60 \cdot 10^{21}$
Gerold type $\alpha_1 = 0.800$	2130	$0.59 \cdot 10^{21}$
Toman type $\sum_{-\infty}^{\infty} m_i = 0.97$	11	$1.14 \cdot 10^{23}$
Toman type $\sum_{-\infty}^{\infty} m_i = 1.86$	7	$1.79 \cdot 10^{23}$

The first model is taken from Gerold (1954, the 6th model); the second is derived from the first by doubling all displacements. The third and fourth are taken from Toman (1957—Table 2, 1st and 3rd column). The \mathcal{N} calculated are based on the experimentally determined value $\mathcal{N} \mathcal{F}^2 = 1.24 \cdot 10^{24}$.

The number of all copper atoms in the alloy of our composition is $1.03 \cdot 10^{21}$ in 1 cm.³; this represents the highest limit for \mathcal{N} . It is evident that all Toman-type zones need an impossible number of copper atoms to explain the observed diffuse intensity. The Gerold models show an essentially better agreement especially when the atomic plane displacements are increased.

References

- GEROLD, V. (1954). *Z. Metallk.* **45**, 599.
 GEROLD, V. (1958). *Acta Cryst.* **11**, 230.
 TOMAN, K. (1957). *Acta Cryst.* **10**, 187.