

angles. Although a somewhat similar arrangement occurs in *p*-aminophenol (Brown, 1951) in which distances of 2.83, 3.13 and 3.18 Å are found at considerably more favourable angles than those shown by hydroxylamine, it seems best to us to leave one hydrogen atom of NH₂OH uninvolved in hydrogen bonding and to assume such bonds only in the 2.74 and 3.07 Å distances.

It is of interest to ask what is the configuration of the molecule, and where are the hydrogen atoms. Considerable effort was made to see if our data were capable of yielding any direct information, with results described in detail elsewhere (Meyers, 1955). In summary, a detailed examination of structure factors, not given here, for three different possible arrangements of hydrogen bonds

- (a) O₁-H...N₂ = 2.74 Å, N₁-H...O₃ = 3.07 Å;
 (b) N₁-H...O₂ = 2.74 Å, O₁-H...N₃ = 3.07 Å;
 (c) N₁-H...O₂ = 2.74 Å, N₁-H...O₃ = 3.07 Å

yielded, respectively, values of $R = 0.16, 0.16$ and 0.17 for all observed reflections, thus supplying no direct evidence regarding the hydrogen positions. Nevertheless, all three of these possible models lead to NH₂OH molecules which, if isolated from the crystal, would have very nearly the *trans* configuration of symmetry C_s . This result lends some support to a model of C_s symmetry in the gas phase, assumed by Giguère & Liu, in so far as extrapolations of from solid to gas are valid.*

* While normally the same geometry occurs in the solid and gas, the binding forces in the solid are occasionally sufficient to produce some modifications of orientation about

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single bonds. In hydrazine an eclipsed form was found. Presumably the singly eclipsed form of hydrazine is only a small deviation from the geometry presumed to exist in the gas phase as indicated in the first drawing of Fig. 1 in the paper by Collin & Lipscomb (1950).

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The Structure of Guinier-Preston Zones. I. The Fourier Transform of the Diffuse Intensity Diffracted by a Guinier-Preston Zone

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The expression for the diffuse intensity diffracted by the Al-Cu alloy with Guinier-Preston zones is derived as a trigonometrical series with coefficients dependent on the structure. It is shown that the coefficients can be determined with the aid of the Fourier transform of the integrated diffuse intensity in relrod (00 l). From these coefficients it is possible to deduce the features which are characteristic of the structure of Guinier-Preston zones.

1. Introduction

The anomalous diffraction effects in Al-Cu and Al-Cu-Mg alloys in the age-hardened stage are well known (Preston, 1938; Guinier, 1938). They corre-

spond approximately to diffraction by a two-dimensional lattice and they are usually connected with the formation of two-dimensional copper-rich regions in the (001) planes of the matrix. The asymmetrical intensity distribution around the reciprocal lattice

points can be explained by distortions in the crystal in the neighbourhood of Guinier-Preston (G.-P.) zones due to the difference in atomic sizes of Cu and Al (Guinier, 1952). The data in the literature concerning the structure of G.-P. zones are based on calculations of scattered intensity on adequately chosen models and their comparison with the experimentally determined variation of intensity.

In this paper it is shown that the structure of G.-P. zones can be determined directly by interpretation of the Fourier transform of the diffuse intensity on the basis of a quite general model (Fig. 1).

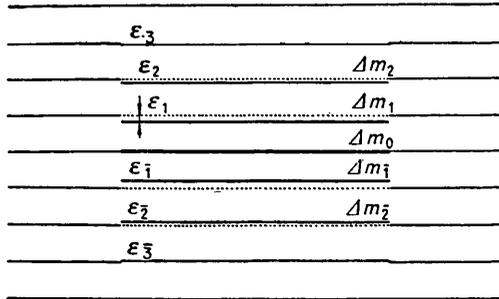


Fig. 1. Model of G.-P. zone used as a basis for the interpretation of scattered diffuse intensity.

We suppose a G.-P. zone to be formed by rectangular atomic planes (001), characterized by $\Delta m_r \neq 0$ and $\varepsilon_r \neq 0$. Here Δm_r is the difference between the copper-atom fraction in the r th plane of the G.-P. zone and that in the matrix; ε_r is the displacement of the r th plane of the G.-P. zone from its position in the matrix and this is measured in $\frac{1}{2}a$ as a unit of distance. The lattice of the G.-P. zone is face-centred cubic and the distribution of copper atoms within each atomic plane is assumed random. The phase relations between the individual G.-P. zones are neglected.

2. Intensity calculation

The amplitude of radiation diffracted by a G.-P. zone and by its neighbourhood is given by the expression (Guinier, 1952).

$$A = \sum_{(M)} f_A \exp(-2\pi i \mathbf{B} \cdot \mathbf{x}) - \sum_{(Z)} f_A \exp(-2\pi i \mathbf{B} \cdot \mathbf{x}) + \sum_{(Z)} f_B \exp(-2\pi i \mathbf{B} \cdot \mathbf{y}). \quad (1)$$

The first summation is taken over all atoms in the whole crystal including the G.-P. zone, the second and the third over the G.-P. zone only. \mathbf{x} and \mathbf{y} are the position vectors of atoms at the lattice points of the undistorted crystal and in the crystal with distortions respectively, f_A is the average atomic factor of atoms outside the G.-P. zone, f_B is the atomic factor of atoms within the G.-P. zone.

Let us begin with the calculation of the last term of the right-hand side of equation (1):

$$\sum_{(Z)} f_B \exp(-2\pi i \mathbf{B} \cdot \mathbf{y}) = \sum_{-\infty}^{+\infty} \Phi_r(h, k) M(r) \exp[-\pi i l(r + \varepsilon_r)], \quad (2)$$

where h, k, l are continuous variables and $\Phi_r(h, k)$ is the Fourier transform of the r th plane in the G.-P. zone. We define the function $M(r)$ as follows:

$$M(r) = \exp(-2\pi i h), \quad r = 2n; \\ M(r) = \exp(-\pi i h), \quad r = 2n + 1.$$

Then we have

$$\Phi_r(h, k) = [f_A + (f_{\text{Cu}} - f_{\text{Al}}) \Delta m_r] \times \{1 + \exp[-\pi i(h + k)]\} \sum_{0,0}^{N_1-1, N_2-1} \exp[-2\pi i(hu + kv)],$$

where f_{Cu} and f_{Al} are the atomic factors of Cu and Al atoms respectively, and N_1 and N_2 are the dimensions of the G.-P. zone in the [100] and [010] directions. For simplicity we will write $\alpha_r = (f_{\text{Cu}} - f_{\text{Al}}) \Delta m_r$; thus

$$\Phi_r(h, k) = (f_A + \alpha_r) \{1 + \exp[-\pi i(h + k)]\} \times \frac{\exp(-2\pi i h N_1) - 1}{\exp(-2\pi i h) - 1} \frac{\exp(-2\pi i k N_2) - 1}{\exp(-2\pi i k) - 1} = (f_A + \alpha_r) \eta(h, k). \quad (3)$$

By introducing expression (3) into equation (2) and considering $\varepsilon_r \ll 1$ we obtain

$$F(h, k, l) = \eta(h, k) \left[\sum_{-\infty}^{+\infty} f_A M(r) \exp(-\pi i l r) + \sum_{-\infty}^{+\infty} M(r) (\alpha_r - \pi i l \varepsilon_r f_r - \frac{1}{2} \pi^2 l^2 f_r \varepsilon_r^2) \exp(-\pi i l r) \right] \quad (4)$$

where

$$f_r = f_A + \alpha_r.$$

The first term on the right-hand side of (4) obviously corresponds to diffraction by the undistorted lattice of the same size and orientation as the G.-P. zone and it has the same meaning as the second term in (1). By inserting (4) in (1) the second term of (1) and the first term of (4) cancel. The amplitude of radiation diffracted by the G.-P. zone and its neighbourhood is accordingly given by the first term on the right-hand side of (1), which corresponds to the sharp Bragg reflexion, and by the second term of (4), which appears due to the irregularities in G.-P. zones ($\Delta m_r \neq 0$ and $\varepsilon_r \neq 0$). The latter term corresponds to diffuse scattering.

The diffuse intensity diffracted by the G.-P. zone is given by

$$|F_{\text{diff}}(h, k, l)|^2 = |\eta(h, k)|^2 \left\{ \pi^2 l^2 \sum_{r,s} (f_r \varepsilon_r f_s \varepsilon_s - f_r \alpha_s \varepsilon_r^2) \times M(r) M^*(s) \exp[-\pi i l(r - s)] - \pi i l \sum_{r,s} (f_r \varepsilon_r \alpha_s - f_s \varepsilon_s \alpha_r) M(r) M^*(s) \exp[-\pi i l(r - s)] + \sum_{r,s} \alpha_r \alpha_s M(r) M^*(s) \exp[-\pi i l(r - s)] \right\}. \quad (5)$$

For simplicity we write

$$\begin{aligned} A_{rs}w_{rs} &= (f_r\varepsilon_r f_s\varepsilon_s - f_r\alpha_r\varepsilon_r^2)M(r)M^*(s), \\ B_{rs}w_{rs} &= (f_r\varepsilon_r\alpha_s - f_s\varepsilon_s\alpha_r)M(r)M^*(s), \\ C_{rs}w_{rs} &= \alpha_r\alpha_s M(r)M^*(s), \\ w_{rs} &= M(r)M^*(s) = \exp(-\pi i\varphi_{rs}). \end{aligned}$$

On account of the relations

$$\begin{aligned} A_{rs}w_{rs} &= A_{sr}w_{sr}^*, \\ B_{rs}w_{rs} &= -B_{sr}w_{sr}^*, \\ C_{rs}w_{rs} &= C_{sr}w_{sr}^*, \end{aligned}$$

equation (5) becomes

$$\begin{aligned} |F_{\text{diff.}}(h, k, l)|^2 &= |\eta(h, k)|^2 \left\{ \pi^2 l^2 \sum_{r,s} A_{rs} \cos \pi[l(r-s) + \varphi_{rs}] \right. \\ &\quad - \pi l \sum_{r,s} B_{rs} \sin \pi[l(r-s) + \varphi_{rs}] \\ &\quad \left. + \sum_{r,s} C_{rs} \cos \pi[l(r-s) + \varphi_{rs}] \right\}, \end{aligned} \quad (6)$$

where

$$|\eta(h, k)|^2 = 2[1 + \cos \pi(h+k)] \frac{\sin^2 \pi h N_1}{\sin^2 \pi h} \frac{\sin^2 \pi k N_2}{\sin^2 \pi k}.$$

$|F_{\text{diff.}}(h, k, l)|^2$ as a function of continuous variables h, k, l is not adequate for practical application. The integrated intensity of diffuse radiation in the relrod with l as variable is more adequate for further analysis of the structure of G.-P. zones.

$$I(l)_{\text{diff.}} = \iint |F(h, k, l)_{\text{diff.}}|^2 dh dk.$$

The function $|F(h, k, l)_{\text{diff.}}|^2$ depends on h and k through the functions $|\eta(h, k)|^2$ and φ_{rs} . Having regard to the fact that $|\eta(h, k)|^2$ is appreciable only for h and k both not far from integers, we introduce instead of h and k the quantities $H + \xi_1, K + \xi_2$, where H and K are integers both even or odd, and ξ_1 and ξ_2 are variables ≤ 1 . The function $|\eta(h, k)|^2$ in this notation then becomes $|\eta(\xi_1, \xi_2)|^2$. The functions φ_{rs} are

$$\varphi_{rs} = (H + \xi_1) \times \begin{cases} \text{even integer } (r, s \text{ equal parity}) \\ \text{odd integer } (r, s \text{ unequal parity}). \end{cases}$$

In the integration of (6) with respect to ξ_1 and ξ_2 the cosine and sine terms can be supposed constant and equal to their mean value in the integration range because of the rapid variation of the function $|\eta(\xi_1, \xi_2)|^2$.

Two separate cases are possible:

(a) *H and K both even.*—In this case φ_{rs} are always equal to even integers. Equation (6) may then be written

$$\begin{aligned} I(l)_{\text{diff.}} &= 4N_1N_2 \left\{ \pi^2 l^2 \sum_{-\infty}^{+\infty} A_n \cos \pi ln \right. \\ &\quad \left. - \pi l \sum_{-\infty}^{+\infty} B_n \sin \pi ln + \sum_{-\infty}^{+\infty} C_n \cos \pi ln \right\}, \end{aligned} \quad (7)$$

where $n = r - s$ and the coefficients A_n, B_n and C_n are given by

$$\begin{aligned} A_n &= \sum_{-\infty}^{+\infty} (f_r\varepsilon_r f_{r-n}\varepsilon_{r-n} - f_r\alpha_r\varepsilon_r^2), \\ B_n &= \sum_{-\infty}^{+\infty} (f_r\varepsilon_r\alpha_{r-n} - f_{r-n}\varepsilon_{r-n}\alpha_r), \\ C_n &= \sum_{-\infty}^{+\infty} \alpha_r\alpha_{r-n}. \end{aligned}$$

(b) *H and K both odd.*—For r and s of equal parity φ_{rs} are even integers, for unequal parity φ_{rs} are equal to odd integers. The detailed calculation leads to

$$\begin{aligned} I(l)_{\text{diff.}} &= 4N_1N_2 \left\{ \pi^2 l^2 \sum_{-\infty}^{+\infty} (-1)^n A_n \cos \pi ln \right. \\ &\quad \left. - \pi l \sum_{-\infty}^{+\infty} (-1)^n B_n \sin \pi ln + \sum_{-\infty}^{+\infty} (-1)^n C_n \cos \pi ln \right\}, \end{aligned} \quad (8)$$

where A_n, B_n and C_n are defined as before.

3. Fourier transform of integrated diffuse intensity in relrod (00l)

The intensity diffracted by G.-P. zones was expressed in the preceding section as a trigonometrical series with coefficients A_n, B_n and C_n . These include Δm_r and ε_r , characteristic of the structure of the G.-P. zone. In this section we will deal with the determination of A_n, B_n and C_n on the basis of analysis of the integrated diffuse intensity in relrod (00l) obtained experimentally.

The cosine Fourier transform of $I(00l)_{\text{diff.}}$ is accordingly (7) given by

$$\begin{aligned} T(x) &\equiv \int_0^{l_0} I(00l)_{\text{diff.}} \exp(-\beta l^2) \cos \pi lx dl \\ &= K \left\{ \pi^2 \int_0^{l_0} l^2 \sum_{-\infty}^{+\infty} A_n \exp(-\beta l^2) \cos \pi ln \cos \pi lx dl \right. \\ &\quad - \pi \int_0^{l_0} l \sum_{-\infty}^{+\infty} B_n \exp(-\beta l^2) \cos \pi lx \sin \pi ln dl \\ &\quad \left. + \int_0^{l_0} \sum_{-\infty}^{+\infty} C_n \exp(-\beta l^2) \cos \pi ln \cos \pi lx dl \right\}, \end{aligned} \quad (9)$$

where $\exp(-\beta l^2)$ has the meaning of the usual artificial temperature factor and l_0 is the upper limit of integrated intensity measured. K , here used as meaning the scale factor, should not be confused with the integer K in the preceding section.

The coefficients A_n, B_n and C_n can be divided into one part not depending on variable l and containing merely Δm_r and ε_r , and a second part containing functions of l alone.

Following the definition in § 1, we have

$$f_r = f_A + (f_{Cu} - f_{\Delta}) \Delta m_r.$$

Owing to the small concentration of copper in solid solutions we can replace f_A by f_{Δ} and Δm_r by the

atomic fraction of copper. Using further the approximation $f_{\text{Cu}} = Z_{\text{Cu}}f(l)$, $f_{\text{Al}} = Z_{\text{Al}}f(l)$, where Z_{Cu} and Z_{Al} are equal to the number of electrons in the copper and aluminium atoms respectively, these approximations lead to

$$\begin{aligned} f_r &= [Z_{\text{Al}} + (Z_{\text{Cu}} - Z_{\text{Al}})m_r]f(l) = Z_r f(l), \\ \alpha_r &= [Z_{\text{Cu}} - Z_{\text{Al}}]m_r f(l) = (Z_r - Z_{\text{Al}})f(l). \end{aligned} \quad (10)$$

By inserting (10) in the expressions for A_n , B_n and C_n we obtain

$$A_n = a_n f^2(l), \quad B_n = b_n f^2(l), \quad C_n = c_n f^2(l),$$

where a_n , b_n and c_n are independent of the variable l and are as follows:

$$\begin{aligned} a_n &= \sum_{-\infty}^{+\infty} [\varepsilon_r \varepsilon_{r-n} Z_r Z_{r-n} - \varepsilon_r^2 Z_r (Z_{r-n} - Z_{\text{Al}})], \\ b_n &= \sum_{-\infty}^{+\infty} (Z_r - Z_{\text{Al}}) (Z_{r+n} \varepsilon_{r+n} - Z_{r-n} \varepsilon_{r-n}), \\ c_n &= \sum_{-\infty}^{+\infty} (Z_r - Z_{\text{Al}}) (Z_{r-n} - Z_{\text{Al}}). \end{aligned} \quad (11)$$

The function $f(l)$ is so chosen that $Z_{\text{Cu}}f(l)$ and $Z_{\text{Al}}f(l)$ represent the atomic factors at the temperature of measurement.

Equation (9) takes the form

$$T(x) = K \left\{ \pi^2 \sum_{-\infty}^{+\infty} a_n \psi(n-x) - \pi \sum_{-\infty}^{+\infty} b_n \chi(n-x) + \sum_{-\infty}^{+\infty} c_n \gamma(n-x) \right\}, \quad (12)$$

where

$$\begin{aligned} \psi(n-x) &= \int_0^{l_0} l^2 f^2(l) \exp(-\beta l^2) \cos \pi l(n-x) dl, \\ \chi(n-x) &= \int_0^{l_0} l f^2(l) \exp(-\beta l^2) \sin \pi l(n-x) dl, \\ \gamma(n-x) &= \int_0^{l_0} f^2(l) \exp(-\beta l^2) \cos \pi l(n-x) dl. \end{aligned}$$

4. Interpretation of the Fourier transform

The Fourier transform of the integrated diffuse scattering according to (12) is represented as the sum of three functions ψ , χ , γ having non-zero values only in the immediate neighbourhood of $x = n$. We determine the coefficients a_n , b_n and c_n by the method of Flinn, Averbach & Rudman (1954).

The function $\chi(n-x)$ has a non-zero first moment with respect to $x = n$ and a zero area. Functions $\psi(n-x)$ and $\gamma(n-x)$ have a zero first moment and a non-zero area (Fig. 2).

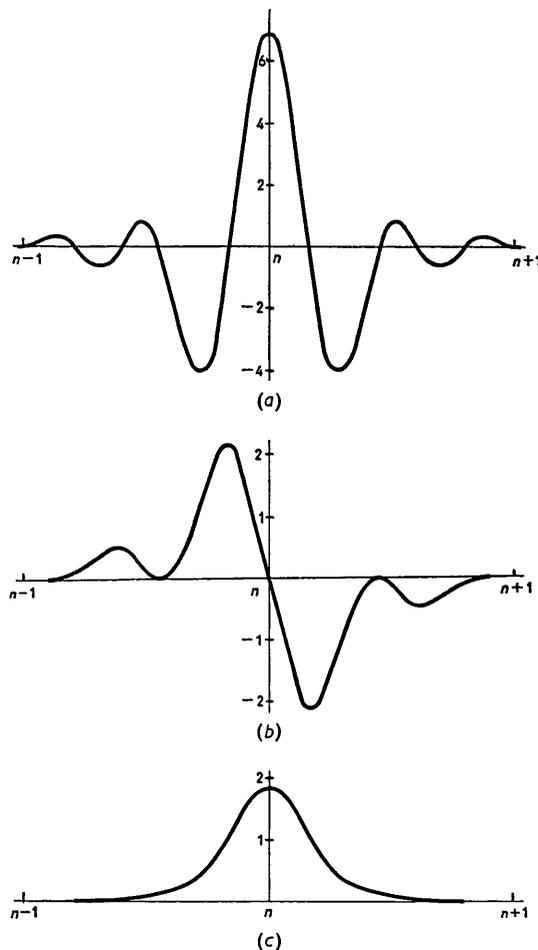


Fig. 2. Functions (a) ψ , (b) χ , (c) γ calculated without artificial temperature factor; $l_0 = 5$.

$$\left. \begin{aligned} \int_{n-\delta_1}^{n+\delta_1} (n-x)T(x) dx &= -K\pi b_n \int_{-\delta_1}^{\delta_1} \xi \chi(\xi) d\xi \\ &= -K\pi b_n M(\delta_1), \\ \int_{n-\delta_2}^{n+\delta_2} T(x) dx &= K[\pi^2 a_n \int_{-\delta_2}^{\delta_2} \psi(\xi) d\xi + c_n \int_{-\delta_2}^{\delta_2} \gamma(\xi) d\xi] \\ &= K[\pi^2 a_n A_1(\delta_2) + c_n A_2(\delta_2)], \\ \int_{n-\delta_3}^{n+\delta_3} T(x) dx &= K[\pi^2 a_n \int_{-\delta_3}^{\delta_3} \psi(\xi) d\xi + c_n \int_{-\delta_3}^{\delta_3} \gamma(\xi) d\xi] \\ &= K[\pi^2 a_n A_1(\delta_3) + c_n A_2(\delta_3)]. \end{aligned} \right\} (13)$$

The limits of integration δ_2 , δ_3 are chosen with advantage at the first and the second zero point of the function ψ . This enables the coefficients a_n and c_n to be separated.

The equations (13) allow us in principle to determine the coefficients a_n , b_n , c_n except for a scale factor K . Therefore we suppose the coefficients (Ka_n) , (Kb_n) , (Kc_n) to be known and we look for the possibility of determining m_r and ε_r . We begin by analysing the coefficients c_n according to (11).

These coefficients contain m_r only. According to the literature dealing with the structure of the G.-P. zones (Jagodzinski & Laves, 1949; Guinier, 1952; Gerold, 1954) we suppose m_r to be appreciable only in one or two neighbouring planes of the G.-P. zone. We distinguish, therefore, further the G.-P. zones odd and even (Fig. 3). In the case of the odd G.-P. zones

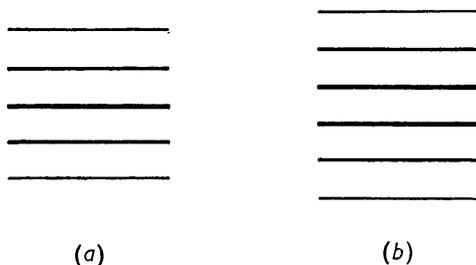


Fig. 3. (a) Odd G.-P. zone. (b) Even G.-P. zone.

we suppose that only m_0 is appreciable and that m_r decreases rapidly as r goes away from zero. In the case of even G.-P. zones m_0 and m_1 are appreciable and m_r decreases rapidly in both directions. In the following we carry out the analysis for the odd G.-P. zones only, this being more probable owing to the strong interaction of copper and aluminium atoms, as stated by Jagodzinski & Laves (1949). That this assumption is true is shown in the Appendix on the basis of experimental data.

If the odd G.-P. zone is symmetrical, it holds $m_r = m_{\bar{r}}$. If asymmetrical we may introduce \bar{m}_r by definition

$$\bar{m}_r = \frac{1}{2}(m_r + m_{\bar{r}}).$$

By assuming the rapid decrease of m_r from a maximum as r goes away from zero the coefficient c_n is given approximately for both symmetrical and asymmetrical zones by

$$c_n = (Z_{\text{Cu}} - Z_{\text{Al}}) \sum_{-\infty}^{+\infty} \bar{m}_r \bar{m}_{r-n}. \quad (14)$$

The accuracy of (14) exceeds that of experimentally determined c_n . It is therefore not possible to determine from the analysis of coefficients c_n the separate values of coefficients m_r and $m_{\bar{r}}$; we can obtain their average values \bar{m}_r only. For the same reason only the determination of $\bar{\varepsilon}_r$, the average of $|\varepsilon_r|$ and $|\varepsilon_{\bar{r}}|$, is possible.

In the first approximation the formula (11) gives

$$\left. \begin{aligned} (Kc_0) &= K(Z_{\text{Cu}} - Z_{\text{Al}})^2 \bar{m}_0'^2, \\ (Kc_1) &= 2(Kc_0)^{\frac{1}{2}} (Z_{\text{Cu}} - Z_{\text{Al}}) \bar{m}_1' / K, \\ (Kc_2) &= 2(Kc_0)^{\frac{1}{2}} (Z_{\text{Cu}} - Z_{\text{Al}}) \bar{m}_2' / K. \end{aligned} \right\} \quad (15)$$

The coefficients (Kc_n) are used owing to the impossibility of determining the coefficients c_n on the absolute scale. For this reason also \bar{m}_r cannot be expressed on the absolute scale. If more precise \bar{m}_r/K is required we make use of the second approximation

$$\begin{aligned} (Kc_0) &= (Z_{\text{Cu}} - Z_{\text{Al}})^2 (K\bar{m}_0''^2 + 2K\bar{m}_1'^2), \\ (Kc_1) &= 2(Z_{\text{Cu}} - Z_{\text{Al}})^2 \bar{m}_1'' / K (\bar{m}_0'' / K + \bar{m}_2' / K), \\ (Kc_2) &= (Z_{\text{Cu}} - Z_{\text{Al}})^2 (2\bar{m}_0'' \bar{m}_2'' / K + \bar{m}_1'^2 / K). \end{aligned}$$

The \bar{m}_r' and \bar{m}_r'' correspond to the first and to the second approximation respectively.

The $\bar{\varepsilon}_n$ can be determined from the coefficients b_n . The first approximation of (11) gives

$$(Kb_n) = 2\bar{\varepsilon}_n' / K \cdot Z_{\text{Al}} (Z_{\text{Cu}} - Z_{\text{Al}}) \bar{m}_0' / K; \quad (16)$$

in the second approximation

$$(Kb_n) = 2(Z_{\text{Cu}} - Z_{\text{Al}}) \cdot Z_{\text{Al}} [\bar{\varepsilon}_n'' / K \cdot \bar{m}_0' / K + \bar{m}_1' / K \cdot (\bar{\varepsilon}_{n+1}' + \bar{\varepsilon}_{n-1}') / K].$$

The $\bar{\varepsilon}_n'$ and $\bar{\varepsilon}_n''$ correspond to the values of $\bar{\varepsilon}_n$ in the first and in the second approximation. The scale factor cannot be directly determined from the experimental data.

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APPENDIX

For an even zone we have

$$\sum_{-\infty}^{+\infty} (-1)^n c_n = 0. \quad (17)$$

The diffuse intensity in relpoint (110) according to (8) and (17) is

$$I(110)_{\text{diff.}} = \sum (-1)^n c_n = 0$$

which is in disagreement with experiment.

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