However, the fragment-development component is not available with *SAYTAN*87 as yet. The test results we report have been carried out with a program based on *MULTAN*80 which stores information, including data, in a way different from that in *SAYTAN*87.

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Equations for Diffuse Scattering from Disordered Alloys with H.C.P. Structure

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Abstract

General equations are presented for the diffuse scattering due to local atomic arrangements and displacements in disordered alloys having h.c.p. structure. The scattering due to static and dynamic displacements is treated separately. The calculations show that the second-order terms in displacements are sufficient for observing the direct effect of temperature factors, common to all contributions of diffuse scattering. A new data analysis scheme, using asymmetry of diffuse scattering around superlattice reflections, is presented for a complete separation of various components.

Introduction

Since the early experiments of Wilchinsky (1944) and Cowley (1950), most quantitative studies of diffuse X-ray or thermal neutron scattering to reveal local atomic arrangements in disordered alloys have been carried out on systems having f.c.c. structure. The techniques for interpreting the diffraction pattern, data and error analysis are still evolving; see Borie & Sparks (1971), Gragg, Hayakawa & Cohen (1973), Hayakawa & Cohen (1975), Tibballs (1975), Khanna (1984) for the latest procedures. Although there are a large number of alloy phases which possess h.c.p. structure at high temperatures and which undergo ordering on cooling, general equations for diffuse scattering from such alloys have not yet been presented. Development of these equations and the separation procedures will be the principal subject of this paper.

After a brief review of the diffraction theory for disordered alloys, general equations are derived for the diffuse scattering due to short-range order and displacements (both static and dynamic) from h.c.p. alloys. Dynamic displacements due to thermal vibrations are treated separately to account properly for their effect on other components of diffuse scattering. Procedures for data analysis and separation of various diffuse scattering components are also discussed.

1. Diffraction theory

From kinematic theory, the total scattered intensity from a disordered binary alloy can be written as

$$I_{\rm tot} = \sum_{\substack{l,l'\\k,k'}} f_{lk} f_{l'k'} \exp\left[i\mathbf{Q}\,.\,(\mathbf{r}_{lk}-\mathbf{r}_{l'k'})\right]. \tag{1}$$

f_{lk} represents the atomic form factor of an atom located at position $\mathbf{r}_{lk}$. l and k are lattice and sublattice indices respectively. $\mathbf{Q}$ is the diffraction vector. Let x^i_k be the sublattice fraction of atom i on sublattice k and let $p^{ij}_{kk'}$ represent the conditional probability of finding a j-type atom on the k'th sublattice of the l'th lattice point if there is an i-type atom on the kth sublattice of the lth lattice point. Equation (1) may then be written as (Hayakawa & Cohen, 1975)

$$I_{\rm tot} = \sum_{\substack{l,l'\\k,k'\\i,j}} x^i_k f_{lk} f_{l'k'} P^{ij}_{kk'} \exp\left[i\mathbf{Q}\,.\,(\mathbf{r}_{lk}-\mathbf{r}_{l'k'})\right]. \tag{2}$$

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Owing to static and dynamic displacements, the atomic positions $\mathbf{r}_{lk}$ differ slightly from the average lattice vector $\mathbf{R}_{lk}$ of the disordered alloy. With the decomposition $\mathbf{r}_{lk}=\mathbf{R}_{lk}+\mathbf{u}_{lk}+\boldsymbol{\delta}_{lk}$, where $\mathbf{u}$ and $\boldsymbol{\delta}$ are respectively the static and dynamic displacements, I_{tot} reduces to

$$\begin{aligned}I_{\text{tot}}=\sum_{\substack{l,l'\\k,k'\\i,j}} & x_k^i f_{lk} f_{l'k'} P_{kk'}^{ij}\\ & \times\exp[i\mathbf{Q}\,.\,(\mathbf{R}_{lk}-\mathbf{R}_{l'k'})]\\ & \times\langle\exp[i\mathbf{Q}\,.\,(\mathbf{u}_{lk}^i-\mathbf{u}_{l'k'}^j)]\rangle\\ & \times\langle\exp[i\mathbf{Q}\,.\,(\boldsymbol{\delta}_{lk}^i-\boldsymbol{\delta}_{l'k'}^j)]\rangle.\end{aligned}\tag{3}$$

Let us first evaluate the contribution due to dynamic effects. For small displacements we have

$$\begin{aligned}&\langle\exp[i\mathbf{Q}\,.\,(\boldsymbol{\delta}_{lk}^i-\boldsymbol{\delta}_{l'k'}^j)]\rangle\\ &\quad\sim\exp[-\tfrac{1}{2}\langle|\mathbf{Q}\,.\,(\boldsymbol{\delta}_{lk}^i-\boldsymbol{\delta}_{l'k'}^j)|^2\rangle].\end{aligned}\tag{4}$$

Since, in a random solid solution, thermal vibrations are determined only from the averaged interatomic potential of the alloy, the space and time average in (4) will depend only on the interatomic vectors and not on the individual atomic pairs of the alloy. If we express the value of thermal displacements (Willis & Pryor, 1975) in terms of lattice vibration modes and assume the phases of all modes to be independent, the average in (4) reduces to

$$\exp[-\omega_k(\mathbf{Q})]\exp[-\omega_{k'}(\mathbf{Q})][1+I_1(\mathbf{Q})+\ldots]\tag{5}$$

where

$$\omega_k(\mathbf{Q})=\frac{1}{2Nm_k}\sum_{j\mathbf{q}}|\mathbf{Q}\,.\,\mathbf{e}(k/j\mathbf{q})|^2\frac{E_j(\mathbf{q})}{\omega_j^2(\mathbf{q})}\tag{6a}$$

$$\begin{aligned}I_1(\mathbf{Q})=\frac{1}{2N[m(k)m(k')]^{1/2}}\sum_{j\mathbf{q}}\frac{E_j(\mathbf{q})}{\omega_j^2(\mathbf{q})}\\ \times\{[\mathbf{Q}\,.\,\mathbf{e}(k|j\mathbf{q})][\mathbf{Q}\,.\,\mathbf{e}^*(k'|j\mathbf{q})]\\ \times\exp[i\mathbf{q}\,.\,(\mathbf{R}_{lk}-\mathbf{R}_{l'k'})]\\ +[\mathbf{Q}\,.\,\mathbf{e}^*(k|j\mathbf{q})][\mathbf{Q}\,.\,\mathbf{e}(k'|j\mathbf{q})]\\ \times\exp[-i\mathbf{q}\,.\,(\mathbf{R}_{lk}-\mathbf{R}_{l'k'})]\}.\end{aligned}\tag{6b}$$

m_k is the mass of an average atom in the kth sublattice in the random solid solution and N is the total number of unit cells in the lattice. $E_j(\mathbf{q})$, $\omega_j(\mathbf{q})$ and $\mathbf{e}(k|j\mathbf{q})$ are, respectively, the energy, frequency and polarization of the vibration mode $(j\mathbf{q})$. $I_1(\mathbf{Q})$ represents terms due to first-order thermal diffuse scattering. Contributions due to higher-order terms have been neglected.

Substituting (5) in (3) we have

$$\begin{aligned}I_{\text{tot}}=\sum_{\substack{l,l'\\k,k'\\i,j}} & x_k^i f'_{l'k} f'_{l'k'} P_{kk'}^{ij}\exp[i\mathbf{Q}\,.\,(\mathbf{R}_{lk}-\mathbf{R}_{l'k'})]\\ & \times\langle\exp[i\mathbf{Q}\,.\,(\mathbf{u}_{lk}^i-\mathbf{u}_{l'k'}^j)]\rangle[1+I_1(\mathbf{Q})]\end{aligned}\tag{7}$$

where

$$f'_{lk}=f_{lk}\exp[-\omega_k(\mathbf{Q})].$$

Note that the thermal Debye-Waller factor extends over all reciprocal space and is not restricted to the volume just near Bragg peaks. Expanding $\exp[i\mathbf{Q}\,.\,(\mathbf{u}_{lk}^i-\mathbf{u}_{l'k'}^j)]$ as a Taylor series and retaining terms up to the second order in dispacement, we have

$$\begin{aligned}I_{\text{tot}}=\sum_{\substack{l,l'\\k,k'\\i,j}} & x_k^i x_{k'}^j f'_i f'_j\exp[i\mathbf{Q}\,.\,(\mathbf{R}_{lk}-\mathbf{R}_{l'k'})]\\ & +(I_{LM}/N)\left(\sum_{\substack{l,l'\\k,k'\\i>j}}\{x_k^i x_{k'}^j (f'_i-f'_j)^2\alpha_{kk'}^{ij}\right.\\ & \times\exp[i\mathbf{Q}\,.\,(\mathbf{R}_{lk}-\mathbf{R}_{l'k'})]\\ & \times[\sum_{k''}\sum_{i>j}x_{k''}^i x_{k''}^j(f'_i-f'_j)^2]^{-1}\}\\ & +i\sum_{\substack{l,l'\\k,k'\\i,j}}F_{kk'}^{ij}\langle\mathbf{Q}\,.\,(\mathbf{u}_k^i-\mathbf{u}_{k'}^j)\rangle\exp[i\mathbf{Q}\,.\,(\mathbf{R}_{lk}-\mathbf{R}_{l'k'})]\\ & +\tfrac{1}{2}\sum_{\substack{l,l'\\k,k'\\i,j}}F_{kk'}^{ij}\langle[\mathbf{Q}\,.\,(\mathbf{u}_k^i-\mathbf{u}_{k'}^j)]^2\rangle\\ & \times\exp[i\mathbf{Q}\,.\,(\mathbf{R}_{lk}-\mathbf{R}_{l'k'})]\\ & \left.+\sum_{\substack{l,l'\\k,k'\\i,j}}x_k^i f'_i f'_j P_{kk'}^{ij}\exp[i\mathbf{Q}\,.\,(\mathbf{R}_{lk}-\mathbf{R}_{l'k'})]I_1(\mathbf{Q})\right)\end{aligned}\tag{8}$$

where

$$\alpha_{kk'}^{ij}=1-(P_{kk'}^{ij}/x_k^j)\tag{9a}$$

$$F_{kk'}^{ii}=x_k^i f_i'^2\left(x_{k'}^i+\sum_{j\neq i}x_{k'}^j\alpha_{kk'}^{ij}\right)\times\left[\sum_{\substack{k''\\i>j}}x_{k''}^i x_{k''}^j(f'_i-f'_j)^2\right]^{-1}\tag{9b}$$

$$F_{kk'}^{ij}=x_k^i x_{k'}^j f'_i f'_j(1-\alpha_{kk'}^{ij})\times\left[\sum_{\substack{k''\\i>j}}x_{k''}^i x_{k''}^j(f'_i-f'_j)^2\right]^{-1}\tag{9c}$$

$$I_{LM}=N\sum_k\sum_{i>j}x_k^i x_k^j(f'_i-f'_j)^2.\tag{9d}$$

The first and second sums in (8) represent contributions due to Bragg reflections and short-range order (SRO) respectively. α represents the Warren-Cowley order parameter. The third and fourth sums represent diffuse scattering due to static displacements and the fifth one is due to first-order thermal diffuse scattering. I_{LM} gives the Laue monotonic scattering. For simplicity, the primes on the form factors will no longer be employed.

2. Scattering equations for a h.c.p. lattice

We first introduce some notation. In Cartesian coordinates, a position vector $\mathbf{R}(l, m, n)$ in a h.c.p. lattice can be represented as (Khanna, 1982)

$$\mathbf{R}(l, m, n) = l(a/2\sqrt{3})\hat{\mathbf{x}} + m(a/2)\hat{\mathbf{y}} + n(c/2)\hat{\mathbf{z}}$$

where l, m and n have integer values. a and c are respectively the basal lattice constant and the separation between two atomic planes parallel to the basal plane. The symmetry of a h.c.p. lattice permits a set of eight vectors $\mathbf{R}(\pm l, \pm m, \pm n)$ (having identical absolute values of l, m and n) for connecting two points lying on the same sublattice (n even). For connecting two points lying on different sublattices (n odd), only a set of four vectors $\mathbf{R}(l, \pm m, \pm n)$ is permitted. Another geometric feature of a h.c.p. lattice is that the reciprocal-lattice vector $\mathbf{Q}$ may be represented as

$$\begin{aligned}\mathbf{Q}(h_1', h_2', h_3') &= (2\pi/\sqrt{3}a)h_1'\hat{\mathbf{x}} + (2\pi/a)h_2'\hat{\mathbf{y}} \\ &\quad + (2\pi/c)h_3'\hat{\mathbf{z}} \\ &= h_1\mathbf{b}_1 + h_2\mathbf{b}_2 + h_3\mathbf{b}_3 \qquad (10)\end{aligned}$$

where $h_1' = h_2'$, $h_2 = -\frac{1}{2}(h_1' + h_2')$ and $h_3 = h_3'$. The $\mathbf{b}$ vectors represent reciprocal-lattice unit vectors.

From (8), the diffuse intensity from a disordered h.c.p. alloy can then be written in a form similar to that for cubic lattices as

$$\begin{aligned}I_D' &= I_D/I_{LM} \\ &= I_{SRO} + h_1Q_x(h_1, h_2, h_3) + h_2Q_y(h_1, h_2, h_3) \\ &\quad + h_3Q_z(h_1, h_2, h_3) + h_1^2R_x(h_1, h_2, h_3) \\ &\quad + h_2^2R_y(h_1, h_2, h_3) + h_3^2R_y(h_1, h_2, h_3) \\ &\quad + h_1h_2S_{xy}(h_1, h_2, h_3) + h_2h_3S_{yz}(h_1, h_2, h_3) \\ &\quad + h_1h_3S_{xz}(h_1, h_2, h_3) + I_{TDS}/I_{LM} \qquad (11)\end{aligned}$$

$$\begin{aligned}I_{SRO} &= 4\sum_m\left[2\sum_n^{\text{even}}\sum_l \cos \pi h_1 l + \sum_n^{\text{odd}}\sum_l \exp(i\pi h_1 l)\right] \\ &\quad \times \cos \pi h_2 m \cos \pi h_3 n\bar{\alpha}_{lmn} \\ Q_x(h_1, h_2, h_3) &= 4\sum_m\left[2\sum_n^{\text{even}}\sum_l \sin \pi l h_1 \right. \\ &\quad \left. + a_1\sum_n^{\text{odd}}\sum_l \exp(i\pi h_1 l)\right] \\ &\quad \times \cos \pi m h_2 \cos \pi n h_3 \varepsilon_{lmn}^x \\ R_x &= 4\sum_m\left[2\sum_n^{\text{even}}\sum_l \cos \pi l h_1 + \sum_n^{\text{odd}}\sum_l \exp(i\pi l h_1)\right] \\ &\quad \times \cos \pi m h_2 \cos \pi n h_3 \delta_{lmn}^x \\ S_{xy} &= 4\sum_m\left[2\sum_n^{\text{even}}\sum_l \sin \pi l h_1 - a_1\sum_n^{\text{odd}}\sum_l \exp(i\pi l h_1)\right] \\ &\quad \times \sin \pi m h_2 \cos \pi n h_3 \gamma_{lmn}^{xy} \qquad (12)\end{aligned}$$

and similarly for other terms.

$$a_1 = \begin{cases} -i & \text{for } x \text{ components} \\ +1 & \text{for } y \text{ and } z \text{ components.}\end{cases}$$

The coefficients for these series are defined as

$$\begin{aligned}\bar{\alpha}_{lmn} &= \sum_{i>j} \frac{x_k^i x_{k'}^j (f_i' - f_j')^2}{\sum_{k''}\sum_{i>j} x_{k''}^i x_{k''}^j (f_i' - f_j')^2}\alpha_{kk'}^{ij}(lmn) \\ \varepsilon_{lmn}^x &= 2\pi i\left[\sum_i\sum_j F_{kk'}^{ij}\langle(\Delta_{kk'}^x)^{ij}\rangle_{lmn}\right]_{kk'} \\ \delta_{lmn}^x &= 4\pi^2\left[\sum_i\sum_j F_{kk'}^{ij}\langle(\Delta_k^x)^i(\Delta_{k'}^x)^j\rangle_{lmn}\right]_{kk'} \qquad (13) \\ \gamma_{lmn}^{xy} &= 8\pi^2\left[\sum_i\sum_j F_{kk'}^{ij}\langle(\Delta_k^x)^i(\Delta_{k'}^y)^j\rangle_{lmn}\right]_{kk'}\end{aligned}$$

where

$$\Delta_{kk'}^x = u_k^{x,i} - u_{k'}^{x,j} \quad \text{and} \quad \Delta_k^{x,i} = u_k^{x,i}.$$

3. Separation of components

For a complete separation of contributions from different sources, the diffuse scattering data should be analysed in two steps.

3.1. *Borie-Sparks method*

As a first step, the data should be analysed according to the Borie & Sparks (1971) (B-S) method, making use of the periodic nature of terms in (11). For this purpose, the TDS contribution can be clubbed along with the second-order static displacement scattering (R and S terms). As I_{SRO}, Q, R and S terms are Fourier series (variation of the ratio of the atomic scattering factor with the scattering vector $\mathbf{Q}$ being neglected) with a periodicity of two, their contribution may be separated as follows:

$$\begin{aligned}R_x &= \tfrac{1}{8}\{[I_D(h_1, h_2, h_3) - I_D(h_1 - 2, h_2, h_3)] \\ &\quad - [I_D(h_1 - 2, h_2, h_3) - I_D(h_1 - 4, h_2, h_3)]\} \\ S_{xy} &= \tfrac{1}{4}\{[I_D(h_1, h_2, h_3) - I_D(h_1 - 2, h_2, h_3)] \\ &\quad - [I_D(h_1, h_2 - 2, h_3) - I_D(h_1 - 2, h_2 - 2, h_3)]\} \\ Q_x &= \tfrac{1}{2}\{[I_D(h_1, h_2, h_3) - I_D(h_1 - 2, h_2, h_3)] \\ &\quad - 4(h_1 - 1)R_x(h_1, h_2, h_3) \\ &\quad - 2h_2S_{xy}(h_1, h_2, h_3) - 2h_3S_{xz}(h_1, h_2, h_3)\} \qquad (14)\end{aligned}$$

and similarly for other terms. Once Q, R and S are known, I_{SRO} can be obtained from (11).

As the basic periodicity is two for cubic and h.c.p. crystals, the separation expressions for both these structures have a similar form. But there are some subtle differences between the two. For example, in a cubic crystal we have

$$Q_y(h_1, h_2, h_3) = Q_x(h_2, h_1, h_3) \tag{15a}$$

$$Q_z(h_1, h_2, h_3) = Q_x(h_3, h_2, h_1). \tag{15b}$$

These equalities arise due to the following assumption regarding the displacements:

$$u^x_{lmn} = u^y_{mln} = u^z_{nml}. \tag{15c}$$

As the lattice response of a cubic crystal is identical along three crystallographic axes, the distorting forces are assumed to be radial in nature for (15*c*) to hold. For a h.c.p. crystal, while the assumption regarding forces is still true, the lattice response is no longer identical along different crystallographic axes. Equation (15*a*) still holds due to the isotropy in the basal plane, but (15*b*) holds only for crystals having the ideal c/a ratio and not for highly anisotropic crystals like zinc and cadmium.

3.2. *Separation of the thermal component*

As a second step we look at the asymmetry of each term in (11) about the (H00) superlattice points along the [H00] direction in reciprocal space.

3.2.1

$I_{\rm SRO}$ symmetric about reciprocal-lattice points. S terms vanish along the [H00] direction.

3.2.2

To evaluate the contribution of R terms to the asymmetry of diffuse scattering, we consider the microdomain model for disordered alloys (Das & Thomas, 1974). According to this model, a disordered binary alloy with persisting short-range order can be viewed as consisting of a large number of highly ordered microdomains embedded in a randomly disordered matrix. The anti-site size effect in these ordered domains/clusters causes a static displacement of atoms in the cluster itself and affects the atoms of the disordered matrix in the continuum limit. As far as scattering around reciprocal-lattice points is concerned, these clusters can be treated as defects. A main contribution to diffuse scattering in this region arises due to the elastic displacement field of the defect and can be quite intense. However, this contribution vanishes around superlattice reflections due to space-group reflection conditions. The only contribution to diffuse scattering is then due to the strongly distorted neighbourhood of the defect. This is very small, especially near Bragg peaks, as a small number of atoms (in contrast to the elastic field) participates in scattering. R terms, which are due to the second power in static displacements, will in general be quite small and their contribution to asymmetry can be neglected.

3.2.3

Q_x terms are asymmetric about reciprocal-lattice points.

$$\begin{aligned} I^Q_{\rm AS} &= (H+q)Q_x(H+q,0,0) - (H-q)Q_x(H-q,0,0) \\ &= 8H\sum_l\sum_m\left[2\sum_m^{\rm even}\varepsilon^x_{lmn}\cos\pi lH\sin\pi lq \right.\\ &\qquad \left. +2\sum_n^{\rm odd}\varepsilon^x_{lmn}\exp(i\pi Hl)\sin\pi lq\right] \\ &\simeq 16\pi Hq\sum_l\sum_m\left[\sum_n^{\rm even}\varepsilon^x_{lmn}l(-1)^{Hl}\right.\\ &\qquad \left.+\sum_n^{\rm odd}\exp(i\pi Hl)\varepsilon^x_{lmn}\right]. \end{aligned} \tag{16}$$

The coefficients ε^x are independent of the wavevector and remain unaffected.

3.2.4

$$\begin{aligned} I^{(\mathbf{Q})}_{\rm TDS} = \sum_{\substack{ll'\\kk'\\ij}}\frac{x^i_k}{2N}\frac{x^j_{k'}f_if_{j'}}{(m_km_{k'})^{1/2}}\sum_{j\mathbf{q}}\frac{E_i(\mathbf{q})}{\omega^2_j(\mathbf{q})} &\times\{[\mathbf{Q}\,.\,\mathbf{e}(k|j\mathbf{q})][\mathbf{Q}\,.\,\mathbf{e}^*(k'|j\mathbf{q})] \\ &\times\exp[i\mathbf{q}\,.\,(\mathbf{R}_{lk}-\mathbf{R}_{l'k'})] \\ &+[\mathbf{Q}\,.\,\mathbf{e}^*(k|j\mathbf{q})][\mathbf{Q}\,.\,\mathbf{e}(k'|j\mathbf{q})] \\ &\times\exp[-i\mathbf{q}\,.\,(\mathbf{R}_{lk}-\mathbf{R}_{l'k'})]\}. \end{aligned} \tag{17}$$

The contribution from first-order TDS can be split into two parts: the continuously varying background due to the Q^2 terms in (17) and the fairly sharp peaks at Bragg reflections due to the $1/\omega^2(\mathbf{q})$ term. Since in the disordered phase the average structure consists of a randomly disordered alloy the peaks in TDS will appear only near fundamental reflections. Near the superlattice positions, we have a contribution mainly from the continuously varying background. Near a superlattice reflection: $\mathbf{Q}=\mathbf{H}+\mathbf{q}$, where $\mathbf{H}$ is a reciprocal-lattice vector and $\mathbf{q}\ll\mathbf{H}$, $I_{\rm TDS}$ can be written as

$$I_{\rm TDS} = Q^2 f(\mathbf{q}) \tag{18}$$

where $f(\mathbf{q})$, symmetric with respect to $\mathbf{q}\rightarrow-\mathbf{q}$, can be obtained from (17) in a straightforward manner. The asymmetric part of TDS about (H00) reflections can then be written as

$$[I_{\rm TDS}]_{\rm AS} = 4Hqf(\mathbf{q}). \tag{19}$$

3.2.5

Total asymmetric diffuse scattering $T^{\rm tot}_{\rm AS}(\mathbf{q})$ can now be written as

$$\begin{aligned} I^{\rm tot}_{\rm AS}(\mathbf{H},\mathbf{q}) = 4Hqf(\mathbf{q}) + 16\pi Hq\sum_{l,m}&\left[\sum_n^{\rm even}l\varepsilon^x_{lmn}(-1)^{Hl}\right.\\ &\left.+\sum_n^{\rm odd}\exp(i\pi Hl)l\varepsilon^x_{lmn}\right]. \end{aligned} \tag{20}$$

The contribution to asymmetry from hQ_x terms can be calculated analytically from the coefficients obtained in step 1 using B–S analysis (§ 3.1). These coefficients are not affected in the present scheme of separating thermal and static components. $f(\mathbf{q})$ can then be obtained from the experimentally observed asymmetry of diffuse scattering. In a similar manner $f(\mathbf{q})$ and hence $I_{\rm TDS}$ can be evaluated in different directions of reciprocal space. In this way the contribution from TDS can be obtained in a straightforward manner without actually computing mode frequencies using elastic constants. This method has the further advantage of yielding $I_{\rm TDS}$ over a range of temperatures, and an additional knowledge regarding the temperature dependence of various physical parameters is no longer required.

Once the contribution from TDS has been subtracted, the remaining diffuse intensity can be reanalysed using the method outlined in step 1 (§ 3.1). The coefficients thus obtained will have contributions only from static displacements.

Concluding remarks

Hayakawa, Bardhan & Cohen (1975) suggest the inclusion of higher powers of $\mathbf{u}$ in the expansion of $\exp(i\mathbf{K}.\mathbf{u})$ for observing the direct effect of temperature factors, common to all contributions of diffuse scattering. This is not strictly true [see equation (7)] as δ^2 terms due to thermal vibrations suffice to produce the above mentioned effect and higher powers are not in general required. u^2 terms included in the present formalism correspond to static distortions and they are expected to yield information about the strongly distorted neighbourhood around the core of the SRO domain/cluster.

We should also note a basic difference between static and dynamic Debye–Waller (DW) factors. Static distortions attenuate atomic form factors only near fundamental reflections and do not modify scattering elsewhere in the reciprocal space (Khanna, 1984). On the other hand, the dynamic DW factor, in addition to affecting Bragg peaks, attenuates diffuse scattering from other sources as well. This result has an important implication. According to (7) the experimental diffuse scattering data have to be weighted by the thermal DW factor $\exp[-\omega_k(\mathbf{Q})]$. Since it is rather difficult to calculate $\exp[-\omega_k(\mathbf{Q})]$ accurately, Bardhan & Cohen (1976) employed the ratio $I(100)/I(300)$ (for f.c.c. crystals) to obtain $\exp[-2\omega(\mathbf{Q})]$. Their claim, that the DW factor thus obtained contains both static and dynamic contributions, is however not correct. $I(100)/I(300)$, the ratio of scattered intensity at superlattice reflections, contains only dynamic contributions and yields the correct DW factor needed to reduce the experimental diffuse scattering data.

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On the Effective Physical Properties of Polycrystalline Materials

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Abstract

An iteration method is presented for calculation of the gross physical properties of polycrystals in terms of the physical properties of the crystals. No assumptions are made concerning the shape or behaviour of the crystallites. The only mathematical condition to be fulfilled is that the product of the matrix of a gross physical property with its inverse must give a unit matrix if the same is valid for the crystals. The method is demonstrated by the calculation of the effective elastic tensor of a hypothetical texturized polycrystal

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