Intrinsic Inequalities Among the Partial Intensities of the Short-Range-Order Diffuse Scattering from a Disordered Ternary Alloy

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Abstract

An inequality relation has been derived from two different points of view. The first is according to a sum rule of the partial structure factors for individual atomic species or static concentration waves in the terminology of Khachaturyan [*Phys. Status Solidi B* (1973), **60**, 9–37] and the second is based on the condition that the total intensity must be positive. The two methods lead to the same result. That is, among α_1 [$\equiv x_B x_C \alpha^{BC}(\mathbf{q})$], α_2 [$\equiv x_C x_A \alpha^{CA}(\mathbf{q})$] and α_3 [$\equiv x_A x_B \alpha^{AB}(\mathbf{q})$] for an A-B-C ternary alloy [x_A being the fraction of atom A and $\alpha^{AB}(\mathbf{q})$ the Fourier transform of the Warren–Cowley parameters, *i.e.* the partial intensity for the pair A-B], the following restriction condition has been achieved: $\alpha_p + \alpha_q \geq 0$ ($p \neq q$), and simultaneously $\sum\sum_{p<q} \alpha_p \alpha_q \geq 0$. This should be helpful for judging whether the partial intensities obtained are in principle possible or forbidden.

1. Introduction

Three independent interatomic correlation functions (for pairs A-B, B-C and C-A) are necessary for describing the short-range-ordered state in a ternary (A-B-C) alloy and are associated with their own partial X-ray diffuse-scattering intensities through the Fourier transformation. In experiments, however, the X-ray diffuse intensity is observed as a superposition of the three partials and, if the individual interatomic correlations are required to be known, they must be theoretically separated by handling the data collected with different kinds of radiation.

Recently synchrotron radiation ·from an electron storage ring has been actively used for diffraction and spectroscopy experiments as a strong white X-ray source. Experimental application of the anomalous scattering of the radiation to the short-range-order (SRO) diffuse scattering from ternary alloys has begun to be reported (Hashimoto, Iwasaki, Ohshima, Harada, Sakata & Terauchi, 1985) as well as a theoretical analysis of such intensity data (Cenedese, Bley & Lefebvre, 1984).

Cenedese *et al.* (1984) suggested criteria for testing the reliability of deducing the partial intensities from the viewpoint of the propagation of observational errors through the theoretical calculation. The importance of such a discussion is closely related to the fact that the intensity analysis is based on a recognition of very small variations of contrast in the intensity data obtained with the use of several kinds of radiation (Hashimoto *et al.*, 1985; Cenedese *et al.*, 1984). We here try to find another criterion to judge whether any given set of partial intensities is in principle possible or forbidden. Such a criterion may be helpful in avoiding mistakes caused by unexpected errors in the observations and physical constants used in the analysis and in constraining the intensity analysis so that it does not result in a physically forbidden set of values for the partials.

In the present work, we derive a formula for the restriction relation among the partial intensity values using a sum rule for the partial structure factors of the individual atomic species (defined in § 3.1) or static concentration waves in the terminology of Khachaturyan (1973). We further show another method (leading to the same result) based on the condition that the total diffuse intensity must be positive or zero, even though any kind of radiation is adopted for measurement fictitiously.

2. Basic equation of the SRO diffuse intensity in a multi(N)-component alloy system

We shall give a derivation of the intensity equation in detail so that the assumptions used can be made apparent. We here ignore both the static displacements of atoms from the average lattice points and the dynamic ones, *i.e.* the thermal vibrations of atoms.

The kinematic X-ray intensity scattered from a crystal can generally be expressed as (Guinier, 1963)

$$I(\mathbf{q}) = \sum_m \sum_n f_m f_n^* \exp\left[-2\pi i \mathbf{q} \cdot (\mathbf{R}_m - \mathbf{R}_n)\right], \quad (1)$$

where $\mathbf{q}$ is the scattering vector, f_m the atomic scattering factor of an atom at the mth lattice site and $\mathbf{R}_m$ the lattice vector. We first define σ_m^i ($i = 1, \ldots, N$, specifying the atomic species in the N-component alloy) as

$$\sigma_m^i = \begin{cases} 1 & \text{if an atom of type } i \text{ is at site } m, \\ 0 & \text{otherwise,} \end{cases} \quad (2)$$

and then define a concentration deviation parameter η^i_m (Taggart, 1973; de Fontaine, 1979†) as

$$\eta^i_m = \sigma^i_m - x_i, \tag{3}$$

where x_i is the fraction of the ith type of atom. f_m referred to the m site is expressed as

$$f_m = \sum_{i=1}^{N} \sigma^i_m f_i = \sum_{i=1}^{N} (x_i + \eta^i_m) f_i, \tag{4}$$

where f_i is the atomic scattering factor of atom i. Inserting (4) into (1), we have

$$I(\mathbf{q}) = \sum_m \sum_n |\sum_i x_i f_i|^2 \exp[-2\pi i \mathbf{q} \cdot (\mathbf{R}_m - \mathbf{R}_n)]$$

$$+ \sum_m \sum_n \left(\sum_i \eta^i_m f_i\right)\left(\sum_j \eta^j_n f^*_j\right)$$

$$\times \exp[-2\pi i \mathbf{q} \cdot (\mathbf{R}_m - \mathbf{R}_n)], \tag{5}$$

where a conservation relation

$$\sum_m \eta^i_m = 0 \tag{6}$$

is used. The first term in (5) represents the fundamental reflection intensity and the second term the SRO diffuse scattering intensity. Both terms can be rewritten in the form $|\dots|^2$, indicating that they are individually positive. From another conservation rule,

$$\sum_j \eta^j_n = 0, \tag{7}$$

the second term in (5) is developed as

$$I_{\text{SRO}}(\mathbf{q}) = \sum_m \sum_n \left(\sum_i \eta^i_m f_i\right)\left(\eta^i_n f^*_i + \sum_{j(\neq i)} \eta^j_n f^*_j\right)$$

$$\times \exp[-2\pi i \mathbf{q} \cdot (\mathbf{R}_m - \mathbf{R}_n)$$

$$= \sum_m \sum_n \left(\sum_i \eta^i_m f_i\right)\left(-\sum_{j(\neq i)} \eta^j_n f^*_i + \sum_{j(\neq i)} \eta^j_n f^*_j\right)$$

$$\times \exp[-2\pi i \mathbf{q} \cdot (\mathbf{R}_m - \mathbf{R}_n)]$$

$$= \sum_m \sum_n \sum_{i \neq j} \eta^i_m \eta^j_n (-|f_i|^2 + f_i f^*_j)$$

$$\times \exp[-2\pi i \mathbf{q} \cdot (\mathbf{R}_m - \mathbf{R}_n)]. \tag{8}$$

From the relation

$$\langle \eta^i_m \eta^j_n \rangle = \langle \eta^j_m \eta^i_n \rangle \quad \text{or} \quad \langle \eta^i_m \eta^j_n \rangle = \langle \eta^i_n \eta^j_m \rangle, \tag{9}$$

which indicates the equality of the number of ij and ji pairs in the crystalline solid solution,‡ we can write

$$I_{\text{SRO}}(\mathbf{q}) = -\sum_{i<j} |f_i - f_j|^2 \sum_m \sum_n \eta^i_m \eta^j_n$$

$$\times \exp[-2\pi i \mathbf{q} \cdot (\mathbf{R}_m - \mathbf{R}_n)], \tag{10a}$$

and then

$$I_{\text{SRO}}(\mathbf{q}) = -\sum_{i<j} |f_i - f_j|^2 \sum_m \sum_n \eta^i_m \eta^j_n$$

$$\times \cos[2\pi \mathbf{q} \cdot (\mathbf{R}_m - \mathbf{R}_n)]. \tag{10b}$$

Here, if we put

$$\langle \eta^i_m \eta^j_n \rangle \equiv -x_i x_j \alpha^{ij}_{mn}, \tag{11}$$

we can rewrite (10b) as

$$I_{\text{SRO}}(\mathbf{q}) = n_a \sum_{i<j} x_i x_j |f_i - f_j|^2 \alpha^{ij}(\mathbf{q}), \tag{12}$$

$$\alpha^{ij}(\mathbf{q}) \equiv \sum_l \alpha^{ij}_l \cos(2\pi \mathbf{q} \cdot \mathbf{R}_l), \tag{13}$$

where n_a is the total number of atoms in the crystal. The double summation with respect to m and n in (10) was replaced by a single summation over l ($\mathbf{R}_l$ indicating the interatomic vector $\mathbf{R}_n - \mathbf{R}_m$), since the interatomic correlation length is much smaller than the coherent length of X-rays. We call $x_i x_j |f_i - f_j|^2 \times \alpha^{ij}(\mathbf{q})$ (in electron units) or $\alpha^{ij}(\mathbf{q})$ (in Laue units) the 'SRO partial intensity' for the ij pair of atomic species.

Equation (11) is in accordance with the definition of the Warren–Cowley SRO parameter (Cowley, 1950; Hayakawa & Cohen, 1975), i.e.

$$\alpha^{ij}_l \text{ (or } \alpha^{ij}_{mn}) \equiv 1 - (P^{ij}_l / x_j), \tag{14}$$

where P^{ij}_l is the probability of finding atom j at the extremity of $\mathbf{R}_l$ with the origin on an i atom, i.e. the so-called conditional probability.

As is readily seen from (10a), the partial intensity never has the form $|\dots|^2$. This suggests that the partial intensities are not necessarily all positive.* Of course, the superposition of those partials must be positive, even if the f_i's take an arbitrary set of complex values. Thus, we can expect the existence of some restriction condition among the $\alpha^{ij}(\mathbf{q})$'s. The derivation of such a condition will be made in the next section.

Before going to the next section, we briefly mention how the separation of the composed intensity as observed into the partials is performed. The intensity is expressed as a linear equation including $N(N-1)/2$ unknowns for an N-component alloy [see (12)], for example, α^{BC}, α^{CA} and α^{AB} in an A–B–C ternary alloy, and their weighting factors ($|f_B - f_C|^2$ etc.) are functions of the atomic scattering factors, which are variable through the anomalous scattering effect near the X-ray absorption edges of the elements. Once we have at least $N(N-1)/2$ kinds of $I_{\text{SRO}}(\mathbf{q})$ measured with different wavelengths of radiation at the same point $\mathbf{q}$ in reciprocal space, we can solve the linear-equation system in principle.

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† de Fontaine used a notation $\gamma_i(m)$ for the parameter in his paper.

‡ For example, see p. 265 in Gunier's (1963) text, in which a binary case is treated.

* In an A–B binary alloy system, (10a) or (12) consists of a single term only for the A–B pair. From (7), we have $\eta^B_m = -\eta^A_m$ and (10a) has the form $|\dots|^2$. The diffuse intensity is necessarily positive.

3. Relation between the partial intensity values

3.1. *Based on a sum rule of the partial structure factors*

In § 2 we obtained an intensity equation represented in terms of η_m^i's in (10). Here, we define a sort of structure factor

$$S^i(\mathbf{q}) \equiv \sum_m \eta_m^i \exp(-2\pi i \mathbf{q} \cdot \mathbf{R}_m), \qquad (15)$$

and call $S^i(\mathbf{q})$ the 'partial structure factor'. For the $S^i(\mathbf{q})$'s ($i = A, B$ and C), we have a sum rule, from the conservation rule (7),

$$\sum_i S^i(\mathbf{q}) = 0 \qquad (16)$$

at any point $\mathbf{q}$ in reciprocal space.

We notice here that the process for deriving (10a) obeys the symmetry condition (9), which implies that the interatomic correlation function has an inversion symmetry in the real lattice. Then $S^i(\mathbf{q})S^{j*}(\mathbf{q})$ becomes real and we can rewrite (10a) as

$$I_{SRO}(\mathbf{q}) = -\sum_{i<j} |f_i - f_j|^2 \operatorname{Re}[S^i(\mathbf{q})S^{j*}(\mathbf{q})] \qquad (17)$$

explicitly so as to make the meaning apparent. By comparing (17) with (12), we have

$$n_a x_i x_j \alpha^{ij}(\mathbf{q}) = -\operatorname{Re}[S^i(\mathbf{q})S^{j*}(\mathbf{q})]. \qquad (18)$$

Thus, we can regard $-\operatorname{Re}(S^i S^{j*})$ as a partial intensity for the pair ij, hereafter represented as α_p.

From (16), we can put

$$S^A = -(S^B + S^C) \qquad (19a)$$

in the ternary case and obtain α_1 as follows. We first calculate

$$S^A S^{A*} = (S^B + S^C)(S^B + S^C)^*, \qquad (19b)$$

and then derive

$$\alpha_1 \equiv -\operatorname{Re}(S^B S^{C*}) = (|S^B|^2 + |S^C|^2 - |S^A|^2)/2. \qquad (20a)$$

Similarly we have

$$\alpha_2 \equiv -\operatorname{Re}(S^C S^{A*}) = (|S^C|^2 + |S^A|^2 - |S^B|^2)/2, \qquad (20b)$$

$$\alpha_3 \equiv -\operatorname{Re}(S^A S^{B*}) = (|S^A|^2 + |S^B|^2 - |S^C|^2)/2. \qquad (20c)$$

From $(20b) + (20c)$, we have

$$\alpha_2 + \alpha_3 = |S^A|^2. \qquad (21)$$

The right-hand side is positive or zero, and so we have

$$\alpha_2 + \alpha_3 \geq 0. \qquad (22a)$$

Similarly, we have

$$\alpha_3 + \alpha_1 \geq 0, \qquad (22b)$$

$$\alpha_1 + \alpha_2 \geq 0. \qquad (22c)$$

Since $S^i(\mathbf{q})$ can be regarded as a vector in a complex coordinate system, (16) can be drawn by a closed loop as illustrated in Fig. 1. $|S^i|$ represents the length of a side of the triangle, and the following inequalities must be satisfied:

$$|S^i| \leq |S^j| + |S^k| \quad (i \neq j \neq k \neq i). \qquad (23)$$

By expressing the $|S^i|$'s in terms of the α_p's through (21) and the other two corresponding equations for B and C atoms, and inserting them into (23), we can obtain an inequality among the α_p's. From (21) and the corresponding equations, we have

$$|S^A| = (\alpha_2 + \alpha_3)^{1/2}, \qquad (24a)$$

$$|S^B| = (\alpha_3 + \alpha_1)^{1/2}, \qquad (24b)$$

$$|S^C| = (\alpha_1 + \alpha_2)^{1/2}. \qquad (24c)$$

Substituting (24) into (23), we get

$$(\alpha_q + \alpha_r)^{1/2} \leq (\alpha_q + \alpha_p)^{1/2} + (\alpha_p + \alpha_r)^{1/2}$$
$$(p \neq q \neq r \neq p). \qquad (25)$$

Squaring both sides of (25), we obtain

$$-\alpha_p \leq [(\alpha_q + \alpha_p)(\alpha_p + \alpha_r)]^{1/2}.$$

This is always satisfied when $\alpha_p \geq 0$ for all kinds of p. For $\alpha_p < 0$, by squaring both sides we have

$$\alpha_1 \alpha_2 + \alpha_2 \alpha_3 + \alpha_3 \alpha_1 \geq 0. \qquad (26)$$

Since this is also satisfied in the case that the α_p's are all positive or zero, we finally have the result

$$x_C x_A \alpha^{CA}(\mathbf{q}) + x_A x_B \alpha^{AB}(\mathbf{q}) \geq 0 \qquad (27a)$$

[from (22a)] and simultaneously

$$x_C \alpha^{BC}(\mathbf{q})\alpha^{CA}(\mathbf{q}) + x_A \alpha^{CA}(\mathbf{q})\alpha^{AB}(\mathbf{q})$$
$$+ x_B \alpha^{AB}(\mathbf{q})\alpha^{BC}(\mathbf{q}) \geq 0 \qquad (27b)$$

[from (26)]. Equations (22b) and (22c) are naturally satisfied under the conditions of (22a) and (26) [or (27a) and (27b)], but (22a–c) enable us easily to find that *two or more of the partial intensities α_p ($p = 1$–3) must be positive and that the absolute value of a negative partial, if present, is smaller than the other two positive ones*. Fig. 2 shows sections ($\alpha_3 = $ constant) of the region limited by (22a) and (26) in α_p space. Fig. 2(a) is for the case of $\alpha_3 > 0$ and (b) for $\alpha_3 < 0$. Fig. 2 shows the possibility of the presence of a negative partial intensity and shows that two or more kinds of partial intensity are not simultaneously negative as mentioned just above.
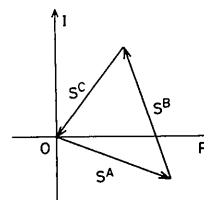

Fig. 1. Closed-loop construction with three 'partial structure factors' in the complex coordinate system.

This aspect is geometrically understood from Fig. 3. The factor $\mathrm{Re}\,(S^iS^{j*})$ implies a scalar product of the S^i and S^j vectors and three typical cases are possible. Case (a) in Fig. 3 indicates that the three vectors make an acute-angled triangle, where all the $-\mathrm{Re}\,(S^iS^{j*})$'s are positive, corresponding to the case of all $\alpha^{ij}(\mathbf{q})$'s being positive. In case (b), both $-\mathrm{Re}\,(S^BS^{C*})$ and $-\mathrm{Re}\,(S^CS^{A*})$ are positive, but $-\mathrm{Re}\,(S^AS^{B*})$ equals zero. That is, one of the partial intensities vanishes and the other two are positive. Case (c) has one obtuse angle, and we have $-\mathrm{Re}\,(S^AS^{B*})$ negative and the other two positive.

In the following subsection, we will turn to another procedure for obtaining the restriction condition in order to gain further insight into the SRO properties in a ternary alloy.

3.2. Based on the positive condition of the total intensity

The second term in (5) has the form $|\ldots|^2$ and must be positive. Therefore, the total diffuse intensity (12) must also take a positive value at every point $\mathbf{q}$ in reciprocal space.

Here, we start by considering that (12) must be positive for any kind of radiation. We make the following replacements, for simplicity:

$$x \equiv f_B - f_C, \qquad (28a)$$

$$y \equiv f_C - f_A, \qquad (28b)$$

where the atomic scattering factors can be treated as real numbers. This should lead to a true conclusion, since the real and imaginary parts contribute independently to the intensity equation in the same algebraic
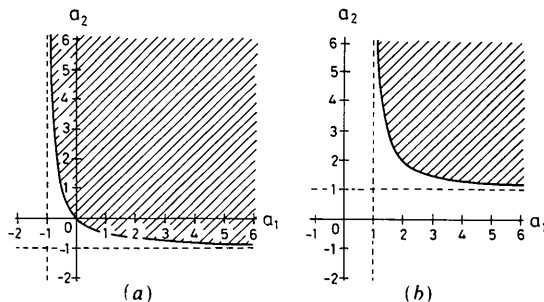
form (see Appendix). Then we have, instead of (12),

$$I_{\mathrm{SRO}}(\mathbf{q}) = \alpha_1 x^2 + \alpha_2 y^2 + \alpha_3 (x+y)^2, \qquad (29)$$

where $\alpha_1 \equiv n_a x_B x_C \alpha^{BC}(\mathbf{q})$ etc., as defined in the preceding subsection, are used. If $x \neq 0$ (i.e. $f_B \neq f_C$), division of (29) by x^2 gives

$$I_{\mathrm{SRO}}(\mathbf{q})/x^2 = (\alpha_2 + \alpha_3)t^2 + 2\alpha_3 t + (\alpha_1 + \alpha_3), \qquad (30)$$

where $t = y/x$. The condition that $I_{\mathrm{SRO}}(\mathbf{q})$ must be positive or zero leads to the following two cases, since the right-hand side of (30) is in a quadratic form with respect to t. Firstly,

$$\alpha_2 + \alpha_3 > 0 \qquad (31)$$

and simultaneously the discriminant must be negative, i.e.

$$D = \alpha_3^2 - (\alpha_2 + \alpha_3)(\alpha_1 + \alpha_3)$$
$$= -(\alpha_1\alpha_2 + \alpha_2\alpha_3 + \alpha_3\alpha_1) \leq 0; \qquad (32)$$

or, secondly, $(\alpha_2 + \alpha_3) = 0$, $\alpha_3 = 0$ and $(\alpha_1 + \alpha_3) \geq 0$, i.e.

$$\alpha_2 = \alpha_3 = 0$$

and

$$\alpha_1 \geq 0.$$

The latter case is included in the former, except for

$$\alpha_1 = \alpha_2 = \alpha_3 = 0. \qquad (33)$$

However, this is compatible with the conditions (31) and (32) by rewriting (31) as

$$\alpha_2 + \alpha_3 \geq 0. \qquad (34)$$

Thus, we achieve the same result as that [(22a) and (26)] obtained in § 3.1.

4. Discussion

The results in §§ 3.1 and 3.2 suggest the equivalence of the two methods. We shall not prove this, because it is not the aim of the present work. We insist here that the requirement of a geometrical possibility of atomic configuration on the crystal lattice ($\equiv$ consideration of the sum rule for the S^i's) is consistent with the fact that the total diffuse intensity is a positive quantity. We have further found that there is a possibility of the existence of a negative partial intensity.

The criterion achieved in the present work is available for judging whether the partial intensities deduced are in principle possible or forbidden. It is a restriction condition and is different from the criteria proposed by Cenedese et al. (1984), which were based on an error analysis. Scientists sometimes experience the risk of mistake caused by unexpected uncertainties in the measured values and in the physical (theoretical and experimental) constants used in the analysis. In the experimental studies considered

Fig. 2. Sections of the possible region of partial intensity values in α_p space. (a) The case of α_3 [$\equiv n_a x_A x_B \alpha^{AB}(\mathbf{q})$] positive, here taken as unity. (b) The case of α_3 negative.
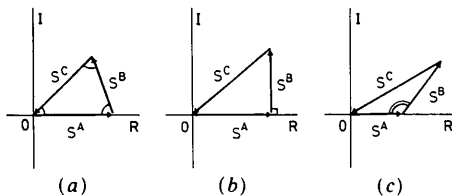
Fig. 3. Three typical relations among the 'partial structure factors' $S^i(\mathbf{q})$ ($i = A$, B and C), which are complex quantities. The vectors are drawn with respect to the phase of S^A.

here, this kind of mistake may occur when the contrast matrix of the linear equation system of diffuse intensity is not well conditioned, *i.e.* in the case that the anomalous scattering factors are much smaller than $|f_i - f_j|$ for the normal scattering. For example, the given result has the possibility of being spoiled by uncertainties in the anomalous scattering factors near the absorption edges and in the absorption coefficients of the alloy, due to EXAFS, very slight mis-setting of the monochromator for selecting wavelength, energy shifts of the absorption edges by alloying and so on, if the theoretical constants are used for analysis.

In practice, thus, many (or much more than three) kinds of radiation need to be adopted for intensity measurements and then the three partial intensities should be deduced as the optimum set from the SRO intensity data. This is conventionally performed by the least-squares fitting method. In such a method, application of the restriction condition is particularly efficient when the convergence of the fitting process is very slow and two or more sets of partial intensity values become candidates for a solution. Of those sets, the optimum ones are to be associated by abandoning the forbidden sets which never satisfy the restriction condition (27). In the next stage, we can obtain the best set of partial intensities by rejecting the intensity data measured with any radiation which leads to a result failing the criterion and then by performing the least-squares fitting analysis again with use of the remaining justifiable intensity data. We can finally give confidence to the result after exposing the sources of the uncertainties involved in the bad data rejected.

It is interesting that there can be a negative partial intensity in a ternary alloy system. We discuss its model of SRO structure and energetics elsewhere (Hashimoto, 1987a, b).

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APPENDIX

The atomic scattering factor f_i is generally expressed, with the anomalous dispersion effect taken into account, as

$$f_i = f_i^0 + f_i' + if_i'', \qquad (A1)$$

where f_i^0 implies the normal scattering factor, f_i' the real part of the anomalous scattering factor and f_i'' the imaginary part. Therefore, $|f_i - f_j|^2$ in (12) can be calculated as

$$|f_i - f_j|^2 = |(f_i^0 + f_i') - (f_j^0 + f_j')|^2 + |f_i'' - f_j''|^2. \qquad (A2)$$

The first term on the right-hand side is contributed from the real parts of the scattering factors and the second term from the imaginary parts. Let us insert this expression into (12) for the ternary alloy case. Then we have

$$I_{\text{SRO}}(\mathbf{q}) = x^2[(\alpha_2 + \alpha_3)t^2 + \alpha_3 t + (\alpha_3 + \alpha_1)]$$
$$+ X^2[(\alpha_2 + \alpha_3)T^2 + \alpha_3 T + (\alpha_3 + \alpha_1)], \qquad (A3)$$

where the partial intensities α_p are defined in § 3 and the identities

$$x \equiv (f_B^0 + f_B') - (f_C^0 + f_C'),$$
$$y \equiv (f_C^0 + f_C') - (f_A^0 + f_A'),$$
$$X \equiv f_B'' - f_C'',$$
$$Y \equiv f_C'' - f_A'',$$

and

$$t \equiv y/x,$$
$$T \equiv Y/X$$

are used. Since x^2 and X^2 are positive and independent of each other, their coefficients must both be positive in order to make $I_{\text{SRO}}(\mathbf{q})$ positive in (A3).

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