

4.2. DISORDER DIFFUSE SCATTERING OF X-RAYS AND NEUTRONS

The correction term may be important in the case of relatively small (1D) domains. As mentioned above, the structure factor of a chain molecule was neglected. The \mathbf{H} dependence of F_m , of course, obscures the intensity variation of the diffuse layers as described by (4.2.4.47a).

The matrix method developed for the case of planar disorder was adapted to 2D disorder by Scaringe & Ibers (1979). Other models and corresponding expressions for diffuse scattering are developed from specific microscopic models (potentials), e.g. in the case of $\text{Hg}_{3-6}\text{AsF}_6$ (Emery & Axe, 1978; Radons *et al.*, 1983), hollandites (Beyeler *et al.*, 1980; Ishii, 1983), iodine chain compounds (Endres *et al.*, 1982) or urea inclusion compounds (Forst *et al.*, 1987).

4.2.4.3.3. Correlations between different almost collinear chains

In real cases there are more or less strong correlations between different chains at least within small domains. Deviations from a strict (3D) order of chain-like structural elements are due to several reasons: shape and structure of the chains, varying binding forces, thermodynamical or kinetic considerations.

Many types of disorder occur. (1) Relative shifts parallel to the common axis while projections along this axis give a perfect 2D ordered net ('axial disorder'). (2) Relative fluctuations of the distances between the chains (perpendicular to the unique axis) with short-range order along the transverse \mathbf{a} and/or \mathbf{b} directions. The net of projected chains down to the ab plane is distorted ('net distortions'). Disorder of types (1) and (2) is sometimes correlated owing to non-uniform cross sections of the chains. (3) Turns, twists and torsions of chains or parts of chains. This azimuthal type of disorder may be treated similarly to the case of azimuthal disorder of single-chain molecules. Correlations between axial shifts and torsions produce 'screw shifts' (helical structures). Torsion of chain parts may be of dynamic origin (rotational vibrations). (4) Tilting or bending of the chains in a uniform or non-uniform way ('conforming/non-conforming'). Many of these types and a variety of combinations between them are found in polymer and liquid crystals and are treated therefore separately. Only some simple basic ideas are discussed here in brief.

For the sake of simplicity the paracrystal concept in combination with Gaussians is used again. Distribution functions are given by convolution products of next-nearest-neighbour distribution functions. As long as averaged lattice directions and lattice constants in a plane perpendicular to the chain axis exist, only two functions $a_{100} = a_1(xyz)$ and $a_{010} = a_2(xyz)$ are needed to describe the arrangement of next-nearest chains. Longitudinal disorder is treated as before by a third distribution function $a_{001} = a_3(xyz)$. The phenomena of chain bending or tilting may be incorporated by an x and y dependence of a_3 . Any general fluctuation in the spatial arrangement of chains is given by

$$a_{mpq} = a_1 * \dots * a_1 * a_2 * \dots * a_2 * a_3 * \dots * a_3. \quad (4.2.4.50)$$

(m -fold, p -fold, q -fold self-convolution of a_1, a_2, a_3 , respectively.)

$$w(\mathbf{r}) = \delta(\mathbf{r}) \sum_m \sum_p \sum_q [a_{mpq}(\mathbf{r}) + a_{-mpq}(\mathbf{r})]. \quad (4.2.4.51)$$

a_ν ($\nu = 1, 2, 3$) are called fundamental functions. If an averaged lattice cannot be defined, more fundamental functions a_ν are needed to account for correlations between them.

By Fourier transformations the interference function is given by

$$G(\mathbf{H}) = \sum_m \sum_p \sum_q F_1^m F_2^p F_3^q = G_1 G_2 G_3; \quad (4.2.4.52)$$

$$G_\nu = \text{Re}\{(1 + |F_\nu|)/(1 - |F_\nu|)\}.$$

If Gaussian functions are assumed, simple pictures are derived. For example:

$$a_1(\mathbf{r} + \langle \mathbf{a} \rangle) = 1/(2\pi)^{3/2} \cdot 1/(\Delta_{11}\Delta_{12}\Delta_{13}) \times \exp\{-\frac{1}{2}[(x^2/\Delta_{11}^2) + (y^2/\Delta_{12}^2) + (z^2/\Delta_{13}^2)]\} \quad (4.2.4.53)$$

describes the distribution of neighbours in the x direction (mean distance $\langle a \rangle$). Parameter Δ_{13} concerns axial, Δ_{11} and Δ_{12} radial and tangential fluctuations, respectively. Pure axial distribution along \mathbf{c} is given by projection of a_1 on the z axis, pure net distortions by projection on the $x - y$ plane. If the chain-like structure is neglected the interference function

$$G_1(\mathbf{H}) = \exp\{-2\pi^2(\Delta_{11}^2 H^2 + \Delta_{12}^2 K^2 + \Delta_{13}^2 L^2)\} \quad (4.2.4.54)$$

describes a set of diffuse planes perpendicular to \mathbf{a}^* with mean distance $1/\langle a \rangle$. These diffuse layers broaden along H with $m\Delta_{11}$ and decrease in intensity along K and L monotonically. There is an ellipsoidal-shaped region in reciprocal space defined by main axes of length $1/\Delta_{11}, 1/\Delta_{12}, 1/\Delta_{13}$ with a limiting surface given by $|F| \simeq 0.1$, beyond which the diffuse intensity is completely smeared out. The influence of a_2 may be discussed in an analogous way.

If the chain-like arrangement parallel to \mathbf{c} [equation (4.2.4.12)] is taken into consideration,

$$l(z) = \sum_{n_3} \delta(z - n_3 c);$$

the set of planes perpendicular to \mathbf{a}^* (and/or \mathbf{b}^*) is subdivided in the L direction by a set of planes located at $l \cdot 1/c$ [equation (4.2.4.15)].

Longitudinal disorder is given by $a_3(z)$ [equation (4.2.4.48), $\Delta_{33} = \Delta$] and leads to two intersecting sets of broadened diffuse layer systems.

Particular cases like pure axial distributions ($\Delta_{11}, \Delta_{12} \sim 0$), pure tangential distributions (net distortions: $\Delta_{11}, \Delta_{13} \sim 0$), uniform bending of chains or combinations of these effects are discussed in the monograph of Vainshtein (1966).

4.2.4.4. Disorder with three-dimensional correlations (defects, local ordering and clustering)

4.2.4.4.1. General formulation (elastic diffuse scattering)

In this section general formulae for diffuse scattering will be derived which may best be applied to crystals with a well ordered average structure, characterized by (almost) sharp Bragg peaks. Textbooks and review articles concerning defects and local ordering are by Krivoglaz (1969), Dederichs (1973), Peisl (1975), Schwartz & Cohen (1977), Schmatz (1973, 1983), Bauer (1979), and Kitaigorodsky (1984). A series of interesting papers on local order is given by Young (1975) and also by Cowley *et al.* (1979). Expressions for polycrystalline sample material are given by Warren (1969) and Fender (1973).

Two general methods may be applied:

(a) the average difference cluster method, where a representative cluster of scattering differences between the average structure and the cluster is used; and

(b) the method of short-range-order correlation functions where formal parameters are introduced.

Both methods are equivalent in principle. The cluster method is generally more convenient in cases where a single average cluster is a good approximation. This holds for small concentrations of clusters with sufficient space in between. The method of short-range-order parameters is optimal in cases where isolated clusters are not realized and the correlations do not extend to long distances. Otherwise periodic solutions are more convenient in most cases.

In any case, the first step towards the solution of the diffraction problem is the accurate determination of the average structure. As

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described in Section 4.2.3.2 important information on fractional occupations, interstitials and displacements (unusual thermal parameters) of atoms may be derived. Unfortunately all defects contribute to diffuse scattering; hence one has to start with the assumption that the disorder to be interpreted is predominant. Fractional occupancy of certain lattice sites by two or more kinds of atoms plays an important role in the literature, especially in metallic or ionic structures. Since vacancies may be treated as atoms with zero scattering amplitude, structures containing vacancies may be formally treated as multi-component systems.

Since the solution of the diffraction problem should not be restricted to metallic systems with a simple (primitive) structure, we have to consider the structure of the unit cell – as given by the average structure – and the propagation of order according to the translation group separately. In simple metallic systems this difference is immaterial. It is well known that the thermodynamic problem of propagation of order in a three-dimensional crystal can hardly be solved analytically in a general way. Some solutions have been published with the aid of the so-called Ising model using next-nearest-neighbour interactions. They are excellent for an understanding of the principles of order–disorder phenomena, but they can scarcely be applied quantitatively in practical problems. Hence, methods have been developed to derive the propagation of order from the diffraction pattern by means of Fourier transformation. This method has been described qualitatively in Section 4.2.3.1, and will be used here for a quantitative application. In a first approximation the assumption of a small number of different configurations of the unit cell is made, represented by the corresponding number of structure factors. Displacements of atoms caused by the configurations of the neighbouring cells are excluded. This problem will be treated subsequently.

The finite number of structures of the unit cell in the disordered crystal is given by

$$F_\nu(\mathbf{r}) = \sum_j \sum_\mu \pi_{j\mu}^\nu f_\mu(\mathbf{r} - \mathbf{r}_j). \quad (4.2.4.55)$$

Note that $F_\nu(\mathbf{r})$ is defined in real space, and \mathbf{r}_j gives the position vector of site j ; $\pi_{j\mu}^\nu = 1$ if in the ν th structure factor the site j is occupied by an atom of kind μ , and 0 elsewhere.

In order to apply the laws of Fourier transformation adequately, it is useful to introduce the distribution function of F_ν

$$\pi_\nu(\mathbf{r}) = \sum_{\mathbf{n}} \pi_{\mathbf{n}\nu} \delta(\mathbf{r} - \mathbf{n}) \quad (4.2.4.56)$$

with $\pi_{\mathbf{n}\nu} = 1$, if the cell $\mathbf{n} = n_1\mathbf{a} + n_2\mathbf{b} + n_3\mathbf{c}$ has the F_ν structure, and $\pi_{\mathbf{n}\nu} = 0$ elsewhere.

In the definitions given above $\pi_{\mathbf{n}\nu}$ are numbers (scalars) assigned to the cell. Since all these are occupied we have

$$\sum_\nu \pi_\nu(\mathbf{r}) = l(\mathbf{r})$$

with $l(\mathbf{r}) =$ lattice in real space.

The structure of the disordered crystal is given by

$$\sum_\nu \pi_\nu(\mathbf{r}) * F_\nu(\mathbf{r}). \quad (4.2.4.57)$$

$\pi_\nu(\mathbf{r})$ consists of $\alpha_\nu N$ points, where $N = N_1 N_2 N_3$ is the total (large) number of unit cells and α_ν denotes the *a priori* probability (concentration) of the ν th cell occupation.

It is now useful to introduce

$$\Delta\pi_\nu(\mathbf{r}) = \pi_\nu(\mathbf{r}) - \alpha_\nu l(\mathbf{r}) \quad (4.2.4.58)$$

with

$$\sum_\nu \Delta\pi_\nu(\mathbf{r}) = \sum_\nu \pi_\nu(\mathbf{r}) - l(\mathbf{r}) \sum_\nu \alpha_\nu = l(\mathbf{r}) - l(\mathbf{r}) = 0.$$

Introducing (4.2.4.58) into (4.2.4.57):

$$\begin{aligned} \sum_\nu \pi_\nu(\mathbf{r}) * F_\nu(\mathbf{r}) &= \sum_\nu \Delta\pi_\nu(\mathbf{r}) * F_\nu(\mathbf{r}) + l(\mathbf{r}) \sum_\nu \alpha_\nu F_\nu(\mathbf{r}) \\ &= \sum_\nu \Delta\pi_\nu(\mathbf{r}) * F_\nu(\mathbf{r}) + l(\mathbf{r}) \langle F(\mathbf{r}) \rangle. \end{aligned} \quad (4.2.4.59)$$

Similarly:

$$\Delta F_\nu(\mathbf{r}) = F_\nu(\mathbf{r}) - \langle F(\mathbf{r}) \rangle \quad (4.2.4.60)$$

$$\sum_\nu \alpha_\nu \Delta F_\nu(\mathbf{r}) = \sum_\nu \alpha_\nu F_\nu(\mathbf{r}) - \sum_\nu \alpha_\nu \langle F(\mathbf{r}) \rangle = 0.$$

Using (4.2.4.60) it follows from (4.2.4.58) that

$$\begin{aligned} \sum_\nu \pi_\nu(\mathbf{r}) * F_\nu(\mathbf{r}) &= \sum_\nu \Delta\pi_\nu(\mathbf{r}) * \Delta F_\nu(\mathbf{r}) \\ &\quad + \sum_\nu \Delta\pi_\nu(\mathbf{r}) * \langle F(\mathbf{r}) \rangle + l(\mathbf{r}) * \langle F(\mathbf{r}) \rangle \\ &= \sum_\nu \Delta\pi_\nu(\mathbf{r}) * \Delta F_\nu(\mathbf{r}) + l(\mathbf{r}) * \langle F(\mathbf{r}) \rangle. \end{aligned} \quad (4.2.4.61)$$

Comparison with (4.2.4.59) yields

$$\sum_\nu \Delta\pi_\nu(\mathbf{r}) * F_\nu(\mathbf{r}) = \sum_\nu \Delta\pi_\nu(\mathbf{r}) * \Delta F_\nu(\mathbf{r}).$$

Fourier transformation of (4.2.4.61) gives

$$\sum_\nu \Pi_\nu(\mathbf{H}) F_\nu(\mathbf{H}) = \sum_\nu \Delta\Pi_\nu(\mathbf{H}) \Delta F_\nu(\mathbf{H}) + L(\mathbf{H}) \langle F(\mathbf{H}) \rangle$$

with

$$\sum_\nu \Delta\Pi_\nu(\mathbf{H}) = 0; \quad \sum_\nu \Delta F_\nu(\mathbf{H}) = 0.$$

The expression for the scattered intensity is therefore

$$\begin{aligned} I(\mathbf{H}) &= \left| \sum_\nu \Delta\Pi_\nu(\mathbf{H}) \Delta F_\nu(\mathbf{H}) \right|^2 + |L(\mathbf{H}) \langle F(\mathbf{H}) \rangle|^2 \\ &\quad + L(\mathbf{H}) \left\{ \langle F^+(\mathbf{H}) \rangle \sum_\nu \Delta\Pi_\nu(\mathbf{H}) F_\nu(\mathbf{H}) \right. \\ &\quad \left. + \langle F^+(\mathbf{H}) \rangle \sum_\nu \Delta\Pi_\nu^+(\mathbf{H}) F_\nu^+(\mathbf{H}) \right\}. \end{aligned} \quad (4.2.4.62)$$

Because of the multiplication by $L(\mathbf{H})$ the third term in (4.2.4.62) contributes to sharp reflections only. Since they are correctly given by the second term in (4.2.4.62), the third term vanishes. Hence, the diffuse part is given by

$$I_d(\mathbf{H}) = \left| \sum_\nu \Delta\Pi_\nu(\mathbf{H}) \Delta F_\nu(\mathbf{H}) \right|^2. \quad (4.2.4.63)$$

For a better understanding of the behaviour of diffuse scattering it is useful to return to real space:

$$\begin{aligned} i_d(\mathbf{r}) &= \sum_\nu \Delta\pi_\nu(\mathbf{r}) * \Delta F_\nu(\mathbf{r}) * \sum_{\nu'} \Delta\pi_{\nu'}(-\mathbf{r}) * \Delta F_{\nu'}(-\mathbf{r}) \\ &= \sum_\nu \sum_{\nu'} \Delta\pi_\nu(\mathbf{r}) * \Delta\pi_{\nu'}(-\mathbf{r}) * \Delta F_\nu(\mathbf{r}) * \Delta F_{\nu'}(-\mathbf{r}) \end{aligned} \quad (4.2.4.64)$$

and with (4.2.4.58):

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$$i_d(\mathbf{r}) = \sum_{\nu} \sum_{\nu'} [\pi_{\nu}(\mathbf{r}) - \alpha_{\nu} l(\mathbf{r})] * [\pi_{\nu'}(-\mathbf{r}) - \alpha_{\nu'} l(\mathbf{r})] * \Delta F_{\nu}(\mathbf{r}) * \Delta F_{\nu'}(-\mathbf{r}). \quad (4.2.4.65)$$

Evaluation of this equation for a single term yields

$$[\pi_{\nu}(\mathbf{r}) * \pi_{\nu'}(-\mathbf{r}) - \alpha_{\nu} l(\mathbf{r}) * \pi_{\nu'}(-\mathbf{r}) - \alpha_{\nu'} l(\mathbf{r}) * \pi_{\nu}(\mathbf{r}) + \alpha_{\nu} \alpha_{\nu'} l(\mathbf{r}) * l(\mathbf{r})] * \Delta F_{\nu}(\mathbf{r}) * \Delta F_{\nu'}(\mathbf{r}). \quad (4.2.4.66)$$

Since $l(\mathbf{r})$ is a periodic function of points, all convolution products with $l(\mathbf{r})$ are also periodic. For the final evaluation the decrease of a number of overlapping points (maximum N) in the convolution products with increasing displacements of the functions is neglected (no particle-size effect). Then (4.2.4.66) becomes

$$[\pi_{\nu}(\mathbf{r}) * \pi_{\nu'}(-\mathbf{r}) - N \alpha_{\nu} \alpha_{\nu'} l(\mathbf{r}) - N \alpha_{\nu} \alpha_{\nu'} l(\mathbf{r}) + N \alpha_{\nu} \alpha_{\nu'} l(\mathbf{r})] * \Delta F_{\nu}(\mathbf{r}) * \Delta F_{\nu'}(-\mathbf{r}) = [\pi_{\nu}(\mathbf{r}) * \pi_{\nu'}(-\mathbf{r}) - N \alpha_{\nu} \alpha_{\nu'} l(\mathbf{r})] * \Delta F_{\nu}(\mathbf{r}) * \Delta F_{\nu'}(-\mathbf{r}). \quad (4.2.4.67)$$

If the first term in (4.2.4.67) is considered, the convolution of the two functions for a given distance \mathbf{n} counts the number of coincidences of the function $\pi_{\nu}(\mathbf{r})$ with $\pi_{\nu'}(-\mathbf{r})$. This quantity is given by $Nl(\mathbf{r})\alpha_{\nu}p_{\nu\nu'}(-\mathbf{r})$, where $\alpha_{\nu}p_{\nu\nu'}(\mathbf{r})$ is the probability of a pair occupation in the \mathbf{r} direction.

Equation (4.2.4.67) then reads:

$$[Nl(\mathbf{r})\alpha_{\nu}p_{\nu\nu'}(-\mathbf{r}) - N \alpha_{\nu} \alpha_{\nu'} l(\mathbf{r})] * \Delta F_{\nu}(\mathbf{r}) * \Delta F_{\nu'}(-\mathbf{r}) = N \alpha_{\nu} [\alpha_{\nu'} p_{\nu\nu'}(-\mathbf{r}) l(\mathbf{r})] * [\Delta F_{\nu}(\mathbf{r}) * \Delta F_{\nu'}(-\mathbf{r})] \quad (4.2.4.68)$$

with $p'_{\nu\nu'}(\mathbf{r}) = p_{\nu\nu'}(\mathbf{r}) - \alpha_{\nu'}$. The function $\alpha_{\nu} p'_{\nu\nu'}(\mathbf{r})$ is usually called the pair-correlation function $g \leftrightarrow \alpha_{\nu\nu'} |_{\mathbf{nn}'}$ in the physical literature.

The following relations hold:

$$\sum_{\nu} \alpha_{\nu} = 1 \quad (4.2.4.69a)$$

$$\sum_{\nu'} \alpha_{\nu} p_{\nu\nu'}(\mathbf{r}) = \alpha_{\nu'}; \quad \sum_{\nu'} \alpha_{\nu} p'_{\nu\nu'}(\mathbf{r}) = 0 \quad (4.2.4.69b)$$

$$\sum_{\nu} \alpha_{\nu} p_{\nu\nu'}(\mathbf{r}) = \alpha_{\nu'}; \quad \sum_{\nu} \alpha_{\nu} p'_{\nu\nu'}(\mathbf{r}) = 0 \quad (4.2.4.69c)$$

$$\alpha_{\nu} p_{\nu\nu'}(\mathbf{r}) = \alpha_{\nu'} p_{\nu'\nu}(-\mathbf{r}). \quad (4.2.4.69d)$$

Also, functions normalized to unity are in use. Obviously the following relation is valid: $p'_{\nu\nu'}(0) = \delta_{\nu\nu'} - \alpha_{\nu'}$.

Hence:

$$\alpha_{\nu\nu'} |_{\mathbf{nn}'} = \alpha_{\nu'} p'_{\nu\nu'}(\mathbf{r}) / (\delta_{\nu\nu'} - \alpha_{\nu'})$$

is unity for $\mathbf{r} = 0$ ($\mathbf{n} = \mathbf{n}'$). This property is especially convenient in binary systems.

With (4.2.4.68), equation (4.2.4.64) becomes

$$i_d(\mathbf{r}) = N \sum_{\nu} \sum_{\nu'} [\alpha_{\nu} p'_{\nu\nu'}(-\mathbf{r}) l(\mathbf{r})] * [\Delta F_{\nu}(\mathbf{r}) * \Delta F_{\nu'}(-\mathbf{r})] \quad (4.2.4.70)$$

and Fourier transformation yields

$$I_d(\mathbf{H}) = N \sum_{\nu} \sum_{\nu'} [\alpha_{\nu} P'_{\nu\nu'}(-\mathbf{H}) * L(\mathbf{H})] \Delta F_{\nu}(\mathbf{H}) \Delta F_{\nu'}^+(\mathbf{H}). \quad (4.2.4.71)$$

It may be concluded from equations (4.2.4.69) that all functions $p'_{\nu\nu'}(\mathbf{r})$ may be expressed by $p'_{11}(\mathbf{r})$ in the case of two structure factors F_1, F_2 . Then all $p'_{\nu\nu'}(\mathbf{r})$ are symmetric in \mathbf{r} ; the same is true for the $P'_{\nu\nu'}(\mathbf{H})$. Consequently, the diffuse reflections described by (4.2.4.71) are all symmetric. The position of the diffuse peak depends strongly on the behaviour of $p'_{\nu\nu'}(\mathbf{r})$; in the case of cluster formation Bragg peaks and diffuse peaks coincide. Diffuse superstructure reflections are observed if the $p'_{\nu\nu'}(\mathbf{r})$ show some damped periodicities.

It should be emphasized that the condition $p'_{\nu\nu'}(\mathbf{r}) = p'_{\nu\nu'}(-\mathbf{r})$ may be violated for $\nu \neq \nu'$ if more than two cell occupations are involved. As shown below, the possibly asymmetric functions may be split into symmetric and antisymmetric parts. From equation (4.2.3.8) it follows that the Fourier transform of the antisymmetric part of $p'_{\nu\nu'}(\mathbf{r})$ is also antisymmetric. Hence, the convolution in the two terms in square brackets in (4.2.4.71) yields an antisymmetric contribution to each diffuse peak, generated by the convolution with the reciprocal lattice $L(\mathbf{h})$.

Obviously, equation (4.2.4.71) may also be applied to primitive lattices, occupied by two or more kinds of atoms. Then the structure factors F_{ν} are merely replaced by the atomic scattering factors f_{ν} and the α_{ν} are equivalent to the concentrations of atoms c_{ν} . In terms of the $\alpha_{\nu\nu'} |_{\mathbf{nn}'}$ (Warren short-range-order parameters) equation (4.2.4.71) reads

$$I_d(\mathbf{H}) = N(\bar{f}^2 - \bar{f}^2) \sum_{\mathbf{n}} \sum_{\mathbf{n}'} \alpha_{\nu\nu'} |_{\mathbf{nn}'} \exp\{2\pi i \mathbf{H}(\mathbf{n} - \mathbf{n}')\}. \quad (4.2.4.71a)$$

In the simplest case of a binary system A, B

$$\alpha_{\mathbf{nn}'} = (1 - p_{AB|\mathbf{nn}'})/c_B = (1 - p_{BA|\mathbf{nn}'})/c_A; \\ c_A p_{AB} = c_B p_{BA}; \quad p_{AA} = 1 - p_{AB};$$

$$I_d(\mathbf{H}) = N c_A c_B (f_A - f_B)^2 \sum_{\mathbf{n}} \sum_{\mathbf{n}'} \alpha_{\mathbf{nn}'} \times \exp\{2\pi i \mathbf{H}(\mathbf{n} - \mathbf{n}')\}. \quad (4.2.4.71b)$$

[The exponential in (4.2.4.71b) may even be replaced by a cosine term owing to the centrosymmetry of this particular case.]

It should be mentioned that the formulations of the problem in terms of pair probabilities, pair correlation functions, short-range-order parameters or concentration waves (Krivoglaz, 1969) are equivalent. Using continuous electron (or nuclear) density functions where site occupancies are implied, the Patterson function may be used, too (Cowley, 1981).

4.2.4.4.2. Random distribution

As shown above in the case of random distributions all $p'_{\nu\nu'}(\mathbf{r})$ are zero, except for $\mathbf{r} = 0$. Consequently, $p'_{\nu\nu'}(\mathbf{r})l(\mathbf{r})$ may be replaced by

$$\alpha_{\nu} p'_{\nu\nu'}(\mathbf{r}) = \alpha_{\nu} \delta_{\nu\nu'} - \alpha_{\nu} \alpha_{\nu'}. \quad (4.2.4.72)$$

According to (4.2.4.59) and (4.2.4.61) the diffuse scattering can be given by the Fourier transformation of

$$\sum_{\nu} \sum_{\nu'} \Delta \pi_{\nu}(\mathbf{r}) * \Delta \pi_{\nu'}(-\mathbf{r}) * F_{\nu}(\mathbf{r}) * F_{\nu'}(-\mathbf{r}) = \sum_{\nu} \sum_{\nu'} p'_{\nu\nu'}(\mathbf{r}) * F_{\nu}(\mathbf{r}) * F_{\nu'}(-\mathbf{r})$$

or with (4.2.4.72):