An empirical test of a convolution-type structure-factor equation.

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Results of Sayre and Woolfson can be used to derive a structure-factor equation of type: $F(h) = \sum A(h,m)F(m)F(h-m)$, where the coefficients $A(h,m)$ can be calculated from the form factors of the atoms present in the structure. The equation will be discussed and an empirical test will be given.

The equation

Sayre's equation (Sayre, 1952), which holds strictly for structures consisting of one kind of non-overlapping atom, is:

$$F(h) = A(h) \sum_m F(m)F(h-m) , \qquad (1a)$$

where

$$A(h) = f(h)/[\sum_m f(m)f(h-m)] . \qquad (1b)$$

The summations in (1) are taken over the points m of the reciprocal lattice, $F(h)$ is the structure factor at the reciprocal-lattice point h and $f(h)$ is the form factor, which is the same for all the atoms of the structure. The denominator of $(1b)$ represents the form factor of the squared atom multiplied by the volume V of the elementary cell.

We will now restrict ourselves to the case where (1) is valid and construct a mapping of the crystal under consideration by replacing all its congruent atoms by parallel-orientated, congruent, artificial scatterers, which are not more extensive than the replaced atoms. The structure factors of this new model will be denoted by $F'(h)$ and the form factor of the artificial scatterer by $f'(h)$.

Now let the new form factor be derived from the old one by multiplying by a function $G(h)$

$$f'(h) = G(h)f(h) . \qquad (2)$$

Hence, as there is only one species of parallel-oriented scatterer in each of the two isotypic structures,

$$F'(h) = G(h)F(h) \qquad (3)$$

is valid, e.g. to $G(h) = -2\pi i h v$ corresponds the replacement of the scattering density $\varrho(x)$ of the structure by its derivative along the vector v:

$$\varrho(x) = 1/V \sum_h F(h) \exp (-2\pi i h x)$$

$$d\varrho(x)/dv = 1/V \sum_h (-2\pi i h v)F(h) \exp (-2\pi i h x) .$$

The scatterers of the mapping cannot penetrate each other because they are assumed to be not more extensive than the scatterers of the original structure. Therefore equation (1) applies also to the structure factors of the mapping:

$$F'(h) = A'(h) \sum_m F'(m)F'(h-m)$$
$$A'(h) = f'(h)/ [\sum_m f'(m)f'(h-m)] .$$

Inserting (2) and (3), we get a new structure-factor equation for the original structure.

$$G(h)F(h) = A'(h) \sum_m G(m)G(h-m)F(m)F(h-m) \qquad (4a)$$

$$A'(h) = G(h)f(h)/[\sum_m G(m)G(h-m)f(m)f(h-m)] . \qquad (4b)$$

Therefore every artificial scatterer which is not more extensive than the atoms of the structure under consideration

and with a form factor that can be derived by multiplying the form factor of the original structure by a function $G(m)$ over the points m of the reciprocal lattice creates a new structure-factor equation, which contains additional constraints for the determination of the phases.

We can easily generalize equation (4) to structures with different kinds of atoms (Rothbauer, 1975, p. 133) and get

$$F(h) = \sum_m A(h,m)F(m)F(h-m) . \qquad (5)$$

The coefficients $A(h,m)$ can be calculated from the form factors, $f_j(m)$, $j = 1,2, \ldots$, of the atomic species present in the structure by introducing a formalism which makes use of a method described by Woolfson (1958). For this we have to find functions $G(m)$ which transform the form factors $f_j(m)$, $j = 1,2, \ldots$, to new ones $G(m)f_j(m)$ whose Fourier transform is only different from zero where the Fourier transform of $f_j(m)$ so differs.

Empirical test

In order to test the practical usefulness of equation (5) for phase determination, equations (1) and (5) were checked empirically for several values of h using the calculated structure factors with temperature factor $B = 0$ of bayerite (Rothbauer, Zigan and O'Daniel, 1967), $Al(OH)_3$, with the series terminated at $\sin (\theta)/\lambda = 0.72$ Å^{-1}. As we have two species of scatterers Al and (OH) we need two generating mappings Γ_1 and Γ_2 (Rothbauer, 1975, pp. 125 and 133) with the property:

$$F[h,\Gamma_1(\varrho)] = 1/V \sum_m G_{11}(m)G_{12}(h-m)F(m,\varrho)F(h-m,\varrho)$$

$$F[h,\Gamma_2(\varrho)] = 1/V \sum_m G_{21}(m)G_{22}(h-m)F(m,\varrho)F(h-m,\varrho)$$

to calculate one function $A(h,m)$.

Three sets of G's were chosen as shown in Table 1, where mv is the scalar product of the vector m and a vector v.

Table 1. *The three sets of G's*

	I	II	III
$G_{11}(m)$	1	1	1
$G_{12}(m)$	1	1	1
$G_{21}(m)$	mv	$\tanh (0.3\ mv)$	$1 - 1/\cosh (0.3\ mv)$
$G_{22}(m)$	mv	1	1

Hence three functions $A(h,m)$ could be calculated to insert in the right-hand side of equation (5). In Table 2 the result of this calculation for several values of h and v is compared with the left-hand side $F(h)$ of equation (5) and with the result of Sayre's equation using averaged form factors of the atoms and squared atoms in $(1b)$.

Table 2. *Comparison of the results of equation* (5) *with those of Sayre's equation*

h (reciprocal lattice)	$F(h)$	(1)	At sin $(\theta)/\lambda = 0.72$ Å^{-1} terminated right-hand side of equation:			v (direct lattice)
			(5,I)	(5,II)	(5,III)	
(001)	54	98	50	55	55	[001]
			67		63	[100]
(110)	−29	−43	−26	−31	−30	[110]
			−24		−26	[001]
(011)	4	7	1	9	7	[011]
			2		1	[100]
(200)	3	40	20	15	17	[100]
			4		5	[001]
(202)	68	73	80	70	75	[101]
			75		70	[010]
(1$\bar{3}$2)	41	55	43	42	43	[010]
			53	48	49	[110]
(330)	61	61	71	64	63	[110]
			65		66	[001]

No solution exists for case II if h is orthogonal to v because tanh is antisymmetric and therefore $F[h, \Gamma_2(\varrho)]$ is zero and no function $A(h, m)$ can be derived.

The examples show that for practical purposes appropriate functions $G(m)$ and hence generating mappings Γ can be found which keep the errors in applying equation (5) sufficiently low.

The errors are caused by termination of the series and by using functions $G(m)$ which do not exactly fulfil the suppositions, e.g. $G_{21}(m)$, of cases II and III.

In practice, these two sources of error cannot be clearly separated because many functions can be fitted very well by allowed functions $G(m)$ in the range of reciprocal space which can be reached by measurement (Rothbauer, 1975, p. 133).

The problem of finding functions $G(m)$ which are adapted to the scatterers of a structure and to the termination of the series in order to minimize the errors must be the content of further investigations.

From the example given above we may conclude that equation (5) contains important constraints for the determination of the phases.

References

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Internal strain of GaAs. I. Longitudinal case: erratum. By C. N. KOUMELIS and E. K. ROZIS, *Department of Physics, University of Athens, Athens 144, Greece*

The results for ζ and α/β of Koumelis & Rozis [*Acta Cryst.* (1975). A**31**, 84–88] should read: $\zeta = 0.77 \pm 0.04$, $\alpha/\beta = 1.20 \pm 0.04$.

In the paper by Koumelis & Rozis (1975), the value $s_{44} = 18.6 \ 10^{-12}$ cm^2/dyne of GaAs given by Huntington (1958) is incorrect by an order of magnitude. With $s_{44} = 1.692 \times 10^{-12}$ cm^2/dyne (Cottam & Saunder, 1973), the values of ζ and α/β are: $\zeta = 0.77 \pm 0.04$, $\alpha/\beta = 1.20 \pm 0.04$. Hence, in GaAs there exists strong internal strain.

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Analysis of orientationally disordered structures. II. Examples: erratum. By WERNER PRESS, *Institut für Festkörperforschung der Kernforschungsanlage Jülich, 517 Jülich, Germany (BRD)*

Corrections are given to Press [*Acta Cryst.* (1973). A**29**, 257–263]. Two misprints in Table 2 should be corrected to $c_{61}^T = \sqrt{26} \cdot \frac{4}{9}$ and $c_{71}^T = -\sqrt{455}/9$. In the 3rd line of equation (2.1) $j_5(Q\varrho)$ should be changed to $j_6(Q\varrho)$.

All information is given in the abstract.