not involve the real characteristics of a specimen except its dispersion capability. The components associated with the real characteristics of the specimen crystal, namely the mosaic spread and its physical dimensions, must belong to a different group whose interactions are modelled by convolution.

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Extinction Corrections from Equivalent Reflections

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Abstract

Corrections for secondary extinction evaluated from the diffraction intensities for equivalent reflections with different path lengths provide an independent check on values that minimize differences between observed and calculated structure factors. Comparison of equivalent intensities also avoids any extinction-parameter bias, which originates in correlation of the extinction corrections with bonding-electron contributions to X-ray structure factors. Corrections from the comparison of equivalent reflections for several X-ray diffraction studies on small crystals of ionic compounds are markedly less than those that minimize differences between observed and calculated structure factors. The discrepancies that originate in extinction-parameter bias are exacerbated by the unfavourable form of the statistical distribution function for the residuals when differences between observed and calculated structure factors are minimized. Analysis of intensities for equivalent reflections, although more demanding experimentally, provides least-squares residuals closer to the normal distribution required for reliability in nonlinear least-squares processes.

Introduction

The kinematic theory of diffraction, readily derived from the first Born approximation, assumes that the radiation is diffracted no more than once in a crystal. At the Bragg condition, the diffracted beam is necessarily oriented so that second- and higher-order elastic coherent scattering occurs. Kinematic theory assumes the scattering contributions to be so small that second- and higher-order processes can be neglected. This assumption is valid and accurate for weak reflections from small crystals. In principle, measured structure factors for stronger reflections may be corrected for high-order components to the scattering by perturbation techniques, if kinematic theory is obeyed approximately.

Estimates of extinction corrections independent of any structural model have been reported for crystals in the form of large slabs cut parallel to a desired

face (Bragg, James & Bosanquet, 1921; Göttlicher, 1968; Göttlicher & Knöchel, 1980; Göttlicher & Vegas, 1988). As it is assumed that extinction can be modelled by an exponential function, these estimates involve a linear extrapolation to zero path length from a plot of log I *versus* t, the total beam path length. This method can be applied to measurements from small crystals using standard diffractometry, but the extended extrapolations required in that case limit the accuracy of the technique (Spadaccini, 1989).

One aspect of the Göttlicher & Vegas (1988) study of $MgCO_3$ is particularly relevant here. In data corrected for secondary extinction by extrapolation, the calculated structure factor F_c for the strong reflections was systematically larger than the observed value F_o. The authors attributed this to primary extinction but did not provide independent evidence to support the diagnosis.

A number of correction formulae for analysing extinction in small crystals, based on different descriptions of the scattering process, have been devised. The widely applied treatment given by Zachariasen (1967) has been extended by Becker & Coppens (1974). Their correction formulae for secondary extinction contain parameters related to the mosaic distribution of microdomains, such as its angular half-width, which must be determined in order to evaluate the extinction corrections.

In most analyses of extinction for small crystals so far, the parameters in the correction formulae have been determined by least-squares minimization of a weighted sum of squares of differences between observed and calculated structure factors. The premises that justify least-squares processes (Yamane, 1973) are not necessarily valid when determining extinction corrections as part of the structure refinement. Thus, it is not uncommon for a modest change to the weight of a strong reflection to change the extinction corrections by amounts that standard tests indicate to be significant.

On one hand, inaccurate extinction corrections are of minor importance when determining structural geometry, because correlation between extinction parameters and atomic coordinates in least-squares analyses of diffraction data is weak. On the other hand, the accuracy of Fourier coefficients for strong low-order Bragg reflections, which are crucial when measuring deformation densities, depends strongly on the extinction corrections. These corrections must be reliable for charge-density studies.

Reliable extinction corrections, which require high accuracy in the measured diffraction intensities, also depend on the validity of the statistical procedures used when determining extinction-parameter values from the measurements. The principles are not restricted to any particular form of extinction formula. Their consequences can therefore be illustrated by reference to the Zachariasen (1967) treatment, which is mathematically convenient because of its simplicity.

Zachariasen's theory

The basic expression is

$$F_k^2 = y^{-1} F_m^2,$$

where F_k^2 is the kinematic structure factor squared, y^{-1} the extinction correction and F_m^2 the measured structure factor squared before correction.

In the isotropic secondary (type I) theory of Zachariasen employed in this illustration, the extinction factor has the simple form

$$y = (1+2x)^{-1/2} = (1+2r^*\bar{T}Q)^{-1/2}, \qquad (1)$$

where $\bar{T}$ is the mean path length and, for unpolarized X-rays,

$$Q = (e^4/m^2c^4V^2)(\lambda^3/\sin 2\theta) \times [(1+\cos^4 2\theta)/(1+\cos^2 2\theta)]F_k^2,$$

where e, m, c, V, λ and θ are the electron charge, electron mass, velocity of light, unit-cell volume, radiation wavelength and Bragg angle, respectively.

Thus, $x = r^*\bar{T}G(s)F_k^2$, where s is the reciprocal-lattice vector and all the geometric factors and conversion constants are contained in the factor

$$G(s) = (e^2/mc^2V)^2\lambda^3(p_2L/p_1).$$

Here, L is the Lorentz factor, $1/\sin 2\theta$, and $p_n = 1+\cos^{2n} 2\theta$. This analysis readily extends to polarized X-rays and neutron diffraction, by substitution of the appropriate expression for $G(s)$.

Least-squares structure refinements

The standard least-squares procedure for analysing crystal structures minimizes a residual of the type

$$R(F) = \sum_i w(F)(|F_o| - |F_c|)^2$$

or

$$R(F^2) = \sum_i w(F^2)(F_o^2 - F_c^2)^2,$$

where the summations are over the independent reflections and the weights are reciprocals of the variances

$$w(F) = \sigma^{-2}(F_o) \quad \text{and} \quad w(F^2) = \sigma^{-2}(F_o^2).$$

The conditions that apply to such analyses are those described by Yamane (1973). Structural parameters determined from the corresponding normal equations

will be best linear unbiased estimates with minimum variance if the residuals $w^{1/2}(F)(|F_o|-|F_c|)$ or $w^{1/2}(F^2)(F_o^2-F_c^2)$ are distributed randomly about zero, by the Gauss–Markov theorem. If the residuals obey the stronger condition of being normally distributed about zero, the minimum-variance parameters satisfy the principle of maximum likelihood. The stronger condition can be guaranteed if the residuals fulfil the premises of the central limit theorem, which are that each residual receives comparable contributions from a large number of sources, with minimal constraints on the statistical distribution for each component.

It can reasonably be argued that the central limit theorem holds for least-squares refinements of sets of structure factors with errors dominated by Poisson counting statistics, having comparable contributions from systematic errors in the measurements and from the shortcomings of the theoretical model for the structure factors. In standard crystal structure analyses, this holds well for the high-order Bragg reflections, which predominantly determine atomic positions and vibration amplitudes. As high-order reflections are not much affected by extinction, or by the redistribution of electron density due to chemical bonding, standard methods of statistical inference apply to most determinations of atomic positions and vibration amplitudes.

It is less obvious that the central limit theorem applies to strong low-order structure factors with large extinction contributions that dominate a parameter determination. The effect of extinction on structure factors is very far from normally distributed. Every extinction contribution to $(|F_o|-|F_c|)$ has a negative sign. It is evident from Zachariasen's derivation that the $(1+2x)^{-1/2}$ form for y in (1) holds only in the limit that $2x<1$, for all structure factors. If that inequality is satisfied for the strong Bragg reflections, which are very limited in number for most structures, then $2x \ll 1$ for most structure factors. The effects of extinction will be appreciable only for the few large structure factors.

What is relevant to the reliability of the nonlinear least-squares analysis, of course, is not the total extinction correction, but the distribution of the residuals after extinction corrections have been applied. For the statistical analysis to be valid, the residuals must be linear functions of errors of the order of the uncertainty in the extinction parameters. Hampel, Ronchetti, Rousseeuw & Stahel (1986), when discussing conditions under which the Gauss–Markov condition could provide the minimum variance for all unbiased estimators, comment: 'Linearity is a drastic restriction. The least squares estimator is optimal in the class of all unbiased estimators only if the errors are normally distributed. Restriction to linear estimators can be justified only by normality (or simplicity). The normal model is never exactly true, and in the presence of small departures from the normality assumption on the errors the least squares procedures (estimators and tests) lose efficiency drastically'.

The residuals for the weak reflections are small. For the strong reflections, very precise corrections are necessary if all their residuals are to fall within the linear range. How can we determine whether the extinction corrections are sufficiently accurate to ensure that an unbiased normal distribution has been achieved? In the case of X-ray diffraction, the parameters for the standard method of determining extinction corrections will be biased to some degree by real differences between $|F_o|$ and $|F_c|$ for the strong reflections, resulting from the redistribution of electrons by bonding. It is unreasonable to argue that such differences are small when correcting for extinction in a charge-density experiment that has their precise measurement as its principal objective. This difficulty is further compounded if the term F_k^2 within the extinction factor $y=(1+2r^*F_k^2Q)^{-1/2}$ is approximated by F_c^2 when r^* is determined as part of a crystal-structure-factor refinement – an approximation that is sometimes used to simplify the normal equations when determining r^* during standard least-squares structure analyses.

We seek a check of the validity of the extinction parameters from standard structure refinements that is independent of model structure factors. Given any extinction formalism such that the kinematic structure can be expressed as an explicit function of the measured structure factor, extinction corrections with that independence can be determined. These provide a check on extinction corrections determined by standard methods. These unbiased estimators may be useful in their own right, if they are sufficiently precise.

r^* from equivalents

The first stage in seeking model-independent extinction corrections is to eliminate any dependence of the extinction formula on a model for the structure. The basic Zachariasen type-I equation rearranges to

$$x^2=(1+2x)[r^*\bar{T}G(s)F_m^2]^2,$$

which solves for $x=\chi^2+\chi(\chi^2+1)^{1/2}$, where $\chi=r^*\bar{T}G(s)F_m^2$.

In this form, the extinction factor $y=(1+2x)^{-1/2}$ is independent of the calculated structure factor.

If the intensities for symmetry-equivalent reflections with different path lengths have been measured, the Zachariasen secondary-extinction coefficient r^* may be determined by analysing the variation among the absorption-corrected intensities. The least-

squares sum to be minimized in this procedure is

$$R_e = \sum_i \left\{ \sum_e w_e [F_k^2(e) - \langle F_k^2 \rangle_e]^2 \right\}$$
$$= \sum_i \left(\sum_e (w_e F_k^2 F_k^2) - \left\{ \left[\sum_e w_e F_k^2(e) \right]^2 \Big/ \sum_e w_e \right\} \right), \quad (2)$$

where $\langle F_k^2 \rangle_e = \sum_e w_e F_k^2(e) / \sum_e w_e$ and $w_e = \sigma^{-2}(F_m^2)_e$ is the reciprocal of the variance of the measured structure factor squared. The inner summations are over the equivalent reflections. The outer summations are over all independent reflections in the sample. The minimum variance occurs for a value of r^* at which the first derivative of the variance quadratic R_e vanishes.

For simplicity, r^* is first assumed to be isotropic and so is a scalar variable. Minimizing R_e with respect to r^* requires that $\partial R_e / \partial r^* = 0$, which on expanding R_e about a trial value of r^* yields the correction

$$\delta r^* = \sum_i [(\Sigma_1 \Sigma_3 / \Sigma_2) - \Sigma_4] \times \left(\sum_i \{ \Sigma_5 + \Sigma_6 - [(\Sigma_3^2 + \Sigma_1 \Sigma_7)/\Sigma_2] \} \right)^{-1}, \quad (3)$$

which updates the r^* value assumed initially. The procedure can be iterated to convergence. After inversion of the normal-equations matrix for the least-squares procedures, the reciprocal of the variance is

$$\sigma^{-2}(r^*) = \sum_i \Sigma_5 + \Sigma_6 - [(\Sigma_3^2 + \Sigma_1 \Sigma_7)/\Sigma_2]. \quad (4)$$

The summations in (3) and (4) are

$$\Sigma_1 = \sum_e w_e F_k^2 = \sum_e w_e F_m^2 (x/\chi)$$

$$\Sigma_2 = \sum_e w_e$$

$$\Sigma_3 = \sum_e w_e (\partial F_k^2 / \partial r^*) = \sum_e w_e F_m^2 [x / r^* (\chi^2 + 1)^{1/2}]$$

$$\Sigma_4 = \sum_e w_e F_k^2 (\partial F_k^2 / \partial r^*) = \sum_e w_e F_m^2 F_m^2 [x^2 / \chi r^* (\chi^2 + 1)^{1/2}]$$

$$\Sigma_5 = \sum_e w_e (\partial F_k^2 / \partial r^*)(\partial F_k^2 / \partial r^*) = \sum_e w_e F_m^2 F_m^2 [x^2 / r^{*2} (\chi^2 + 1)]$$

$$\Sigma_6 = \sum_e w_e F_k^2 (\partial^2 F_k^2 / \partial r^{*2}) = \sum_e w_e F_m^2 F_m^2 [x\chi / r^{*2} (\chi^2 + 1)^{3/2}]$$

$$\Sigma_7 = \sum_e w_e (\partial^2 F_k^2 / \partial r^{*2}) = \sum_e w_e F_m^2 [\chi^2 / r^{*2} (\chi^2 + 1)^{3/2}].$$

As each term Σ_4, Σ_5, Σ_6, $\Sigma_1\Sigma_3$, Σ_3^2 and $\Sigma_1\Sigma_7$ in these expressions is quadratic in F_m^2, the stronger reflection intensities should dominate the analysis.

To apply this method to an alternative extinction formula, r^* is replaced by the appropriate alternative extinction parameter and the right-hand expressions for Σ_1, Σ_3, Σ_4, Σ_5, Σ_6 and Σ_7 are adapted to include the corresponding derivative expression. To extend the treatment to anisotropic extinction, r^* is replaced by the equivalent second-rank tensor, derivatives of F_k^2 with respect to the unique elements of that tensor are formed, sums corresponding to terms Σ_3, Σ_4, Σ_5, Σ_6 and Σ_7 are evaluated and the set of simultaneous equations equivalent to (3) is solved.

In the application of the Zachariasen procedure, it is convenient to rearrange the expression for F_m^2 to obtain F_k^2 as

$$F_k^2 = [1 + 2r^* \bar{T} G(s) F_k^2]^{1/2} F_m^2 = [\chi + (\chi^2 + 1)^{1/2}] F_m^2,$$

while the variance in the squared kinematic structure factor determined is

$$\sigma^2(F_k^2) = \{2\chi + [\chi^2/(\chi^2+1)^{1/2}] + (\chi^2+1)^{1/2}\}^2 \sigma^2(F_m^2) + F_m^2 F_m^2 (\chi / r^*)^2 \times \{1 + [\chi/(\chi^2+1)^{1/2}]\}^2 \sigma^2(r^*).$$

The validity of the method was verified by analysing simulated data with a stand-alone program. Intensities were generated for a range of independent kinematic structure factors assuming various degrees of extinction for equivalent reflections with different $\bar{T}$ values. Equation (3) was iterated until the shift δr^* was less than 0.001 times $\sigma(r^*)$. In all cases, minimization of the expression defined in (2) converged rapidly towards the correct r^* value. Tests with noise added to the initial data confirmed that the r^* determination was not excessively sensitive to random error.

The stand-alone routine was then tested on real diffraction data for several crystals, including small sets consisting of strong reflections only and larger sets consisting of both strong and weak intensities. The results confirmed that the refinement process is dominated by the extinction-affected intense reflections. The much larger number of weaker reflections contribute very little to the least-squares normal equations in these analyses, as expected.

Applications

This procedure, re-implemented by du Boulay (1992) to the specifications of the *XTAL* system of crystallographic programs (Hall & Stewart, 1990), has been

applied to X-ray diffraction studies of α-Al_2O_3, $KZnF_3$, $SrTiO_3$, $CaTiO_3$, $YAlO_3$, $YFeO_3$, $LaAlO_3$, K_2SiF_6, K_2PdCl_4 and Y_2BaCuO_5. The maximum dimension of each crystal specimen was of the order of 50 μm. Crystal dimensions determined optically for the absorption corrections in these analyses were verified by carefully measuring the specimens with a scanning electron microscope.

For the structures containing atoms with atomic number 30 or less, none of the extinction corrections determined by the comparison of equivalent reflections differed markedly from unity, whereas minimizing the residual based on calculated structure factors gave what appeared to be appreciable corrections in most cases.

Data derived from strong Mo $K\alpha$ reflections given in Table 1 are for the following compounds containing heavier atoms:

$LaAlO_3$, $a=b=c=7.582$ (2) Å, pseudocubic, space group $Fm\bar{3}m$, $R_{int}=0.027$ for 6890 measured reflections, $R=0.029$, $wR=0.029$ for 155 unique reflections;

$YAlO_3$, $a=5.331$ (2), $b=7.370$ (2), $c=5.179$ (3) Å, orthorhombic, space group *Pnma*, $R_{int}=0.056$ for 6890 measured reflections, $R=0.057$, $wR=0.021$ for 1122 unique reflections;

$YFeO_3$, $a=5.594$ (2), $b=7.601$ (2), $c=5.281$ (3) Å, orthorhombic, space group *Pnma*, $R_{int}=0.069$ for 7562 measured reflections, $R=0.062$, $wR=0.029$ for 1240 unique reflections.

The higher R_{int} and R indices for the *Pnma* strucures reflect the high proportion of systematically weak reflections for these distorted perovskite compounds.

Typically, 2% precision in the extinction factor y is achieved with a ±25% variation in the path length $\bar{T}$. The method is not hypersensitive to the weights of particular independent reflections. In the absence of strong extinction anisotropy, the residuals for each of the reflections equivalent to the same independent reflection have comparable expansion values, which fulfils the premises of the central limit theorem.

Results for the ten structures have the general characteristics that:

(i) extinction parameters determined as part of the structure refinement are hypersensitive to the weights of the strong reflections with large $w^{1/2}(F)(|F_o|-|F_c|)$ residuals, which dominate the least-squares structure refinement and have a non-normal distribution;

(ii) extinction corrections from the comparison of equivalent reflections are usually less severe than those determined from minimizing $R(F)$, as occurs for $YAlO_3$ and $LaAlO_3$, the first and second examples in Table 1. The third example, $YFeO_3$, where the two types of correction are comparable, is the only exception encountered so far. High significance should not be attached to one exception because of the uncertainties identified in (i).

Table 1. *Miller indices, absorption-corrected intensities I, path lengths, extinction factors y for independent Bragg reflections from the comparison of equivalent reflections and mean extinction factors $\bar{y}$ from standard least-squares refinements for perovskite structures*

h	k	l	I	$\bar{T}(\mu)$	y	$\bar{y}$
$LaAlO_3$						
−4	0	0	857692	37	0.982 (12)	
0	−4	0	852560	36	0.982 (12)	
0	0	−4	837064	45	0.978 (14)	0.92
4	0	0	850656	37	0.982 (12)	
0	4	0	838469	36	0.982 (11)	
0	0	4	815571	45	0.979 (14)	
$YAlO_3$						
−1	−2	−1	1067376	44	0.931 (23)	
−1	2	−1	1031622	45	0.932 (23)	
1	−2	−1	1038928	52	0.921 (26)	
1	2	−1	969223	59	0.917 (27)	0.77
−1	−2	1	970630	59	0.916 (27)	
1	−2	1	1032689	45	0.932 (23)	
−1	2	1	1016095	52	0.922 (26)	
1	2	1	1089939	44	0.929 (23)	
$YFeO_3$						
−1	−2	−1	425114	34	0.809 (18)	
−1	2	−1	468997	20	0.868 (13)	
1	−2	−1	455220	24	0.849 (14)	
1	2	−1	433802	29	0.829 (16)	0.85
−1	−2	1	433414	29	0.825 (16)	
1	−2	1	474866	20	0.866 (13)	
−1	2	1	476012	24	0.842 (15)	
1	2	1	435901	34	0.804 (18)	

Fig. 1(*a*) depicts secondary-extinction contributions ΔF_{ext} to the structure-factor magnitudes $|F_o|$ determined by analysing intensities of equivalent reflections for the small crystal of $SrTiO_3$ (Maslen, Spadaccini, Ito, Marumo & Satow, 1993*b*), an ideal perovskite with a cubic $Pm3m$ structure. The likelihood that refinement of that structure would satisfy the Gauss–Markov conditions for validity of the least squares can be roughly assessed from Fig. 1(*a*). If extinction corrections are determined by least-squares minimization of differences between observed and model structure factors, the least-squares refinement will be dominated by the few strong reflections for which ΔF_{ext} is large. Unless extinction is modelled with exceptional accuracy, it is unlikely that their residuals will be distributed randomly, as assumed when the least-squares principle is invoked. It is correspondingly unlikely that extinction corrections determined using coefficients distributed like those in Fig. 1(*a*) would be reliable.

Fig. 1(*b*) depicts the difference coefficients $\Delta F=|F_o|-|F_c|$ to $SrTiO_3$ X-ray structure factors after experimental extinction corrections from equivalent reflections have been applied, to generate F_o values by averaging the equivalent reflections. The distribution function for ΔF broadly resembles that for ΔF_{ext} in Fig. 1(*a*), to within a scale factor. This will result in a high degree of correlation of the extinction correction with structure-factor changes caused by bonding. Because of that correlation, the coefficients

determining the extinction correction are biased significantly by the signal that is being measured. It is correspondingly difficult to distinguish unreliable extinction corrections from errors in measured deformation densities when the electron density and extinction are determined simultaneously.

Those who prefer the standard least-squares-refinement procedure may contend that the form of the residuals depicted in Fig. 1(*b*) is due to underestimation of extinction resulting from undiagnosed bias in the determination of r^* by the minimization of differences between equivalent reflections. That argument implies a preference for the hypothesis of equality of F_o to F_c, for which there is no clear theoretical justification, *versus* that of the equality of intensities for equivalent reflections, which is firmly supported by theory.

The low r^* vaues determined from equivalent intensities measured with Mo $K\alpha$ radiation for α-Al_2O_3 (Maslen, Streltsov, Streltsova, Ishizawa, Marumo & Satow, 1993), the ideal cubic perovskites $KZnF_3$ and $SrTiO_3$ (Maslen, Spadaccini, Ito, Marumo & Satow, 1993*a*, *b*) and for K_2PdCl_4 (Hester, Maslen, Spadaccini, Ishizawa & Satow, 1993) have been checked with diffraction measurements using synchrotron radiation at two wavelengths. Scaled structure factors for the strong reflections were not diminished appreciably at longer wavelengths, as would be expected if the measurements were affected as strongly by extinction as is indicated by the standard structure refinements. Because the extinction corrections do not change with wavelength, the hypothesis that the discrepancies between extinction corrections from equivalent reflections and those from structure refinements are due to extinction is unconvincing. A more unified picture of the electron density in $KZnF_3$ and $SrTiO_3$ emerges when the F_o values corrected for extinction by comparison of equivalent reflections are taken at face value (Maslen, Spadaccini, Ito, Marumo & Satow, 19983*a*, *b*).

After correcting their $MgCO_3$ data for extinction using linear extrapolation with large crystals, Göttlicher & Vegas (1988) reported that F_c was usually larger than F_o for the stronger reflections. Because this phenomenon also occurs for our small perovskite crystals to an extent that is independent of wavelength, Göttlicher & Vegas's explanation of the F_o *versus* F_c discrepancies in $MgCO_3$ in terms of primary extinction must therefore be questioned.

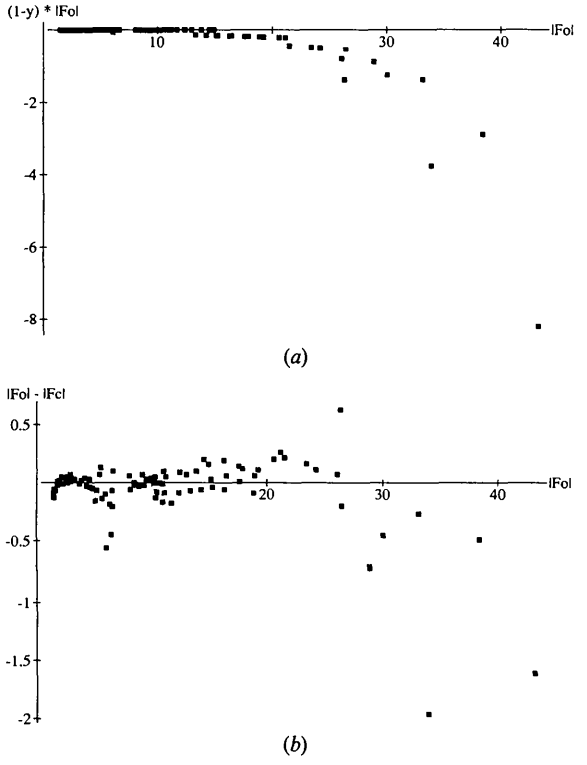

Fig. 1. (*a*) Extinction correction $\Delta F_{ext} = (1-y)F_o$ and (*b*) difference density coefficient $\Delta F = |F_o| - |F_c|$, in electrons, *versus* $|F_o|$ for the symmetry-independent reflections in $SrTiO_3$, with y determined from the symmetry-related reflections.

Concluding remarks

Minimization of the differences between intensities for equivalent reflections allows extinction corrections to be determined directly from the intensities for reflections with the same structure factor but with different path lengths. This procedure eliminates any dependence of the extinction correction on the structure model and the difference density redistribution. It requires data with precision sufficient to describe the variation of extinction with path length. It can be adapted to any extinction model, isotropic or anisotropic.

The formulation presented above is suited to high-symmetry structures with a large number of equivalent reflections, for which the Gauss-Markov conditions for validity in a least-squares procedure are approximated closely. For lower symmetry structures, equivalent information can be obtained from ψ scans for the strong reflections, provided the crystal shape is sufficiently anisotropic to provide a satisfactory range of $\bar{T}$ values for the larger structure factors.

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One-Dimensional Quasilattices: Fractally Shaped Atomic Surfaces and Homometry

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Abstract

The section method was used to determine the atomic surfaces of one-dimensional quasilattices generated by means of deflation rules with the scale factor $\mu=\tau^{-n}$, where $\tau=(1+5^{1/2})/2$ and $1\le n\le 3$. The quasilattices satisfy the condition that the distances between neighboring points take on just the two values of the original Fibonacci quasilattice. Evidence suggests that the atomic surfaces are regular fractals, whose width depends on both length and frequency of periodic inclusions. The frequencies of interpoint distances as well as squared Fourier transforms and simulated diffraction patterns of the quasilattices have been calculated and will be discussed. Generalization of the fractal development of atomic surfaces yields homometric quasicrystals.

1. Introduction

Since the discovery of tiles that force nonperiodic tilings (Penrose, 1974, 1979) and of quasicrystals (Shechtman, Blech, Gratias & Cahn, 1984), much experimental and theoretical work has been focused on the discovery of new types of quasicrystals [for a review the reader is referred to Steurer (1990)] and on several methods for the generation of quasilattices:

(i) deflation procedures (Penrose, 1974, 1979; de Bruijn, 1981; Socolar, 1989);

(ii) grid methods (de Bruijn, 1981; Gähler & Rhyner, 1986; Socolar & Steinhardt, 1986; Korepin, Gähler & Rhyner, 1988);

(iii) the projection and section method (de Bruijn, 1981; Kramer & Neri, 1984; Duneau & Katz, 1985; Kalugin, Kitaev & Levitov, 1985; Elser, 1986; Bak, 1986; Janssen, 1986).

One direction of theoretical research is to increase understanding of the higher-dimensional space-group symmetries (Janner, 1991; Janssen, 1991, 1992). Another direction is to investigate the possibilities of decorating the quasilattices in physical space (Henley, 1986; Kumar, Sahoo & Athithan, 1986) constructed by means of either the projection or the section method. However, surprisingly little attention has been paid to modified window functions (the projection method) or atomic surfaces (the section method) (Zia & Dallas, 1985; Bak, 1986; DiVincenzo, 1986; Elser, 1986). The purpose of this paper is to investigate which kinds of windows (atomic surfaces) correspond to quasilattices obtained by means of 'simple' deflation rules* and what the corresponding effects are on the squared Fourier transforms and diffraction patterns of these quasilattices.

2. Deflation rules

The one-dimensional quasilattices described in this paper have been generated by means of deflation rules with the scale factor $\mu=\tau^{-n}$ $[\tau=(1+5^{1/2})/2]$ with $1\le n\le 3$. They satisfy the condition that the lengths of line segments joining adjacent points take

* 'Simple' deflation rule means that every line segment of a given length is decomposed in the same way.