RESEARCH PAPERS

Acta Cryst. (1994). A**50**, 686–690

A Unified Treatment of Small-Angle X-ray Scattering, X-ray Refraction and Absorption using the Rytov Approximation

By T. J. Davis

CSIRO Division of Materials Science and Technology, Private Bag 33, *Rosebank MDC, Clayton, Victoria* 3169, *Australia*

(*Received* 31 *January* 1994; *accepted* 30 *March* 1994)

Abstract

The Helmholtz wave equation for X-rays in a dielectric medium is solved using the Rytov approximation for the X-ray phase perturbation. It is shown that under appropriate limits the solution yields the equations for small-angle X-ray scattering, X-ray refraction and absorption. This demonstrates that the Rytov approximation provides a unified treatment of small-angle X-ray phenomena.

Introduction

Small-angle X-ray scattering provides information about the size and the distribution of particles in a scattering medium. The usual formulation describing this scattering (Guinier & Fournet, 1955; Porod, 1982) is equivalent to that obtained in the first Born approximation in the quantum theory of scattering (Gottfried, 1966). As the particle size increases, the scattering angle decreases and it becomes increasingly difficult to separate the scattered X-rays from the unscattered beam. In this regime, the first Born approximation begins to fail. For particles very much larger than the X-ray wavelength, it is more realistic to describe the interaction in terms of refraction rather than scattering.

In the early years of small-angle scattering, it was unclear whether the divergence of an X-ray (or neutron) beam as it passed through a finely divided material was due to diffraction or refraction (Weiss, 1951). The two competing theories were that of Rayleigh–Gans (Rayleigh, 1911; Gans, 1925), in which the scattering was due to diffraction, and that of von Nardroff (1926), in which refraction was deemed to be responsible. The problem was solved in 1946 by Van de Hulst (1957), who showed that both effects were limiting cases of the correct approach to the problem. More recently, a unified treatment of small-angle neutron scattering was developed for the single-particle cross section, encompassing the transition from diffraction to refraction (Berk & Hardman-Rhyne, 1986).

In this paper, an alternative treatment of the problem is given using the Rytov approximation (Rytov, 1937; from reference 11 in Chernov, 1960) for the phase shift in the X-ray beam as it traverses a dielectric medium. This approximation is well known in wave theory and optics and has similarities with the Born approximation (Devaney, 1981), although it is generally considered to be more accurate (Keller, 1969; Oristaglio, 1985). The phase perturbation is obtained as a solution to the Helmholtz wave equation for the medium. It is shown that the Rytov approximation leads to small-angle scattering in the limit of far-field observation and that it describes X-ray refraction and absorption in large particles at short wavelengths. In this way, the relationship between X-ray scattering and X-ray refraction is emphasized.

The Helmholtz wave equation

The Helmholtz equation for the interaction of X-rays in a non-magnetic dielectric material can be obtained from the following Maxwell equations:

$$\mathbf{D} = (1+\chi)\mathbf{E}, \tag{1}$$

$$(1/c)\partial\mathbf{D}/\partial t = \nabla\times\mathbf{H}, \tag{2}$$

$$(1/c)\partial\mathbf{H}/\partial t = -\nabla\times\mathbf{E}, \tag{3}$$

$$\nabla\cdot\mathbf{D} = 0. \tag{4}$$

The dielectric susceptibility $\chi(\mathbf{r})$ for X-rays is very small and it is taken here in an average sense over a large volume of the dielectric, such that its variations with position $\mathbf{r}$ are very much smaller than the X-ray wavenumber k, *i.e.* $|\nabla\chi/\chi| << k$. This is equivalent to expanding $\chi(\mathbf{r})$ as a Fourier series in reciprocal-lattice vectors over a local region about $\mathbf{r}$, as is done in Takagi's (1969) theory of imperfect crystal diffraction, and retaining only the zeroth-order coefficient $\chi_0(\mathbf{r})$. This assumes that the incident X-rays are far

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from a lattice diffraction condition. Then, the spatial derivatives of $\chi(\mathbf{r})$ can be neglected and (1), (2) and (3) lead to the wave equation

$$(1+\chi)(1/c^2)\partial^2\mathbf{D}(\mathbf{r},t)/\partial t^2 = -\nabla\times\nabla\times\mathbf{D}(\mathbf{r},t) = \nabla^2\mathbf{D}(\mathbf{r},t), \tag{5}$$

where the vector identity $\nabla\times\nabla\times\mathbf{D} = \nabla(\nabla\cdot\mathbf{D}) - \nabla^2\mathbf{D}$ and (4) have been used.

In the usual way, $\mathbf{D}(\mathbf{r},t)$ is written as a product of a space-dependent amplitude $\mathbf{D}(\mathbf{r})$ and a time-dependent phase with angular frequency ω. If the vacuum wave number is defined as $k=\omega/c$, then the equation for the wave amplitude is the Helmholtz equation

$$\nabla^2\mathbf{D}(\mathbf{r}) + k^2[1+\chi(\mathbf{r})]\mathbf{D}(r) = 0. \tag{6}$$

This equation must be satisfied for both vector components separately, so that only the scalar Helmholtz equation need be considered. Furthermore, it is assumed that the scattering angles are small so that polarization effects can be ignored. The factor $(1+\chi)$ is the square of the refractive index, n. In a homogeneous material, (6) yields a plane-wave solution with a modified wave vector $k(1+\chi)^{1/2}$.

Eikonal equation and the Rytov approximation

An approximate solution to (6) can be found by introducing a position-dependent optical path $\varphi(\mathbf{r})$, or eikonal (Born & Wolf, 1964; Gottfried, 1966),

$$D(\mathbf{r}) = D_0\exp[ik\varphi(\mathbf{r})], \tag{7}$$

where D_0 is the wave amplitude specified at some fixed point. In general, the eikonal is complex and controls both the phase and the amplitude variations induced by the medium. When (7) is inserted in (6), it is found that the eikonal obeys a Riccati equation in $\nabla\varphi(\mathbf{r})$,

$$(i/k)\nabla^2\varphi(\mathbf{r}) - [\nabla\varphi(\mathbf{r})]^2 + [1+\chi(\mathbf{r})] = 0. \tag{8}$$

This equation is impossible to solve exactly when $\chi(\mathbf{r})$ is an arbitrary function of $\mathbf{r}$. Instead, consider the phase perturbation

$$\varphi(\mathbf{r}) = \varphi_0(\mathbf{r}) + \delta\varphi(\mathbf{r}), \tag{9}$$

where $\varphi_0(\mathbf{r})$ satisfies the vacuum eikonal equation,

$$(i/k)\nabla^2\varphi_0(\mathbf{r}) - [\nabla\varphi_0(\mathbf{r})]^2 + 1 = 0. \tag{10}$$

Since this equation describes the vacuum propagation of the wave, its solution is trivial:

$$k\varphi_0(\mathbf{r}) = \mathbf{k}\cdot\mathbf{r}. \tag{11}$$

The normal to the wave front defines the direction of propagation of the wave so that the gradient $\nabla\varphi_0(\mathbf{r}) = \hat{\mathbf{k}}$ is the unit vector in the propagation direction of the X-ray beam in a vacuum.

The Rytov approximation is obtained when (9) is inserted in (8) and only first-order terms in $\delta\varphi(\mathbf{r})$ are retained. Then, the phase perturbation is governed by

$$(i/k)\nabla^2\delta\varphi - 2\nabla\varphi_0\cdot\nabla\delta\varphi + \chi = 0, \tag{12}$$

where, for convenience, the position dependences are assumed and are no longer shown. The Rytov approximation requires that $|\nabla\delta\varphi| << 1$. Since $|\nabla\delta\varphi| \simeq |\chi|$ [see (13) below], the condition is met when $|\chi| << 1$. This is usually the case for X-rays.

Before proceeding with the solution to (12), it is worth considering the short-wavelength limit, $1/k\rightarrow 0$. Then, (12) becomes

$$\hat{\mathbf{k}}\cdot\nabla\delta\varphi = \chi/2 \tag{13}$$

or

$$\mathrm{d}\delta\varphi/\mathrm{d}s = \chi(s)/2, \tag{14}$$

where s represents the distance travelled by the X-ray beam along the vacuum propagation direction, $\hat{\mathbf{k}}$. Then, the phase perturbation is given by

$$\delta\varphi = \tfrac{1}{2}\textstyle\int\chi(s)\mathrm{d}s. \tag{15}$$

The phase of the X-ray beam is shifted by an amount $k\delta\varphi$ as a result of the dielectric medium in the path of the beam. If there is a variation in χ transverse to $\hat{\mathbf{k}}$, then the phase will also have a transverse variation. Since the propagation direction is defined by $\nabla\varphi$, the transverse variation in $\delta\varphi$ leads to a change in the direction of propagation, relative to $\hat{\mathbf{k}}$. This is the refraction of waves by the medium. A derivation of Snell's law of refraction of X-rays using the phase perturbation is given below. The refraction of optical waves at a plane interface in the Rytov approximation is discussed by Oristaglio (1985).

An exact solution to (12) can be found by making use of the transformation

$$\delta\varphi(\mathbf{r}) = \exp[-ik\varphi_0(\mathbf{r})]F(\mathbf{r}), \tag{16}$$

where $F(\mathbf{r})$ is a function to be determined. Substituting (16) into (12) and making use of (10) yields for $F(\mathbf{r})$

$$\nabla^2F(\mathbf{r}) + k^2F(\mathbf{r}) = ik\chi(\mathbf{r})\exp[ik\varphi_0(\mathbf{r})], \tag{17}$$

which is the inhomogeneous Helmholtz equation. The solution to this is (Morse & Feshbach, 1953)

$$F(\mathbf{r}) = -(ik/4\pi)\int_{V'}\chi(\mathbf{r}')\exp[ik\varphi_0(\mathbf{r}')]G(\mathbf{r}-\mathbf{r}')\mathrm{d}V', \tag{18}$$

where the free-space Green's function in three dimensions is

$$G(\mathbf{r}-\mathbf{r}') = \exp(ik|\mathbf{r}-\mathbf{r}'|)/|\mathbf{r}-\mathbf{r}'|. \tag{19}$$

With (16), (18), (19) and the vacuum eikonal (11), the phase perturbation is described by

$$\delta\varphi(\mathbf{r}) = -(ik/4\pi)\exp(-i\mathbf{k}\cdot\mathbf{r}) \times \int_{V'} \chi(\mathbf{r}')[\exp(i\mathbf{k}\cdot\mathbf{r}' + ik|\mathbf{r}-\mathbf{r}'|)/|\mathbf{r}-\mathbf{r}'|]\mathrm{d}V'. \quad (20)$$

This equation gives the perturbation in the phase of the vacuum wave as it traverses a dielectric medium. In the following sections, it is shown that the first Born approximation is obtained when the phase perturbation is small and this yields the equation for small-angle scattering in the far-field region. Under the conditions where the wave number k is very large, (20) also describes the refraction of X-rays, as given by (15).

Small-angle X-ray scattering

The derivation here follows that of Gottfried (1966) for the quantum-mechanical scattering of particles observed in the far-field region, $r\rightarrow\infty$. For observations of the X-ray beam far from the scattering point, $r >> r'$ and

$$\begin{aligned} |\mathbf{r}-\mathbf{r}'| &= r(1 + r'^2/r^2 - 2\mathbf{r}\cdot\mathbf{r}'/r^2)^{1/2} \\ &\simeq r(1 - \mathbf{r}\cdot\mathbf{r}'/r^2). \end{aligned} \quad (21)$$

Then,

$$k|\mathbf{r}-\mathbf{r}'| \simeq kr - \mathbf{k}'\cdot\mathbf{r}', \quad (22)$$

where $\mathbf{k}' = k\hat{\mathbf{r}}$ is the wave vector in the direction of scattering. Since the wave number is unaltered, this represents elastic scattering of the X-rays to the point of observation. With the scattering vector defined as

$$\mathbf{q} = \mathbf{k}' - \mathbf{k} \quad (23)$$

and $\mathbf{r}'$ ignored in the denominator, (20) becomes

$$\delta\varphi(\mathbf{r}) = -(ik/4\pi r)\exp(-i\mathbf{k}\cdot\mathbf{r} + ikr) \times \int_{V'} \chi(\mathbf{r}')\exp(-i\mathbf{q}\cdot\mathbf{r}')\mathrm{d}V'. \quad (24)$$

If the phase perturbation is small, then

$$\exp(ik\delta\varphi) \simeq 1 + ik\delta\varphi. \quad (25)$$

This is equivalent to the first Born approximation. The wave at the observation point is given by

$$D(\mathbf{r}) = D_0\exp(i\mathbf{k}\cdot\mathbf{r}) + D_0(k^2/4\pi r)\exp(ikr) \times \int_{V'} \chi(\mathbf{r}')\exp(-i\mathbf{q}\cdot\mathbf{r}')\mathrm{d}V'. \quad (26)$$

The first term in (26) is the unscattered vacuum wave at $\mathbf{r}$ and the second term is the wave scattered from the volume V'. To make an explicit connection with small-angle scattering, note that the dielectric susceptibility for a wave with wavelength λ is related to the electron density $\rho(\mathbf{r})$ by (see *e.g.* Azároff, Kaplow, Kato, Weiss, Wilson & Young, 1974)

$$\chi(\mathbf{r}) = -(e^2\lambda^2/\pi mc^2)\rho(\mathbf{r}). \quad (27)$$

Then, the wave amplitude arising from the scattering of X-rays is

$$D_s = C\int_{V'} \rho(\mathbf{r}')\exp(-i\mathbf{q}\cdot\mathbf{r}')\mathrm{d}V', \quad (28)$$

where C is a constant at a fixed observation point. This expression forms the basis of small-angle X-ray scattering calculations in the continuum approximation (Guinier & Fournet, 1955; Porod, 1982).

X-ray refraction and absorption

In this section, it is demonstrated that, for scatterers very much larger than the wavelength of the X-ray and in which the X-ray beam is almost a plane wave, the asymptotic solution to the phase perturbation (20) leads directly to the refraction of the transmitted beam. In the case of an absorbing medium, χ is complex and the transmitted X-ray intensity decays exponentially with distance (Beer's law).

The derivation is based on the method of stationary phase (Van Kampen, 1949; Born & Wolf, 1964, Appendix III). For this purpose, it is convenient to choose a set of coordinate axes such that the Z axis is aligned with the direction of propagation. Consider again

$$F(\mathbf{r}) = -(ik/4\pi)\int_{V'} \chi(\mathbf{r}')\exp(i\mathbf{k}\cdot\mathbf{r}' + ikR)/R\,\mathrm{d}V', \quad (29)$$

where

$$\mathbf{r}-\mathbf{r}' = (x-x')\hat{\mathbf{x}} + (y-y')\hat{\mathbf{y}} + (z-z')\hat{\mathbf{z}} \quad (30)$$

and

$$R = [(x-x')^2 + (y-y')^2 + (z-z')^2]^{1/2}. \quad (31)$$

The integral in (29) is first taken over the $X'Y'$ plane at some fixed position z' along the path of the beam. Over a region in the medium small enough for R to be almost constant, the exponential factor in the integrand changes sign many times, provided k is large. Then, the contribution of this small region to the integral is negligible. This is not true where the phase is constant or stationary. To form an asymptotic solution in this case, consider the integral in the form

$$\int\int g(x,y)\exp[ikf(x,y)]\mathrm{d}x\mathrm{d}y, \quad (32)$$

where g and f are independent of k, which is large. Now, let (x_0,y_0) be the point of stationary phase where $\partial f/\partial x = \partial f/\partial y = 0$ and perform a Taylor-series expansion about this point to second order,

$$f(x,y) = f(x_0,y_0) + (\alpha/2)\xi^2 + (\beta/2)\eta^2 + \gamma\xi\eta, \quad (33)$$

where

$$\alpha = \partial^2 f/\partial x^2|_{x_0,y_0}; \quad \beta = \partial^2 f/\partial y^2|_{x_0,y_0}; \quad \gamma = \partial^2 f/\partial y \partial x|_{x_0,y_0}; \tag{34}$$

and

$$\xi = (x - x_0); \quad \eta = (y - y_0). \tag{35}$$

Then, the stationary terms can be brought outside the integral (32), with the result

$$g(x_0,y_0)\exp[ikf(x_0,y_0)] \times \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \exp[ik(\alpha\xi^2 + \beta\eta^2 + 2\gamma\xi\eta)/2]\mathrm{d}\xi\mathrm{d}\eta = g(x_0,y_0)\exp[ikf(x_0,y_0)](2\pi i/k)|\alpha\beta - \gamma^2|^{-1/2}, \tag{36}$$

provided $\alpha\beta > \gamma^2$ and $\alpha > 0$.

Now, comparison of (32) and (29), with the reminder that $\mathbf{k} = k\hat{\mathbf{z}}$, gives

$$f(x',y',z') = z' + [(x - x')^2 + (y - y')^2 + (z - z')^2]^{1/2} \tag{37}$$

and the point of stationary phase occurs when $x' = x$ and $y' = y$. At this point,

$$\alpha = \beta = 1/|z - z'|, \quad \gamma = 0, \tag{38}$$

$$R = |z - z'| \tag{39}$$

and

$$f(x' = x,\ y' = y,\ z') = z' + [(z - z')^2]^{1/2} = z, \tag{40}$$

provided $z > z'$. Thus, the asymptotic result for large k is

$$F(x,y,z) = \tfrac{1}{2}\int \chi(x,y,z')\exp(ikz)\mathrm{d}z' \tag{41}$$

and the phase perturbation becomes

$$\delta\varphi = \tfrac{1}{2}\int \chi(x,y,z')\mathrm{d}z', \tag{42}$$

which is identical to the phase (15) obtained directly from the eikonal equation.

To demonstrate that (42) gives rise to refraction, consider two homogeneous media, with dielectric susceptibilities χ_1 and χ_2, separated by a common boundary with its normal inclined at an angle θ to the Z axis (Fig. 1). The direction of propagation in medium 1 is along the Z axis, $\mathbf{k} = k\hat{\mathbf{z}}$. Because of this boundary, the phase perturbation at some point (x,z) in medium 2 is

$$\delta\varphi = (z - x\tan\theta)\chi_2/2 + x\tan\theta\chi_1/2. \tag{43}$$

The propagation direction at (x,z) is then

$$\nabla\varphi_0 + \nabla\delta\varphi = \hat{\mathbf{z}}(1 + \chi_2/2) + \hat{\mathbf{x}}\tan\theta(\chi_1 - \chi_2)/2. \tag{44}$$

The angular deviation with respect to $\mathbf{k} = k\hat{\mathbf{z}}$ associated with this change in direction is

$$\delta\theta \simeq [\tan\theta(\chi_1 - \chi_2)/2]/[1 + \chi_2/2], \tag{45}$$

since the χ are small. Rearrangement and the addition of $\sin\theta$ to both sides, gives

$$(1 + \chi_1/2)\sin\theta = (1 + \chi_2/2)(\sin\theta + \cos\theta\delta\theta) \simeq (1 + \chi_2/2)\sin(\theta + \delta\theta), \tag{46}$$

since $\delta\theta$ is small. This is recognized as Snell's law of refraction with a refractive index

$$n = (1 + \chi)^{1/2} \simeq 1 + \chi/2. \tag{47}$$

Now suppose that χ is constant in the dielectric medium and consider the imaginary component that determines the absorption in the medium. Then, the absorption per unit length is defined by

$$\mu \equiv k\mathrm{Im}(\chi) \tag{48}$$

and the intensity change with distance z is obtained from (42), (7) and (9):

$$|D(z)|^2 = |D_0|^2\exp(-\mu z). \tag{49}$$

This exponential decay of the beam with distance in the medium is Beer's law. The expression for absorption in an inhomogeneous medium, expressed by (15) or (42), has the form of a Radon transform, which is used extensively in solving inverse problems (Deans, 1983). In particular, it forms the basis of X-ray computed tomography. The more general expression (20) has been proposed as the basis of reconstructive tomography using ultrasonic wave fields (Devaney, 1986).

Concluding remarks

In X-ray scattering from large particles, the phase perturbation (20) provides a more realistic description of the scattering process, as it contains both diffraction and refraction effects. It is valid when the dielectric susceptibility varies slowly over the scale of the X-ray wavelength and it allows for large cumula-

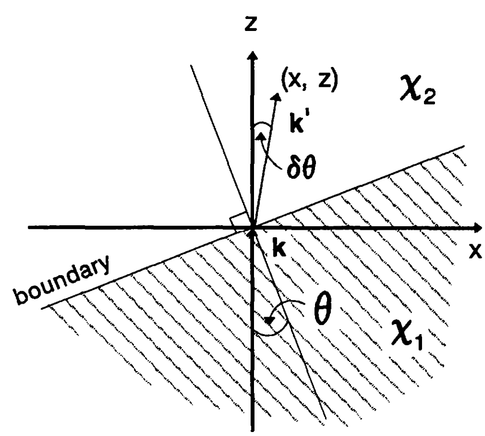

Fig. 1. The geometry for deriving Snell's law of refraction from the perturbation in the X-ray phase as it crosses a boundary.

tive phase shifts in the scattered wave. This contrasts with the first Born approximation and the usual formulation of small-angle scattering, which require the scattered field to be small. Furthermore, the first Born approximation breaks down if the scattering is weak but extends over a region that is large compared with the incident wavelength (Gottfried, 1966). In this case, (25) is not valid.

The fact that refraction phenomena and scattering are intimately related is not new. Ewald and Oseen (Born & Wolf, 1964) have provided rigorous derivations of the laws of refraction and reflection of light from considerations of scattering of electromagnetic radiation from electric dipoles in optical media (the Ewald–Oseen extinction theorem). Here, a unified treatment of small-angle scattering and refraction of X-rays has been obtained using the Rytov approximation for the X-ray phase.

References

AZÁROFF, L. V., KAPLOW, R., KATO, N., WEISS, R. J., WILSON, A. J. C. & YOUNG, R. A. (1974). *X-ray Diffraction*, pp. 180–183. Sydney: McGraw-Hill.

BERK, N. F. & HARDMAN-RHYNE, K. A. (1986). *Physica* (*Utrecht*), **136**B&C, 218–222.

BORN, M. & WOLF, E. (1964). *Principles of Optics*, 2nd. ed. New York: Pergamon.

CHERNOV, L. A. (1960). *Wave Propagation in a Random Medium.* New York: McGraw-Hill.

DEANS, S. R. (1983). *The Radon Transform and some of its Applications.* New York: Wiley.

DEVANEY, A. J. (1981). *Opt. Lett.* **6**, 374–376.

DEVANEY, A. J. (1986). *Inverse Probl.* **2**, 161–183.

GANS, R. (1925). *Ann. Phys.* **76**, 29–38.

GOTTFRIED, K. (1966). *Quantum Mechanics.* Vol. I. *Fundamentals.* Sydney: Benjamin.

GUINIER, A. & FOURNET, G. (1955). *Small-Angle Scattering of X-rays.* New York: Wiley.

KELLER, J. B. (1969). *J. Opt. Soc. Am.* **59**, 1003–1004.

MORSE, P. M. & FESHBACH, H. (1953). *Methods of Theoretical Physics*, Part I, Section 7.2, pp. 803–834. New York: McGraw-Hill.

NARDROFF, R. VON (1926). *Phys. Rev.* **28**, 240–246.

ORISTAGLIO, M. L. (1985). *J. Opt. Soc. Am.* **2**, 1987–1993.

POROD, G. (1982). *Small Angle X-ray Scattering*, edited by O. GLATTER & O. KRATKY, ch. 2. New York: Academic Press.

RAYLEIGH, LORD (1911). *Proc. R. Soc.* (*London*). *Ser. A*, **84**, 25–46.

RYTOV, S. M. (1937). *Izv. Akad. Nauk SSSR Ser. Fiz.* No. 2, p. 223.

TAKAGI, S. (1969). *J. Phys. Soc. Jpn*, **26**, 1239–1253.

VAN DE HULST, H. C. (1957). *Light Scattering by Small Particles.* New York: Wiley.

VAN KAMPEN, N. G. (1949). *Physica* (*Utrecht*), **14**, 575–589.

WEISS, R. J. (1951). *Phys. Rev.* **83**, 379–389.

Acta Cryst. (1994). A**50**, 690–703

A More General Expression for the Average X-ray Diffraction Intensity of Crystals with an Incommensurate One-Dimensional Modulation

BY ERWIN J. W. LAM AND PAUL T. BEURSKENS

Crystallography Laboratory, Research Institute for Materials, University of Nijmegen, Toernooiveld, 6525 ED Nijmegen, The Netherlands

AND SANDER VAN SMAALEN

Laboratory of Chemical Physics, Materials Science Center, University of Groningen, Nijenborgh 4, 9747 AG Groningen, The Netherlands

(*Received* 1 *February* 1994; *accepted* 5 *April* 1994)

Abstract

Statistical methods are used to derive an expression for the average X-ray diffraction intensity, as a function of $(\sin\theta)/\lambda$, of crystals with an incommensurate one-dimensional modulation. Displacive and density modulations are considered, as well as a combination of these two. The atomic modulation functions are given by truncated Fourier series that may contain higher-order harmonics. The resulting expression for the average X-ray diffraction intensity is valid for main reflections and low-order satellite reflections. The modulation of individual atoms is taken into account by the introduction of overall modulation amplitudes. The accuracy of this expression for the average X-ray diffraction intensity is illustrated by comparison with model structures. A definition is presented for normalized structure factors of crystals with an incommensurate one-dimensional modulation that can be used in direct-methods procedures for solving the phase problem in X-ray crystallography. A numerical fitting procedure

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ISSN 0108-7673 © 1994