will severely distort the ideal interaction considered here. Such a suppression of the TDS divergence was not obtained by Afanas'ev *et al.* (1968), based on a somewhat different formulation that still led to a log (q) dependence. The differences in formulation have already been discussed in WJ.

Finally, dynamical modifications of the kind discussed here should also manifest themselves in the interaction of X-rays with other types of waves. Apart from any specific details of the interaction, the expression replacing $\langle f/q_0\rangle$ will have to take into account that the density of states of these waves may differ from the $1/q$ dependence for thermal phonons underlying the form of (6).

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Reciprocal-Lattice Interpretation of the Interaction of Crystal-Monochromated X-radiation with a Small Single Crystal

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Abstract

When dealing with X-radiation of two near wavelengths, λ_1 and λ_2, from a crystal monochromator, M, incident on a small single crystal, c, interpretation of the interaction between the radiation and the specimen crystal is usually based on a single reciprocal lattice and two reflecting circles (spheres) of radii $1/\lambda_1$ and $1/\lambda_2$ whose centres do not coincide. If one uses the alternative Ewald construction of a single reflecting circle (sphere) of unit radius (which uniquely defines the specimen crystal location) and two reciprocal lattices mutually parallel but dimensionally scaled as $\lambda_1:\lambda_2$ and with displaced origins, then this allows a more ready appreciation of the special relationships between the dispersion of the specimen crystal and that of the monochromator as θ_c changes, in particular, when θ_c equals arctan $(0{\cdot}5 \tan\theta_M)$, arctan $(0{\cdot}6 \tan\theta_M)$ or θ_M.

To illustrate the interaction of a small single crystal with monochromated radiation corresponding to a wavelength band $\Delta\lambda = \lambda_2 - \lambda_1$, the more usual Ewald construction, *e.g.* Zachariasen (1945), Schoenborn (1983), involves (Fig. 1) a single reciprocal lattice and a range of reflecting circles (spheres) of radius $1/\lambda_2$ to $1/\lambda_1$ whose centres, c_2 to c_1, (and hence the effective location of the specimen crystal, c) are continually displaced as λ changes. This construction

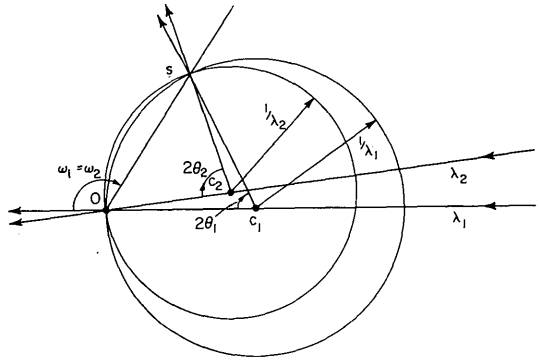

Fig. 1. The interaction of a small single crystal with monochromated X-radiation corresponding to a wavelength band, $\Delta\lambda = \lambda_2 - \lambda_1$, demonstrated by an Ewald construction based on a single reciprocal lattice, origin O, and a range of reflecting circles of radius $1/\lambda_2$ to $1/\lambda_1$, with centres c_2 to c_1. The point s corresponds to the 'focusing' condition.

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does offer ready identification of the so-called 'focusing' condition at s when $\theta_c = \theta_M$ (Fig. 1) but otherwise tends to obscure special relationships between the dispersion of the specimen crystal and that of the monochromator crystal for certain specific values of θ_c, in relation to θ_M.

The alternative construction (Fig. 2) has a single reflecting circle (sphere) with unit radius, the location of the specimen crystal, c_{12}, being coincident with the circle centre and therefore uniquely defined. For each wavelength, a different reciprocal lattice is generated, with direct-lattice constants normalized by $1/\lambda$ (Arndt & Willis, 1966). Here, the beams from the monochromator crystal, corresponding to the limit wavelengths λ_1 and λ_2, pass through the small specimen crystal c (and the centre of the reflecting circle c_{12}) with an interbeam angle $\Delta\theta_M = k \tan \theta_M$, where $k = \Delta\lambda/\lambda_m$, $\lambda_m = \frac{1}{2}(\lambda_1 + \lambda_2)$, θ_M being the monochromator Bragg angle. Take λ_1 as the reference beam and RL1 and its origin O_1 as the reference in reciprocal space. Then RL2 is located with its origin at O_2 on the circumference of the reflecting circle, such that $\angle O_1 c_{12} O_2 = -\Delta\theta_M$. Since RL1 and RL2 derive from the same crystal, the orientation of RL2, relative to RL1, is such that O_1p_1 and O_2p_2 are parallel, p_1 and p_2 corresponding to equivalent points (but one *hkl* order) in the two reciprocal lattices. The $\Delta\omega$, $\Delta 2\theta$ coordinates of O_2 relative to O_1 are therefore $-\Delta\theta_M$, $-\Delta\theta_M$ (or $-k \tan \theta_M$, $-k \tan \theta_M$). Hence, in moving from the condition that point p_1 of RL1 intersects the reflecting circle to the condition that point p_2 of RL2 intersects the reflecting circle, two conditions apply, that O_1p_1 and O_2p_2 are held parallel and that the ratio $O_2p_2 : O_1p_1 = \lambda_2 : \lambda_1 = (1+k) : 1$ (λ_m and λ_1 are effectively identical). As one moves outwards in reciprocal space, the situation is demonstrated in Fig. 2 by the points O_1O_2, p_1p_2, q_1q_2, (r_1r_2), s_1s_2, t_1t_2, while Fig. 3 shows the equivalent points in the corresponding diagram in $\Delta\omega, \Delta 2\theta$ space (Mathieson, 1985). Since the $\Delta\omega$, $\Delta 2\theta$ diagram refers to the *local* differential distribution, the origin points O_1, p_1, q_1, r_1, s_1, t_1 are coincident in Fig. 3.

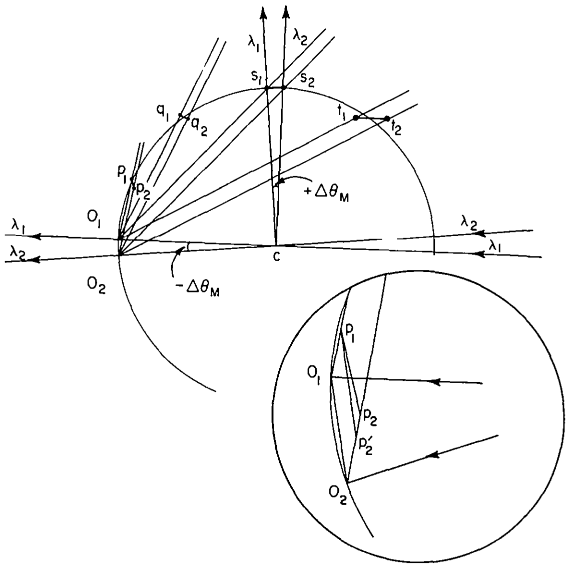

Fig. 2. The alternative Ewald construction involves a reflecting circle of unit radius, with the location of the specimen crystal, c, coincident with the circle centre, c_{12}, and therefore uniquely defined. For each wavelength in the band, $\Delta\lambda$, a different reciprocal lattice (RL) is generated. $\Delta\theta_M$ is the interbeam angle between the limit wavelengths λ_1, λ_2. O_1, O_2 are the origins of the λ_1, λ_2 reciprocal lattices, O_1 being taken as reference. The points p_1p_2, q_1q_2 *etc.* correspond to points on RL1 and RL2, respectively, at progressively greater Bragg angles θ_c. The insert shows the region near O_1O_2 in more detail. If the wavelength of the beams through O_1 and O_2 was λ_1, then the point p_1 relative to O_1 would correspond to the point p_2' relative to O_2 and p_1p_2' would be parallel to O_1O_2. If, however, the beam through O_2 is of a different wavelength, λ_2, the reciprocal-lattice point corresponding to p_1 is p_2 and the slope of p_1p_2 relative to O_1O_2 changes as O_1p_1 increases in length.

In respect of this Ewald construction (comparing Figs. 2 and 3), one sees how the sequence of λ_1, λ_2 components changes as one moves out in θ_c. Corresponding to the clockwise rotation of the reciprocal lattices, the sequence of intersection of the pairs of points with the reflecting circle is O_2O_1, then p_2p_1 and so on. In respect of q_2q_1, all wavelengths fall on the same position at the detector, *i.e.* $\Delta 2\theta = 0°$, over a $\Delta\omega$ range $= -\frac{1}{2}k \tan \theta_M$. The appropriate value of θ_c is given by $\tan \theta_c = \frac{1}{2} \tan \theta_M$. r_2r_1 corresponds to the position of minimum wavelength dispersion, $(1/5^{1/2})k \tan \theta_M$, with $\Delta\omega = -(2/5)k \tan \theta_M$, $\Delta 2\theta = +(1/5)k \tan \theta_M$. At this point, the value of θ_c is given by $\tan \theta_c = 0{\cdot}6 \tan \theta_M$. This case is not illustrated in Fig. 2 as it lies rather close to the right of q_2q_1. In respect of s_2s_1, they both intersect with the reflecting circle for one setting of ω, *i.e.* $\Delta\omega = 0°$, while $\Delta 2\theta = +k \tan \theta_M$. The value of θ_c is given by $\tan \theta_c = \tan \theta_M$.

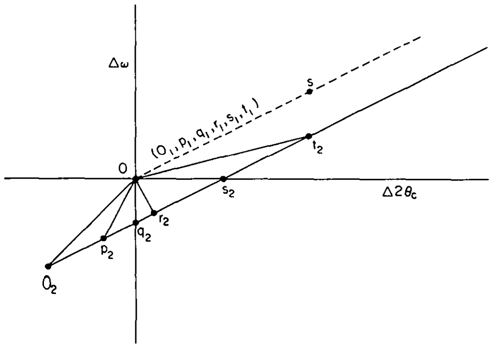

Fig. 3. The $\Delta\omega$, $\Delta 2\theta$ diagram of the dispersion of the wavelength band, λ_1 to λ_2. The points (and loci) O_1O_2, p_1p_2, q_1q_2 *etc.* correspond to those in Fig. 2. Since the $\Delta\omega$, $\Delta 2\theta$ diagram deals with local differential distributions adjacent to a Bragg reflection, the origin points O_1, p_1, q_1 *etc.* are coincident, at O. At $\theta_c = 0°$, the locus is O_1O_2 and as θ_c increases the locus progressively becomes p_1p_2 ($\tan \theta_c < 0{\cdot}5 \tan \theta_M$), q_1q_2 ($\tan \theta_c = 0{\cdot}5 \tan \theta_M$), r_1r_2 ($\tan \theta_c = 0{\cdot}6 \tan \theta_M$), s_1s_2 ($\tan \theta_c = \tan \theta_M$) and t_1t_2 ($\tan \theta_c > \tan \theta_M$). The dashed line corresponds to the wavelength dispersion in the non-monochromator case, Os corresponding to O_2s_2 in the monochromator case.

Table 1. *Special relationships between dispersion of specimen crystal and dispersion of monochromator*

θ_c	$\Delta\omega$	$\Delta 2\theta$	Comments
$\arctan(0{\cdot}5 \tan\theta_M)$	$-\frac{1}{2}k\tan\theta_M$	0	All wavelengths enter the detector in parallel but are not diffracted simultaneously
$\arctan(0{\cdot}6 \tan\theta_M)$	$-\frac{2}{5}k\tan\theta_M$	$\frac{1}{5}k\tan\theta_M$	Minimum wavelength dispersion in $\Delta\omega$, $\Delta 2\theta$ space
θ_M	0	$k\tan\theta_M$	All wavelengths enter the detector simultaneously but as a divergent beam

This corresponds to the 'focusing' condition (Arndt & Willis, 1966) where all wavelengths, λ_2 to λ_1, diffract simultaneously. Note, however, that while the dispersion is zero in respect of $\Delta\omega$ it is not zero in respect of $\Delta 2\theta$. When one goes beyond s_2s_1, the sequence of intersection with the reflecting circle inverts to t_1t_2, *i.e.* first t_1 then t_2. The special relationships are summarized in Table 1.

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From a Partial to the Complete Crystal Structure. II. The Procedure and Its Applications

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Abstract

A multisolution procedure, based on the probabilistic formulas obtained by Giacovazzo [*Acta Cryst.* (1983). A39, 685-692] is described, which aims at recovering the complete crystal structure from a partial one. A new weighted tangent formula develops starting phases: the correct solution among others is found by means of two revised figures of merit. The procedure is successfully applied to some practical cases.

Symbols and abbreviations

Throughout the paper a number of symbols will find frequent application. For most of them the reader is referred to the first paper of this series (Giacovazzo, 1983), from now on referred to as paper I. Other symbols not used in I are listed below.

$\Sigma_p, \Sigma_q, \Sigma_N = \sum f_i^2$	The summation is extended to the *p*, *q*, *N* atoms. Atomic thermal factors are included.
$\Sigma_p^0, \Sigma_q^0, \Sigma_N^0 = \sum^0 f_i^2$	The summation is extended to the *p*, *q*, *N* atoms. Atomic thermal factors are excluded.
$F_{p,\mathbf{h}}^0$	Structure factor for the partial structure. Atomic thermal factors are not considered.
$I_\mathbf{h}$	$\lvert F_\mathbf{h}\rvert^2$ on an arbitrary scale.
$E'_\mathbf{h}$	Pseudo-normalized structure factor with vectorial index **h** defined by $E'_\mathbf{h} = F_\mathbf{h}/\Sigma_q^{1/2}$.
$E'_{p,\mathbf{h}}$	Pseudo-normalized structure factor of the partial structure with *p* atoms in the unit cell, defined by $E'_{p,\mathbf{h}} = F_{p,\mathbf{h}}/\Sigma_q^{1/2}$.