Resolution in diffraction. An outline of the method of conjugate diameters

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RESOLUTION IN DIFFRACTION

An Outline of the Method of Conjugate Diameters.
Lecture Notes for Summer School on Synchrotron Radiation,
Vienna 1980

Jens Als-Nielsen

Abstract. The in-plane resolution of a diffraction apparatus is discussed in the Gaussian approximation. This approximation is generally adequate to find half-widths of the resolution function, but the detailed resolution line-shape may differ from a Gaussian line-shape for instance in using perfect crystals as monochromator or analyzer. In combining the contributions from different elements in the apparatus to the resolution function we find the method of conjugate diameters useful. The resulting resolution widths are not given in explicit formulae but by means of a few simple subroutines in a computer program, e.g. transforming a set of conjugate diameters to another set with a prescribed direction of one diameter, the method seems to be readily applicable ot a variety of instruments.

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PREFACE

These notes for a lecture on the 1980 Vienna Summer School on Synchrotron Radiation deal with the general problem of resolution in a diffraction experiment. The approach taken here builds on the method of conjugate diameters invented in 1969 by H.B. Møller and Mourits Nielsen (Acta Cryst. A25, 547). The first edition contained an error with respect to Darwin width and perfect crystals. Additional examples, including the source line-width from an X-ray tube, may be found in Finn Christensen's thesis, Risø Report R-459.

1. INTRODUCTION

Structures with a length scale of the order of atomic dimensions (Å) can be studied by diffraction of radiation (neutrons, X-rays or electrons) with a wavelength of a similar order of magnitude. The principles of diffraction is simple. A volume element $d\vec{r}$ at position $\vec{r}$ in the structure scatters the incident plane-wave beam described by its wavevector $\vec{k}_1$.

Looking at scattering into the direction of the scattered wavevector $\vec{k}_2$ the phase of the beam scattered from the volume element is $(\vec{k}_1-\vec{k}_2)\cdot\vec{r} \equiv \vec{Q}\cdot\vec{r}$ and the amplitude is $\rho(\vec{r})d\vec{r}$, where $\rho(\vec{r})$ indicate the scattering length density, so the total scattered amplitude is proportional to $\int\rho(\vec{r})e^{i\vec{Q}\cdot\vec{r}}d\vec{r}$. To the extent that the scattering density reflects the structure, the latter can be determined by measuring the scattered intensity versus wavevector transfer $\vec{Q}$. We assume here that the scattering is very nearly elastic, $|\vec{k}_2| \approx |\vec{k}_1|$, an approximation which is excellent for X-ray diffraction due to the relatively large energy of X-ray photons.

The experimental uncertainty is partly due to the finite count rate at a certain wavevector and partly due to the accuracy with which the wavevector $\vec{Q}$ is determined by the diffraction apparatus. These two sources of uncertainty are complementary in the sense that one generally has to sacrifice a loss of intensity in improving the $\vec{Q}$-resolution, but sharp features in the cross section are smeared in a diffraction apparatus with broad wavevector resolution. For a given experiment there is an optimum between the requirements of high intensity and narrow resolution and it is therefore of importance to be able to calculate the resolution in order to design an experiment properly.

The scattering process to be studied is conveniently depicted in reciprocal space, Fig. 1a. The incident beam is given by the wavevector $\vec{k}_1$ and the scattered beam by wavevector $\vec{k}_2$. The elastic scattering cross section depends only on the wavevector difference $\vec{Q} \equiv \vec{k}_1 - \vec{k}_2$, not on $\vec{k}_1$ and $\vec{k}_2$ separately.

The scattering diagram of Fig. 1a may be obtained by the set-up shown in Fig. 1b. The X-ray source may be synchrotron radiation. A monochromatic beam is obtained by Bragg reflection from the monochromator crystal M. The degree of monochromatization depends on the aperture A together with the source size as well as the mosaic width and/or Darwin-width of the monochromator crystal. The monochromatic beam is scattered by the sample S and

in Fig. 1b is shown a set-up where only scattered radiation in a certain direction defined by the multislit collimator C (a so-called Soller collimator) is detected. It should be emphasized that there is a great variety of ways to obtain a certain scattering diagram. Let us just mention a few examples. Synchrotron radiation is very well collimated, typical to 0.1 mrad and the incident direction of k_1 is therefore typically defined within 0.1 mrad corresponding to 2 slits 1 meter apart and each 1/10 of a millimeter wide! If the direction of the scattered beam should be defined to a similar degree of accuracy a Soller collimator is not practical (in practice the lower limit for a Soller collimator is 1 mrad). Instead one can insert an analyzer crystal in front of the detector. In that case we have a triple axis spectrometer (1 axis = monochromator, 2 axis = sample, 3rd axis = analyzer). The analyzer crystal analyzes the direction of the scattered beam, not its wavelength or frequency, since we have

presumed that the scattering is practically elastic. The angular resolution of the analyzer device depends in this case on the incident wavelength band-width. Another possibility is to detect the entire angular distribution of scattered radiation using a position sensitive detector. The spatial resolution is typically 0.1 mm and if the apparent width of scattering volume is of the same order of magnitude an angular resolution of 0.1 mrad is obtained by a detector distance of 1 meter which is quite practical.

In general, the monochromatic beam is neither perfectly monochromatic nor perfectly well collimated. Similarly, the scattered beam reaching the detector has a small but finite angular spread. As a consequence, for a given setting of a spectrometer one samples the scattering cross section over a finite region of Q-space. It is the purpose of this lecture to discuss a rather general method to calculate the size of the region in Q-space over which the scattering cross section is sampled, or to be more specific: the resolution function is approximated by a two-dimensional Gaussian and we discuss how to obtain the corresponding widths. Whether the actual resolution function is more or less Gaussian-like depends on the individual components of the diffractometer. The advantage of assuming Gaussian resolution is of course the great simplification in carrying out folding integrals.

2. GAUSSIAN APPROXIMATION

All individual components of the instrument determing the final resolution will be approximated by Gaussian functions of the same width as the true distribution function. For example, although the angular resolution of two slits of width w_1 and w_2 ($w_2 > w_1$) at distance L apart (Fig. 2) is of trapezoidal shape

with a full width at half height (FWHM) of w_2/L it will be approximated by a Gaussian having the same FWHM and the same area (not the same maximum height!).

The advantage of assuming individual Gaussian distributions is that any combination of two distributions is also Gaussian:

$$P(x_o) \equiv c' \int \exp[-(x/\sigma_1)^2 - ((x-x_o)/\sigma_2)^2]dx = c \exp[-(x_o/\sigma)^2] \quad (1)$$

with

$$\sigma^2 \equiv \sigma_1^2 + \sigma_2^2 \quad (2)$$

so the combined distribution is also Gaussian with a width σ simply to be found by the rule of sum-of-squares as given in Eq. (2). In equation (1) c' and c are normalization constants which we shall not always write out explicitly.

Equation 1 describing the folding of two Gaussians holds only in one dimension, whereas the resolution function we are seeking is two-dimensional. As a matter of fact it is three-dimensional, the third dimension being perpendicular to the scattering plane, but this third component is usually uncorrelated with the components in the scattering plane. The general question for calculating a two-dimensional distribution function is the following:

Suppose a certain two-dimensional, Gaussian distribution function is given by its half-contour ellipse E_1 in the x-y plane, Fig. 3. In the Cartesian x-y coordinates the half-contour is given by equating a second order polynomium in x and y, including cross terms, with unity. Suppose now that this distribution has to be folded with a one-dimensional distribution along

a certain line D_1. How do we find the folded distribution? One convenient way, which utilizes the rule of sum-of-squares, is to abandon a description in the Cartesian coordinate system with its cross terms, and instead express the distribution function as the product of two independent distributions along the diameter D_1 and along its conjugate diameter D_2:

$$P_o(\bar{r}) \sim \exp(-u^2/\sigma_1^2)\ \exp(-v^2/\sigma_2^2) \tag{3}$$

$$\text{with } \bar{r} = u/\sigma_1\ \hat{D}_1 + v/\sigma_2\ \hat{D}_2 \tag{4}$$

$\hat{D}_1$ and $\hat{D}_2$ denoting unit vectors along the diameters D_1 and D_2. The distribution $P_o(\bar{r})$ folded with a Gaussian along the $\hat{D}_1$ unit vector with a width σ_3 is simply

$$P(\bar{r}) \sim \exp(-u^2/\sigma^2)\ \exp(-v^2/\sigma_2^2) \tag{5}$$

$$\text{with } \bar{r} = (u/\sigma)\ \hat{D}_1 + (v/\sigma_2)\ \hat{D}_2 \tag{6}$$

$$\text{and } \sigma^2 = \sigma_1^2 + \sigma_3^2 \tag{7}$$

The resulting ellipse is shown as E in Fig. 3.

In the following section we shall consider the rules of conjugate diameters in ellipses.

3. CONJUGATE DIAMETERS

The ellipse E is considered as the projection of a circle C as shown in Fig. 4. Explicitly, the coordinate along axis 1 in the circle is left unchanged during the projection, but the coordinate along the orthogonal axis is multiplied by a certain

number b/a < 1. Two arbitrary orthogonal diameters in the circle, say O'A'-O'B', are projected as two conjugate diameters in the ellipse, OA-OB. From this definition it follows immediately that diameter $\vec{OB}$ conjugate to $\vec{OA}$ is colinear with the tangent to the ellipse in point A. An arbitrary point C' on the circle is given by two numbers c_1 and c_2:

$$\vec{O'C'} = c_1\vec{O'A'} + c_2\vec{O'B'} \tag{8}$$

with $$c_1^2 + c_2^2 = 1 \tag{9}$$

The point C in the ellipse corresponding to C' on the circle is given by

$$\vec{OC} = c_1\vec{OA} + c_2\vec{OB} \tag{10}$$

As the point C' on the circle is given by the coordinates (c_1,c_2) the orthogonal diameter point D' must have the coordinates $(-c_2,+c_1)$ and the corresponding point D on the ellipse is given by

$$\vec{OD} = -c_2\vec{OA} + c_1\vec{OB} \tag{11}$$

The vector product $\vec{OC} \times \vec{OD}$ becomes

$$\vec{OC} \times \vec{OD} = (c_1\vec{OA}+c_2\vec{OB}) \times (-c_2\vec{OA}+c_1\vec{OB})$$
$$= c_1^2\vec{OA} \times \vec{OB} - c_2^2\vec{OB} \times \vec{OA}$$
$$= (c_1^2+c_2^2)\vec{OA} \times \vec{OB} \quad \text{i.e.}$$
$$\vec{OC} \times \vec{OD} = \vec{OA} \times \vec{OB} \tag{12}$$

Any set of conjugate diameters in the ellipse has identical vector products.

Suppose that we instead of Eq. (10) giving the ellipse in terms of the basis $\vec{OA}$, $\vec{OB}$ want another basis-set $\vec{OC}$, $\vec{OD}$ where for instance the direction of $\vec{OC}$ is given. This transformation is carried out as follows: Let the projections of $\vec{OA}$ and $\vec{OB}$ on a line (x-axis) perpendicular to the given direction $\vec{OC}$ be A_x and B_x, respectively. It follows from Eq. (10) that

$$0 = c_1A_x + c_2B_x \text{ and using } 1 = c_1^2 + c_2^2 \text{ we find}$$
$$c_1^2 = B_x^2/W_x^2 \text{ and } c_2^2 = A_x^2/W_x^2 \tag{13}$$

with

$$W_x^2 \equiv A_x^2 + B_x^2 \tag{14}$$

Furthermore

$$\vec{OC}\cdot\vec{OC} = (c_1\vec{OA}+c_2\vec{OB})\cdot(c_1\vec{OA}+c_2\vec{OB})$$
$$= c_1^2OA^2+c_2^2OB^2+2c_1c_2\vec{OA}\cdot\vec{OB}$$

and using Eq. (13) we find

$$W_x^2OC^2 = B_x^2(A_x^2+A_y^2) + A_x^2(B_x^2+B_y^2) - 2A_xB_x(A_xB_x+A_yB_y) \tag{15}$$
$$= (A_xB_y-A_yB_x)^2 = |OA\times OB|^2 \quad \text{or}$$
$$OC = |\vec{OA}\times\vec{OB}|/W_x \tag{16}$$

Let us finally consider the ratio between the vector product and the scalar product of $\vec{OC}$ and $\vec{OD}$ in order to determine the angle α between the given direction $\vec{OC}$ and the conjugate diameter $\vec{OD}$:

$$\operatorname{tg}\alpha = \frac{|\vec{OC}\times\vec{OD}|}{\vec{OC}\cdot\vec{OD}}$$

The scalar product is easily seen to fulfil

$$W_x^2(\vec{OC}\cdot\vec{OD}) = -|\vec{OA}\times\vec{OB}|\,(A_xA_y+B_xB_y)$$

and utilizing (12) we find

$$\operatorname{tg}\alpha = -\frac{W_x^2}{A_xA_y+B_xB_y} \qquad (17)$$

The length of OD is finally given by

$$|\vec{OD}| = \frac{|\vec{OC}\times\vec{OD}|}{OC\sin\alpha} = \frac{W_x}{\sin\alpha} \qquad (18)$$

Formulae (14), (16)-(18) constitute the wanted transformation $(\vec{OA},\vec{OB}) \rightarrow (\vec{OC},\vec{OD})$.

Note that OD $\sin\alpha$ is the projection on the x-axis of the diameter OD and we conclude from Eq. (18):

The projection W_x of an ellipse on an arbitrary axis (x-axis) is the square root of the sum of squared projections of any set of conjugate diameters, $W_x^2 = A_x^2+B_x^2$.

From a set of conjugate diameters, $\vec{OA}$ and $\vec{OB}$, one readily finds the major and minor axis. Without less of generality we define

$|\vec{OA}| \equiv A$ to be larger than $|\vec{OB}| \equiv B$ and their orientation so that the angle from $\vec{OA}$ to $\vec{OB}$, v, is less than $\pi/2$. Let the major axis be $\vec{OM}_1$ and minor axis $\vec{OM}_2$ along an x-axis and a y-axis, respectively. The major axis (x-axis) must be in between $\vec{OA}$ and $\vec{OB}$ with say angle m from $\vec{OA}$ to $\vec{OM}_1$. It follows from eq. (17) that $A_xA_y+B_xB_y = 0$ or $-A^2\cos m\sin m + B^2\cos(v-m)\sin(v-m) = 0$, i.e.

$$\tan 2m = \frac{\sin 2v}{A^2/B^2+\cos 2v} \qquad (17a)$$

$$\text{and } OM_1 = [(A\cos m)^2 + (B\cos(v-m))^2]^{1/2} \qquad (18a)$$

$$\text{and } OM_2 = [(A\sin m)^2 + (B\sin(v-m))^2]^{1/2} \qquad (16a)$$

4. MONOCHROMATIZATION BY SINGLE BRAGG REFLECTION IN A WHITE BEAM

As an example of using the basis of conjugate diameters to describe distribution functions in reciprocal space we consider in Fig. 5 a monochromator crystal in a collimated white beam.

For simplicity let us first assume that the monochromator crystal is perfect, no mosaic width, no Darwin width. An angular deviation of u in the exit collimator necessitates an angular deviation of -u, Fig. 5a, in the incident collimator, so the probability for this ray is

$$P(u) = c\exp(-[(-u/\sigma_o)^2+(u/\sigma_1)^2])$$

$$\text{or} \quad P(u) = c\exp(-(u/\sigma)^2) \text{ with } \sigma^{-2} \equiv \sigma_o^{-2}+\sigma_1^{-2} \qquad (19)$$

This ray has a smaller Bragg angle than the central ray and consequently a larger wavevector by an amount Δk following from the Bragg equation:

$$\Delta k = \frac{k}{tg\theta_M} \cdot u$$

With $u = \sigma$ we find the 1/e width

$$X_1 = \frac{k\sigma}{sinv_1} \tag{20}$$

and

$$tgv_1 = \frac{k\sigma}{\Delta k(u=\sigma)} = tg\theta_M \quad \text{i.e. } v_1 = \theta_M \tag{21}$$

and we conclude $v_1 = \theta_M$, so the $\bar{k}$-distribution is in this case degenerated to be along a straight line parallel to the monochromator planes with a 1/e width of $k\sigma/sin\theta_M$.

Next we consider the general case, Fig. 5b, allowing for a finite mosaic width of the monochromator crystal.
Consider a ray with an exit angular deviation of u, scattered from a mosaic block with deviation angle m. The incident ray must therefore have had an angular deviation of (-u+2m) and the probability P(u,m) for this ray is given by

$$-\ell nP(u,m) = (u/\sigma_1)^2 + (m/\eta)^2 + (2m-u)^2/\sigma_o^2 \tag{22}$$

This quadratic form in (u,m) leads of course to a distribution of $\bar{k}$-vectors with an ellipse half-contour.

We want to find this ellipse in terms of two conjugate diameters, and since the ellipse degenerates to the line $\bar{X}_1$ for a perfect crystal, it is natural to let $\bar{X}_1$ be the first of the two conjugate diameters. Since m = 0 for the $\bar{X}_1$ axis it coincides with the u-axis in the (u,m) plane. We shall now find its conjugate $\bar{X}_2$. In the (u,m) plane the direction of $\bar{X}_2$ must be given by $u = \gamma m$ where γ is some dimensionless combination of σ_o, σ_1 and probably η. We shall therefore rewrite Eq. (22) in the form

$$- \ell nP = \alpha^2 m^2 + \beta^2 (u-\gamma m)^2 \tag{23}$$

and by comparison with Eq. (22) we find

$$\alpha^2 = \frac{4}{\sigma_o^2+\sigma_1^2} + 1/\eta^2, \quad \beta^2 = \sigma_o^{-2} + \sigma_1^{-2}, \gamma = 2\sigma_1^2/(\sigma_o^2 + \sigma_1^2)$$

The length of X_2 is found in the same way as X_1 in Eq. (20) and Eq. (21). We consider a deviation in the exit angle of $u = \gamma m$, and since we want the 1/e contour the value of m must be α^{-1} according to Eq. (23). The situation is depicted in Fig. 6. The direction of X_2 is given by the angle v_2 and the length of X_2 is $ku/\sin v_2$, that is $k(\gamma\alpha^{-1})/\sin v_2$ or explicitly:

$$X_2 = \frac{k}{\sin v_2} \frac{2\sigma_1^2}{\sigma_o^2+\sigma_1^2} \left[\frac{4}{\sigma_o^2+\sigma_1^2} + \frac{1}{\eta^2}\right]^{-\frac{1}{2}} \tag{24}$$

The angle v_2 is determined by the corresponding change in wavevector, Δk, as $\mathrm{tg}v_2 = k(\gamma m)/\Delta k$. The quantity Δk is given by differentiation of the Bragg law as $\Delta k = (k/\mathrm{tg}\theta_M)(\Delta\theta_M)$ and in the present case $\Delta\theta_M$ is the difference between deviations in exit

angle $u = \gamma m$ and mosaic angle m, i.e. $\Delta\theta_M = (\gamma-1)m$, so the formula for tgv_2 becomes

$$tgv_2 = \frac{k(\gamma m)}{(k/tg\theta_M)(\gamma-1)m} = \frac{\gamma}{\gamma-1}\, tg\theta_M = \frac{2\sigma_1^2}{\sigma_1^2-\sigma_o^2}\, tg\theta_M \qquad (25)$$

$$(0 < v_2 \leq \pi)$$

Equations (20), (21), (24) and (25) determine the conjugate diameters $\vec{X}_1$, $\vec{X}_2$ in terms of the collimations σ_o, σ_1 and the mosaic width η.

Let us now consider a perfect crystal (no mosaic width) but take into account the so-called Darwin-width. The finite Darwin width expresses the fact that a perfectly monochromatic ray may be Bragg scattered from the perfect crystal, even if the incident angle deviates slightly from the Bragg angle by an amount m. In the Gaussian approximation the probability for reflection from the crystal is $\exp[-(m/\sigma_D)^2]$, σ_D denoting the Darwin width. In this case also the reflected ray deviates by m from the central ray. In addition we now consider a slightly different wavevector, $k+\Delta k$, which then have the maximum chance of being reflected if it also has an angular deviation u from the central ray related to Δk by $\Delta k = ku/tg\theta_M$. The general (u,m) ray has the probability P(u,m) of being transmitted by collimotors 0 and 1 as well as being Bragg reflected from the perfect crystal and the analogue of eq. (22) becomes:

$$-\ln P(u,m) = \left(\frac{u+m}{\sigma_o}\right)^2 + \left(\frac{u+m}{\sigma_1}\right)^2 + \left(\frac{m}{\sigma_D}\right)^2 \qquad (22a)$$

By identifying this with the form

$$-\ln P(u,m) = \alpha^2 m^2 + \beta^2 (u-\gamma m)^2 \qquad (23a)$$

we find simply

$$\gamma = -1, \quad \beta^2 = \sigma_O^{-2} + \sigma_1^{-2}, \quad \alpha^2 = \sigma_D^{-2}$$

The length of X_2 becomes

$$|\bar{X}_2| = k\sigma_D / \mathrm{tg}\,\theta_M \qquad (24a)$$

and its direction coincides with the reflected ray.

5. ELASTIC SCATTERING

We shall in this section see how the distribution of incident wavevectors, given by the conjugate diameters $\vec{X}_1$ and $\vec{X}_2$, is transformed to a resolution function in wavevector transfer $\vec{k}_1 - \vec{k}_2$ assuming the scattering process $\vec{k}_1 \rightarrow \vec{k}_2$ to be elastic. Consider Fig. 7. It turns out to be convenient first to transform the set (X_1, X_2) into a set Y_1, Y_2 where Y_1 is perpendicular to the scattering vector AB. The transformation was explicitly derived in section 3.

Let us first assume that the collimation σ_2 is infinitesimal. In the <u>elastic</u> scattering process, the endpoint of Y_1 is transferred to the point C' on a line at angle θ with respect to AB so $BC' = Y_1 \sin\theta$. The endpoint of Y_2 is transferred to the point Z_2. Consider the triangle BB'D in Fig. 7. The piece $Z_2 D = Y_2 \sin(\alpha-\theta)$. The angle γ is determined by

$$tg\gamma = Z_2D/DB = Z_2D/(BB'\sin\theta)$$

That the scattering is elastic implies

$$BB' = 2M'M = 2Y_2\cos(\alpha-90) \quad \text{so}$$

$$tg\gamma = \tfrac{1}{2}(\cot\theta-\cot\alpha) \tag{26}$$

The length $BZ_2 = DZ_2/\sin\gamma$ or

$$Z_2 = Y_2\sin(\alpha-\theta)/\sin\gamma \tag{27}$$

For infinitesimal σ_2 the resolution ellipse is given by (Z_1, Z_2) where Z_1 is perpendicular to k_2. It is therefore straight forward to include a finite σ_2 as that implies a smearing perpendicular to k_2, that is along one of the conjugate diameters. Applying the rule of sum-of-squares we simply find

$$Z_1 = [(Y_1\sin\theta)^2 + (k\sigma_2)^2]^{\frac{1}{2}} \tag{28}$$

whereas the formulae for γ and Z_2 are unaltered by including finite σ_2, cf. Figure 3.

Finally, we shall consider the vertical resolution. Let the vertical collimation before and after the monochromator be β_1 and β_2. Consider rays incident with a divergence angle of v_1 being Bragg reflected from a mosaic block with vertical divergence angle m. They will leave the monochromator with a vertical divergence angle $v_2 = v_1+2m\sin\theta_M$. This expression is just the vertical component part of the vectorial Bragg condition $\underline{k}_2 = \underline{k}_1 + \underline{\tau}$ to-

gether with the ralation $|\underline{\tau}| = 2k\sin\theta_M$. It is then straightforward to find the 1/e-vertical width X_3:

$$X_3 = k\beta_2[(\beta_1^2 + 4\eta_M^2\sin^2\theta_M)/(\beta_1^2 + \beta_2^2 + 4\eta_M^2\sin^2\theta_M)]^{\frac{1}{2}} \qquad (29)$$

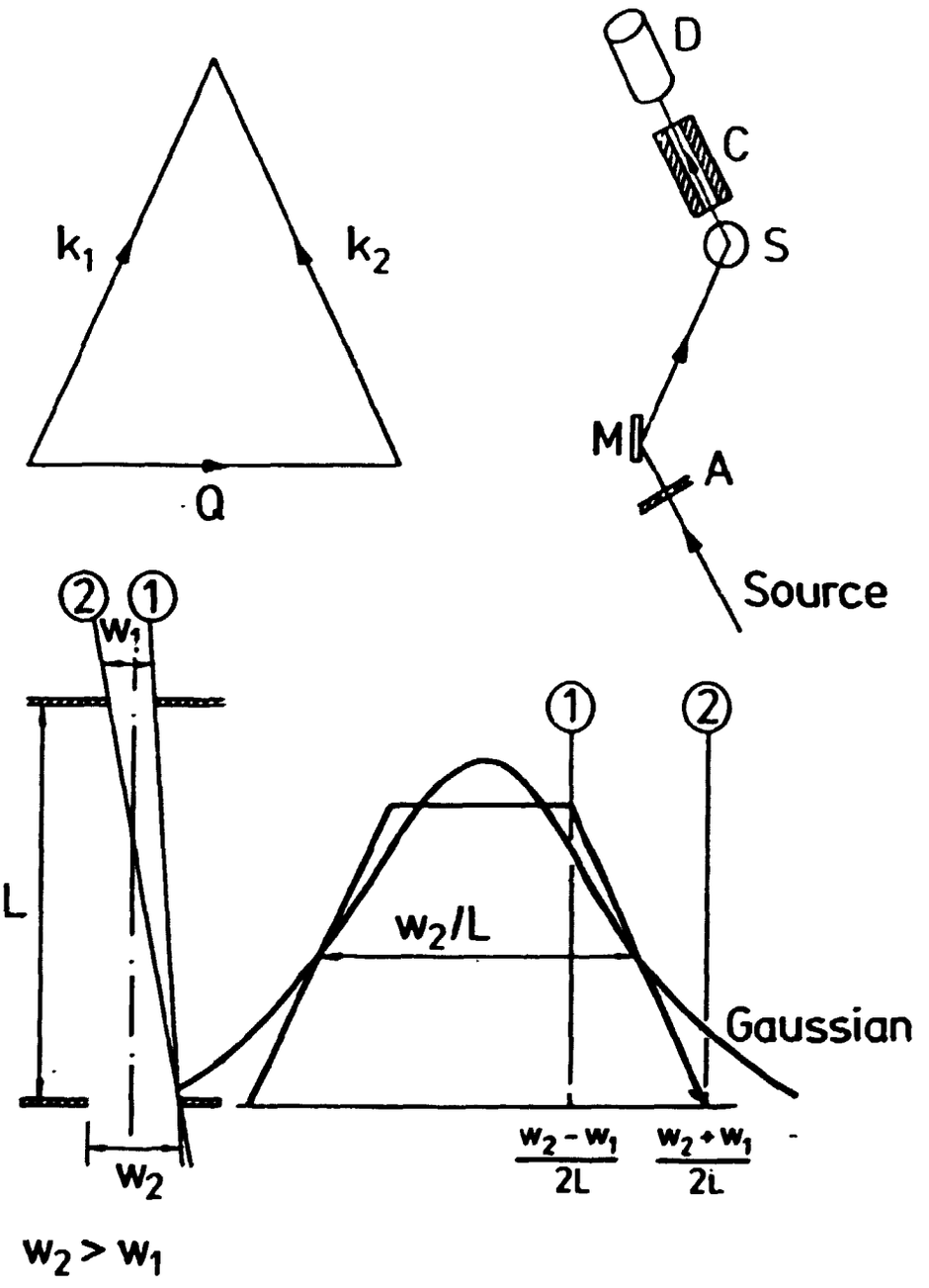
The final vertical resolution X_v is

$$X_v = [X_3^2 + (k\beta_3)^2]^{\frac{1}{2}} \qquad (30)$$

where β_3 is the vertical collimation after the sample.

SUMMARY

The in-plane resolution of a diffraction apparatus has been discussed in the Gaussian approximation. This approximation is generally adequate to find half-widths of the resolution function, but the detailed resolution line-shape may differ from a Gaussian line-shape for instance in using perfect crystals as monochromator or analyzer. In combining the contributions from different elements in the apparatus to the resolution function we find the method of conjugate diameters useful. The resulting resolution widths are not given in explicit formulae but by means of a few simple subroutines in a computer program, e.g. transforming a set of conjugate diameters to another set with a prescribed direction of one diameter, the method seems to be readily applicable to a variety of instruments.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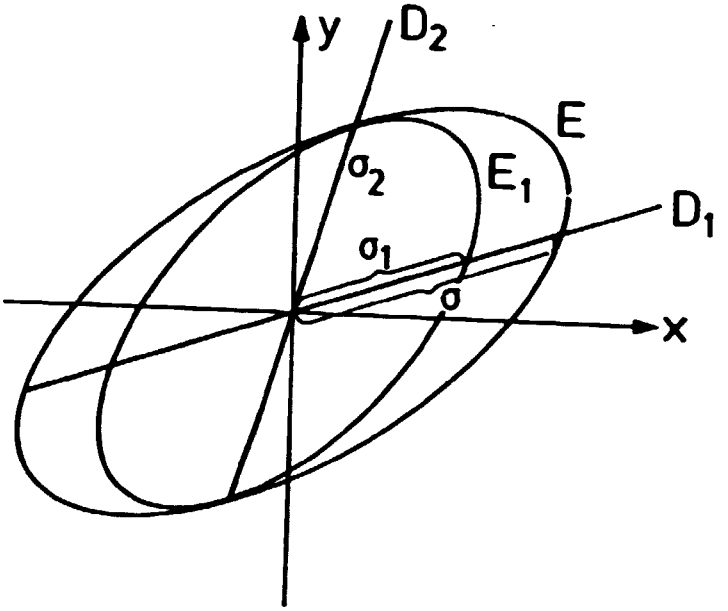
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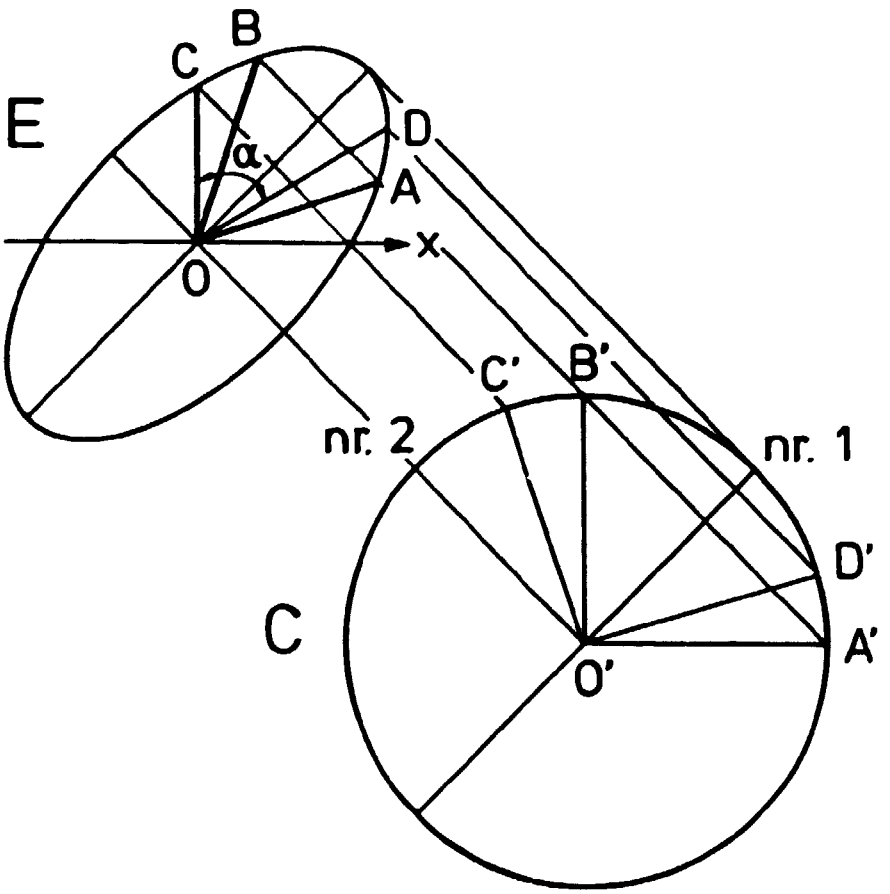
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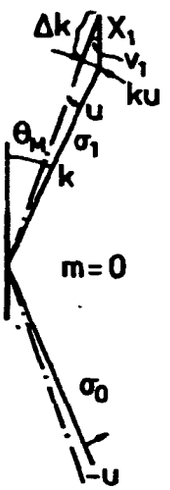

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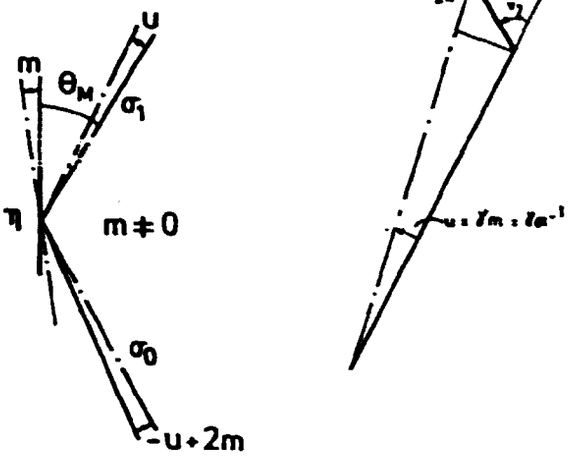


$\ln P = (-u/\sigma_0)^2 + (u/\sigma_1)^2 \equiv (u/\sigma)^2$

$\Delta k = k/tg\theta_M - u$ (Bragg)

$tgv_1 = \frac{ku}{\Delta k} \Longrightarrow v_1 = \theta_M$

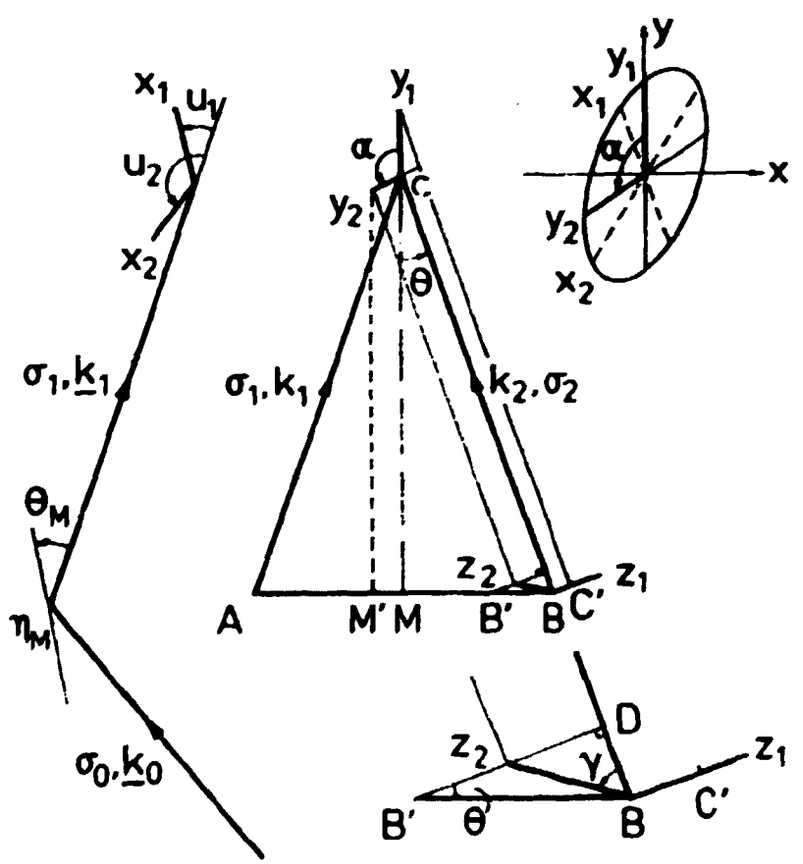
$X_1 = \frac{k\sigma}{tg\theta_M} \frac{1}{\cos\theta_M} = (k\sigma)/\sin\theta_M$

$\sigma^{-2} \equiv \sigma_0^{-2} + \sigma_1^{-2}$

$\ln P = (u/\sigma_1)^2 + (m/\eta)^2 + (2m-u)^2/\sigma_0^2$

$= [u - 2m\sigma^2\sigma_1^{-2}]^2\sigma^{-2}$

$+ m^2\left[\frac{4}{\sigma_0^2+\sigma_1^2} + \frac{1}{\eta^2}\right]$



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Title and author(s)

Resolution in Diffraction

An Outline of the Method of Conjugate Diameters. Lecture Notes for Summer School on Sunchrotron Radiation, Vienna 1980.

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Department or group: Solid State Physics

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Abstract

The in-plane resolution of a diffraction apparatus is discussed in the Gaussian approximation. This approximation is generally adequate to find half-widths of the resolution function, but the detailed resolution line-shape may differ from a Gaussian line-shape for instance in using perfect crystals as monochromator or analyzer. In combining the contributions from different elements in the apparatus to the resolution function we find the method of conjugate diameters useful. The resulting resolution widths are not given in explicit formulae but by means of a few simple subroutines in a computer program, e.g. transforming a set of conjugate diameters to another set with a prescribed direction of one diameter, the method seems to be readily applicable to a variety of instruments.

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