ΦΥΣΙΚΗ.— **The focusing error in the X-Ray Johann Spectrometer**,

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ABSTRACT

The focusing error in the Johann X-ray spectrometer is calculated step by step for an ideal crystal completely opaque to the radiation. Parameters are given which permit choices to be made between source size and energy resolution.

INTRODUCTION

The achievement of an intense a monochromatic X-ray beam as possible has been of interest since the earliest days of the X-ray spectroscopy[1]. The simplest method of selecting a wavelenght is to use a flat single crystal as a monochromator. With flat crystals an incident but divergent X-ray beam remains divergent after diffraction so that the radiation diverging from a point source is dispersed in space, and the energy must be selected by fine slits reducing the intensity collected by a counter. In spite of this great disadvantage, flat crystal monochromators are still used in various spectrometers[2]. Many devices have been proposed to maximize the intensity in a diffracted beam. The most common are those using a bent single crystal in both the transmission[3] and reflection[4] geometry. In the reflection geometry of a Johann spectrometer, the focusing properties of a cylindrically curved crystal are not perfect. A bent crystal spectrometer which gi-

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ves perfect focusing for the case of strictly monochromatic radiation from a point source is the so-called Johhanson spectrometer[5–6]: A single crystal bent to a radius 2·R and then its face ground to a radius R. In both Johann and Johhanson spectrometer, the reflecting crystal planes may or may not be parallel to the crystal face. Other types, are described for a perfect focusing[7–9]. Because of the great difficulty in bending and grinding a crystal, the singly bent crystal spectrometer (Johann) is still widely used for its simplicity. The main reason of the focusing error (broadening of the lines) in a spectrometer are generally the following:

1.-The natural width of the X-ray line.

2.-The X-ray source dimensions

3.-The mosaic spread of the crystal

4.-The depth of the penetrating radiation

Ignoring the two last cases, we will calculate step by step the focusing error in the Johann X-ray spectrometer for an ideal crystal completely opaque to the radiation.

I. POINT SOURCE - STRICTLY MONOCHROMATIC RADIATION

In all the following cases, we accept that the reflecting crystal planes intercept the entire X-ray beam and are parallel to the crystal face. When a crystal is bent to a radius 2-R to form a cylindrical surface, the crystal planes are also bent to the same radius 2·R (Fig. 1). If the crystal is completely opaque to radiation, its surface is shown by a thin circular line in coincidence with the reflecting plane (hkl). We will analyze only the errors in the equator rays as they are the ones of interest. For a wavelenght λ of a strictly monochromatic radiation, the proper angle θ for reflection from the crystal is defined by Bragg's law:

$$2 \cdot d \cdot \sin\theta = \lambda \qquad (1)$$

where d is the spacing of the crystal planes (hkl).

For a given source-crystal distance SC, a circle (focusing circle) passing through the points S and C is completely defined, or for a given ra-

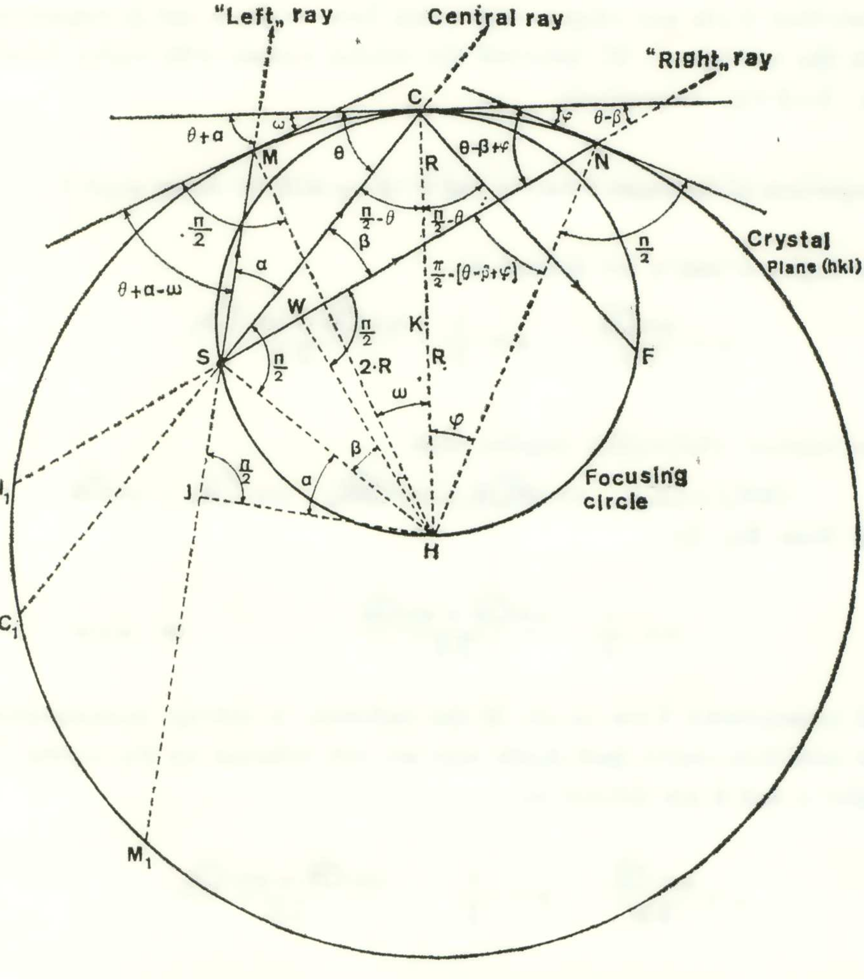

Fig. 1. The geometry for a divergent X-ray beam incident on a cylindrically bent crystal.

dius R of the focusing circle, the distance (SC) is completely defined by the relation

$$(SC)=2\cdot R\cdot \sin\theta \tag{2}$$

A point source S of divergent radiation exists on the focusing circle in a position for Bragg reflection of the ray SC (c e n t r a l r a y). We examine the behavior for the «Left» and «Right» rays on the crystal. Figure 1 shows that «Left» and «Right» rays which form angles α and β, respectively, with the central ray SC intersect the crystal surface with angles $\theta+\alpha-\omega$ and $\theta-\beta+\varphi$, respectively.

Comparison of the angles $\theta+\alpha-\omega$ and $\theta-\beta+\varphi$ with the Bragg angle θ

The angles ω and α are defined as:

$$\omega=\frac{\mathrm{arc}\widehat{CM}}{2\cdot R} \qquad \alpha=\frac{1}{2}\cdot\frac{\mathrm{arc}\,\widehat{CM}+\mathrm{arc}\,\widehat{C_1M_1}}{2\cdot R} \tag{3}$$

The relation (HJ)<(HS) implies that:

$$(MM_1)>(CC_1)\ ,\quad \mathrm{arc}\,\widehat{MC_1M_1}>\mathrm{arc}\,\widehat{CMC_1}\ ,\quad \mathrm{arc}\,\widehat{C_1M_1}>\mathrm{arc}\widehat{CM}$$

And from Eq. (3):

$$\alpha>\frac{1}{2}\cdot\frac{\mathrm{arc}\widehat{CM}+\mathrm{arc}\widehat{CM}}{2\cdot R} \qquad \text{or} \quad \alpha>\omega$$

and consequently $\theta+\alpha-\omega>\theta$. If the radiation is strictly monochromatic, this condition imples that «Left» rays are not reflected by the crystal. The angles φ and β are defined as:

$$\varphi=\frac{\mathrm{arc}\,\widehat{CN}}{2\cdot R} \qquad \beta=\frac{1}{2}\cdot\frac{\mathrm{arc}\,\widehat{CN}+\mathrm{arc}\,\widehat{CN_1}}{2\cdot R} \tag{4}$$

The relation (HW)<(HS) implies that:

$$(NN_1)>(CC_1) \qquad \mathrm{arc}\,\widehat{NCN_1}>\mathrm{arc}\,\widehat{CN_1C_1} \qquad \mathrm{arc}\,\widehat{CN}>\mathrm{arc}\widehat{C_1N_1}$$

And from Eq. (4):

$$\beta<\frac{1}{2}\cdot\frac{\mathrm{arc}\,\widehat{CN}+\mathrm{arc}\,\widehat{CN}}{2\cdot R} \qquad \text{or } \beta<\varphi$$

and consequently $\theta-\beta+\varphi>\theta$. That means, «Right» rays are not reflected from the crystal. Therefore, in the ideal case of strictly monochromatic radiation from a point source, no broadening occurs.

II. POINT SOURCE - LINE HAVING A NATURAL FWHM $2 \cdot \Delta E_{FWHM}$

Only a divergent beam exists. A «Left» ray reflects from the crystal at the wavelength λ_L difined by the equation:

$$2 \cdot d \cdot \sin(\theta + \alpha - \omega) = \lambda_L$$

In as much as $\theta + \alpha - \omega > \theta$, then $\lambda_L > \lambda$, where λ is the wavelength corresponding to the angle θ (Fig. 1). We can write:

$$2 \cdot d \cdot \sin \cdot (\theta + \alpha - \omega) = \lambda + \Delta\lambda_L \qquad (\Delta\lambda_L > 0) \tag{5}$$

Similarly, a «Right» ray reflects from the crystal at wavelenght λ_R defined by the equation:

$$2 \cdot d \cdot \sin(\theta - \beta + \varphi) = \lambda_R$$

In as much as $\theta - \beta + \varphi > \theta$, then $\lambda_R > \lambda$, so we write:

$$2 \cdot d \cdot \sin(\theta - \beta + \varphi) = \lambda + \Delta\lambda_R \qquad (\Delta\lambda_R > 0) \tag{6}$$

Therefore, only the r i g h t h a l f of the curve of Fig. 2 permits reflections both for «Left» and «Right» rays. For a line having a given full width at half maximum (FWHM), the angles α, β, ω, and φ have values limited by this width, thus the divergent beam accepted by the crystal has one limit for the «Left» and one limit for the «Right» ray. The positions of these limit rays are dependent on the $\Delta\lambda_{L_{max}}$ and $\Delta\lambda_{R_{max}}$. For most characteristic lines (Fig. 2):

$$\Delta\lambda_{L_{max}} = \Delta\lambda_{R_{max}} = 3 \cdot \Delta\lambda_{FWHM} = \Delta\lambda_{max}$$

We put for convenience $\Delta\theta_{max} = \Delta\theta$, $\Delta\lambda_{max} = \Delta\lambda$, $\Delta E_{max} = \Delta E$*

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*It can be shown that $\frac{\Delta\lambda}{E} = \left|\frac{\Delta E}{E}\right|$

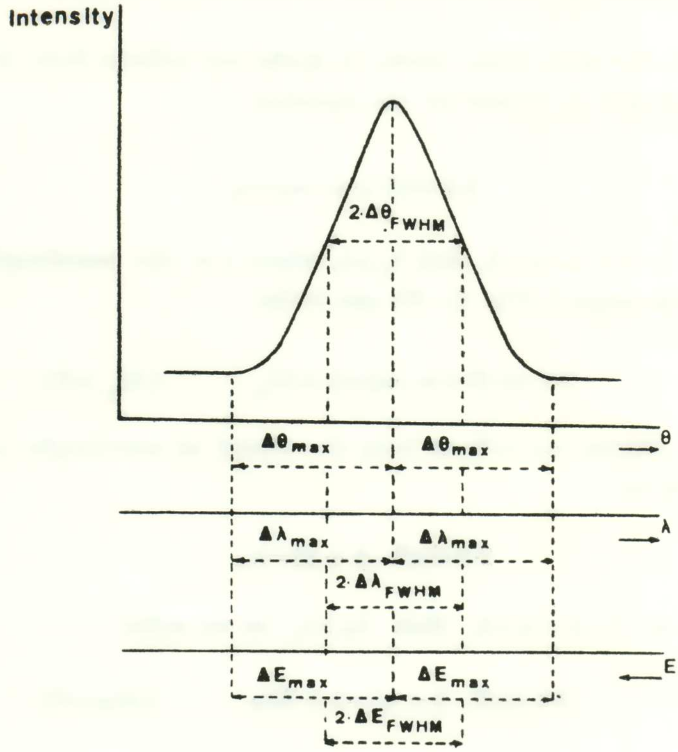

Fig. 2. X-ray line having a natural FWHM of $2\cdot\Delta E_{FWHM}$.

Equations (1), (5), and (6) give for the limit «Left» and «Right» rays:

$$\sin(\theta + \alpha - \omega) = \left(1 + \frac{\Delta\lambda}{\lambda}\right) \cdot \sin\theta \tag{7}$$

and

$$\sin(\theta - \beta + \varphi) = \left(1 + \frac{\Delta\lambda}{\lambda}\right) \cdot \sin\theta. \tag{8}$$

From Fig. 1 we have:

$$(HJ) = (HS)\cdot\cos\alpha, \qquad (HS) = (OC).\sin\left[\frac{\pi}{2} - \theta\right] = 2\cdot R\cdot\cos\theta$$

$$(HJ)=2\cdot R\cdot\cos\theta\cdot\cos\alpha,\quad (HJ)=(HM)\cdot\sin\left[\frac{\pi}{2}-(\theta+\alpha-\omega)\right]=2.R.\cos(\theta+\alpha-\omega)$$

$$\cos(\theta+\alpha-\omega)=\cos\theta\cdot\cos\alpha \tag{9}$$

Equations (7) and (9) imply:

$$\cos\alpha=\sqrt{1-\frac{\Delta\lambda}{\lambda}\cdot\left[2+\frac{\Delta\lambda}{\lambda}\right]\cdot\tan^2\theta} \tag{10}$$

Similarly, from Fig. 1:

$$(HW)=(HS)\cdot\cos\beta=2\cdot R\cdot\cos\theta\cdot\cos\beta$$

$$(HW)=(HN)\cdot\sin\left[\frac{\pi}{2}-(\theta-\beta+\varphi)\right]=2\cdot R\cdot\cos(\theta-\beta+\varphi)$$

$$\cos(\theta-\beta+\varphi)=\cos\theta\cdot\cos\beta \tag{11}$$

Equations (8) and (11) imply:

$$\cos\beta=\sqrt{1-\frac{\Delta\lambda}{\lambda}\cdot\left[2+\frac{\Delta\lambda}{\lambda}\right]\cdot\tan^2\theta} \tag{12}$$

For the same $\frac{\Delta\lambda}{\lambda}$ Eqs. (7), (8), (10), and (12) give:

$\alpha=\beta$ (Rays symmetrical to the central ray) and $\omega+\varphi=2\cdot\alpha$ (13)

For θ very large, it is possible that:

$$1-\frac{\Delta\lambda}{\lambda}\cdot\left[2+\frac{\Delta\lambda}{\lambda}\right]\cdot\tan^2\theta<\theta$$

In this case, the $\Delta\lambda$ is smaller than $3\cdot\Delta\lambda_{FWHM}$, i.e., a small part of the right half of the curve of Fig. 2 permits reflections. In as much as the ratio $\Delta\lambda/\lambda$ for characteristic X — rays remains between 0.00037 and 0.0016[10], the last condition is valid for $\theta>86.8°$.

Path of the «Left» and «Right» Rays after Reflection

We examine the intersection of the «Left» and «Right» rays with the focusing circle (Fig. 3). It is easy to show that:

$$\text{arc}\widehat{BD} < \text{arc}\widehat{DE} \qquad \text{arc}\widehat{ZG} < \text{arc}\widehat{GI}. \tag{14}$$

From Fig. 3 we have:

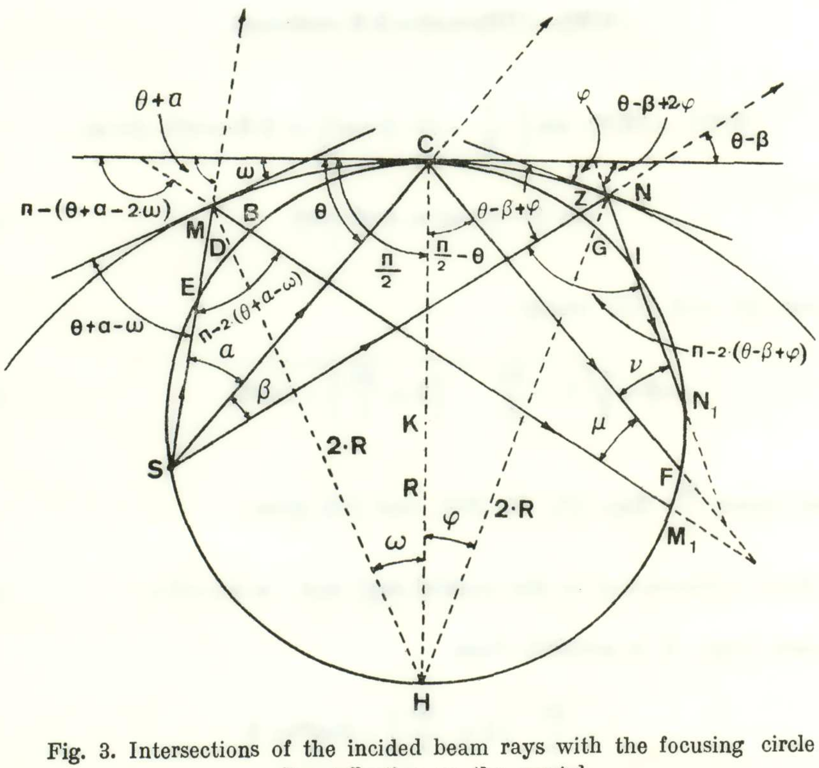

Fig. 3. Intersections of the incided beam rays with the focusing circle after reflection on the crystal.

$\pi - (\theta + \alpha - 2\cdot\omega) = \frac{\pi}{2} + (\frac{\pi}{2} - \theta) + \mu$ or that $\mu = 2\cdot\omega - \alpha$ and:

$$\mu = 2\cdot\omega - \alpha = 2\cdot\frac{\text{arc}\,\widehat{CD}}{2\cdot R} - \frac{\text{arc}\,\widehat{CE}}{2\cdot R} = \frac{\text{arc}2\cdot\widehat{CD} - \text{arc}\widehat{CE}}{2\cdot R}$$

$$= \frac{\text{arc}\widehat{CB} + \text{arc}(\widehat{BD} - \widehat{DE})}{2\cdot R}$$

And according to the first of Eq. (14):

$$\mu < \frac{\text{arc}\,\widehat{CB}}{2\cdot R}$$

This relation implies that the intersection of the rays CF and MM_1 do not lie on the focusing circle, i.e., the intersection M_1 of the ray CM_1 with the focusing circle lies «under» the point F, so that the ray SM causes after reflection the broadening $\text{arc}\widehat{M_1F}$, focusing error. Also, we have from Fig. 4:

$$\theta - \beta + 2\cdot\varphi = \theta + \nu \quad \text{or} \quad \nu = 2\cdot\varphi - \beta \qquad \text{And:}$$

$$\nu = 2\cdot\varphi - \beta = 2\cdot\frac{\text{arc}\,\widehat{CG}}{2\cdot R} - \frac{\text{arc}\,\widehat{CZ}}{2\cdot R} = \frac{\text{arc}2\cdot\widehat{CG} - \text{arc}\,\widehat{CZ}}{2\cdot R}$$

$$= \frac{\text{arc}\widehat{CZ} + \text{arc}\widehat{ZG} + \text{arc}\widehat{ZG}}{2\cdot R}$$

And according to the second relationship of Eq. (14):

$$\nu < \frac{\text{arc}\,\widehat{CI}}{2\cdot R}$$

The last equation implies that the intersection of the rays CF and NN_1 lies off the focusing circle so that the ray SN after reflection causes the broadening denoted by $\text{arc}\widehat{N_1F}$.

Calculation of the Broadening from a «Left» Ray

To calculate the angle δ, we use the relationships from Fig. 4:

$$(HL) = (HM)\cdot\sin\left[\frac{\pi}{2} - (\theta + \alpha - \omega)\right] = 2\cdot R\cdot\cos(\theta + \alpha - \omega)$$

$$= 2\cdot R\cdot\cos\theta\cdot\cos\alpha$$

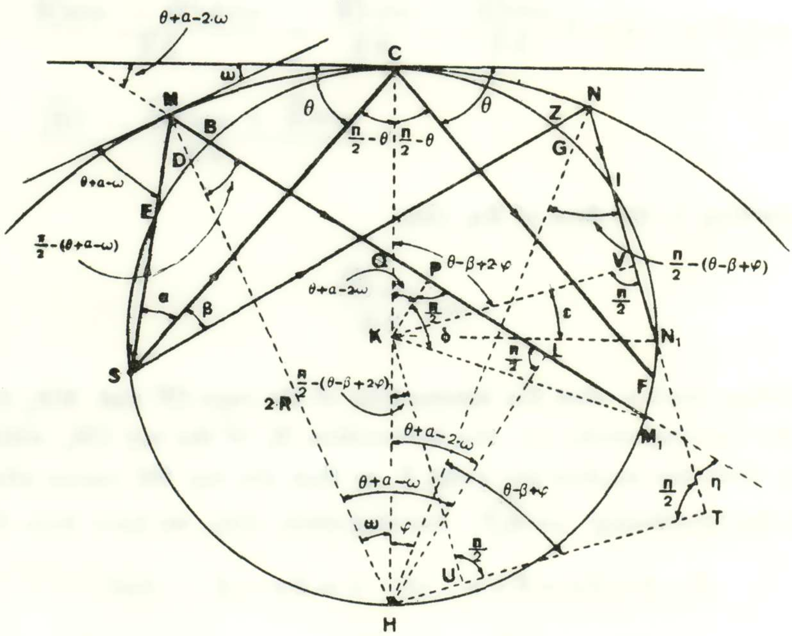

Fig. 4. Path of the rays of a divergent beam before and after reflection on the crystal.

$$(HQ) = \frac{(HL)}{\cos(\theta + \alpha - 2\cdot\omega)} = \frac{2\cdot R\cdot\cos\theta\cdot\cos\alpha}{\cos(\theta + \alpha - 2\cdot\omega)}$$

$$(KQ) = (HQ) - (HK) = \left[\frac{2\cdot\cos\theta\cdot\cos\alpha}{\cos(\theta + \alpha - 2\cdot\omega)} - 1\right]\cdot R$$

$$(KP) = (KQ)\cdot\cos(\theta + \alpha - 2\cdot\omega) = [2\cdot\cos\theta\cdot\cos\alpha - \cos(\theta + \alpha - 2\cdot\omega)]\cdot R$$

$$(KP) = R\cdot\cos\delta \quad \text{and} \quad \cos\delta = 2\cdot\cos\theta\cdot\cos\alpha - \cos(\theta + \alpha - 2\cdot\omega) \qquad (15)$$

Equations (9) and (15) define the angle δ for given angles θ and α.

From Fig. 4 we conclude that:

$$\text{arc}\widehat{M_1C} + \text{arc}\widehat{CB} = 2\cdot\delta\cdot R\ , \qquad \text{arc}\widehat{M_1C} - \text{arc}\widehat{CB} = 2\cdot(\theta + \alpha - 2\cdot\omega)\cdot R$$

and $$\mathrm{arc}\widehat{M_1C} = (\theta + \alpha + \delta - 2 \cdot \omega) \cdot R$$

The broadening $\mathrm{arc}\widehat{M_1F}$ is:

$$\mathrm{arc}\widehat{M_1F} = \mathrm{arc}\widehat{M_1C} - \mathrm{arc}\widehat{FC} = (\theta + \alpha + \delta - 2 \cdot \omega) \cdot R - 2 \cdot \theta \cdot R$$

And finally $$\frac{\mathrm{arc}\widehat{M_1F}}{R} = \alpha + \delta - \theta - 2 \cdot \omega \qquad \text{Angular broadening from the «Left» ray SM} \qquad (16)$$

where α, ω, and δ are defined by Eqs. (9), (10), and (15) respectively.

Calculation of the Broadening from a «Right» Ray

To calculate the angle ε, we derive from Fig. 4 that:

$$(HT) = (HN) \cdot \sin\left[\frac{\pi}{2} - (\theta - \beta + \varphi)\right] = 2 \cdot R \cdot \cos(\theta - \beta + \varphi)$$
$$= 2 \cdot R \cdot \cos\theta \cdot \cos\beta$$

$$(HU) = (HK) \cdot \sin\left[\frac{\pi}{2} - (\theta - \beta + 2 \cdot \varphi)\right] = R \cdot \cos(\theta - \beta + 2 \cdot \varphi)$$

$$(KV) = (UT) = [2 \cdot \cos\theta \cdot \cos\beta - \cos(\theta - \beta + 2 . \varphi)] \cdot R\,,\ (KV) = R \cdot \cos\varepsilon$$

$$\cos\varepsilon = 2 \cdot \cos\theta \cdot \cos\beta - \cos(\theta - \beta + 2 \cdot \varphi) \qquad (17)$$

For $\varepsilon = 0$ (NN_1 tangent to the focusing circle), Eq. (17) gives:

$$2 \cdot \cos\theta \cdot \cos\beta - \cos\,(\theta - \beta + 2 \cdot \varphi) = 1$$

This equation defines the g e o m e t r i c a l β_{max}^{Geom} If $\beta > \beta_{max}^{Geom}$, the reflected ray NN_1 d o e s n o t t o u c h the focusing circle.

The broadening $\mathrm{arc}\widehat{FN_1}$ is:

$$\mathrm{arc}\widehat{FN_1} = \mathrm{arc}\widehat{FN_1C} - \mathrm{arc}\widehat{N_1C} = 2 \cdot \theta \cdot R - (\theta - \beta + 2 \cdot \varphi + \varepsilon) \cdot R$$

And $$\frac{\mathrm{arc}\widehat{FN_1}}{R} = \theta + \beta - 2 \cdot \varphi - \varepsilon \qquad \text{Angular broadening from the «Right» ray SN} \qquad (18)$$

where β, φ, and ε are defined by Eqs. (12). (11), and (17) respectively.

Total Broadening from «Left» and «Right» Rays

The total broadening is (Fig. 4):

$$\mathrm{arc}\widehat{M_1N_1} = \mathrm{arc}\widehat{M_1F} + \mathrm{arc}\widehat{FN_1}$$

$$\frac{\mathrm{arc}\widehat{M_1N_1}}{R} = \alpha + \beta + \delta - \varepsilon - 2 \cdot (\omega + \varphi)$$ Total angular broadening from «Left» and «Right» rays

For $\alpha = \beta$ when $\omega + \varphi = 2\alpha$:

$$\frac{\mathrm{arc}\widehat{M_1N_1}}{R} = \delta - \varepsilon - 2 \cdot \alpha \qquad (19)$$ Total angular broadening from «Left» and «Right» rays when $\alpha = \beta$

Perceptive Broadening

The counter of the spectrometer is rotated about an axis perpendicular to the equator at point C on the focusing circle; therefore, it is very useful to know the angle η (Fig. 4) which defines the perceptive total broadening:

$$\eta = \frac{\mathrm{arc}\widehat{BCI} - \mathrm{arc}\widehat{N_1M_1}}{2 \cdot R} = \frac{\mathrm{arc}\widehat{BCM_1} - \mathrm{arc}\widehat{IN_1} - \mathrm{arc}\widehat{N_1M_1} - \mathrm{arc}\widehat{N_1M_1}}{2 \cdot R}$$

Or $$\eta = 2 \cdot (\omega + \varphi) - (\alpha + \beta)$$

For $\alpha = \beta$ when $\omega + \varphi = 2 \cdot \alpha$ we have $\eta = 2 \cdot \alpha$

III. SOURCE HAVING A GIVEN LENGTH ALONG THE FOCUSING CIRCLE - STRICTLY MONOCHROMATIC RADIATION

From such a source, divergent, convergent, and parallel beams exist. Only divergent beam rays have the possibility of making the proper Bragg angle θ with the crystal.

If the source S with a length of $\mathrm{arc}2.\widehat{SS_1}$ along the focusing circle is in a reflection position for the ray SC [wavelenght λ, Fig. (5)], then:

$$(HS) = (HF) = (HC) \cdot \sin\left[\frac{\pi}{2} - \theta\right] = 2 \cdot R \cdot \cos\theta$$

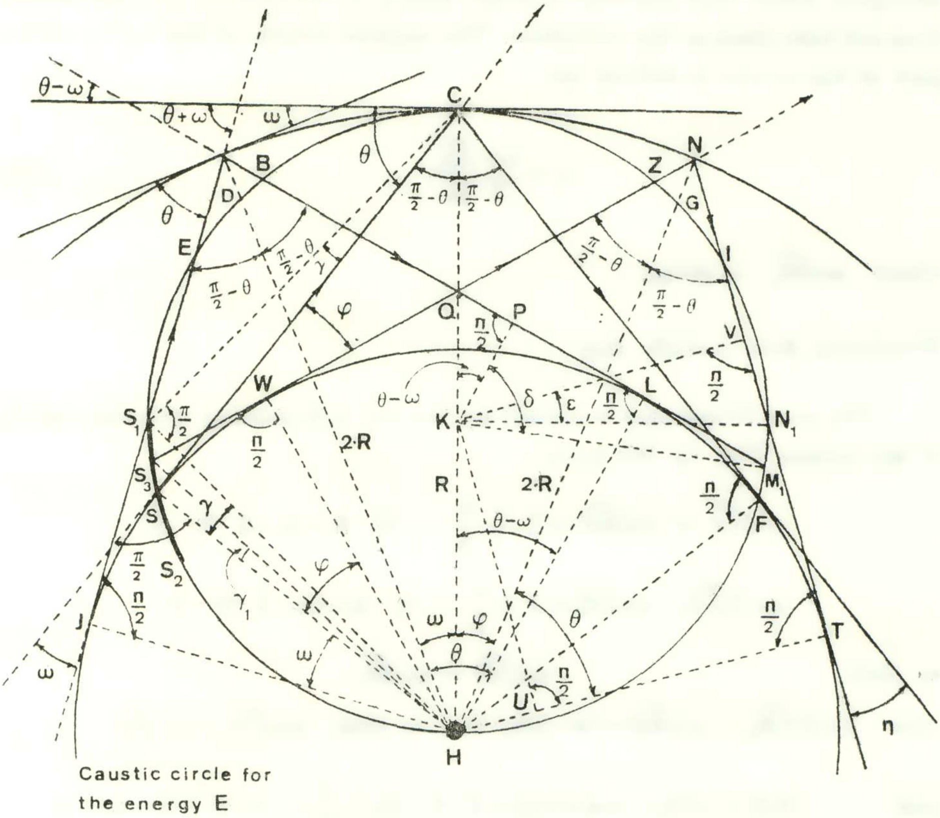

Fig. 5. Broadening from «Left» and «Right» rays from an extended source.

The points S and F lay on a circle having center H and radius (HS) which defines the c a u s t i c c i r c l e*. Every other ray S_3W tangent to the caustic circle intersects the crystal surface with the angle θ as is evident from Fig. 5. The supplement of this angle is π/2—θ, and this is possible only for

*If the crystal planes are not parallel to the crytal face, there are two different caustic circles, one for the incident and one for the differacted ray: Both have their centers at H.

divergent beam rays starting from the $\mathrm{arc}\widehat{SS_1}$ of the source, i.e., the $\mathrm{arc}\widehat{SS_2}$ does not take place in the reflection. The angular length of this e f f e c t i v e part of the source is defined as:

$$\gamma = \frac{\mathrm{arc}\ \widehat{SS_1}}{2 \cdot R} \tag{20}$$

where $\mathrm{arc}\widehat{SS_1}$ is given.

Broedening from a «Left» Ray

The max broadening is caused by the ray S_1M starting from the end S_1 of the source (Fig. 5). We have:

$$\mathrm{arc}\widehat{SH} = \mathrm{arc}\widehat{HF} = 2 \cdot \left[\frac{\pi}{2} - \theta\right] \cdot R = (\pi - 2 \cdot \theta) \cdot R$$

$$\mathrm{arc}\ \widehat{S_1SH} - \mathrm{arc}\widehat{DE} = 2 \cdot \left(\frac{\pi}{2} - \theta\right) \cdot R = (\pi - 2 \cdot \theta) \cdot R$$

so that $\mathrm{arc}\widehat{DE} = \mathrm{arc}\widehat{SS_1}$

Also $\mathrm{arc}\widehat{HFM_1} - \mathrm{arc}\widehat{BD} = (\pi - 2 \cdot \theta) \cdot R$ so that $\mathrm{arc}\widehat{FM_1} = \mathrm{arc}\widehat{BD}$

and $$(HJ) = (HS_1) \cdot \cos(\omega+\gamma) = 2 \cdot R \cdot \sin\left[\frac{\pi}{2} - \theta + \gamma\right] \cdot \cos\ (\omega+\gamma)$$

$$(HJ) = (HS_1) \cdot \cos(\omega+\gamma) = 2 \cdot R \cdot \cos\ (\theta-\gamma) \cdot \cos(\omega+\gamma)$$

$$(HJ) = (HM) \cdot \sin\left[\frac{\pi}{2} - \theta\right] = 2 \cdot R \cdot \cos\theta$$

$$\cos(\omega+\gamma) = \frac{\cos\theta}{\cos(\theta-\gamma)} \tag{21}$$

which defines the angle ω.

Also $$(HQ) = \frac{(HL)}{\cos(\theta-\omega)} = \frac{2 \cdot R \cdot \cos\theta}{\cos(\theta-\omega}$$

$$(KQ) = (HQ) - (HK) = \left[\frac{2 \cdot \cos\theta}{\cos(\theta-\omega)} - 1\right] \cdot R$$

$(KP)=(KQ)\cdot\cos(\theta-\omega)=[2\cdot\cos\theta-\cos(\theta-\omega)]\cdot R\,,\qquad (KP)=R\cdot\cos\delta$

$$\cos\delta=2\cdot\cos\theta\;(\theta-\omega) \tag{22}$$

which defines the angle δ.

For the broadening of $\mathrm{arc}\widehat{FM_1}$ we have that $\mathrm{arc}\widehat{M_1C}+\mathrm{arc}\widehat{CB}=2\cdot\delta\cdot R$

$\mathrm{arc}\widehat{M_1C}-\mathrm{arc}\widehat{CB}=2\cdot(\theta-\omega)\cdot R$ and $\mathrm{arc}\widehat{M_1C}=(\theta+\delta-\omega)\cdot R$

Also $\mathrm{arc}\widehat{FM_1}=\mathrm{arc}\widehat{FC}-\mathrm{arc}\widehat{M_1C}=2\cdot\theta\cdot R-(\theta+\delta-\omega)\cdot R$

And finally: $$\frac{\mathrm{arc}\widehat{FM_1}}{R}=\theta+\omega-\delta \quad \text{Angular broadening from the «Left» ray } S_1M \tag{23}$$

where ω and δ are defined by Eqs. (21) and (22).

Broadening from a «Right» Ray

We examine generally the broadening $\mathrm{arc}\widehat{FN_1}$ caused by a «Right» ray starting from a point S_3 of the source (Fig. 5).
It is easy to show that $\mathrm{arc}\widehat{SS_3}=\mathrm{arc}\widehat{ZG}$, $\mathrm{arc}\widehat{FN_1}=\mathrm{arc}\widehat{GI}$

For the case shown in Fig. 5 the broadening $\mathrm{arc}\widehat{FN_1}$ of the «Right» ray S_3N includes the broadening $\mathrm{arc}\widehat{FM_1}$ from the limit «Left» ray S_1C. Thus the broadening $\mathrm{arc}\widehat{FN_1}$ is also the total broadening. In every case both broadenings from «Left» and «Right» rays are «above» the point F.

From Fig. 5 we have that $\gamma_1=\dfrac{\mathrm{arc}\,\widehat{SS_3}}{2\cdot R}$

$(HW)=(HN)\cdot\sin\left[\dfrac{\pi}{2}-\theta\right]=2\cdot R\cdot\cos\theta\,,\qquad (HW)=(HS_3)\cdot\cos(\varphi-\gamma_1)$

* $(HS_3)=(HC)\cdot\sin\left[\dfrac{\pi}{2}-\theta+\gamma_1\right]=2\cdot R\cdot\cos(\theta-\gamma_1)$

$$(HW)=2\cdot R\cdot\cos(\theta-\gamma_1)\cdot\cos(\varphi-\gamma_1)\,,\qquad \cos(\varphi-\gamma_1)=\frac{\cos\theta}{\cos(\theta-\gamma_1)} \tag{24}$$

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*In Fig. 5 the line CS_3 is not plotted.

which defines the angle φ. Also:

$$(HT) = (HN)\cdot\sin\left[\frac{\pi}{2}-\theta\right] = 2\cdot R\cdot\cos\theta\ ,\quad (HU)=(HK)\cdot\cos(\theta+\varphi) = R\cdot\cos\,(\theta+\varphi)$$

$$(KV)=(UT)=(HT)-(HU)=[2\cdot\cos\theta-\cos(\theta+\varphi)]\cdot R$$

$$(KV)=(KN_1)\cdot\cos\varepsilon=R\cdot\cos\varepsilon$$

$$\cos\varepsilon=2\cdot\cos\theta-\cos\,(\theta+\varphi) \tag{25}$$

which defines the angle ε. For the broadening $\mathrm{arc}\widehat{FN_1}$ we have that:

$$\mathrm{arc}\widehat{FN_1}+\mathrm{arc}\widehat{N_1I}+\mathrm{arc}\ \widehat{IG}+\mathrm{arc}\widehat{GC}=2\cdot\theta\cdot R$$

or
$$\mathrm{arc}\widehat{FN_1}+2\cdot\varepsilon\cdot R+\mathrm{arc}\widehat{FN_1}+2\cdot\varphi\cdot R=2\cdot\theta\cdot R$$

And finally $$\frac{\mathrm{arc}\widehat{FN_1}}{R}=\theta-\varepsilon-\varphi \qquad \text{Angular broadening from the «Right» ray } S_3N \text{ (Total)} \tag{26}$$

Maximum Total Broadening

The broadening becomes a maximum when the ray NN_1 is tangent to the focusing circle; then $\varepsilon=0$, and Eq. (25) gives for the angle φ:

$$2\cdot\cos\theta-\cos\,(\theta+\varphi_{max})=1 \tag{27}$$

so that $$\left[\frac{\mathrm{arc}\ FN_1}{R}\right]_{max}=\theta-\varphi_{max} \qquad \text{Maximum total angular broadening} \tag{28}$$

From Eqs. (27) and (28) it is evident that for Case III, the maximum total angular broadening in a Johann spectrometer depends only on the Bragg angle θ*.

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*The φ_{max} corresponding to the maximum permissible broadening does not mean that it is maximum itself.

Adequate Lenght of the Source for Maximum Broadening

We calculate the angle ζ using the geometry shown in Fig. 6.

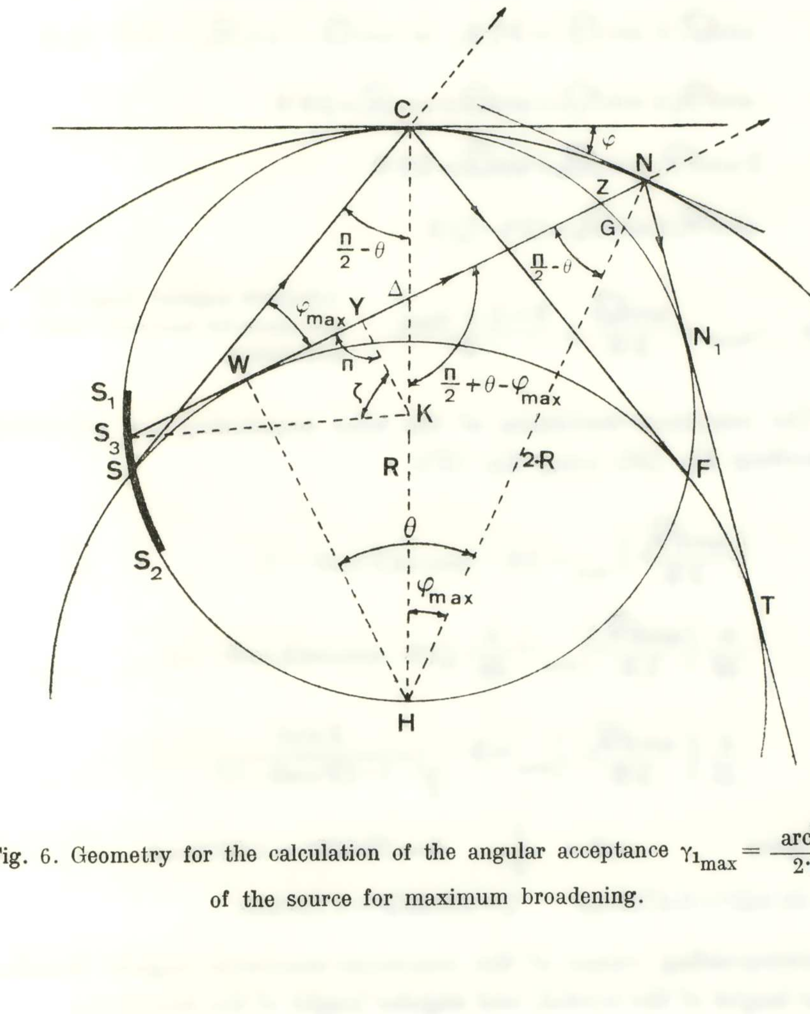

Fig. 6. Geometry for the calculation of the angular acceptance $\gamma_{1_{max}} = \dfrac{\operatorname{arc}\widehat{S_3S}}{2 \cdot R}$ of the source for maximum broadening.

$$(H\Delta) = \frac{(HW)}{\cos(\theta - \varphi_{max})} = \frac{2 \cdot R \cdot \cos\theta}{\cos(\theta - \varphi_{max})}$$

$$(K\Delta) = (H\Delta) - (HK) = \left[\frac{2 \cdot \cos\theta}{\cos(\theta - \varphi_{max})} - 1\right] \cdot R$$

$(KY)=(K\Delta)\cdot\cos(\theta-\varphi_{max})=[2\cdot\cos\theta-\cos\theta-\varphi_{max})\cdot R,\quad (KY)=(KS_3)\cdot\cos\zeta$

$$\cos\zeta=2\cdot\cos\theta-\cos(\theta-\varphi_{max}) \qquad (29)$$

which defines the angle ζ when $\varepsilon=0$.

Also $\quad \mathrm{arc}\widehat{S_3C}+\mathrm{arc}\,\widehat{CZ}=2\cdot\zeta\cdot R,\;$ or $\;\mathrm{arc}\,\widehat{CZ}-\mathrm{arc}\,\widehat{SS_3}=2\cdot(\zeta-\theta).R$

And $\quad \mathrm{arc}\widehat{FN_1}+\mathrm{arc}\widehat{N_1G}+\mathrm{arc}\widehat{GZ}+\mathrm{arc}\widehat{ZC}=2\cdot\theta\cdot R$

Or $\quad 2\cdot\mathrm{arc}\widehat{FN_1}+\mathrm{arc}\widehat{SS_3}+\mathrm{arc}\widehat{CZ}=2\cdot\theta\cdot R$

and $\quad \mathrm{arc}\widehat{FN_1}+\mathrm{arc}\widehat{SS_3}=(2\cdot\theta-\zeta)\cdot R$

Finally $\quad \gamma_{1max}=\dfrac{\mathrm{arc}\widehat{S_3S}}{2\cdot R}=\dfrac{\theta-\zeta+\varphi_{max}}{2}$ Adequate angular lenght of the source for maximum total broadening (30)

The maximum-maximum of the total broadening can be calculated by rewriting Eq. (28) using Eq. (27):

$$\left[\frac{\mathrm{arc}\widehat{FN_1}}{2\cdot R}\right]_{max}=2\cdot\theta-\arccos[2\cdot\cos\theta-1]$$

and $$\frac{d}{d\theta}\left[\frac{\mathrm{arc}\widehat{FN_1}}{2.R}\right]_{max}=\frac{d}{d\theta}\cdot[2\cdot\theta-\arccos(2.\cos\theta-1)]$$

$$\frac{d}{d\theta}\left[\frac{\mathrm{arc}\widehat{FN_1}}{2\cdot R}\right]_{max}=2-\frac{2\cdot\sin\theta}{\sqrt{1-[2\cdot\cos\theta-1]^2}}=0$$

which gives $\qquad \cos\theta=\dfrac{1}{3} \qquad \theta=70\cdot529^{o}=1\cdot2310\mathrm{rad},$

$\varphi_{max}=38.942^{o}=0.6797\mathrm{rad}\;,\quad \zeta=100.672^{o}=1.7574\mathrm{rad}$

The corresponding values of the maximum-maximum angular broadening, angular lenght of the crystal, and angular lenght of the source are:

$\left[\dfrac{\mathrm{arc}\widehat{FN_1}}{R}\right]_{max\text{-}max.}=0.5513\ \mathrm{rad}\;,\;\varphi_{max\text{-}max}=0.6797\ \mathrm{rad}\;\;\gamma_{1_{max\text{-}max}}=0.078\ \mathrm{rad}^*,$

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*The $\gamma_{1_{max\text{-}max}}$ corresponds to the maximum-maximum broadening but this does not mean that it is maximum itself.

The above very large values are not practical. Generaly, in Case III we need to first calculate from Eq. (30) the angle $\gamma_{1_{max}}$ for the given θ and compare it with the given γ of the source. If $\gamma > \gamma_{1_{max}}$* Eq. (28) gives the total broadening. If $\gamma < \gamma_{1_{max}}$, Eq. (26) gives the total broadening by substituting γ for γ_1.

Perceptive Total Angular Broadening

The perceptive total angular broadening is (see Fig. 5):

$$\eta = \frac{\text{arc}\widehat{CI} - \text{arc}\widehat{N_1F}}{2 \cdot R} = \frac{\text{arc}\widehat{CG} + \text{arc}\widehat{GI} - \text{arc}\widehat{N_1F}}{2 \cdot R} = \frac{\text{arc}\widehat{CG}}{2 \cdot R} = \varphi$$

where φ is defined by Eq. (24).

Matching the Broadening from the «Right» Ray to that of the «Left» Ray

For a given angular lenght of the source, it is possible to have the contribution to the total broadening arc$\widehat{FN_1}$ the same for both «Left» and «Right» rays.

The matching of the broadening contribution from the «Left» and «Right» rays takes place when the «Right» ray NN_1 passes from the point M_1 (Fig. 5). Then if the lenght of the right part of the crystal is reduced to the arc$\widehat{CN}$, the condition for minimization is fulfilled. Further reduction in the right part of the crystal «below» arc$\widehat{CN}$ does not reduce the broadening arc$\widehat{FM_1}$ but results in a loss of intensity.

From Fig. 5 when NN_1 passes through the point M_1 ($\varphi = \varphi_{miu}$)**, it is concluded that:

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*For $5^o < \theta < 80^o$, it is concluded that $2 \cdot 10^{-2}$ rad $< \gamma_{1_{max}} < 77.10^{-2}$ rad. For this reason, the case $\gamma_1 > \gamma_{1max}$ is rather improbable

**φ_{min} means that it corresponds to the crystal lenght giving the minimum broadening

$$\varphi_{min} = \delta - \omega - \varepsilon \tag{31}$$

The quantities δ and ω are independent of φ_{min}, but ε is not:

$$\cos\varepsilon = 2.\cos\theta - \cos(\theta + \varphi_{min}) \tag{32}$$

Equations (31) and (32) give:

$$\cos\left[\frac{\theta+\omega-\delta}{2} + \varphi_{min}\right] = \frac{\cos\theta}{\cos\frac{\theta+\delta-\omega}{2}}$$

where δ and ω are defined by Eqs. (21) and (22).

IV. SOURCE HAVING A GIVEN LENGTH ALONG THE FOCUSING CIRCLE - RADIATION HAVING A FWHM $2 \cdot \Delta E_{FWHM}$ (GENERAL CASE)

Parallel, covergent, and divergent beams exist. Each ray has an energy spectrum for which the crystal will make the proper Bragg angle for a part of the spectrum.

We suppose that the central ray SC (for which the Bragg angle is θ) starts from point S of the source $\mathrm{arc}\widehat{S_1S_2}$, which is extended along the focusing circle. The angles γ_1 and γ_2 (given) are defined by:

$$\gamma_1 = \frac{\mathrm{arc}\widehat{S_1S}}{2 \cdot R} \qquad \text{and} \qquad \gamma_2 = \frac{\mathrm{arc}\widehat{SS_2}}{2 \cdot R}$$

Parallel Beam

From the infinite systems of parallel beams we examine those beams parallel to the central ray SC (Fig. 7). The ray S_1C starting from the left end S_1 of the source impacts rhe crystal under the angle $\theta - \omega$, so that the left half of the cuvre of Fig. 2 permits reflections from «Left» rays parallel to the central ray SC. The «Right» ray S_2N parallel to the central ray SC impacts the crystal under the angle $\theta + \varphi$, so that the right half of the curve of Fig. 2 permits reflections for «Right» rays.

Broadening from a «Left» Ray

For the broadening arc$\widehat{FM_1}$ we have from Fig. 7 that:

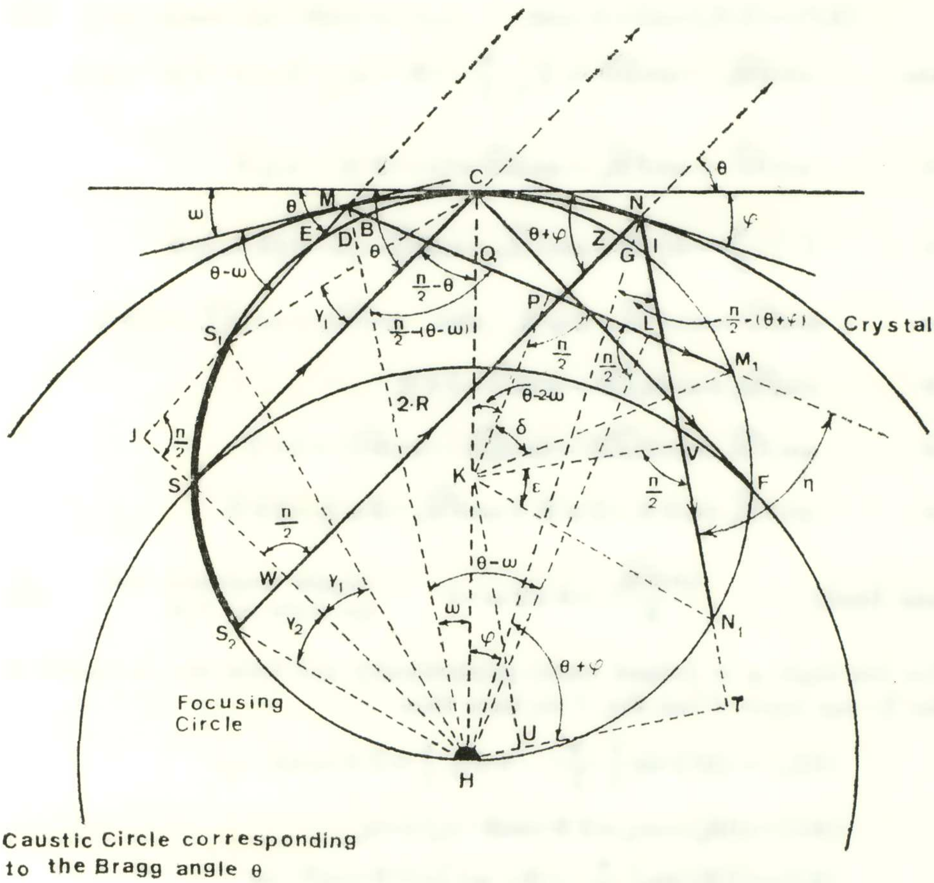

Fig. 7. Broadening from a beam parallel to the central ray SC.

$$(HL)=(HM)\cdot\sin\left[\frac{\pi}{2}-(\theta-\omega)\right]=2\cdot R\cdot\cos(\theta-\omega)$$

$$(HQ)=\frac{(HL)}{\cos(\theta-2\cdot\omega)}=\frac{2\cdot R\cdot\cos(\theta-\omega)}{\cos(\theta-2\cdot\omega)}$$

$$(KQ)=(HQ)-(HK)=\left[\frac{2\cdot\cos(\theta-\omega)}{\cos(\theta-2.\omega)}-1\right]\cdot R$$

$$(KP)=(KQ)\cdot\cos(\theta-2\cdot\omega)=[2\cdot\cos(\theta-\omega)-\cos(\theta-2\cdot\omega)]\cdot R$$

$$(KP)=(KM_1)\cdot\cos\delta=R\cdot\cos\delta,\qquad \cos\delta=2\cdot\cos(\theta-\omega)-\cos(\theta-2\cdot\omega) \tag{33}$$

Also $\quad \text{arc}\widehat{HM_1}-\text{arc}\widehat{BD}=2\cdot\left[\frac{\pi}{2}-(\theta-\omega)\right]\cdot R=[\pi-2\cdot(\theta-\omega)]\cdot R$

Or $\quad \text{arc}\widehat{HF}+\text{arc}\widehat{FM_1}-\text{arc}\widehat{BD}=[\pi-2\cdot(\theta-\omega)].R$

Or $\quad 2\cdot\left[\frac{\pi}{2}-\theta\right]\cdot R+\text{arc}\widehat{FM_1}-\text{arc}\widehat{BD}=[\pi-2\cdot(\theta-\omega)]\cdot R$

So $\quad \text{arc}\widehat{BD}=\text{arc}\widehat{FM_1}-2\cdot\omega\cdot R,\quad$ also $\quad \text{arc}\widehat{FM_1}+\text{arc}\widehat{M_1C}=2\cdot\theta\cdot R$

Or $\quad \text{arc}\widehat{FM_1}+\text{arc}\widehat{M_1CB}-\text{arc}\widehat{CB}=2\cdot\theta\cdot R$

Or $\quad \text{arc}\,\widehat{FM_1}+\text{arc}\widehat{M_1CB}-(\text{arc}\widehat{CD}-\text{arc}\widehat{BD})=2\cdot\theta\cdot R$

Or $\quad \text{arc}\widehat{FM_1}+2\cdot\delta\cdot R-2\cdot\omega\cdot R+\text{arc}\widehat{FM_1}-2\cdot\omega\cdot R=2\cdot\theta\cdot R$

And finally $\quad \dfrac{\text{arc}\widehat{FM_1}}{R}=\theta+2\cdot\omega-\delta \qquad$ Angular broadening from the «Left» ray S_1M $\quad$ (34)

But the angle ω is defined twice: geometrically and from the $\Delta\lambda$ spread of the X- ray beam. From Fig. 7 we have that:

$$(HS_1)=(HC)\cdot\sin\left[\frac{\pi}{2}-\theta+\gamma_1\right]=2\cdot R\cdot\cos(\theta-\gamma_1)$$

$$(HJ)=(HS_1).\cos\gamma_1=2\cdot R\cdot\cos(\theta-\gamma_1)\cdot\cos\gamma_1$$

$$(HJ)=(HM)\cdot\sin\left[\frac{\pi}{2}-(\theta-\omega)\right]=2\cdot R\cdot\cos(\theta-\omega)$$

$$\cos(\theta-\omega)=\cos(\theta-\gamma_1)\cdot\cos\gamma_1 \tag{35}$$

which defines the angle ω from the dimension γ_1 of the source. Also the Bragg equation gives:

$$\sin(\theta-\omega_L)=(1-\frac{\Delta\lambda}{\lambda})\cdot\sin\theta \tag{36}$$

which gives another value ω_L for the angle ω, so that we have to first compare the two values ω and ω_L. If $\omega<\omega_L$, Eq. 34) gives the broadening where the ω and δ are defined by Eqs. (35) and (33) respectively. If $\omega>\omega_L$, the ω and

δ are defined by Eqs. (36) and (33) respectively. In this case ($\omega > \omega_L$), equations (35) and (36) give that:

$$\cos(\theta - \gamma_{1_L}) \cdot \cos\gamma_{1_L} = \sqrt{1 - \left[1 - \frac{\Delta\lambda}{\lambda}\right]^2 \cdot \sin^2\theta}$$

Or $$\cos(\theta - 2\cdot\gamma_{1_L}) = 2\cdot\sqrt{1 - \left[1 - \frac{\Delta\lambda}{\lambda}\right]^2 \cdot \sin^2\theta} - \cos\theta \qquad (37)$$

which defines the part γ_{1_L} of the source which takes place in the reflecrion of a «Left» beam parallel to the central ray SC.

Broadening from «Right» Rays

For the calculation of the broadening $\mathrm{arc}\widehat{FN_1}$ from the «Right» ray S_2N, Fig. 7 gives that:

$$(HT) = (HN)\cdot\sin\left[\frac{\pi}{2} - (\theta + \varphi)\right] = 2\cdot R.\cos(\theta + \varphi)$$

$$(HU) = (HK).\cos(\theta + 2\cdot\varphi) = R\cdot\cos(\theta + 2\cdot\varphi)$$

$$(KV) = (HT) - (HU) = [2\cdot\cos(\theta + \varphi) - \cos(\theta + 2\cdot\varphi)]\cdot R$$

$$(KV) = (KN_1)\cdot\cos\varepsilon = R\cdot\cos\varepsilon$$

$$\cos\varepsilon = 2\cdot\cos(\theta + \varphi) - \cos(\theta + 2\cdot\varphi) \qquad (38)$$

Also $$\mathrm{arc}\widehat{HN_1} - \mathrm{arc}\widehat{IG} = 2\cdot\left[\frac{\pi}{2} - (\theta + \varphi)\right]\cdot R = [\pi - 2\cdot(\theta + \varphi)]\cdot R$$

Or $$\mathrm{arc}\widehat{HF} - \mathrm{arc}\,\widehat{N_1F} - \mathrm{arc}\widehat{IG} = [\pi - 2\cdot(\theta + \varphi]\cdot R$$

Or $$2\cdot\left[\frac{\pi}{2} - \theta\right]\cdot R - \mathrm{arc}\widehat{N_1F} - \mathrm{arc}\widehat{IG} = [\pi - 2\cdot(\theta + \varphi)]\cdot R$$

And $$\mathrm{arc}\widehat{IG} = 2\cdot\varphi\cdot R - \mathrm{arc}\widehat{N_1F}$$

And $$\mathrm{arc}\widehat{HN_1} + \mathrm{arc}\widehat{N_1FI} + \mathrm{arc}\widehat{IG} + \mathrm{arc}\widehat{GC} = \pi\cdot R$$

Or $$\mathrm{arc}\widehat{HF} - \mathrm{arc}\widehat{N_1F} + \mathrm{arc}\widehat{N_1FI} + \mathrm{arc}\widehat{IG} + \mathrm{arc}\widehat{GC} = \pi\cdot R$$

Or $$2\cdot\left[\frac{\pi}{2} - \theta\right]\cdot R - \mathrm{arc}\widehat{N_1F} + 2\cdot\varepsilon\cdot R + 2\cdot\varphi\cdot R - \mathrm{arc}\widehat{N_1F} + 2\cdot\varphi\cdot R = \pi\cdot R$$

And finally $$\frac{\mathrm{arc}\widehat{N_1F}}{R} = \varepsilon + 2\cdot\varphi - \theta$$ Angular broadening from the «Right» ray S_2N (39)

But the angle φ is defined twice: geometrically and from the $\Delta\lambda$ spread of the X-ray beam. From Fig. 7 we have that:

$$(HW)=(HN)\cdot\sin\left[\frac{\pi}{2}-(\theta+\varphi)\right]=2\cdot R\cdot\cos(\theta+\varphi) \qquad (HW)=(HS_2)\cdot\cos\gamma_2$$

$$^{*}(HS_2)=(HC)\cdot\sin\left[\frac{\pi}{2}-\theta-\gamma_2\right]=2\cdot R\cdot\cos(\theta+\gamma_2)$$

$$(HW)=2\cdot R\cdot\cos(\theta+\gamma_2)\cdot\cos\gamma_2$$

$$\cos(\theta+\varphi)=\cos(\theta+\gamma_2)\cdot\cos\gamma_2 \tag{40}$$

which defines the angle φ from the dimension γ_2 of the source. Also, the Bragg equation gives that:

$$\sin(\theta+\varphi_L)=(1+\frac{\Delta\lambda}{\lambda})\cdot\sin\theta \tag{41}$$

so that we have to first compare the angles φ and φ_L, If $\varphi<\varphi_L$, Eq. (39) gives the broadening, where φ and ε are defined by Eqs. (40) and (38) respectively. If $\varphi>\varphi_L$, the φ and ε are defined by Eqs. (41) and (38) respectively. In this case, ($\varphi>\varphi_L$), Eqs. (40) and (41) give that:

$$\cos(\theta+\gamma_{2_L})\cdot\cos\gamma_{2_L}=\sqrt{1-\left[1+\frac{\Delta\lambda}{\lambda}\right]^2\cdot\sin^2\theta}$$

Or

$$\cos(\theta+2\cdot\gamma_{2_L})=2\cdot\sqrt{1-\left[1+\frac{\Delta\lambda}{\lambda}\right]^2\cdot\sin^2\theta}-\cos\theta \tag{42}$$

which defines the part γ_{2_L} of the source which contributes to the reflection od a «Right» beam parallel to the central ray SC so that the angles γ_{1_L} and γ_{2_L} define the widest beam parallel to SC that reflects from the crystal.

Total Broadening

From Eqs. (34) and (39) the total broadening is given by:

$$\frac{arc\widehat{M_1N_1}}{R}=\varepsilon-\delta+2\cdot(\omega+\varphi) \qquad \text{Total angular broadenin8 from abeam parallel to the central ray SC} \tag{43}$$

*In Fig. 7 the line CS_3 is not plotted.

Perceptive Total Angualar Broadening

The perceptive total angular broedening η is given by:

$$2\cdot\eta\cdot R\cdot = \text{arc}\widehat{BCI} + \text{arc}\widehat{M_1N_1} = \text{arc}\widehat{BC} + \text{arc}\widehat{CG} + \text{arc}\widehat{GI} + \text{arc}\widehat{M_1N_1}$$

$$= \text{arc}\widehat{DC} - \text{arc}\widehat{DB} + \text{arc}\widehat{CG} + \text{arc}\widehat{GI} + \text{arc}\widehat{M_1F} + \text{arc}\widehat{FN_1}$$

$$= 2\cdot\omega\cdot R - (\text{arc}\widehat{FM_1} - 2\cdot\omega\cdot R) + 2\cdot\varphi\cdot R + (2\cdot\varphi\cdot R - \text{arc}\widehat{FN_1})$$

$$+ \text{arc}\widehat{M_1F} + \text{arc}\widehat{FN_1}$$

And finally $\qquad \eta = 2\cdot(\omega + \varphi)$

Beam Convergent to C

The «Left» and «Right» rays strating from the points S_1 and S_2 of the source (Fig. 8) and convergent at C are incident on the crystal at angles $\theta - \gamma_1$ and $\theta + \gamma_2$, respectively. These rays are reflected only if:

$$\gamma_1 < \gamma'_{1L} \quad (44), \qquad \gamma_2 < \gamma'_{2L} \quad (45)$$

where the angles γ'_{1L} and γ'_{2L} are defined by the following equations:

$$\sin(\theta - \gamma'_{1L}) = (1 - \frac{\Delta\lambda}{\lambda})\cdot\sin\theta \quad (46), \qquad \sin(\theta + \gamma'_{2L}) = (1 + \frac{\Delta\lambda}{\lambda}).\sin\theta \quad (47)$$

The angles γ'_{1L} and γ'_{2L} determined by the FWHM of the line define the widest convergent beam permitted to reflect from point C on the crystal. It is easy to show that the corresponding broadenings are that:

$$\frac{\text{arc}\widehat{FS_{11}}}{R} = 2\cdot\gamma_1 \quad (48), \qquad \frac{\text{arc}\widehat{FS_{21}}}{R} = 2\cdot\gamma_2 \quad (49)$$

and the total angular broadening from both «Left» and «Right» rays convergent to C is given by

$$\frac{\text{arc}\ \widehat{S_{21}S_{11}}}{R} = 2\cdot(\gamma_1 + \gamma_2) \qquad \text{Total angular broadening from a beam convergent to C} \quad (50)$$

If the relations of Eqs. (44) and (45) are not fulfilled, the γ_1 and γ_2 in Eq. (50) must be replaced by γ'_{1L} and γ'_{2L}.

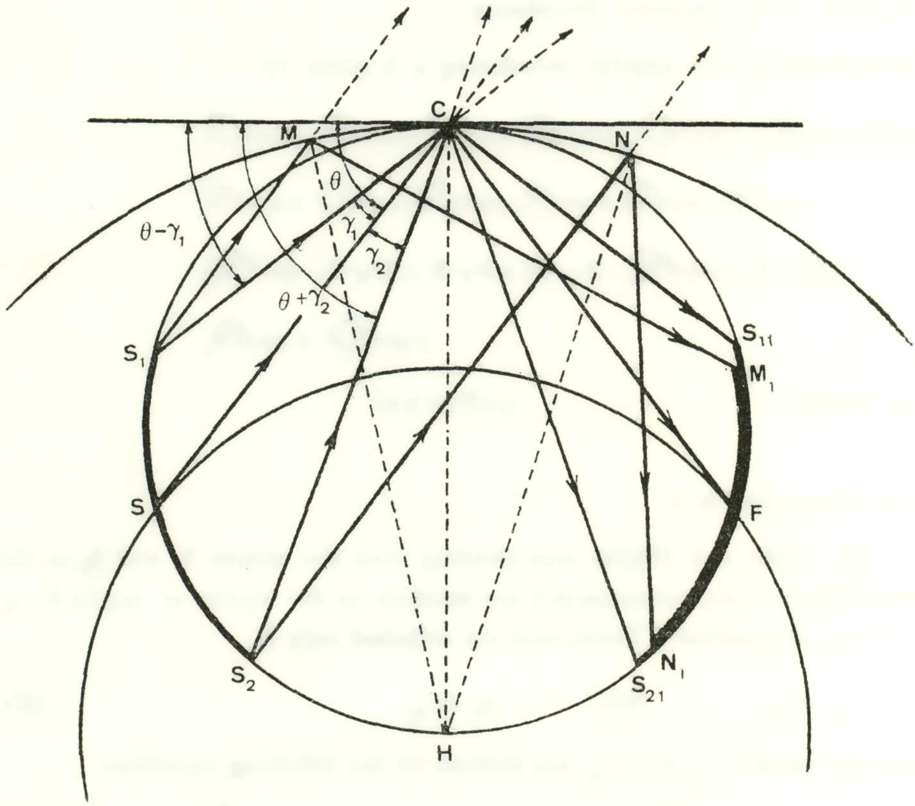

Fig. 8. Broadening from a convergent beam to C ($\gamma_1 < \gamma'_{1_L}$, $\gamma_2 < \gamma'_{2_L}$).

Total Broadening from a Beam Parallel to SC and from a Beam Convergent to C

The widest beam parallel to SC reflected from the crystal is determined by the angles γ_{1_L} and γ_{2_L} defined by Eqs. (37) and (42). Using Eqs. (37) and (46) and Eqs. (42) and (47), we compare the angles γ_{1_L} and γ'_{1_L} and γ_{2_L} and γ'_{2_L} and find that:

$$\gamma'_{1_L} < \gamma_{2_L} \qquad (51), \qquad\qquad \gamma_{2_L} < \gamma'_{2_L} \qquad (52)$$

As shown in Part II, Fig. 3, even if $\gamma'_{2_L} = \gamma_{2_L}$, the point N_1 (Fig. 8) lies «up» the point S_{21}. So the broadening from the «Right» ray S_2C includes the broadening from the «Right» ray S_2N.

Suppose that $$\gamma_1 < \gamma'_{1_L} < \gamma_{1_L} \tag{53}$$

then, both the rays S_1M and S_1C are reflected by the crystal. As it has been shown in Part II, Fig. 3, the point M_1 lies «under» the point S_{11}, so that the broadening from the ray S_1C includes the broadening from the ray S_1M, and the total angular broadening from rays both parallel to SC and convergent to C is:

$$\frac{\mathrm{arc}\widehat{S_{21}S_{11}}}{R} = 2\cdot(\gamma_1+\gamma_2) \tag{54}$$

Total angular broadening from rays both parallel to SC and convergent to C when $\gamma_1 < \gamma'_{1_L} < \gamma_{1_L}$

If $\gamma_2 > \gamma'_{2_L}$ in the above equation, γ_2 must be replaced by γ'_{2_L} as defined by Eq. (47). Now suppose that $\gamma'_{1_L} < \gamma_{1_L} < \gamma_1$. In this case, the limit «Left» ray to C starts from a point of the source corresponding to the angle γ'_{1_L}, and the limit «Left» ray parallel to SC starts from a point corresponding to the angle γ_{1_L}. Let us examine the broadening from each of them. The broadening from the «Left» ray to C is $2\cdot\gamma'_{1_L}$. The broadening from the «Left» ray parallel to SC is [Eq. (34)

$$\frac{\mathrm{arc}\widehat{FM_1}}{R} = \theta + 2\cdot\omega - \delta$$

Equations (36) and (46) give that $\omega_L = \gamma'_{1_L}$ so we can write:

$$\frac{\mathrm{arc}\widehat{FM_1}}{R} = \theta + 2\cdot\gamma'_{1_L} - \delta \tag{55}$$

We will now show that $\theta > \delta$ or $\cos\theta < \cos\delta$. From Eq. (33) we have to show that:

$$\cos\theta < 2\cdot\cos(\theta-\omega) - \cos(\theta-2\cdot\omega)$$

Or $$\cos\theta - \cos(\theta-\omega) < \cos(\theta-\omega) - \cos(\theta-2\cdot\omega)$$

Or $$-2\cdot\sin\left[\theta-\frac{\omega}{2}\right]\cdot\sin\frac{\omega}{2} < -2\cdot\sin\left[\theta-\frac{3\cdot\omega}{2}\right]\cdot\sin\frac{\omega}{2}$$

or $$\sin\left[\theta-\frac{\omega}{2}\right]\rangle\sin\left[\theta-\frac{3\cdot\omega}{2}\right]$$

and, therefore $\theta \rangle \delta$. Equation (55) implies that the broadening caused from the «Left» ray SM, includes in this case the broadening from the «Left» ray S_1C. So the total angular broadening from the rays parallel to SC and convergent to C is:

$$\frac{\mathrm{arc}\widehat{S_{21}M_1}}{R}=2\cdot\gamma_2+\theta+2\cdot\omega-\delta \qquad (56)$$

Total angular broadening from parallel to SC and convergent to C beams, when $\gamma'_{1_L}\langle\gamma_{1_L}\langle\gamma_1$

where ω and δ are defined by Eqs. (36) and (33) respectively, and $\gamma_1=\gamma_{1_L}$ defined by Eq. (37). If $\gamma'_2\rangle\gamma_{2_L}$, in Eq. (56), γ_2 must be replaced by γ'_{2_L} defined by Eq. (47). Now suppose that $\gamma'_{1_L}\langle\gamma_1\langle\gamma_{1_L}$. In this case, the limit «Left ray to C starts from a point on the source corresponding to the angle γ'_{1_L}, and the limit «Left» ray parallel to SC starts from the left end of the source corresponding to the angle γ_1. To examine which is the larger contribution, we will use either Eq. (54) or (56).

Beam Convergent to the Points M and/or N Defined by the Limit Rays S_1M, S_2N Parallel to the Central Ray

Convergent Beam Intersecting at M

The ray S_1M parallel to SC (Fig. 9) intercepts the crystal planes with the angle $\theta-\omega$. The ray S_2M intercepts the crystal planes with the angle $\theta-\omega+\chi$. We will show that $\theta-\omega+\chi \rangle \theta$. We have that:

$$\chi=\frac{\mathrm{arc}\widehat{S_1S_2}}{2\cdot R}-\frac{\mathrm{arc}\widehat{EO}}{2\cdot R}=\gamma_1+\gamma_2-\frac{\mathrm{arc}\widehat{EO}}{R}$$

$$\omega=\frac{\mathrm{arc}\widehat{CD}}{2\cdot R}=\frac{\mathrm{arc}\widehat{CO}}{2\cdot R}-\frac{\mathrm{arc}\widehat{DE}}{2\cdot R}-\frac{\mathrm{arc}\widehat{EO}}{2\cdot R}=\gamma_1-\frac{\mathrm{arc}\widehat{EO}}{2\cdot R}-\frac{\mathrm{arc}\widehat{DE}}{2\cdot R}$$

$$\langle\gamma_1-\frac{\mathrm{arc}\widehat{EO}}{2\cdot R}\langle\chi$$

and consequently $\theta-\omega+\chi>\theta$. The angle χ is determined by the source

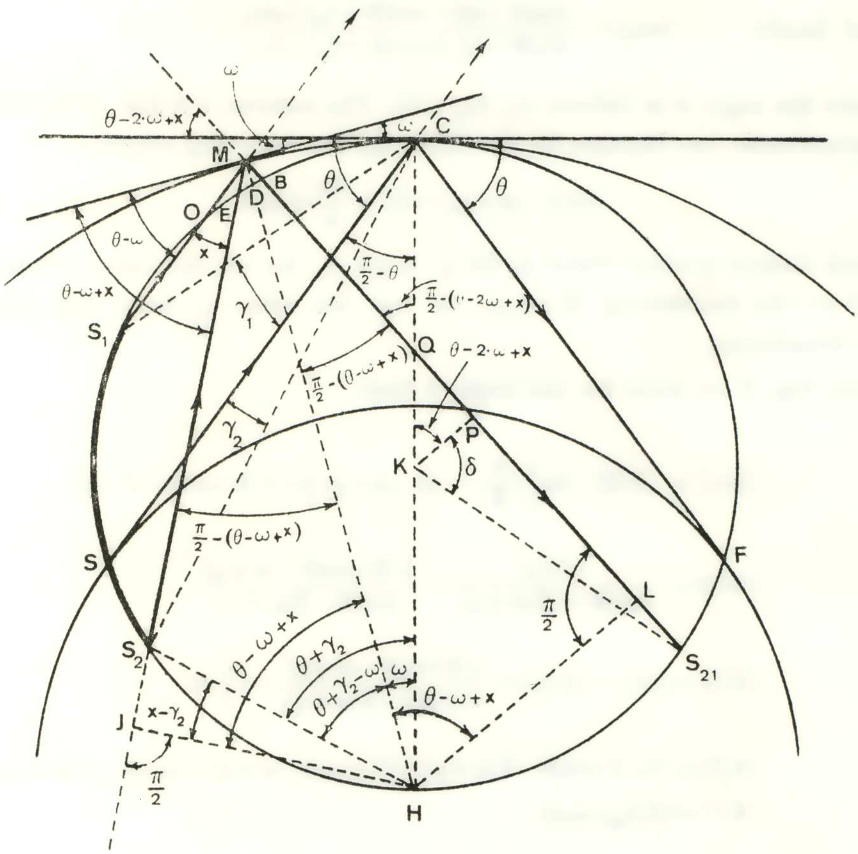

Fig. 9. Broadening from a beam convergent to M.

size and/or from the natural width of the X-ray line. From Fig. 9 we have that:

$$(HJ)=(HM)\cdot\sin\left[\frac{\pi}{2}-(\theta-\omega+\chi\right]=2\cdot R\cdot\cos(\theta-\omega+\chi)$$

$$(HJ)=(HS_2)\cdot\cos(\chi-\gamma_2)$$

$$(HS_2)=(HC)\cdot\sin\left[\frac{\pi}{2}-\varphi-\gamma_1\right]=2\cdot R\cdot\cos(\theta+\gamma_2)$$

$$(HJ)=2\cdot R\cdot\cos(\theta+\gamma_2)\cdot\cos(\chi-\gamma_2)$$

$$\cos(\theta-\omega+\chi)=\cos(\theta+\gamma_2)\cdot\cos(\chi-\gamma_2)$$

And finally $$\tan\chi=\frac{\cos(\theta-\omega)-\cos(\theta+\gamma_2)\cdot\cos\gamma_2}{\sin(\theta-\omega)+\cos(\theta+\gamma_2)\cdot\sin\gamma_2} \quad (57)$$

where the angle ω is defined by Eq. (35). The natural FWHM of the X-ray characteristic line imposes for the limit ray the following relation:

$$\sin(\theta-\omega+\chi_L)=(1+\frac{\Delta\lambda}{\lambda})\cdot\sin\theta \quad (58)$$

which defines another value χ_L for χ. If $\chi<x_L$, we use the value χ from Eq. (57) for the broadening. If $\chi>\chi_L$, we use the value χ_L from Eq. (58) for the broadening.

From Fig. 9 we have for the angle δ that:

$$(HL)=(HM)\cdot\sin\left[\frac{\pi}{2}-(\theta-\omega+\chi)\right]=2\cdot R\cdot\cos(\theta-\omega+\chi)$$

$$(HQ)=\frac{(HL)}{\cos(\theta-2\cdot\omega+\chi)}=\frac{2\cdot R\cdot\cos(\theta-\omega+\chi)}{\cos(\theta-2\cdot\omega+\chi)}$$

$$(KQ)=(HQ-(HK)=\left[\frac{2\cdot\cos(\theta-\omega+\chi)}{\cos(\theta-2\cdot\omega+\chi)}-1\right]\cdot R$$

$$(KP)=(KQ)\cdot\cos(\theta-2\cdot\omega+\chi)=[2\cdot\cos(\theta-\omega+\chi)-\cos(\theta-2\cdot\omega+\chi)]\cdot R$$

$$(KP)=(KS_{21})\cdot\cos\delta$$

$$\cos\delta=2\cdot\cos(\theta-\omega+\chi)-\cos(\theta-2\cdot\omega+\chi) \quad (59)$$

And we have for the broadening that:

$$\text{arc } \overset{\frown}{S_{21}F}+\text{arc } \overset{\frown}{FC}+\text{arc } \overset{\frown}{CB}=2\cdot\delta\cdot R$$

$$\text{arc}\overset{\frown}{S_{21}F}+\text{arc } \overset{\frown}{FC}-\text{arc } \overset{\frown}{CB}=2\cdot(\theta-2\cdot\omega+\chi)\cdot R$$

and $$\text{arc}2\cdot\overset{\frown}{S_{21}F}+\text{arc}2\cdot\overset{\frown}{FC}=2\cdot(\theta-2\cdot\omega+\chi+\delta)\cdot R$$

Or $$\text{arc}\overset{\frown}{S_{21}F}+2\cdot\theta\cdot R=(\theta-2\cdot\omega+\chi+\delta).R$$

And finally $$\frac{\text{arc } \overset{\frown}{S_{21}F}}{R}=\delta+\chi-\theta-2\cdot\omega$$ Angular broadening from the ray S_2M (60)

If $x>x_L$, the ray to M starts from a point S'_2 corresponding to an angle smaller than γ_2.

Convergent Beam Intersecting at N

The ray S_2N parallel to CN intersects the crystal planes with an angle $\theta+\varphi$, and the ray S_1N intersects the crystal planes with an angle $\theta+\varphi-\psi$ (Fig. 10). In this case, every one of the following relations is possible:

$$\theta+\varphi-\psi>\theta \qquad \theta+\varphi-\psi=\theta \qquad \theta+\varphi-\psi<\theta$$
$$(\varphi>\psi) \qquad (\varphi=\psi) \qquad (\varphi<\psi)$$

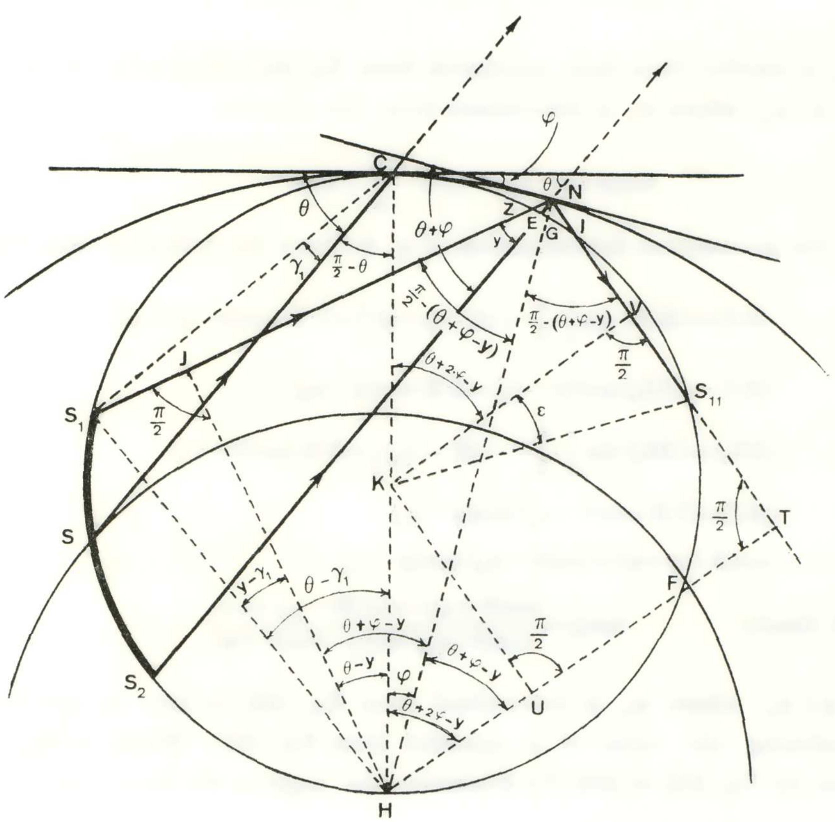

Fig. 10. Broadening from a beam convergent to N.

The angle φ is defined by Eq. (40). We write Eq. (24) as:

$$\cos(\varphi+\theta-2\cdot\gamma_1)=2\cdot(\cos\theta-\sin\theta.\sin\varphi)-\cos(\varphi+\theta) \tag{61}$$

If the angle γ_1 is equal to the angle γ_1 calculated from Eq. (61), then $\theta+\varphi-\psi=\theta$, and the ray S_1N is tangent to the focusing circle with Eq. (26) giving the broadening from that ray. If γ_1 is larger than that calculated from Eq. (61), then $\psi > \theta$, $\theta+\varphi-\psi < \theta$, and $\psi < \psi_L$, where ψ_L is determined from the equation:

$$\sin(\theta+\varphi-\psi_L)=(1-\frac{\Delta\lambda}{\lambda})\cdot\sin\theta \tag{62}$$

If γ_1 is smaller than that calculated from Eq. (61), then $\psi < \theta$; $\theta+\varphi-\psi > \theta$ and $\psi < \psi_L$, where ψ_L is determined from the equation

$$\sin(\theta+\varphi-\psi_L)=(1+\frac{\Delta\lambda}{\lambda})\cdot\sin\theta \tag{63}$$

For the geometrical determination of ψ, we have the following from Fig. 10:

$$(HJ)=(HN)\cdot\sin\left[\frac{\pi}{2}-(\theta+\varphi-\psi)\right]=2\cdot R\cdot\cos(\theta-\varphi+\psi)$$

$$(HJ)=(HS_1).\cos(\psi-\gamma_1)=2\cdot R\cdot\cos(\psi-\gamma_1)$$

$$(HS_1)=(HC)\cdot\sin\left[\frac{\pi}{2}-(\theta-\gamma_1)\right]=2\cdot R\cdot\cos(\theta-\gamma_1)$$

$$(HJ)=2\cdot R\cdot\cos(\theta-\gamma_1)\cdot\cos(\psi-\gamma_1)$$

$$\cos(\theta+\varphi-\psi)=\cos(\theta-\gamma_1)\cdot\cos(\psi-\gamma_1)$$

And finally $$\tan\chi=\frac{\cos(\theta+\varphi)-\cos(\theta-\gamma_1)\cdot\cos\gamma_1}{\cos(\theta-\gamma_1)\cdot\sin\gamma_1-\sin(\theta+\varphi)} \tag{64}$$

If $\psi < \psi_L$ where ψ_L is determined from Eq. (62) or (63), we use for the broadening the value of ψ calcuted from Eq. (64). When $\psi > \psi_L$, ψ_L is given by Eq. (62) or (63). To determine the angle ε, we have from Fig. 10:

$$(HT)=(HN)\cdot\sin\left[\frac{\pi}{2}-(\theta+\varphi-\psi)\right]=2\cdot R\cdot\cos\theta)+\varphi-\psi)$$

$$(HU)=(HK)\cdot\cos(\theta+2\cdot\varphi-\psi)=R\cdot\cos(\theta+2\cdot\varphi-\psi)$$

$$(KV)=(HT)-(HU)=[2\cdot\cos(\theta+\varphi-\psi)-\cos(\theta+2\cdot\varphi-\psi)]\cdot R$$

$$(KV)=(KS_{11})\cdot\cos\varepsilon=R\cdot\cos\varepsilon$$

$$\cos\varepsilon=2\cdot\cos(\theta+\varphi-\psi)-\cos(\theta+2\cdot\varphi-\psi) \qquad (65)$$

And we have for the broadering:

$$\text{arc}\widehat{HF}+\text{arc}\widehat{FS_{11}}-\text{arc}\widehat{IG}=2\cdot\left[\frac{\pi}{2}-(\theta+\varphi-\psi)\right]\cdot R=[\pi-2\cdot(\theta+\varphi-\psi)]\cdot R$$

Or $\quad \text{arc}\widehat{FS_{11}}-\text{arc}\widehat{IG}=2\cdot(\psi-\varphi)\cdot R$

and $\quad \text{arc}\widehat{S_{11}I}+\text{arc}\widehat{IG}+\text{arc}\widehat{GC}=(\theta+2\cdot\varphi-\psi+\varepsilon).R$

and $\quad \text{arc}\widehat{FS_{11}}+\text{arc}\widehat{S_{11}I}+\text{arc}\widehat{GC}=(\theta+2\cdot\varphi-\psi+\varepsilon)\cdot R+2\cdot(\psi-\varphi)\cdot R$

Or $\quad \text{arc}\widehat{FS_{11}}+2\cdot\varepsilon\cdot R+2\cdot\varphi\cdot R=(\theta+\psi+\varepsilon)\cdot R$

And finally $\quad \dfrac{\text{arc}\widehat{FS_{11}}}{R}=\theta+\psi-\varepsilon-2\cdot\varphi \quad$ Angular broadening rom the ray S_1M $\quad$ (66)

Total Broadening from Beams Convergent to M and N

From Eqs. (60) and (66) we have the total angular broadening:

$\dfrac{\text{arc}\widehat{S_{21}S_{11}}}{R}=\chi+\psi+\delta-\varepsilon-2\cdot(\varphi+\omega) \quad$ Total angular broadening from beams convergent to the points M and N $\quad$ (67)

Broadening from a Divergent Beam Generally

«Left» Ray

The «Left» ray S_1M starting from the end S_1 of the source (Fig. 11) intercepts the crystal plane at an angle $\theta+\alpha-\omega$. Every one of the following relations is possible:

$\theta+\alpha-\omega>\theta$	$\theta+\alpha-\omega=\theta$	$\theta+\alpha-\omega<\theta$
$(\alpha>\omega)$	$(\alpha=\omega)$	$(\alpha<\omega)$

We examine the most interesting case $\theta+\alpha-\omega>\theta$. Then, the angles α and ω for the limit ray must fulfill the relation:

$$\sin(\theta+\alpha-\omega)=\left(1+\frac{\Delta\lambda}{\lambda}\right)\cdot\sin\theta \qquad (68)$$

From Fig. 11 we have:

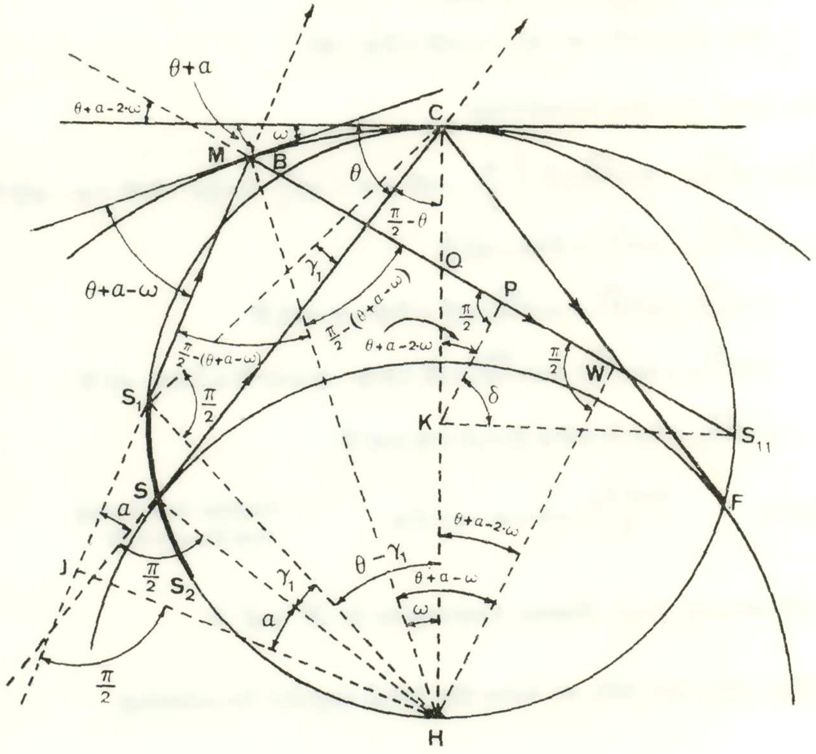

Fig. 11. Broadening from the «Left» ray S_1M.

$$(HJ) = (HM)\cdot\sin\left[\frac{\pi}{2} - (\theta + \alpha - \omega)\right] = 2\cdot R\cdot\cos(\theta + \alpha - \omega)$$

$$(HJ) = (HS_1)\cdot\cos(\alpha + \gamma_1)$$

$$(HS_1) = (HC)\cdot\sin\left[\frac{\pi}{2} - \theta + \gamma_1\right] = 2\cdot R\cdot\cos(\theta - \gamma_1)$$

$$(HJ) = 2\cdot R\cdot\cos(\theta - \gamma_1)\cdot\cos(\alpha + \gamma_1)$$

$$\cos(\theta + \alpha - \omega) = \cos(\theta - \gamma_1)\cdot\cos(\alpha + \gamma_1) \tag{69}$$

which gives with Eq. (68):

$$\cos(\alpha+\gamma_1)=\frac{\sqrt{1-\left[1+\frac{\Delta\lambda}{\lambda}\right]^2\cdot\sin^2\theta}}{\cos(\theta-\gamma_1)} \qquad (70)$$

Equations (69) and (70) define the angles α and ω. For determination of the angle δ we have from Fig. 11:

$$(HW)=(HM)\cdot\sin\left[\frac{\pi}{2}-(\theta+\alpha-\omega)\right]=2\cdot R\cdot\cos(\theta+\alpha-\omega)$$

$$(HQ)=\frac{(HW)}{\cos(\theta+\alpha-2\cdot\omega)}=\frac{2\cdot R\cdot\cos(\theta+\alpha-\omega)}{\cos(\theta+\alpha-2\cdot\omega)}$$

$$(KQ)=(HQ)-(HK)=\left[\frac{2\cdot\cos(\theta+\alpha-\omega)}{\cos(\theta+\alpha-2\cdot\omega)}-1\right]\cdot R$$

$$(KP)=(KQ)\cdot\cos(\theta+\alpha-2\cdot\omega)=[2\cdot\cos(\theta+\alpha-\omega)-\cos(\theta+\alpha-2\cdot\omega)]\cdot R$$

$$(KP)=(KS_{11})\cdot\cos\delta=R\cdot\cos\delta$$

$$\cos\delta=2\cdot\cos(\theta+\alpha-\omega)-\cos(\theta+\alpha-2\cdot\omega) \qquad (71)$$

And for determination of the broadening $\mathrm{arc}\overset{\frown}{FS_{11}}$:

$\mathrm{arc}\,\overset{\frown}{S_{11}C}+\mathrm{arc}\overset{\frown}{CB}=2\cdot\delta\cdot R$ $\qquad$ $\mathrm{arc}\overset{\frown}{S_{11}C}-\mathrm{arc}\overset{\frown}{CB}=2\cdot(\theta+\alpha-2\cdot\omega)\cdot R$

Or $\qquad \mathrm{arc}\overset{\frown}{S_{11}C}=(\theta+\alpha-2\cdot\omega+\delta)\cdot R$

Also $\qquad \mathrm{arc}\overset{\frown}{FS_{11}}+\mathrm{arc}\overset{\frown}{S_{11}C}=2\cdot\theta\cdot R$

Or $\qquad \mathrm{arc}\,\overset{\frown}{FS_{11}}+(\theta+\alpha-2\cdot\omega+\delta)\cdot R=2\cdot\theta\cdot R$

And finally $\qquad \dfrac{\mathrm{arc}\,\overset{\frown}{FS_{11}}}{R}=\theta+2\cdot\omega-\alpha-\delta$ $\qquad$ Angular broadening from the limit «Left» ray S_1M $\qquad$ (72)

«Right» Rays

The «Right» ray S_2N starting from the end S_2 of the source (Fig. 12) intercepts the crystal planes at an angle $\theta-\beta+\varphi$. We see that:

$$\beta<\frac{\mathrm{arc}\overset{\frown}{CZ}}{2\cdot R}<\frac{\mathrm{arc}\overset{\frown}{CG}}{2\cdot R}$$

or $\beta<\varphi$ and $\theta-\beta+\varphi>\theta$, so that for the limit ray S_2N the angles β and φ must fulfill the relation:

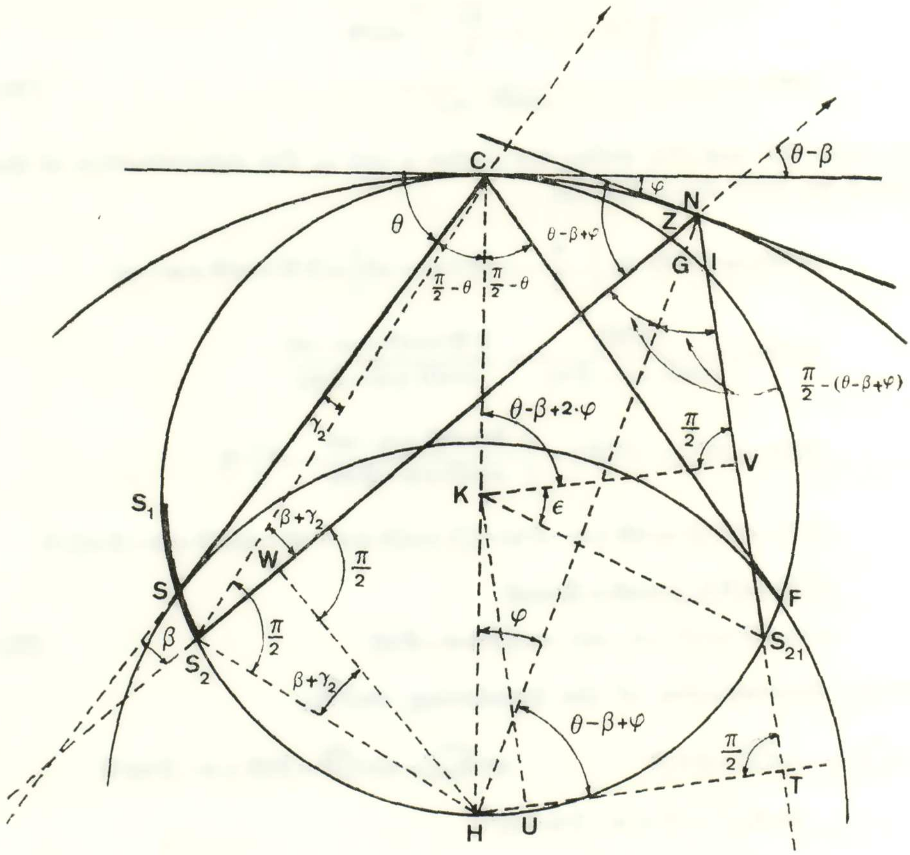

Fig. 12. Broadening from the «Right» ray S_2N.

$$\sin(\theta-\beta+\varphi)=(1+\frac{\Delta\lambda}{\lambda})\cdot\sin\theta \qquad (73)$$

It is also easy to show that on increasing β, the difference $\varphi-\beta$ increases so that $\gamma_2 < \gamma_{2_L}$ · If $\gamma_2 > \gamma_{2_L}$, then $\beta=0$ and Eq. (39) gives the broadening. From Fig. 12 we have:

$$(HW)=(HN)\cdot\sin\left[\frac{\pi}{2}-(\theta-\beta+\varphi)\right]=2\cdot R\cdot\cos(\theta-\beta+\varphi)$$

$$(HW)=(HS_2)\cdot\cos(\beta+\gamma_2)$$

$$(HS_2) = (HC)\cdot\sin\left[\frac{\pi}{2} - \theta - \gamma_2\right] = 2\cdot R\cdot\cos(\theta+\gamma_2)$$

$$(HW) = 2\cdot R\cdot\cos(\theta+\gamma_2)\cdot\cos(\beta+\gamma_2)$$

$$\cos(\theta-\beta+\varphi) = \cos(\theta+\gamma_2)\cdot\cos(\beta+\gamma_2) \tag{74}$$

which gives with Eq. (73):

$$\cos(\beta+\gamma_2) = \frac{\sqrt{1-\left[1+\frac{\Delta\lambda}{\lambda}\right]^2\cdot\sin^2\theta}}{\cos(\theta+\gamma_2)} \tag{75}$$

Equations (74) and (75) define the angles β and φ. For the determination of the angle ε we have from Fig. 12:

$$(HT) = (HN)\cdot\sin\left[\frac{\pi}{2} - (\theta-\beta+\varphi)\right] = 2\cdot R\cdot\cos(\theta-\beta+\varphi)$$

$$(HU) = (HK)\cdot\cos(\theta-\beta+2\cdot\varphi) = 2\cdot R\cdot\cos(\theta-\beta+2\cdot\varphi)$$

$$(KV) = (UT) = [2\cdot\cos(\theta-\beta+\varphi) - \cos(\theta-\beta+2\cdot\varphi)]\cdot R$$

$$(KV) = (KS_{21})\cdot\cos\varepsilon = R\cdot\cos\varepsilon$$

$$\cos\varepsilon = 2\cdot\cos(\theta-\beta+\varphi) - \cos(\theta-\beta+2\cdot\varphi) \tag{76}$$

And for the broadening $\mathrm{arc}\widehat{S_{21}E}$:

$$\mathrm{arc}\,\widehat{S_{21}F} + \mathrm{arc}\widehat{FC} = (\theta-\beta+2\cdot\varphi+\varepsilon)\cdot R$$

And finally $\frac{\mathrm{arc}\widehat{S_{21}F}}{R} = \varepsilon + 2\cdot\varphi - \theta - \beta$ Angular broadening from the limit «Right» ray S_2N (77)

Total Broadening

Equations (72) and (77) give the total angular broadening:

$\frac{\mathrm{arc}\widehat{S_{11}S_{21}}}{R} = 2\cdot(\omega+\varphi) + \varepsilon - \alpha - \beta - \delta$ Total angular broedening from a divergent beam generally

REFERENCES

1. L. De Broglie, Compt. Rend. 158, 944, 1914.
2. C. N. Koumelis, C. A. Londos, Z. I. Kavogli, D. K. Leventouri, A. B. Vassilikou, and G. E. Zardas, Can. J. Phys. 60, 1241, 1982.
3. Y. Cauchois, J. de Pfysique 3, 320, 1932.
4. H. H. Johann, Zeitschr. f. Physik, 69, 185, 1931.
5. Du Mond and Kirkpatrik, Rev. Sci. Instr. 1, 88, 1930.
6. Johansson Naturwiss. 20, 758, 1932.
7. P. M. De Wolff, Selected Topics On X-ray Crystallography, ed. J. Bouman, Amsterdam, North Holland Publishing Co. 1951.
8. J. Witz, Acta Crystallogr. A25, 50, 1969.
9. D. W. Berremann, J. Stamatoff and S. J. Kennedy, Appl. Optics. 16, 2081, 1977.
10. S. I. Salem and P. L. Lee, At. Data Nucl. Data Tables 18, 233, 1976.
11. A. Nilson, Arkiv. Physik 6, 516, 1953.

ΠΕΡΙΛΗΨΙΣ

Τὸ σφάλμα ἑστιάσεως εἰς τὸ φασματοσκόπιον Johann ἀκτίνων Roentgen

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