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CHOICE OF COLLIMATORS FOR A CRYSTAL SPECTROMETER FOR NEUTRON DIFFRACTION

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In this paper we establish some criteria for the choice of the collimators for a crystal spectrometer for neutron diffraction in order to achieve a good compromise between luminosity and resolution.

General expressions for the full width at half maximum and for the luminosity of the diffraction peaks are developed for powder sample. The advantage of the parallel arrangement is also computed.

1. Introduction

The diffraction pattern obtained with a neutron crystal spectrometer shows several peaks due to Bragg reflections of the crystalline sample.

The full width at half maximum and the luminosity of these peaks are related to the angular divergence of the spectrometer collimators and to the crystal mosaic spread.

The purpose of this paper is to show how to choose the most convenient values for the angular divergences of the collimators in order to obtain a good compromise between resolution and luminosity.

2. The Soller Collimators and the Crystal Mosaic Spread

2.1. THE SOLLER COLLIMATORS

In a crystal spectrometer for neutron diffraction, there are three collimators: the first collimator is located inside a beam hole in the reactor shielding, the second one is in the monochromatic beam between the monochromating crystal and the sample, the third one is on the rotating arm, between the sample and the BF_3 detector.

We shall assume the three collimators to be of the Soller type[1]); the horizontal angular divergence α_i ($i = 1, 2, 3$) of the i-th collimator is determined by the ratio $\alpha_i = s_i/l_i$ of the width s_i to the length l_i of its Soller elements.

We shall also assume, in accordance with Sailor *et al.*[2]), that the i-th collimator reduces the intensity of the incident neutron beam by a factor

$$A(\phi_i) = \exp -(\phi_i/\alpha'_i)^2 \qquad (1)$$

where ϕ_i is the angle made by the projection on a horizontal plane, of any individual ray with the centerline of the i-th collimator††, and $\alpha'_i = \alpha_i/2(\ln 2)^{\frac{1}{2}}$. The sign of ϕ_i is chosen so that $+\phi_i$ would tend to increase the Bragg angle of the ray.

It can be shown that, by providing a coarse vertical collimation, any effect due to the vertical angular divergence of i-th collimator can be neglected.

2.2. THE CRYSTAL MOSAIC SPREAD

We shall assume[2]) that the monochromating crystal is actually composed of mosaic blocks, each individually perfect, oriented in a gaussian distribution of the type

$$\Theta(\eta) = K \exp -(\eta/\beta')^2 \qquad (2)$$

where K depends on the properties of the crystal under consideration[2]), η is the angular displacement from the mean of the projection of the

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†† Such an angle is given by $\sigma - \phi_3$ (see sect. 3. eq. (71)) for the third collimator.

1) W. Soller, Phys. Rev. **24** (1924) 158.

2) V. L. Sailor, H. L. Foote, Jr., H. H. Landon and R. E. Wood, Rev. Sci. Instr. **27** (1956) 26.

normal to the reflecting planes of any block upon a horizontal plane, and β' is related to the full width at half maximum of the distribution β, by eq. $\beta' = \beta/2(\ln 2)^{\frac{1}{2}}$. The sign of η is chosen so the Bragg angle would be increased when η is positive.

3. Derivation of the Full Width at Half Maximum and of the Luminosity of the Diffraction Peaks; Powder Sample

In order to calculate the shape and the full width at half maximum of the experimental diffraction peaks due to a powder sample, it will be useful to establish some relations between the angles ϕ_i, the Bragg angles of the monochromating crystal and the Bragg angles of the sample.

Let θ_0 be the Bragg angle for a central ray incident upon the monochromating crystal with $\phi_1 = 0$ and $\eta = 0$, and let θ be the Bragg angle for any individual ray. Hence we have[2]):

$$\theta - \theta_0 \equiv \delta = \phi_1 + \eta \qquad (3)$$

$$\phi_2 = \delta + \eta\,. \qquad (4)$$

Furthermore, let d be the interplanar distance of the monochromating crystal, and let d_B and θ_B be the interplanar distance and the Bragg angle of the sample respectively; setting:

$$a = \frac{(\mathrm{d}\lambda/\mathrm{d}\theta)_{\text{monochromating crystal}}}{(\mathrm{d}\lambda/\mathrm{d}\theta)_{\text{sample}}} = \frac{d\cos\theta_0}{d_B\cos\theta_{B0}},^{\dagger} \qquad (5)$$

in the "parallel position" we get:

$$\phi_3 = 2a\delta - \phi_2\,^{\dagger\dagger}. \qquad (6)$$

For any Bragg angle θ_B, let ρ be the angular displacement of the axis of the BF_3 detector with respect to the angle $2\theta_{B0}$ (for which the diffracted ray intensity has a maximum).

Let us now consider a neutron of wavelength $(\lambda,\ \lambda + \mathrm{d}\lambda)$ and, therefore, having a value of $\theta - \theta_0$ equal to $(\delta,\ \delta + \mathrm{d}\delta)$. The probability $J(\rho, \phi_1, \delta)\,\mathrm{d}\phi_1\,\mathrm{d}\delta\,\mathrm{d}\rho$ of such neutron going through the first collimator with an angle $(\phi_1, \phi_1 + \mathrm{d}\phi_1)$, being reflected by the monochromating crystal with a Bragg angle given by $(\delta,\ \delta + \mathrm{d}\delta)$, going through the second collimator, being reflected by the sample and then finally reaching the BF_3 detector whose axis makes an angle $(\rho,\ \rho + \mathrm{d}\rho)$ with the direction $2\theta_{B0}$, is given by:

$$J(\rho, \phi_1, \delta)\,\mathrm{d}\phi_1\,\mathrm{d}\delta\,\mathrm{d}\rho = H \exp - \left[\left(\frac{\phi_1}{\alpha'_1}\right)^2 + \left(\frac{\eta}{\beta'}\right)^2 + \left(\frac{\phi_2}{\alpha'_2}\right)^2 + \left(\frac{\rho - \phi_3}{\alpha'_3}\right)^2\right] \mathrm{d}\phi_1\,\mathrm{d}\delta\,\mathrm{d}\rho \qquad (7)$$

where H is a constant.

Taking into account eqs. (3), (4), and (6), we get for the total number, $I(\rho)\,\mathrm{d}\rho$, of neutrons reaching the BF_3 detector at the angular position $(\rho,\ \rho + \mathrm{d}\rho)$:

$$I(\rho)\,\mathrm{d}\rho = H\,\mathrm{d}\rho \int_{-\infty}^{+\infty}\mathrm{d}\phi_1 \int_{-\infty}^{+\infty}\mathrm{d}\delta \exp - \left[\left(\frac{\phi_1}{\alpha'_1}\right)^2 + \left(\frac{\delta - \phi_1}{\beta'}\right)^2 + \left(\frac{2\delta - \phi_1}{\alpha'_2}\right)^2 + \left(\frac{\rho - \phi_1 + 2\delta(1 - a)}{\alpha'_3}\right)^2\right]. \qquad (8)$$

In eq. (8) we extend the limits of integration to $\pm\,\infty$ since this doesn't appreciably affect the value of $I(\rho)\,\mathrm{d}\rho$.

By applying the relation:

$$\int_{-\infty}^{+\infty} \exp(-px^2 \pm qx)\,\mathrm{d}x = \left(\frac{\pi}{p}\right)^{\frac{1}{2}} \exp\frac{q^2}{4p} \qquad (9)$$

twice, we obtain from eq. (8):

$$I(\rho)\,\mathrm{d}\rho = M\,\mathrm{d}\rho \frac{\alpha_1\alpha_2\alpha_3\beta}{[\alpha_1^2\alpha_2^2 + \alpha_1^2\alpha_3^2 + \alpha_2^2\alpha_3^2 + 4\beta^2(\alpha_2^2 + \alpha_3^2) - 4a\alpha_2^2(\alpha_1^2 + 2\beta^2) + 4a^2(\alpha_1^2\alpha_2^2 + \alpha_1^2\beta^2 + \alpha_2^2\beta^2)]^{\frac{1}{2}}} \qquad (10)$$

$$\cdot \exp - \left\{\rho^2 \frac{(4\ln 2)(\alpha_1^2 + \alpha_2^2 + 4\beta^2)}{[\alpha_1^2\alpha_2^2 + \alpha_1^2\alpha_3^2 + \alpha_2^2\alpha_3^2 + 4\beta^2(\alpha_2^2 + \alpha^2_3) - 4a\alpha_2^2(\alpha_1^2 + 2\beta^2) + 4a^2(\alpha_1^2\alpha_2^2 + \alpha_1^2\beta^2 + \alpha_2^2\beta^2)]}\right\}.$$

† The quantity a takes into account the fact that in the crystal spectrometer for neutron diffraction, the dispersion of the sample in any Bragg position is, in general, different from the dispersion of the monochromating crystal.

†† In the "antiparallel position" we get: $\phi_3 = 2a\delta + \phi_2\,.$ (6′)

In eq. (10), M contains numerical factors connected with the nature of the monochromating crystal and the sample, the structure factors of their Bragg reflections under consideration, etc.

Eq. (10) shows that any diffraction peak, centered about an angle $2\,\theta_{B0}$ related to a by eq. (5), has a gaussian shape with the full width at half maximum $A_{\frac{1}{2}}$ given by:

$$A_{\frac{1}{2}} = \left[\frac{\alpha_1^2\alpha_2^2 + \alpha_1^2\alpha_3^2 + \alpha_2^2\alpha_3^2 + 4\beta^2(\alpha_2^2 + \alpha_3^2) - 4a\alpha_2^2(\alpha_1^2 + 2\beta^2) + 4a^2(\alpha_1^2\alpha_2^2 + \alpha_1^2\beta^2 + \alpha_2^2\beta^2)}{\alpha_1^2 + \alpha_2^2 + 4\beta^2}\right]^{\frac{1}{2}}. \quad (11)$$

By integration of eq. (10) with respect to ρ, we find for the luminosity L':

$$L' = P\frac{\alpha_1\alpha_2\alpha_3\beta}{(\alpha_1^2 + \alpha_2^2 + 4\beta^2)^{\frac{1}{2}}} \quad (12)$$

where P is a constant factor related to M in a simple way.

We will refer to the quantity $L \equiv L'/P$ as the spectrometer luminosity.

4. Preliminary Discussion of the Results for the Particular Case $\alpha_1 = \alpha_2 = \alpha_3 = \beta \equiv \alpha$

It may be useful to study first the behaviour of $A_{\frac{1}{2}}$ and L, in a particular case of practical interest: i.e. for the case with $\alpha_1 = \alpha_2 = \alpha_3 = \beta \equiv \alpha$.

From eqs. (11) and (12), we obtain for this case:

$$A_{\frac{1}{2}} = \alpha\left(\frac{11 - 12a + 12a^2}{6}\right)^{\frac{1}{2}} \quad (11')$$

$$L = \alpha^3/(6)^{\frac{1}{2}}. \quad (12')$$

We see, therefore, that for any Bragg angle, the full width at half maximum of the diffraction peaks is proportional to α, while the luminosity is proportional to α^3. This fact implies a comparatively large sacrifice of luminosity when resolution has to be improved.

Furthermore, we see that the quantity $A_{\frac{1}{2}}/\alpha$, expressed as a function of a, has a minimum at $a = 0.5$, and then increases with a in a way almost proportional to a.

In fig. 1, curve U shows how $A_{\frac{1}{2}}/\alpha$ should vary with a. We compared this theoretical behaviour with the values of $A_{\frac{1}{2}}/\alpha$ obtained from diffraction peaks by Corliss *et al.*[3,4]), who used $\alpha \simeq 20$ min·arc. Our theoretical values of $A_{\frac{1}{2}}/\alpha$ are in accordance within about 15% with experimental values of $A_{\frac{1}{2}}/\alpha$ obtained from fig. 3 of ref.[4]). The small deviations of our theoretical values from the experimental widths could be partly attributed to our having neglected in the calculations any effect of total reflection of neutrons against the walls of the steel collimators.

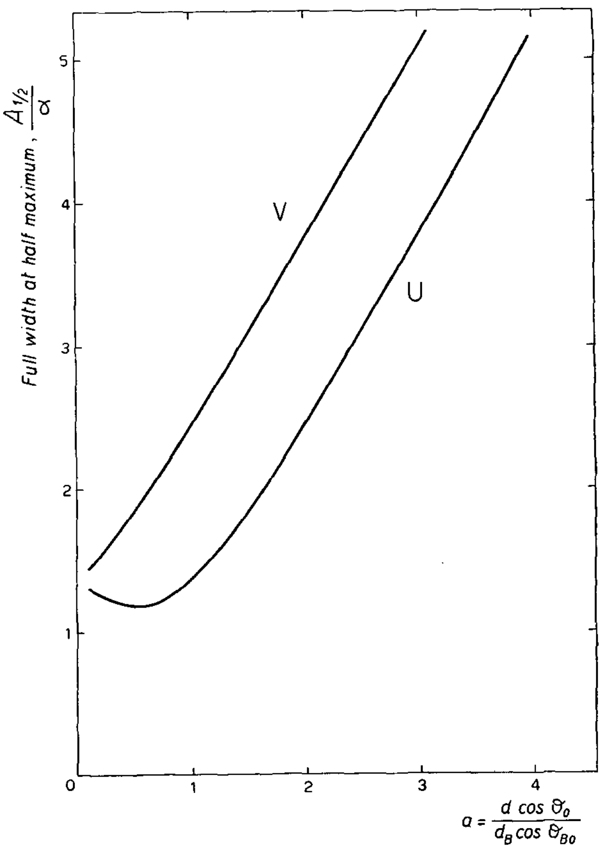

Fig. 1. Full width at half maximum $A_{\frac{1}{2}}$, divided by the horizontal angular divergence of the collimators α, as a function of $a = d \cos \vartheta_0 / d_B \cos \vartheta_{B0}$, for the particular case $\alpha_1 = \alpha_2 = \alpha_3 = \beta \equiv \alpha$. Curves U and V refer to the parallel and antiparallel positions respectively.

[3]) Pasternack, McReynolds, Weiss and Corliss, Phys. Rev. **81** (A) (1951) 326.

[4]) L. M. Corliss, J. M. Hastings and F. G. Brockman, Phys. Rev. **90** (1953) 1013.

It may be interesting to note that, taking into account eqs. (3), (4), (6′) and (7), in the antiparallel position we get:

$$A_{\frac{1}{2}}\,(\text{antiparallel}) = \alpha\left(\frac{11 + 12a + 12a^2}{6}\right)^{\frac{1}{2}} \quad (11'')$$

$$L\,(\text{antiparallel}) = \alpha^3/(6)^{\frac{1}{2}}\,. \quad (12'')$$

Eqs. (11′–12″) show that, the luminosity being the same, $A_{\frac{1}{2}}$ (antiparallel) $> A_{\frac{1}{2}}$ for any a.

In fig. 1, curve V is a plot of eq. (11″). Curves U and V show the focusing action due to the parallel position; they are in satisfactory agreement with experimental results[5]).

5. Discussion

With reference to eqs. (11) and (12), we may state that:

(1) The luminosity L is a symmetrical function of α_1, and α_2.

(2) The luminosity L is a linear function of α_3, so that a convenient way of obtaining a larger luminosity is to increase α_3.

(3) The function $A_{\frac{1}{2}}{}^2$ is a sum of three quantities: the first, which is independent of a, gives the largest contribution to $A_{\frac{1}{2}}{}^2$ for small values of a (or $2\theta_B$). The first term is the only one which depends on α_3, so that an increase in the luminosity as suggested in (2) causes a broadening of the diffraction peaks mainly for small values of a (or $2\theta_B$).

The third term is a symmetrical function of α_1 and α_2, so that α_1 and α_2 are equally important in broadening the diffraction peaks for large values of a (or $2\theta_B$).

In order to show the features of the various possible choices of the horizontal angular divergences of the collimators with reference to L and $A_{\frac{1}{2}}$, we found it convenient to plot in the (L, $A_{\frac{1}{2}}$) plane, for each choice of the values of α_1, α_2, α_3, the three points of co-ordinates

$$L\,(\alpha_1, \alpha_2, \alpha_3; \beta) \text{ and } A_{\frac{1}{2}}\left(\alpha_1, \alpha_2, \alpha_3; \beta; \begin{smallmatrix} a = 3 \\ a = 1.5 \\ a \to 0 \end{smallmatrix}\right).$$

Obviously we will obtain a convenient situation for the points (L, $A_{\frac{1}{2}}$) which lie near the lower right corner of the plot.

We have calculated the quantities L and $A_{\frac{1}{2}}$ for about 150 groups of the values (α_1, α_2, α_3; a) and for the value of practical interest $\beta = 20$ min arc[3]).

In fig. 2 we report typical results.

Looking at fig. 2, we may further observe that for two ordered groups

(4)	(5)	(6)
$\underline{\alpha}^{(1)} \equiv (\alpha_1, \alpha_2, \alpha_3)$	$\underline{\alpha}^{(3)} \equiv (\alpha_1, \alpha_2, \alpha_3)$	$\underline{\alpha}^{(5)} \equiv (\alpha_1, \alpha_2, \alpha_3)$
$\underline{\alpha}^{(2)} \equiv (\alpha_2, \alpha_1, \alpha_3)$	$\underline{\alpha}^{(4)} \equiv (\alpha_1, \alpha_3, \alpha_2)$	$\underline{\alpha}^{(6)} \equiv (\alpha_3, \alpha_2, \alpha_1)$

for which

$\alpha_1 < \alpha_2$,	$\alpha_2 < \alpha_3$,	$\alpha_1 < \alpha_3$,

we have:

$L(\underline{\alpha}^{(1)}) = L(\underline{\alpha}^{(2)})$	$L(\underline{\alpha}^{(3)}) > L(\underline{\alpha}^{(4)})$	$L(\underline{\alpha}^{(5)}) > L(\underline{\alpha}^{(6)})$
$A_{\frac{1}{2}}(\underline{\alpha}^{(1)}) < A_{\frac{1}{2}}(\underline{\alpha}^{(2)})$	$A_{\frac{1}{2}}(\underline{\alpha}^{(3)}) < A_{\frac{1}{2}}(\underline{\alpha}^{(4)})$	$A_{\frac{1}{2}}(\underline{\alpha}^{(5)}) < A_{\frac{1}{2}}(\underline{\alpha}^{(6)})$

where the eqs. for $A_{\frac{1}{2}}(\underline{\alpha})$ hold for a large part of the range of a, and hold definitely as a increases.

On the basis of the above remarks, we believe it would be wise in general to discard a group (α_1, α_2, α_3) for which $\alpha_1 > \alpha_2 > \alpha_3$ (see for example the points (30, 20, 10) and (10, 20, 30) in fig. 2).

We also think it would be convenient to choose a comparatively small value of α_1, which allows us to obtain both a small $A_{\frac{1}{2}}$ (by reducing L), and a comparatively large value of the luminosity (without a big loss of resolution), by changing only α_2 and/or α_3 (see for example the points (10, 10, 10) and (10, 60, 60) in fig. 2).

In figs. 3 and 4, we show the behaviour of other groups of the values (α_1, α_2, α_3); each plot is obtained by varying only the value of α_2.

6. Conclusion

In this paper we have established some criteria which should be of some help in the designing and operation of a crystal spectormeter for neutron diffraction.

In particular we found that the simple choice of three identical collimators may not be the most convenient one, when a good compromise between resolution and luminosity has to be achieved. Instead a suitable choice of the values

[5]) G. E. Bacon, Neutron Diffraction (Oxford at the Clarendon Press, 1955) p. 88, fig. 34.

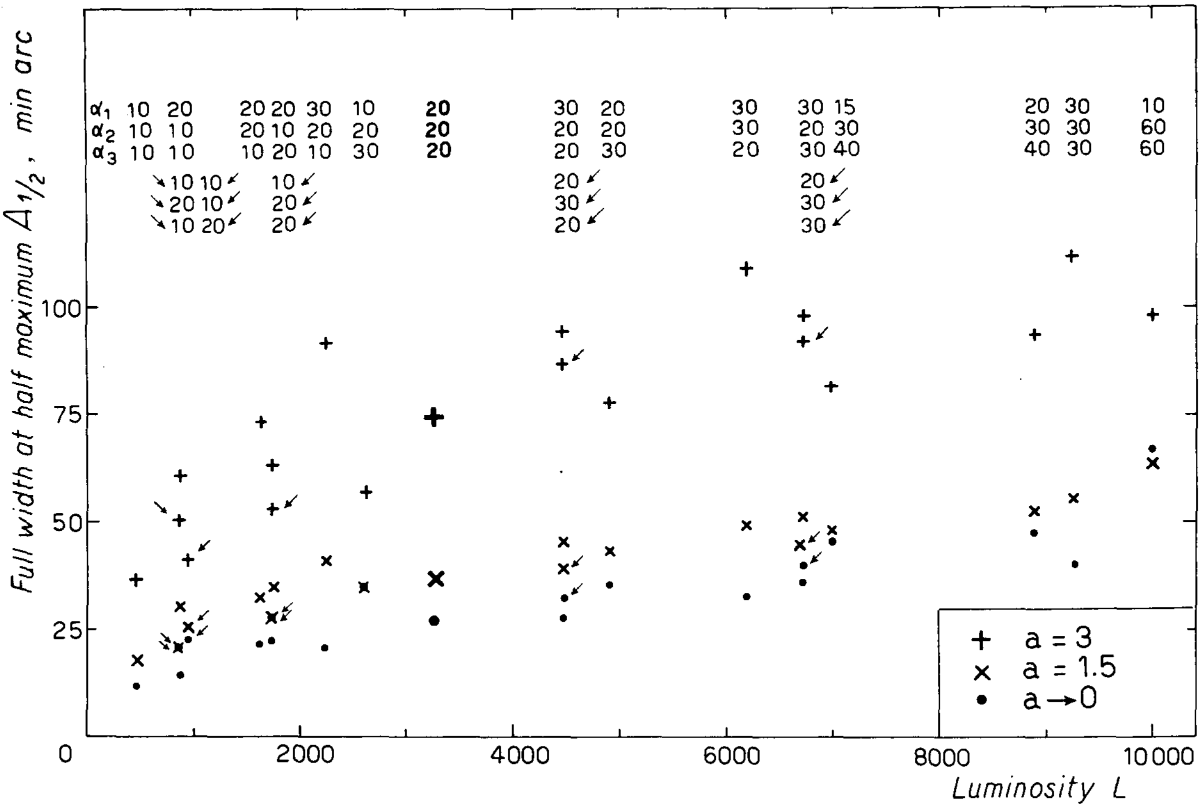

Fig. 2. Full width at half maximum $A_{\frac{1}{2}}$ (min·arc) *vs.* luminosity L for various choices of the horizontal angular divergences (α_1, α_2, α_3) of the three collimators, and for the values $a \to 0$, $a = 1.5$, and $a = 3$. All the points are calculated for a monochromating crystal mosaic spread $\beta = 20$ min·arc.

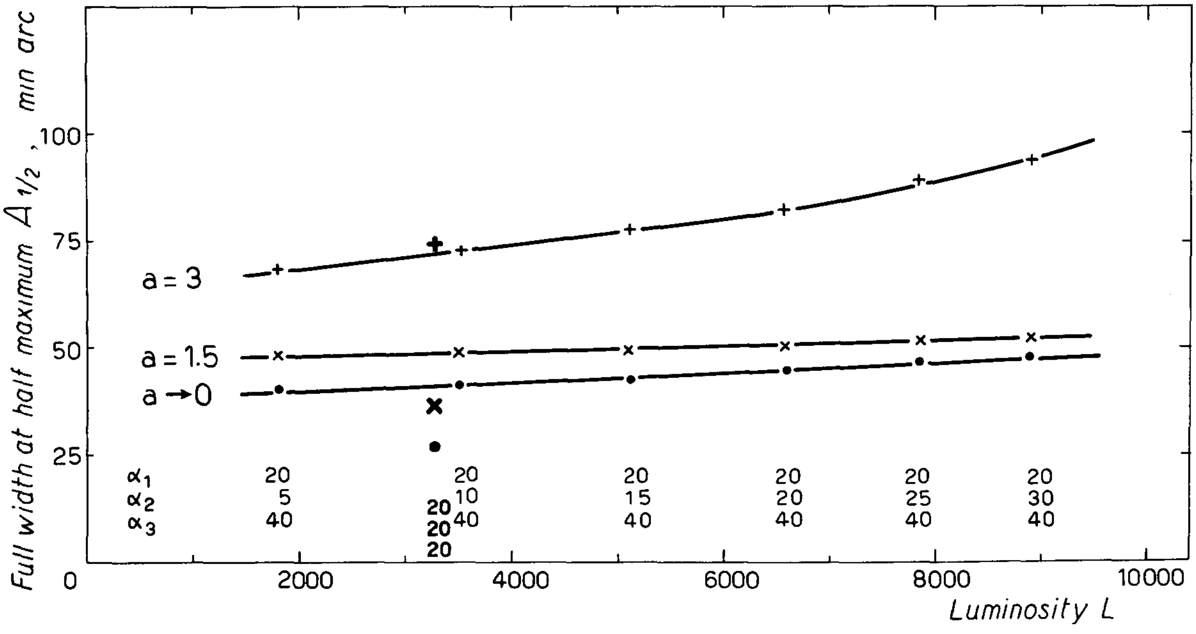

Fig. 3. Full width at half maximum $A_{\frac{1}{2}}$ (min·arc) *vs.* luminosity L, for the choices (20, α_2, 40) of the horizontal angular divergences of the three collimators, and for the values $a \to 0$, $a = 1.5$, $a = 3$, $\beta = 20$ min·arc. Points $\left[L\,(20, 20, 20), A_{\frac{1}{2}}\left(20, 20, 20; \begin{smallmatrix} a = 3 \\ a = 1.5 \\ a \to 0 \end{smallmatrix}\right)\right]$ are also reported.

(α_1, α_2, α_3) of the horizontal angular divergences of the first, second, and third collimators seems to be one for which $\alpha_1 < \alpha_2 < \alpha_3$.

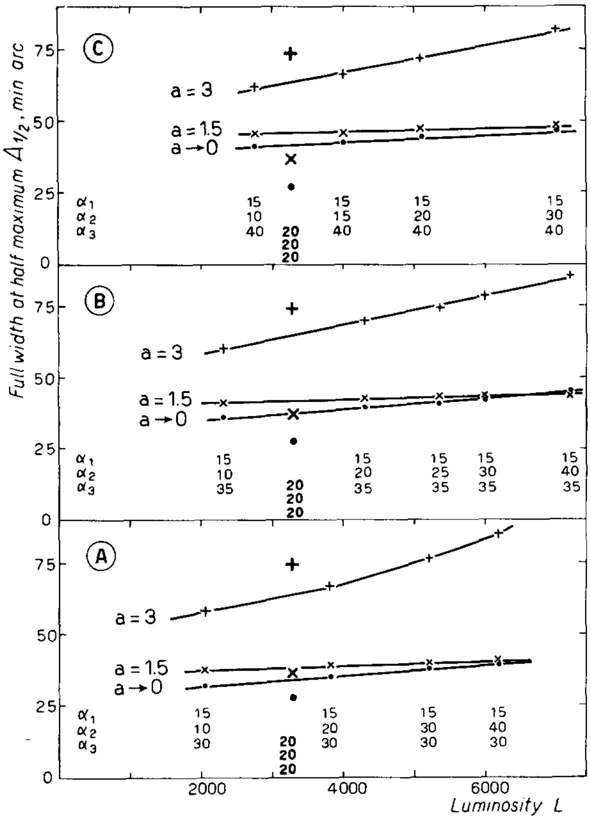

Fig. 4. Full width at half maximum $A_{\frac{1}{2}}$ (min·arc) *vs.* luminosity L, for the following choices of the horizontal angular divergences of the three collimators: (15, α_2, 30), (15, α_2, 35), (15, α_2, 40) respectively in sections A, B, and C, and for the values $a \to 0$, $a = 1.5$, $a = 3$, $\beta = 20$ min·arc. Points $\left[L\,(20, 20, 20), A_{\frac{1}{2}}\left(20, 20, 20; \begin{smallmatrix} a = 3 \\ a = 1.5 \\ a \to 0 \end{smallmatrix}\right)\right]$ are also reported.

Further, we evaluated the focusing action due to the parallel position.

Our calculations refer to collimators in which total reflection of neutrons can be neglected. Nevertheless, the criteria we established can be thought of as holding in general as a first approximation, and could be useful for those cases for which one is interested in a comparison between a possible group of values (α_1, α_2, α_3) and a group of values (for instance the group (20, 20, 20)) of known experimental behaviour[4]).

7. Acknowledgments

We wish to thank Professor E. Amaldi for the interest shown in this work.