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Optimum Geometric Conditions in the Design and Use of X-ray Diffraction Tubes and Cameras

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A theory is developed which enables optimum geometric conditions to be determined under various conditions. The validity of the simplifying assumptions is discussed. The theory shows (*a*) that stationary-anode X-ray tubes should be employed with focal dimensions three times those of the specimen; (*b*) that rotating-anode X-ray tubes should have focal dimensions five times those of the specimen. In each case, the distance between specimen and focus and the film distance are determined by the spacings which it is desired to record. Optimum conditions are also calculated for cases where the focal size, specimen distance, and/or film distance are restricted by experimental conditions. The dosage received by the specimen and the contrast produced at the film are also considered.

The implications of this analysis are discussed, and, in particular, it is concluded that a need exists for X-ray tubes of variable focal size.

1. The problem

1·1 *Introduction*

When conventional techniques are employed, inorganic specimens can generally be obtained of sufficient size to produce an X-ray diffraction photograph in a reasonable time; exposure time is not a limiting factor, and camera dimensions are not usually of crucial importance. In biological studies, however, specimens are likely to be both small and weakly diffracting, and exposure time becomes a limiting factor in the application of the technique. It is of great importance, therefore, to make sure that the dimensions of the X-ray tube and camera are chosen so as to produce a satisfactory photograph in the shortest possible time.

A comprehensive treatment of part of this problem has already been published by Bolduan & Bear (1949) who considered the special slit and pinhole collimation systems suitable for use in low-angle diffraction work, where the specimen size can be selected as required and the film distance is controlled principally by the need to view conveniently very close-spaced patterns.

The present paper deals with wider-angle techniques, where a simpler collimator can be used but where specimen size is a controlling factor in the design of the camera and where the film distance may be altered within fairly wide limits.

1·2. *Assumptions*

In order to make the problem manageable, certain simplifying assumptions have to be introduced. These are:

(1) That the condition of maximum intensity occurs when there is maximum X-ray intensity at the centre of the diffracted image, and is not a function of the distribution of intensity elsewhere in the image.

(2) That absorption in the specimen can be neglected (this is a reasonable approximation for small organic specimens).

(3) That the diffracted image from a crystal, illuminated by a source of X-rays, and rotated through the diffracting angle, is the geometrical image of the crystal cast by the X-ray focal spot; this assumption is justified over the inner region of reciprocal space when the diffraction spread produced by the crystal is small compared with the angle that the crystal subtends at the focus, or that the focus subtends at the crystal.

(4) That only iso-dimensional specimens are to be considered; in practice, a specimen thickness rather greater than the specimen width can be tolerated if diffraction spots with $2\theta < 45°$ are being recorded; this thickness will bear a constant ratio to the specimen width, and the only effect on the general theoretical treatment will be the introduction of a numerical factor.

(5) That the resolution required at the centre of the photograph is sufficiently low for low-angle scattering by the collimator to be neglected. This will be true for distances from the centre corresponding to spacings up to 100 Å approximately. If higher resolutions at the centre of the photograph are required, then a collimator with suitable guarding arrangements should be used; this case has not been considered here, as the introduction of the additional variables necessary renders the problem unmanageable. The paper by Bolduan & Bear (1949) should be consulted for certain types of solution.

It is necessary to specify the resolution required of the camera. In the case of the Buerger precession

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camera, or others where a moderately undistorted picture of a single plane in reciprocal space is produced, the separation of the centres of the spots on the film is determined by the unit-cell dimensions and the film distance; the size of the individual spots will be determined by the geometry of the camera, which must be such that neighbouring spots do not overlap. If the unit-cell dimension is equal to $l\lambda$ (where λ is the wavelength of the X-rays being used) then the condition of the separation of adjacent spots may be conveniently expressed by saying that the resolution of the camera must be equal to l wavelengths. In other types of camera, where overlapping of reciprocal-lattice planes or displacement of the film occurs, a value of the effective resolution required will have to be determined from experience. The general theoretical treatment remains unchanged, as the resolution appears only as a numerical factor.

Finally, it should be emphasised that the treatment is of necessity only an approximate one, and is intended to show the general form of the relationships which exist between the various dimensions of the camera, specimen and X-ray tube; different criteria for resolution or optimum intensity will lead to somewhat different sets of values, but will leave the general form of the relationships essentially unchanged.

1·3. *Notation*

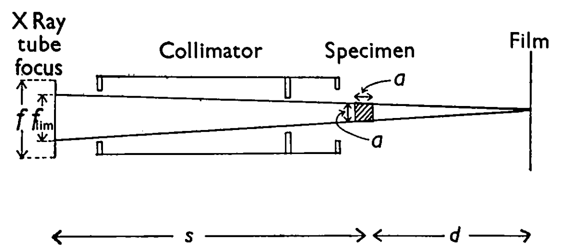

Fig. 1. Typical X-ray diffraction camera arrangement, showing notation used.

f = linear dimensions of focus of X-ray tube.
a = linear dimensions of specimen.
s = distance of focus from specimen.
d = distance of film from specimen.
l = resolution (expressed as length in wavelengths of effective unit cell).
I_0 = specific loading on focus of X-ray tube.
I = intensity of diffracted X-rays.

1·4. *Basic theory*

If the specimen is rotated through the diffracting position, the width of the image from a point focus is $\{(d+s)/s\}a$. As the size of the focus is increased, a series of overlapping images is produced; when the focal size exceeds a certain value, $f_{\text{lim.}}$ (see Fig. 1) the images formed from points at opposite extremities no longer overlap; and beyond this point, while the total size of the image increases, the peak intensity per unit area within the image stays constant.

From assumption (1) it follows that there is no gain in making the focus larger than this limiting size; thus

$$f \leqslant \left(\frac{d+s}{d}\right) a\,. \tag{1}$$

Now, if the camera is to produce separate images corresponding to adjacent points in the reciprocal lattice, then simple geometry shows that the following relation must exist between the camera dimensions and the effective unit-cell dimensions:

$$\frac{d}{l} \geqslant f\left(\frac{d}{s}\right) + a\left(\frac{d+s}{s}\right)$$

and

$$d \geqslant \frac{las}{s-la-lf}, \tag{2}$$

For highest intensity, the smallest possible film distance should be employed: by making (2) an identity, and putting this value of d into (1), the condition for overlap becomes

$$f \leqslant \frac{s}{2l}. \tag{3}$$

If I_0 is the specific loading on to the X-ray focus, then the intensity at the image on the film is readily seen to be

$$I \propto \frac{I_0 f^2 a}{(d+s)^2}.$$

If the smallest possible film distance is used,

$$I \propto \frac{I_0 a f^2 (s-la-lf)^2}{(s^2-lsf)^2}. \tag{4}$$

Equations (3) and (4) are the basic expressions from which all the theory which follows is developed.

In this theory, the value of l (the resolution) will be regarded as given, and the minimum possible film distance will of course always be used. The specimen size (a), the focal distance (s) and the size of the focus (f) will be treated at variables in a number of relevant cases, which may impose various limitations on the variables; in each case, the variables are then adjusted to maximize the value of the intensity I given by (4).

It is necessary to calculate the optimum conditions for three types of X-ray tube:

(1) Where the size of the focus is fixed: f (effective size) could only be varied by stopping down with a collimator (it will however emerge that it never pays to do this). In this case, the specific loading on the anode (I_0) is constant.

(2) Where the size of the focus is variable: in this case, the specific loading will vary approximately as $1/f$ (Müller, 1931).

(3) Where the size of the focus is variable and a rotating anode is also used: in this case, the specific loading will vary approximately as $1/f^{\frac{1}{2}}$ (Müller, 1931).

The details of the calculation are given in the

Appendix, to which reference is made in the discussion that follows.

2. Results

2·1

The first part of the discussion (§§ 2·2–2·4) will be concerned with the optimum conditions when the only limitations are those imposed by the focal size and the specimen size. The further restrictions which may arise due to camera design, X-ray tube dimensions etc. will be reserved until later (§ 3).

2·2. *Fixed-focus tubes* (*size of focus f*)

It is shown in the Appendix:

(i) That in the case where the specimen size may be varied at will, the whole of the focus will always be used. A specimen should be chosen having dimensions one-third those of the focus. The focal distance should have the value $s = 2lf$. The film distance will be half the focal distance, i.e. lf (Appendix 6·2·1, equation (9)).

Some examples are given in Table 1.

Table 1. *Examples*

To resolve a spacing of 60 Å

Focal distance (cm.)	Focal size (μ)	Specimen size (μ)	Film distance (cm.)
1	125	42	0·5
2	250	83	1·0
5	625	208	2·5
10	1250	416	5

To resolve a spacing of 120 Å

Focal distance (cm.)	Focal size (μ)	Specimen size (μ)	Film distance (cm.)
1	62	20	0·25
2	125	42	1·0
5	312	104	2·5
10	625	208	5

(ii) That in the case where the specimen size is fixed it is found (Appendix 6·2·2) that the dimensions should again always be arranged so that the whole of the focus is being used. The form of the solution depends on the relative values of f and a:

(*a*) If $a > f/3$, then the optimum focal distance is given by

$$s = l\{a+f+\sqrt{(a^2+af)}\}$$

(Appendix 6·2·3, equation (11)) and the film distance by

$$d = \frac{la\{a+f+\sqrt{(a^2+af)}\}}{\sqrt{(a^2+af)}}$$

(by substitution in equation (2)).

(*b*) If $a < f/3$, then one uses

$$s = 2lf$$

and

$$d = \frac{4l^2af}{s-2la}$$

(by substitution in equation (2); see Appendix 6·2·3).

A typical example would be $f = 1$ mm., $a = 1$ mm. (i.e. $a > f/3$). To resolve a 60 Å spacing, it follows that optimum focal distance = 13·6 cm. and film distance = 9·6 cm. In this case, conventional camera arrangements are near optimum.

If, however, $f = 1$ mm., as before, but $a = 0{\cdot}1$ mm. (i.e. now $a < f/3$) it is found that optimum focal distance = 8·0 cm. and film distance = 0·9 cm. This is very different from the kind of arrangement usually adopted.

It is a common fallacy that a decrease in the film distance necessarily brings about a fall in the resolution with a focus of conventional size. This is not so, for with small specimens the required resolution can still be obtained, and a great gain in intensity can be achieved, by using a small film distance (which would not of course be possible with large specimens owing to overlap of spots). A further increase in intensity can be obtained by using a variable-focus tube (see § 3). Thus, consider the case above where a 0·1 mm. crystal with a unit cell of 60 Å is being examined. A conventional camera arrangement might have $f=1$ mm., $s = 10$ cm. and $d = 6$ cm.; if the optimum distances are used (including the smallest film distance—0·9 cm. —for resolution to be still possible) then a gain by a factor of 45 in the intensity of the spots is obtained. If a variable-focus were used (300 μ at 2·4 cm.) then a total gain of 75 times is obtained with d now of 1·2 cm.

If it is required to maintain d fixed at 6 cm., then the theory would predict (§ 3·3) that a 0·11 mm. focus should be used at a distance of 0·9 cm.; this would give an intensity gain of 9 times over conventional practice.

2·3. *Variable-focus tubes*

The greatest intensity will always be obtained by adjusting the focal size to be three times the specimen size. The focal distance is given by $s = 2lf$ and the film distance by $d = lf$ (Appendix 6·3, equations (17) and (18)). For reasons which are discussed in the Appendix, it thus turns out that the relations have the same form as was noted above for a fixed-focus tube with a variable specimen size; hence Table 1 may also be used to illustrate optimum sets of conditions for variable-focus tubes. The optimum conditions always lead to the same value of the intensity, whatever the scale of the apparatus, which, if the specimen size is variable, will obviously be adjusted for convenience (but see considerations of contrast etc. §§ 4·2, 4·3).

The condition $f = 3a$ depends on the form of the relation between maximum permissible power loading and focal size ($I_0 \propto 1/f$). Other relations would lead to different conditions, e.g. in the case of a rotating-anode tube ($I \propto 1/f^{\frac{1}{2}}$) the relation is $f = 5a$ (see below). Again, if a tube were available whose loading could be made independent of focal size it would pay to increase the latter without limit, increasing the focal distance accordingly.

2·4. *Rotating-anode tubes*

(i) *Fixed focal size.*—Obviously, the conditions here will be precisely the same as those discussed under fixed-focus tubes (§ 2) and require no separate discussion.

(ii) *Variable focus.*—Where the size of the specimen a is fixed, the focal size f should be adjusted so that $f = 5a$. The focal distance is given by $s = 2lf$ and the film distance by $d = \frac{1}{2}lf$ (Appendix 6·4·2, equation (22)). Typical sets of dimensions are given in Table 2.

Table 2. *Rotating-anode tubes*

To resolve a spacing of 60 Å

Focal distance (cm.)	Focal size (μ)	Specimen size (μ)	Film distance (cm.)
0·6	50	10	0·15
6	500	100	1·5
15	1250	250	3·5
30	2500	500	7·5

To resolve a spacing of 120 Å

Focal distance (cm.)	Focal size (μ)	Specimen size (μ)	Film distance (cm.)
1·2	50	10	0·3
12	500	100	3
30	1250	250	7·5
60	2500	500	15

(iii).—Where the specimen size is variable, the largest available specimen should be used (since the intensity increases with the scale of the apparatus (Appendix, equation (19)) and the focal size should again be made five times the specimen size. If this value of the focal size is not attainable, then the focus should be made as large as possible and the specimen should be one-third its size.

3. Practical limitations

3·1.

In practice, cases will often arise where the optimum conditions described in the previous paragraphs cannot be attained, owing to the limitations of available cameras and X-ray tubes. The best compromise conditions are summarized in Tables 4 and 5. One special case will be discussed briefly below.

3·2. *Maximum specimen size fixed; minimum focal distance fixed*

This is a particularly important case. The optimum focal size will be very small for very small specimens, and even with quite high resolution, the optimum focal distance will also be small. Thus, a 20 μ specimen, under optimum conditions, with a resolution of 120 Å would require the following arrangement (from equations (18) and (22)):

(*a*) With stationary anode and variable focus

Focal size	60 μ
Focal distance	9·6 mm.
Film distance	4·8 mm.

(*b*) With rotating anode

Focal size	100 μ
Focal distance	1·6 cm.
Film distance	4 mm.

While film distances as small as these are quite practicable, it will often be impossible to come within the optimum distance of the focus of the X-ray tube.

If the closest practicable distance of approach is $s_{\text{min.}}$, where $s_{\text{min.}} > 6la$ (stationary anode) or $> 10la$ (rotating anode) then it can be shown that the optimum focal size is given by

$$f = \frac{s_{\text{min.}}}{2l}$$

and the film distance by

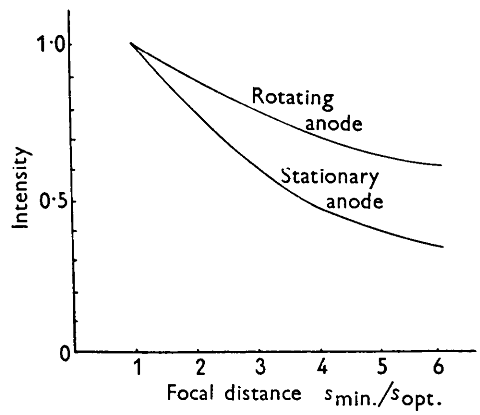

Fig. 2. Variation of intensity with film distance for fixed specimen size.

Table 3. *Optimum conditions with one variable fixed*

Variables	Specimen size (a) fixed		Focal size (f) fixed	Specimen distance (s) fixed	Film distance (d) fixed	
	S.A.	R.A.	All tubes	All tubes	S.A.	R.A.
Specimen size	a	a	$f/3$	$s/6l$	$d/3l$	$2d/5l$
Focal size	$3a$	$5a$	f	$s/2l$	d/l	$2d/l$
Specimen distance	$6la$	$10la$	$2lf$	s	$2d$	$4d$
Film distance	$3la$	$5la$	lf	$s/2$	d	d

S.A. = Stationary anode.
R.A. = Rotating anode.

Table 4. *Optimum conditions with two variables fixed*

Variables	Film distance and focal size fixed		Maximum specimen size (a_m) and focal size fixed		Maximum specimen size and minimum specimen distance fixed			
	All tubes		All tubes		S.A.		R.A.	
Specimen size	If $f \leqslant d/l$ use $a = d/3l$	If $f > d/l$ use $a = df/(2lf+d)$	If $a_m \geqslant f/3$ use $a = f/3$	If $a_m < f/3$ use $a = a_m$	$a_{\max.}$		$a_{\max.}$	
Focal size	f	f	f	f	$s/2l$		$s/2l$	
Specimen distance	$(d+3lf)/2$	$2lf$	$2lf$	$2lf$	If $s_{\min.} > 6la$ use $s = s_{\min.}$	If $s_{\min.} < 6la$ use $s = 6la$	If $s_{\min.} > 10la$ use $s = s_{\min.}$	If $s_{\min.} < 10la$ use $s = 10la$
Film distance	d	d	lf	$4l^2af/(s-2la)$	$2las/(s-2la)$	$s/2$	$2las/(s-2la)$	$s/4$

S.A. = Stationary anode.
R.A. = Rotating anode.

Table 5. *Optimum conditions with film distance and maximum specimen size fixed*

Variables	Maximum specimen size (a_m) and film distance fixed				Maximum specimen size (a_m), focal size and film distance fixed				
					All tubes				
	S.A.		R.A.		$a_m > d/3l$			$a_m < d/3l$	
					If $f > d/l$		If $f < d/l$		
Specimen size	If $a_m > d/3l$ use $a = d/3l$	If $a_m < d/3l$ use $a = a_m$	If $a_m > 2d/5l$ use $a = 2d/5l$	If $a_m < 2d/5l$ use $a = a_m$	If $a_m > fd/(d+2lf)$ use $a = fd/(d+2lf)$	If $a_m < fd/(d+2lf)$ use $a = a_m$	use $a = d/3l$	If $f > ad/(d-2la)$ use $a = a_{\max.}$	If $f < ad/(d-2la)$ use $a = a_{\max.}$
Focal size	d/l	$ad/(d-2la)$	$2d/l$	$ad/(d-2la)$	f	f	f	f	f
Focal distance	$2d$	$2lad/(d-2la)$	$4d$	$2lad/(d-2la)$	$2lf$	$\{(f-a)/a\}d$	$(d+3lf)/2$	$\{(f-a)/a\}d$	$ld(a+f)/(d-la)$
Film distance	d	d	d	d	d	d	d	d	d

$$d = \frac{2las_{\text{min.}}}{s_{\text{min.}}-2la}.$$

The variation of intensity for values of $s_{\text{min.}}$ greater than $s_{\text{opt.}}$ is shown in Fig. 2.

4. Other considerations

4·1. *Dosage of specimen*

The X-ray dosage received by the specimen may produce changes in it which cause the diffracted image to deteriorate.

The dosage rate at the specimen is given by

$$D \propto F\,,$$

where F is the incident flux.

The diffracted intensity at the film is given by

$$I \propto Fa\,.$$

Thus, the dosage received by the specimen for a given film intensity will increase as the specimen grows smaller. This is true whatever type of X-ray tube is used. This effect will fix an absolute lower limit to the size of specimens which can be examined by X-ray diffraction.

4·2. *Contrast on film*

Another important consideration is the contrast produced between the diffracted image and the general background radiation.

For a given incident flux, the diffracted intensity at the film due to Bragg reflexion of the characteristic radiation will be

$$I \propto a^3/d^2\,,$$

and as $d \propto a$ for optimum conditions (see equations (18) and (22))

$$I_{\text{diff.}} \propto a\,.$$

The scattered radiation causing the background on the film may be caused in three ways:

(1) Incoherent scattering, etc., by the specimen; the intensity produced by this will vary as a^3/d^2, so that the contrast ratio $I_{\text{diff.}}/I_{\text{scatt.}}$ will remain constant as a alters.

(2) Air scattering. The total intensity produced (at the centre of the film) by a column of air between the specimen and a backstop at a distance Δ from the film is given by

$$2I_{\text{scatt.}} \propto a^2(1/\Delta-1/d)\,.$$

Thus if the backstop and film distances are both made always proportional to a, then the intensity at the centre of the film due to air scattering will be proportional to a. If we consider a point on the film on which reflexions from a spacing w will fall, then the distance of that point from the centre will be proportional to d (and so to a). Thus a simple calculation shows that the air scattered intensity arriving at that point will always be the same fraction of the intensity arriving at the centre of the film. Thus the contrast ratio for air-scattering is independent of specimen size for all reflexions.

(3) Scattering from specimen mount (if used); the intensity here will be given by

$$3I_{\text{scatt.}} \propto (a^2/d^2)t\,,$$

where t is the thickness of the wall of the specimen holder plus mounting liquid (if any).

For practical reasons, t will in general decrease more slowly than a, so that the contrast ratio here will decrease with a. Thus, the contrast on the film is independent of specimen size, unless the specimen is mounted in a chamber (or in liquid) whose thickness decreases more slowly than that of the specimen as the specimen size is decreased; under these circumstances, the contrast will become poorer when smaller specimens are used.

5. Conclusions

It is most important, when the diffracted intensity is small, to have X-ray tubes with variable sized foci and if possible rotating anodes. For equal resolution in all directions in reciprocal space, the focal spot should appear approximately square after foreshortening, and a range of sizes from 50 μ to 1·0 mm. would be very satisfactory for most purposes. It should also be pointed out that in many cases when only small foci are required it is desirable to modify the present technique of viewing the anode with a foreshortening ratio of 10:1. It is possible to obtain an increase in apparent brightness of focus down to viewing angles of 1° (Bolduan & Bear, 1949), and so a considerable gain would be introduced by using a foreshortening ratio of 40:1 or 50:1 and a focal line of appropriate dimensions.

It is also desirable, when working with very small specimens, to be able to approach close to the focal spot. If a resolution of about 100 Å is required, a 1 cm. focal distance would be adequate for specimens of the order of 30 μ for stationary anodes or 20 μ for rotating anodes. The decline in intensity if this short focal distance is not attainable is, however, moderately slow, particularly in the rotating-anode case. Such small focal distances are not necessary with normal-sized specimens.

For specimens where a lower resolution is permissible, even shorter focal distances are advantageous and a fine-focus tube with a working distance of a few millimetres or less would be most valuable.

It may be said that it is in principle possible with stationary-anode X-ray tubes, by varying the focal spot size of the X-ray tube and adjusting camera dimensions to the optimum, to obtain the same intensity per unit area at the film for all sizes of specimen. With rotating-anode tubes, the intensity will of course always be higher than in the stationary-anode case, but the gain will be greater for larger specimens.

If specimens are used which are adversely affected by X-ray exposure, then an absolute lower limit will be fixed to the usable specimen size. It may also be expected that if any mounting chamber is used for the specimen, then the contrast will fall as the specimen size is reduced.

It should also be pointed out that the design of cameras and X-ray tubes with optimum dimensions for the smaller specimens presents considerable technical problems, since the focal size and focal distance need to be so small, and a balance must be reached between the gain in exposure time and the difficulty of building and operating the equipment needed to produce it. It is necessary then to examine the effect on the intensity of departures from the optimum conditions, and this is best done by numerical evaluation of the particular problem.

Table 3 summarizes the optimum conditions under various circumstances.

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6. Appendix

6·1. *Outline of procedure*

In order to determine the relations between the optimum values of the dimensions, the following procedure is adopted.

(1) A fixed specimen size (a) is considered and, keeping the focal distance (s) constant, a value of focal size (f) is found which maximizes the intensity given by expression (4).

(2) This value of f is then substituted back into (4), and an optimum value of specimen size (a) is found. That is, the specimen size is varied, always keeping the focal size optimum for that particular value of specimen size, and the point at which highest intensity occurs is located. Finally, the variation of intensity with the focal distance s (which has hitherto been constant) is investigated.

In terms of a contour diagram of intensity plotted against a and f, a ridge has been located by moving parallel to the f axis, and then that ridge has been followed to the peak by varying a and f together. The contour diagram is a simple one and this procedure is justified. Finally, the change in the height of the peak with variation in focal distance s is calculated.

This procedure locates the optimum conditions when the focal distance is kept fixed, and then shows how the intensity will vary according to the value of focal distance that has been chosen.

If either the focal size or the specimen size were regarded as the fixed quantities, then the solutions are not necessarily the same. Optimum conditions in these cases are evaluated by a procedure similar to the one above, after making use of results already obtained.

It is necessary to apply this procedure in the three separate cases described above (§ 1·4), i.e. X-ray tubes with fixed focus, with variable focus, and with rotating anodes.

6·2. *Fixed-focus tube*

6·2·1. *Fixed specimen distance.*—By differentiating (4) with regard to f, the value of focal size corresponding to a maximum of intensity is found to be

$$f = (s - \sqrt{las})/l\,. \tag{5}$$

Substituting the value of f given by (5) into (4), and differentiating with regard to a, the optimum specimen size is found to be

$$a = s/9l\,. \tag{6}$$

Furthermore, the value of I falls to zero at $a = 0$ and $a = s/l$ (as can be seen from (4) when f from (5) has been substituted). Hence, the general form of the relation between I and a is as shown by the broken line in Fig. 3.

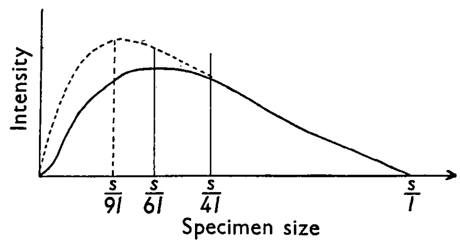

Fig. 3. Variation of intensity with specimen size (focal distance fixed).

If, however, the overlap condition ($f \leqslant s/2l$) is introduced by substituting for f in (5), then one finds

$$a \geqslant s/4l\,. \tag{7}$$

In other words, the maximum I shown in the diagram can never be attained. If f is left at the optimum value given by (5), and a is reduced from s/l, then the overlap condition breaks down below the point $a = s/4l$. The best that can be done is to keep the focal size at the overlap value ($f = s/2l$). To the left of the vertical line the new condition causes the value of I to follow a lower curve shown as a full line. This curve reaches a maximum where

$$a = s/6l \tag{8}$$

(as can be shown by substituting $f = s/2l$ in (4) and differentiating with regard to a).

Thus the optimum conditions, for a given value of the focal distance, s, are

$$f = s/2l,\ a = s/6l,\ d = s/2\,, \tag{9}$$

(by substituting for f and a in (2)).

The intensity formula (4) now reduces to

$$I \propto I_0 s\,. \tag{10}$$

Thus, as long as the power loading, I_0, is kept constant, the intensity at the film increases with increasing focal distance and increasing focal size providing that all the other quantities are kept at optimum. Therefore, if the focal size of the X-ray tube is fixed, the whole of it should be used.

6·2·2. *Effect of using fixed value of focal size, with focal distance and specimen size variable.*—By differentiation of (5) with regard to s, it can be shown that the optimum value of s for a given value of f and a is

$$s = l\{a+f+\sqrt{(a^2+af)}\}\,. \tag{11}$$

If this value of s is substituted into (4), the optimum value of a can now be found by differentiation. It is

$$a = f/3\,.$$

Now, if the overlap condition is to be satisfied, then by substituting the value $f \leqslant s/2l$ into (11), one finds

$$a \geqslant f/3\,.$$

Hence the value above can be reached, and so, when f is fixed, the optimum conditions are

$$a = f/3,\ s = 2lf,\ d = s/2\,. \tag{12}$$

6·2·3. *Effect of fixing specimen size and allowing focal size and focal distance to vary.*—As was found in (11), the optimum value of s for a given value of f and a is

$$s = l\{a+f+\sqrt{(a^2+af)}\}$$

so long as $f \leqslant 3a$. If this value of s is substituted in (4), it can be shown that I increases with increasing f.

When $f > 3a$, s can no longer be given this optimum value without violating the overlap condition. The best that can be done is to use s at the overlap value $s = 2lf$. Substituting this value of s into (4) one readily obtains

$$I \propto \frac{I_0(f-a)^2}{l^2 f^2}, \tag{13}$$

i.e. the intensity increases with f in the region, also tending towards a limit as the f tends to infinity. Thus, when the power loading on the anode is constant, the film intensity for a given specimen size will increase towards a limit with increasing focal size, so long as the focal distance is always given its best value. Therefore, the whole of the focus should always be used.

6·3. *Variable-focus tube*

Expression (4) now becomes

$$I \propto \frac{af(s-la-lf)^2}{(s^2-lsf)^2}. \tag{14}$$

By differentiation with regard to f, the value of focal size for maximum intensity is found to be

$$f = \frac{2s+la-\sqrt{(l^2a^2+8las)}}{2l} \tag{15}$$

Substituting this value of f into (14) it can be shown by differentiation that the optimum value of a is given by

$$a = s/6l\,. \tag{16}$$

Now, if the overlap condition ($f \leqslant s/2l$), and the condition for optimum f (equation (15)) are to be satisfied together, then, by substituting for f in (15), one finds

$$a \geqslant s/6l\,.$$

Thus the overlap condition is satisfied when a and f are adjusted to their optimum values. These are

$$a = s/6l,\ f = s/2l,\ d = s/2\,. \tag{17}$$

Thus, the optimum dimensions for a given value of s are the same in this case as in Case 1 (fixed focus, constant power loading); however, the intensity at the film is now seen to be

$$I \propto \text{constant}$$

and is independent of the value of the focal distance (i.e. independent of the scale of the apparatus). Hence, a contour map of intensity plotted against f and a will show a peak at $f = s/2l$, $a = s/6l$ of the same height for all values of s, and the optimum conditions can therefore always be expressed by the relations

$$f = 3a,\ s = 6la,\ d = s/2\,. \tag{18}$$

If, therefore, the specimen size, or the focal size, were the fixed quantity, the same relationships would hold between the optimum dimensions as in the case where the focal distance was fixed.

6·4. *Rotating-anode tube*

6·4·1. *Fixed specimen distance.*—The optimum conditions may be obtained in this case as follows. In both Case 1 (constant I_0) and Case 2 ($I_0 \propto 1/f$) it was shown that, for a given value of s, the optimum conditions obtained when f was given by $f_{\text{opt.}} = s/2l$ and a was given by $a = f/3$. Thus, in each case the intensity would be reduced by using $f < s/2l$ even though, in Case 2, the power loading could be increased by a factor $(f_{\text{opt.}}/f)$.

Now, in the rotating-anode case, if a value of f is used such that $f < s/2l$ then the power loading can only be increased by a factor $(f_{\text{opt.}}/f)^{\frac{1}{2}}$. Clearly then, a decrease in intensity at the film would be produced.

Thus, in this case also, for a given value of focal distances the optimum conditions are given by

$$f = s/2l,\ a = s/6l,\ d = s/2$$

(cf. equation (18)).

The intensity at the film is now seen to be

$$I \propto s^{\frac{1}{2}} \tag{19}$$

and therefore increases as the scale of the apparatus is increased.

6·4·2. *Effect of fixed specimen size.*—Consider first the dimensions arranged so that the value a at which the specimen size is fixed is the optimum value for the particular focal distance (s) being used, the focal size (f) being also given its optimum value. Then, as in (18),

$$s = 6la,\ f = 3a,\ d = s/2\ .$$

Now, if a smaller value of s were used, and if a and f were adjusted to their optimum values (for this new value of s), then, by (19), the resultant intensity at the film would *decrease*. Therefore, the optimum value of s for a given value of a must be in the region where $s \geqslant 6la$. Consider now values of s in this range.

If the intensity expression (4) (with I_0 now made $\propto 1/f^{\frac{1}{2}}$) is differentiated with regard to f, the optimum value of f for a given value of a and s is seen to be

$$f = \frac{6s+la-\sqrt{(l^2a^2+48las)}}{2l}\ . \tag{20}$$

If the overlap condition is to be obeyed, then by substituting $f \leqslant s/2l$ in (20) one readily obtains

$$s \leqslant \frac{38la}{25}\ .$$

Therefore, the optimum value of focal size given by (20) cannot be reached in the region where $s \geqslant 6la$.

Inspection of (4) shows that the intensity at the film increases from zero when $f = 0$, and would in theory reach a maximum at the value of f given by (20); thus the best value of f is the maximum permissible for overlap, i.e.

$$f = s/2l\ .$$

The intensity expression now reduces to

$$I \propto \frac{(s-2la)^2}{s^{5/2}}\ . \tag{21}$$

Differentiating this expression with regard to s, the maximum value of intensity is found to occur when

$$s = 10la,\ f = 5a,\ d = 5la\ . \tag{22}$$

6·4·3. *Focal size fixed.*—In this case, as the power loading will be constant, the optimum conditions must be the same as for the stationary-anode fixed-focus case. That is,

$$a = f/3,\ s = 2lf,\ d = lf\ ,$$

as in equation (13).

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A Method for the Estimation of Transmission Factors* in Crystals of Uniform Cross Section

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This article presents a method of estimating the transmission factors of crystals with uniform cross section. It synthesizes Albrecht's idea of dividing the section into parallelograms and measuring the path length x for the centre of each, with Howells's loci of points of constant x. Thus, bands of approximately constant x are obtained, which make the computations very quick. An example and a detailed discussion on the accuracy to be expected are also given.

1. Introduction

While working on the determination of the crystal structure of the strongly absorbing sodium–thyroxine (μ = 437 cm.$^{-1}$) the intensities of the diffracted beams had to be corrected for absorption.

The best method known to us for estimating the transmission factors was that of Howells (1950) by which these factors can be calculated very conveniently with any degree of accuracy required. Although it is very quick for some particular advantageous cases, it may become involved in some others, requiring a

* The authors think that the name of transmission factor is more appropriate than the generally accepted name of absorption factor, as it actually gives the fraction of radiation transmitted by the crystal.