THE APPARENT SHAPE OF X-RAY LINES AND ABSORPTION LIMITS[1]

By F. K. Richtmyer[2]

Abstract

Effect of instrumental factors on the observed intensity distribution of x-ray lines and at absorption limits.—(1) *Slit width.* In the case of two slits of equal width, sharp lines reflected from a perfect crystal should give an isosceles triangle distribution. If the two slit widths are unequal, the triangle is truncated; this may shift the relative position of the lines of a partly resolved doublet. (2) *Slit height* widens the isosceles triangles slightly, making the long-wave-length side less steep. (3) *Non-uniform energy distribution over the focal spot* produces corresponding lack of symmetry. An actual distribution curve obtained with very narrow slits showed two unequal maxima near the edges of the spot. The same three factors affect the apparent sharpness of the absorption limit. In particular, the finite slit width results in the rounding off of a sharp discontinuity into a skew-symmetrical S curve consisting of parts of two parabolas whose axes are vertical and separated a distance equal to the angular slit width.

Intensity distribution in the Kα doublet of Mo.—The curves correspond to monochromatic lines of width .0003A or less. The relative intensity is very close to 2 (2.01). There is no line between them with intensity greater than 1 percent that of $K\alpha_1$.

Sharpness of the K absorption limit of Ag.—The curve obtained agrees with that for a limit which is sharp within experimental error, .0002A.

THE x-ray spectrometer used by the writer in studying absorption coefficients needs frequent calibration. For this purpose the several orders of the K series of the target-element (usually tungsten or molybdenum) have been used. In this connection certain peculiarities and characteristics of the x-ray spectrometer have been observed, which seem not without interest and which should be given consideration in studying the actual shape of x-ray lines and absorption edges and in making precision wave-length measurements.

The spectrometer is of the usual Bragg type. The x-ray beam is limited by two slits 38 cm apart placed between crystal and target. Each slit is about 2 cm high and is formed by two lead jaws 1 cm wide, ground plane, and very carefully adjusted to parallelism. The jaws may be moved

[1] This paper is based in part on papers read in February and April, 1924, before meetings of the American Physical Society. (See Richtmyer and Spencer, Phys. Rev. **23**, pp. 550 and 760.) The author takes pleasure in expressing his appreciation of the assistance rendered by Mr. Spencer.

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bi-laterally by micrometer screws reading to .0001 inch (.0025 mm). The tube is adjusted so that the plane of the target makes an angle of about 8° with the line of the slits, the focal spot thus being equivalent to an ellipse approximately 15 mm high and 2 mm wide. The crystal is of calcite, a very perfect one kindly loaned to the writer by Professor Bergen Davis. Ionization currents are read in the usual way, by means of an electrometer of the Compton type.

Factors Affecting the Apparent Shape and Width of Lines

Fig. 1 represents a typical calibration curve showing the first-order lines of Mo and taken with slits .075 mm wide.[3] The abscissas represent

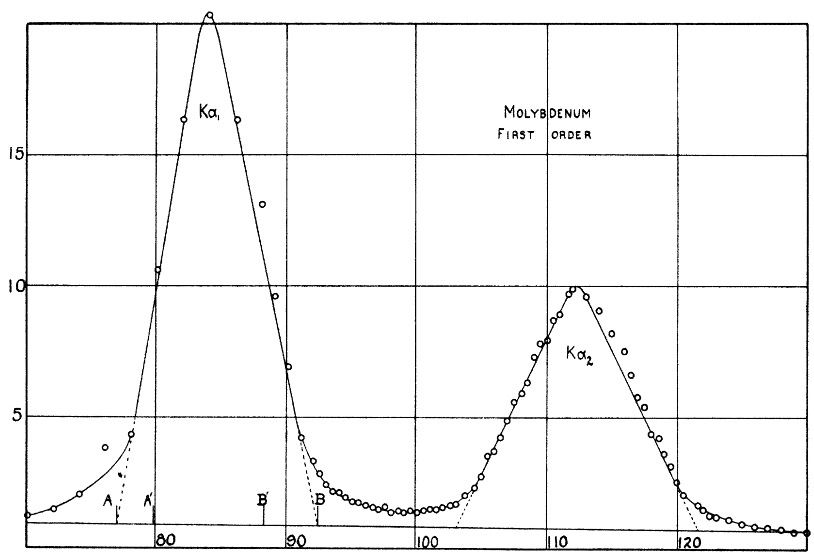

Fig 1. The first order Kα lines of Mo as used in calibrating the spectrometer. The lines are approximately triangles, but are slightly convex outward on the right (long wave-length) side.

arbitrary divisions on the scale of the spectrometer, each division corresponding approximately to .00015A. It will be noted that each line is approximately a triangle *but with the long wave-length side slightly convex outward.* It was this observation which started this investigation of the *instrumental factors* affecting the apparent shape of x-ray lines. Omitting the effect of the crystal[4] these factors are:

[3] This curve was taken with some care in order to investigate the region between $K\alpha_1$ and $K\alpha_2$ where it had been suggested to the author that a faint line might be found. It is quite obvious that no such line of appreciable intensity exists.

[4] See Bergen Davis and W. M. Stempel, Phys. Rev. **19**, p. 504 (1922).

(1) The width (actual and relative) of the slits limiting the beam.
(2) The "brightness" of different parts of the focal spot.
(3) The height of the slit.

The effect of slit width. In what follows we shall assume that we are dealing with a strictly monochromatic line of wave-length λ, and with a *perfect* crystal which reflects λ at the angle θ_λ given by the usual equation

$$n\lambda = 2d \sin \theta_\lambda$$

In Fig. 2A let the two limiting slits be a distance D apart and have the same width s_1. (In any actual case D is very large compared to s_1.) Let TT be the focal spot, the major axis of the ellipse being at right angles to the paper. The crystal, not shown, is at the right of the figure and is capable of rotation about an axis perpendicular to the plane of the

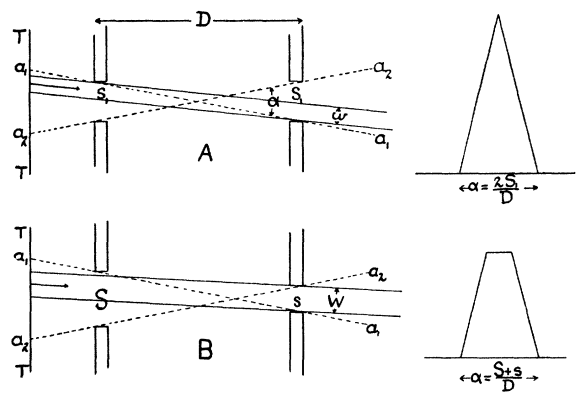

Fig. 2. Showing diagrammatically the effect of finite slit widths on the apparent shape of a line.

figure. Let the angular position of the crystal be measured, in the usual way, by the angle θ which the crystal planes make with the line passing through the centers of the two slits.

Starting from $\theta = 0$ and turning the crystal counter-clockwise, no reflection of the line λ will be observed until the crystal planes make an angle θ_λ with the line a_1a_1 which is defined by the far edge of the left-hand slit and the near edge of the right-hand slit. As the crystal is rotated beyond this position the planes make the angle θ_λ with a beam of *parallel* rays of width w, as shown in the figure. This width w will increase and the *apparent* intensity of the reflected line will accordingly increase until the crystal position is such that w is equal to the slit width s_1. Beyond this point w will decrease to zero when the crystal makes the angle θ_λ with the line a_2a_2. Since s_1 is always very small compared to D this change of w (increase or decrease) is a linear function of the angular position of the crystal. Hence the *observed* shape of the line should be a triangle with a base of which the *angular* width is given by $2s_1/D$.

If the slits be of *unequal* width, say S and s as in Fig. 2B, similar considerations show that the apparent shape of the line will be an isosceles trapezoid of which the base has the angular width $(S+s)/D$.

Parenthetically, it is interesting to point out that the apparent shape of a close doublet will be materially influenced accordingly as the measurements are made with equal or unequal slits. Fig. 3A shows, diagramatically, the apparent shape of a doublet, such as $K\alpha_1$, α_2, when observed by slits of unequal width. The inevitable rounding off of the corners would make this appear as a single line with the maximum at h instead of h_1. Fig. 3B shows the appearance of the doublet when slits of equal width are used. The maximum of the more intense line appears in its correct position, and the presence of the weaker component is indicated by irregularity on the side of the curve.

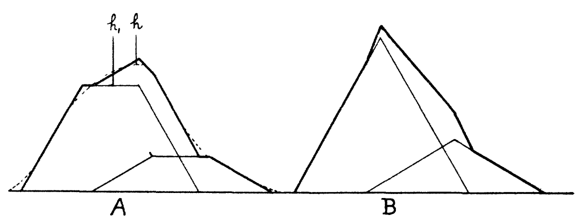

Fig. 3. A. The apparent shape of a doublet when observed by slits of unequal width. B. Same for slits of equal width. Curve A would evidently lead to an incorrect location of the more intense line.

The effect of variation of "brightness" in the focal spot. Referring to Fig. 2A it is readily observed that the apparent shape of the line can be a perfect isosceles triangle only if there is a constant x-ray brightness over that part of the focal spot falling within the solid angle defined by the slits (the angle between the lines a_1a_1 and a_2a_2). There is reason to expect such variation of brightness, partly because of space charge effects within the electron stream from filament to target, partly because of the dissymmetry in field introduced in tubes where the target makes an angle of 45° with the axis of the tube.

To test this point, the slits s were made very narrow (less than .025 mm), thereby isolating a very narrow vertical strip (*aa* Fig. 4) of the focal spot, parallel to its major axis. Using the direct beam, the intensity of the radiation was measured as the tube was moved by micrometer adjustment, so as to cause the focal spot to move past the axis of the slits. The resulting curve is shown in Fig. 4. The distance R on the graph corresponds to the minor axis of the focal spot as seen from the slit system. Two maxima, A and B, are observed indicating that there is a ring of greater intensity just inside the focal spot, but that the one edge of the ring, B, is more intense than the other.

From Fig. 2A it is obvious that dissymmetry will be introduced into the triangle if for example the adjustment of the focal spot should be such that the hump B corresponds to point a_1 and some point midway between the two humps corresponds to a_2. Something like this was apparently the case when the data for Fig. 1 were taken.

To test these two points the slits s were carefully adjusted to .038 mm each, and the tube was so placed that the flat part of the curve, between A and B of Fig. 4, coincided with the region a_1a_2 of the focal spot in Fig.

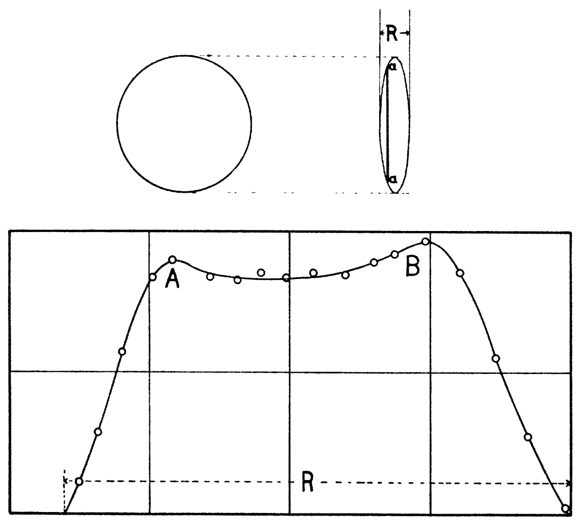

Fig. 4. The unequal distribution of energy across the focal spot of a tube. The focal spot is seen from the spectrometer as an ellipse with minor axis R.

2A. A run was then taken on the line $K\alpha_1$. The result is shown in Fig. 5. It is observed that the sides of this line correspond to the sides of a triangle, and that there is lateral symmetry, instead of the convexity observed in Fig. 1. The width of the base of the triangle is somewhat greater than predicted from the known slit width. But it is rather difficult to measure with high precision slit widths as narrow as .038 mm.

In the case of Fig. 1, the graph shows data taken with slits .076 mm wide. The full line just above the abscissa scale, represents, as nearly as could be estimated, the white radiation in the same region. Therefore one may find the width of the base of the triangle, for α_1 for example, by projecting the sides down to this base line. In this way it is found that with these slits, the width of the base AB corresponds to an equivalent wave-length range of .00232A. The slits were then narrowed to .038 mm and another run taken. The data are not plotted but the base line was observed to be $A'B'$, corresponding to an equivalent wave-length range of .00136A. Extrapolating from these two results, zero slit width would correspond to a wave-length range of .0003A. That is to say, so far as these observations go the line $K\alpha_1$, is monochromatic to this extent. However, because of the difficulty of making precise measures of slit widths as small as these, not too much dependence should be put on this result.

Another point of some little importance when one is concerned with measuring wave-lengths to the highest precision, is brought out by the

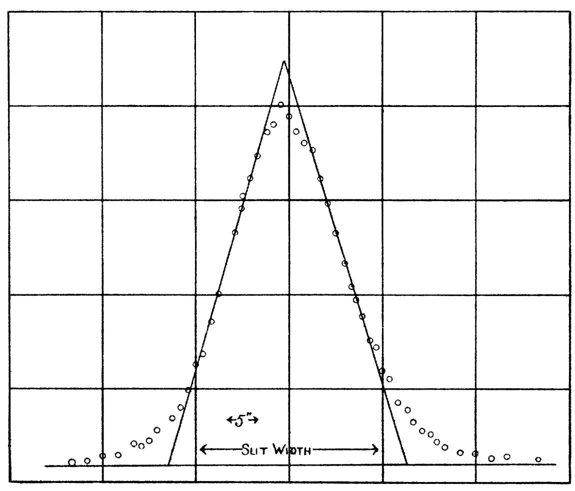

Fig. 5. The $K\alpha_1$ line of Mo (first order), taken with slits of equal width and with the tube so adjusted as to give nearly equal energy distribution over the part of the focal spot used.

$K\alpha_2$ line of Fig. 1. As has been pointed out above, the long wave-length side of the graph is convex outward because of the irregular distribution of energy over the focal spot. Had a smooth graph been drawn through these points and the *maximum* taken as the exact location of the line this maximum would differ from the one shown in the graph by approximately .00015A. While this difference is not large, it shows that the position of a line may be misjudged by an appreciable amount unless care be taken to work with equal energy distribution on the target.

The effect of slit height.[5] For most purposes this effect can be neglected but in work aiming at high precision it is of sufficient importance to be

[5] See also article by H. S. Uhler, Phys. Rev. **11**, p. 11 (1918).

worthy of mention. To simplify discussion, assume that the axis of rotation of the crystal is vertical and that the crystal planes are parallel to this axis; also that the slits limiting the x-ray beam are, as above, between crystal and tube (and are, of course, vertical). It is then usually assumed that the angle θ in the equation

$$n\lambda = 2d \sin\theta$$

is measured by the angle between the *plane* of the crystal face and a second plane passing through the axis of rotation and the two slits. This is obviously the case only for those rays which are *horizontal.* On account of the finite height of the slits there will be other rays, not horizontal, passing through the slit system. For a ray which makes an angle φ with the horizontal, the glancing angle θ at which it meets the crystal planes, is given by the equation

$$\sin\theta' = \sin\theta \cos\varphi.$$

If the wave-length of this ray be λ, then the angle θ_λ at which it will be reflected will be given by

$$\sin\theta_\lambda = \sin\theta' = \sin\theta\cos\varphi,$$

or

$$\sin\theta = \sin\theta_\lambda/\cos\varphi;$$

that is, the greater the divergence of the ray from the horizontal the greater must be the angle θ for reflection to take place. In any actual case φ is small, and its maximum value is given very nearly by the angle which the slit nearest the ionization chamber (or photographic plate) subtends at the slit farthest away from the chamber. The net result of this effect, with very narrow slits and a crystal thin enough to eliminate the penetration error, is to produce a reflected beam, as the crystal is turned, of which the cross section is similar to the cross section of a plano-concave lens, the plane side being sharp and turned toward shorter wave-lengths, while the curved side is slightly diffuse. For this reason the long wave-length side of the triangles, such as in Fig. 1, should be not quite so steep as the short wave-length side. *This effect is observed in practically every case.* To illustrate the magnitude of the effect, it may be pointed out that for a value of φ of 1°, the observed position of the Kα lines of Mo will be shifted about 4″ from the true position, in the first order.

Monochromaticity. A question closely allied to the above is the extent to which the degree of monochromaticity of a reflected beam of white radiation is influenced by the finite width and height of slits. From the law of the crystal grating it follows by differentiation that

$$d\lambda = (2d/n)\cos\theta\, d\theta$$

from which, by knowing the angular divergence $d\theta$ of the reflected beam the value of $d\lambda$ can be obtained. From what has been said above it is obvious that $d\theta$ is made up of two parts, a part α due to the finite width of the slits and a part δ due to finite height of the slits. By reference to Fig. 2 it is readily seen that α is equal to twice the angle subtended by the width of one of the limiting slits at the other, if the slits be of equal width. We can compute δ as follows. From the preceding section

$$\sin \theta' = \sin \theta \cos \varphi_m$$

where φ_m now represents the *maximum* value of φ and is approximately the vertical angle subtended by the slit nearest the chamber at the slit

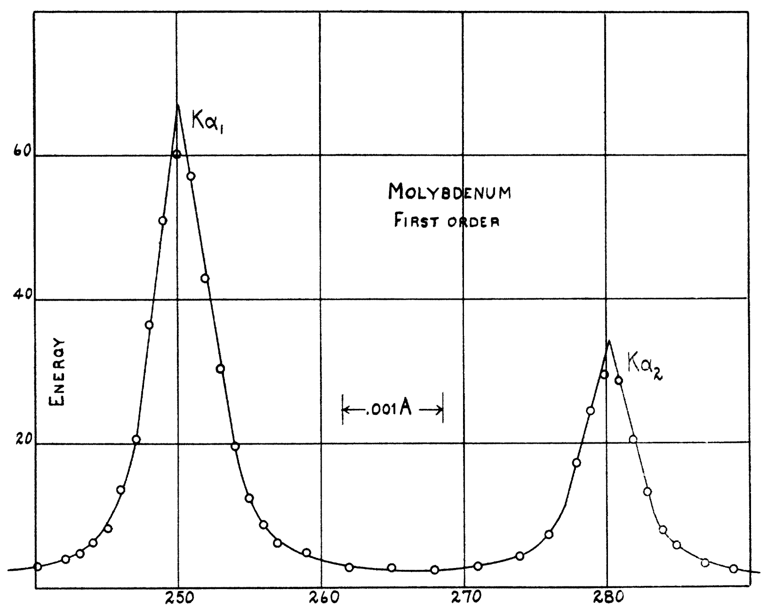

Fig. 6. The Kα lines of Mo (first order), taken with slits .0025 cm wide and 38 cm apart, showing that the curve for each line is an almost symmetrical triangle. Measured from the white radiation in the neighborhood, the height of α_1 is almost exactly twice that of α_2 (65.0/32.3). Note also the high resolving power.

farthest away, assuming the slits to be of equal height. Then

$$\delta = \theta - \theta' \ .$$

Fig. 6 gives observations of the Kα lines of Mo in the first order taken with the spectrometer described above using a calcite prism. The slits were all approximately 2.5 cm high. The slits limiting the beam were .025 mm wide and 38 cm apart. This gives a value of α of .00013 radian. The distance between the slits nearest and farthest from the ionization chamber was about 100 cm, from which it is computed that δ is .000025 radian. Hence

$$d\theta = \alpha + \delta = .000155 \text{ radian}$$

and

$$d\lambda = .00094\text{A}$$

or about one fifth of the distance between the Kα lines. This agrees with the excellent resolution shown in Fig. 6. In spite of this high resolution the radiation between the two lines is slightly greater than is to be expected from the magnitude of the white radiation on either side of the doublet. This may possibly be due to slight crystal imperfections. The effect is much more apparent in Fig. 1.

The Apparent Width of the Absorption Limit

The methods used in determining the effect of the slit system on the apparent shape of x-ray lines may be applied equally well to absorption limits. Assume, as before, that we are dealing with a perfect crystal and further that the absorption limit of the absorber used is infinitely sharp and occurs at wave-length λ_K. We will also assume that the target has no characteristic lines in this neighborhood, so that we are dealing only with the white radiation. Let I be the intensity of this white radiation, practically constant over the very narrow spectral region concerned. Let β_1 and β_2 be the fractional transmission coefficients on the short wave-length side and long wave-length side, respectively, of this absorption limit, and let the corresponding intensities be $\beta_1 I$ and $\beta_2 I$. Then on account of the finite slit widths the apparent absorption break will not be sharp, if high resolving power be used, but the rise from $\beta_1 I$ to $\beta_2 I$ will be gradual.

We can regard the continuous spectrum coming through the absorber as made up of a large number of adjacent lines, the intensity of which (see Fig. 7C) suddenly rises from $\beta_1 I$ to $\beta_2 I$ as the absorption limit is passed. These in turn can be regarded as a series of lines of intensity $(\beta_2 - \beta_1)I$ superimposed on the spectrum $\beta_1 I$. When the crystal is set at such an angle that none of the "lines" $(\beta_2 - \beta_1)I$ are reflected, the observed intensity will be constant and equal to $\beta_1 I$; but when the slit approaches the absorption limit[6] some of the "lines," will be reflected, each line giving rise to a triangle, as previously discussed, the base of the triangle being determined by the slit widths. The actual observed intensity, at any crystal angle, will be the sum of the intensities due to each of the separate triangles (Fig. 7B), i.e. the sum of the intercepts which the sides of the several triangles make on an ordinate erected at the abscissa corresponding to the crystal setting. Thus Fig. 7C repre-

[6] The "lines" are assumed narrow compared to the slit system.

sents the "lines" forming the transmitted spectrum, the absorption break occurring at θ_k. To each line 1, 2, 3, ... there corresponds a triangle 1, 2, 3, ... (Fig. 7B) the base of which is defined by the slit width. If the crystal be set at the angle θ_h, the energy observed at that setting will be proportional to the sum of the intercepts made on that ordinate by the first four triangles. This corresponds to point p of Fig. 7A. The locus of point p, from b to o is a parabola, tangent at b to the line ab and meeting, tangentially at o another similar parabola which is the locus of p from o to c, the latter parabola being tangent to the line

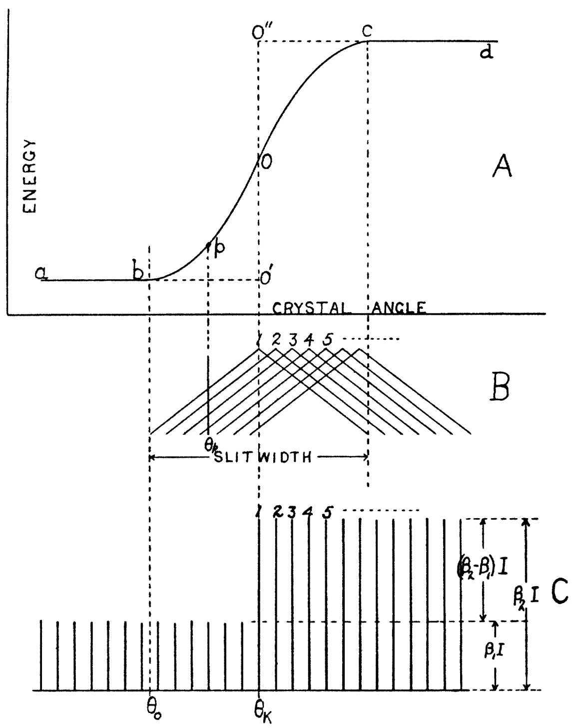

Fig. 7. Showing diagrammatically how the finite slit width determines the apparent shape of an absorption break.

cd at c. The line ab represents the constant intensity $\beta_1 I$, and the line cd the constant intensity $\beta_2 I$. For infinitely narrow slits the absorption break would be given by the line $o'o''$. For slits of finite width the absorption break is given by the line boc, the angular distance bc being exactly equal to the angle of the slits.

Fig. 8 shows such an energy distribution curve taken through the K limit of silver. The points $abocd$ correspond to similar points in Fig. 7A. The full line boc is a *theoretical* curve, made up of two parabolas tangent at a and c to the lines ab and cd respectively, and meeting each other tangentially at point o. The circles are actual observations. The observed points are seen to agree exceptionally well with the theoretical curve between b and c.

Furthermore it is to be noted that the actual observed width of the discontinuity agrees *within the limit of error* with the slit width, the difference being certainly not more than 4 percent. That is to say, the

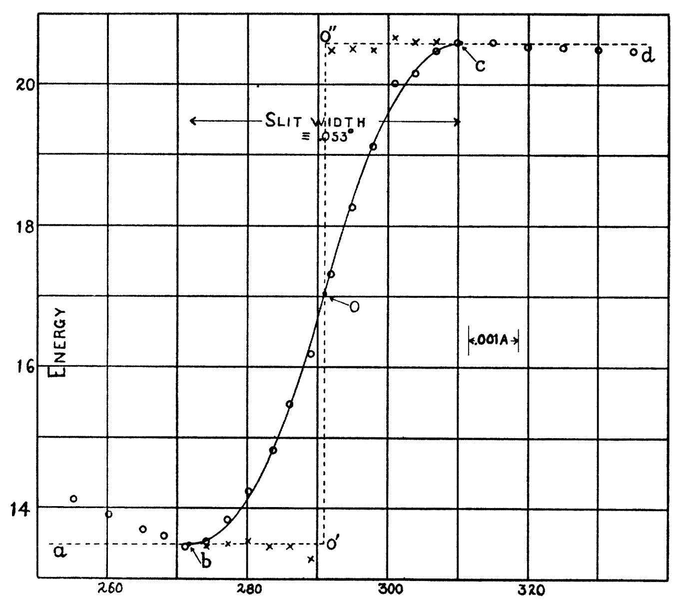

Fig. 8. The K absorption limit of silver, determined by taking an energy distribution curve of the white radiation from a Mo target with a silver absorber in the path of the beam. The curve *abocd* is a theoretical curve based on the known slit widths used. The circles are observed points. The crosses are the result of correcting the readings for slit width error. Note the sharpness of the absorption break.

K discontinuity of silver is sharp to this extent, the real width of the discontinuity, if it is different from zero, being probably less than .0002A.

It is now a very simple matter to plot a corrected discontinuity curve, eliminating the effect due to slit width. It is only necessary to move each observed point between b and o *downward* by the distance between the theoretical curve and the straight line ab, extended at that point. Similarly, each point between o and c should be moved upward. This has been done; the resulting points are represented by crosses. As noted in the preceding paragraph, the discontinuity is sharp within the limits of error of this experiment.

By this method it is possible to get values of the mass absorption coefficient very close to the absorption limit.

The author takes pleasure in expressing his very great obligations to the Research Laboratory of the General Electric Company for making available certain very essential parts of the equipment used in this investigation.

Cornell University,
July 2, 1925.