DOUBLE-CRYSTAL X-RAY SPECTROMETRY

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ABSTRACT

INTRODUCTION

X-ray spectrometry can be divided conveniently into three divisions: (*1*) production of the X-rays, (*2*) spectral analysis of the X-rays, and (*3*) measurement of the X-rays. In this abstract we shall confine our discussion to the analysis of the rays, or the separation of the beam into a spectrum.

Two considerations of prime importance confront us in all spectrometry: How accurately can we segregate a single wave-length from a beam? Will this more or less monochromatic beam have sufficient intensity to allow its study?

SINGLE-CRYSTAL SPECTROMETRY

The resolving power of any X-ray spectrometer is determined by two factors. The first is the imperfect collimating action of the slits, which can be termed the geometrical resolving power. The second is the physical resolving power, as set forth in the theory of crystalline diffraction, and can be expressed as the deviations from the Bragg law $n\lambda = 2d \sin \Theta$. The physical resolving power of a Bragg type single-crystal spectrometer is, for all angles of incidence, much greater than the geometrical resolving power, and we can say that the limit of the instrument is contained in its geometry. (See Phys. Rev. 38, 203 (1931).)

Divergence.—The angle of horizontal divergence of the beam incident upon the crystal may be defined as 2α and the vertical divergence as 2φ. Then $2\alpha = \frac{w_1 + w_2}{L}$ and $2\varphi = \frac{h_1 + h_2}{L}$ where w_1, w_2, h_1 and h_2 are the widths and heights of the confining slits S_1 and S_2 respectively, and L the distance between them. Assume for simplicity strict obeyance of the law $n\lambda = 2d \sin \Theta$, and, for the moment, that the incident beam is composed of purely monochromatic radiation. Considering all possible rays passing through the slits, the limiting divergence being the angles 2α and 2φ, one finds a certain small amount of radiation having the maximum vertical divergence and at the same time striking the crystal at the proper angle Θ for reflection but whose angle projected in the horizontal plane is greater than Θ by an amount ϵ. This particular ray is shown in the diagram by the dotted line. Simple trigonometry gives the value of ϵ as $\frac{\varphi^2}{2} \tan \Theta$. These considerations allow for the horizontal divergence of the incident beam an angular range $(\Theta - \alpha)$ to $(\Theta + \alpha)$ and for the reflected beam an angular range Θ to $(\Theta + \epsilon)$. Consequently, reflection of this wave-length takes place while the crystal is rotated through the range $(2\alpha + \epsilon)$, which is therefore the full width of an ionization or "rocking curve" taken for this wave-length.

Resolving power.—Two lines of wave-length difference $d\lambda$ are arbitrarily defined as resolved if, as in optical spectrometry, the "maximum" of one falls above the "minimum" of the other. This wave-length separation amounts to an angular separation of $d\Theta$, where $d\Theta = \frac{1}{2}(2x + \epsilon) = \frac{1}{2}(2\alpha + \frac{\varphi^2}{2} \tan \Theta)$

Also $d\Theta = \frac{nd\lambda}{2d \cos \Theta}$ from $n\lambda = 2d \sin \Theta$

Therefore $d\lambda = \frac{2d}{n} \cos \Theta \, (\alpha + \frac{1}{4}\varphi^2 \tan \Theta)$ which gives $\frac{\lambda}{d\lambda} = \frac{\tan \Theta}{\alpha + \frac{\varphi^2}{4} \tan \Theta}$

For a given wave-length, the only variables in this expression for the resolving power of a single-crystal spectrometer are α and φ. If the resolving power is to be increased, the widths and heights of the slits must be decreased or the distance between them increased. Either change results in a diminution of intensity, and a compromise between intensity and resolving power must be made. This compromise is inherent in all single-crystal spectrometers.

DOUBLE-CRYSTAL SPECTROMETRY

Instead of allowing the beam reflected from the crystal to pass directly into the ionization chamber let there be placed a second crystal so as to intercept the reflected beam. When this second crystal is properly orientated the beam will strike it at the glancing angle Θ and experience a second reflection. There are obviously two positions of the second crystal for which this orientation is effected. Case I and Case II or the "anti-parallel" and the "parallel" positions.

Geometrical width of a line.—The geometrical width of the line reflected from crystal A we have just seen to be $\epsilon_A = \frac{\varphi^2}{2} tan\ \Theta_A$. This angular range will therefore be the horizontal divergence of the beam incident upon the second crystal, B. The vertical divergence of the beam is unchanged by reflection from crystal A. Just as in the case of the first crystal, there will be an angle ϵ_B for the geometrical width of a single wave-length reflected from crystal B. Consequently, the curve obtained by rocking crystal B will have a full geometrical width of $\Delta\Theta$ given by

Case I	Case II
$\Delta\Theta = \epsilon_A + \epsilon_B$	$\Delta\Theta = \epsilon_A - \epsilon_B$
$\Delta\Theta = \frac{\varphi^2}{2}(tan\ \Theta_A + tan\ \Theta_B)$	$\Delta\Theta = \frac{\varphi^2}{2}(tan\ \Theta_A - tan\ \Theta_B)$

That the positive sign between ϵ_A and ϵ_B in case I must be replaced by the negative sign in case II can be seen from simple analysis of the two cases.

Dispersion.—Consider two lines in the incident beam separated by a wave-length difference $\delta\lambda$. Crystal A will give these lines an angular separation of $\delta\Theta_A$ and crystal B will separate them by $\delta\Theta_B$. It follows that if crystal A remains stationary, crystal B must be turned through an angle $d\Theta_B$ in order to reflect both lines. Now

$$\delta\Theta_B = \frac{n_A\,\delta\lambda}{2d\ cos\ \Theta_A} \quad \text{and} \quad \delta\Theta_B = \frac{n_B\delta\lambda}{2d\ cos\ \Theta_B}$$

$$d\Theta_B = \delta\Theta_A \pm \delta\Theta_B = \delta\lambda\left(\frac{n_A}{2d\ cos\ \Theta_A} \pm \frac{n_B}{2d\ cos\ \Theta_B}\right)$$

which gives for the dispersion

$$D \equiv \frac{d\Theta_B}{\delta\lambda} = \left(\frac{n_A}{2d\ cos\ \Theta_A} \pm \frac{n_B}{2d\ cos\ \Theta_B}\right),$$

the plus and minus sign applying to cases I and II respectively.

Resolving Power.—Applying the same definition of resolving power that we employed for the single-crystal spectrometer, two lines are resolved if they are separated by an angular range for crystal B of an amount equal to one half the geometrical full width of a single line. That is, providing

$$d\Theta_B = \frac{\Delta\Theta}{2} = \frac{\varphi^2}{4}(tan\ \Theta_A \pm tan\ \Theta_B).$$

The expression for D just derived, when multiplied by $n\lambda = 2d\ sin\ \Theta$, gives,

$$D \equiv \frac{d\Theta_B}{d\lambda} = \frac{1}{\lambda}(tan\ \Theta_A \pm tan\Theta_B)$$

Therefore $\frac{\varphi^2}{4d\lambda}(tan\ \Theta_A \pm tan\ \Theta_B) = \frac{1}{\lambda}(tan\ \Theta_A \pm tan\ \Theta_B)$ and $\frac{\lambda}{d\lambda} = \frac{4}{\varphi^2}$

It will be observed that this expression for the geometrical resolving power of a double-crystal spectrometer is identical with that obtained for a single-crystal instrument if $\alpha = 0$. In this sense, the first crystal can be said to act as an extremely effective collimator for the beam incident upon the second crystal. The greatest virtue of the two-crystal instrument lies in the fact that the resolving power is independent of the slit-widths, and a highly resolved beam of relatively large intensity is available. Actually the geometrical resolving power can be made much greater than the physical resolving power, and the limitations of the double-crystal spectrometer are then determined by the state of perfection of the crystals. That practically perfect calcite crystals can be obtained has been shown by the author (Parratt, Phys. Rev. *41*, 561 (1932)).