Sec. 6, is given by

$$a' = a_0 + bx, \tag{A8}$$

where

$$x = \tfrac{1}{2}[(\cos^2\theta/\sin\theta) + \cos^2\theta/\theta].$$

Since the standard error of d and, therefore, of a' depends on the value of θ, a weight inversely proportional to the variance of d was assigned to the a' values. This weight was defined as

$$w_i = [1/(\sigma_{d_i}^*)^2]/\sum(1/\sigma_{d_i}^*)^2, \tag{A9}$$

where

$$(\sigma_{d_i}^*)^2 = \sum_j [(d_{ij} - \bar{d}_i)^2/(n-1)] \tag{A10}$$

and $j = 1 \cdots n_1$, the number of d-spacing determinations for each Bragg angle θ and $i = 1 \cdots k$, the number of Bragg angles (see Fig. 6).

The values of a_0 and b are obtained by minimizing the sum of the squares of the deviations:

$$S = \sum_i n_i w_i (a_i' - a_0 - bx_i)^2.$$

Again, using the results from weighted least squares, we have

$$b = \sum n_i w_i a_i' (x_i - \bar{x}) / \sum n_i w_i (x_i - \bar{x})^2 \tag{A11}$$

and

$$a_0 = \bar{a}' - b\bar{x}, \tag{A12}$$

where

$$\bar{a}' = \sum n_i a_i' w_i / \sum n_i w_i, \tag{A13}$$

$$\bar{x} = \sum n_i x_i w_i / \sum n_i w_i. \tag{A14}$$

The variance of estimate is given by

$$V(a'/x) = \sum n_i w_i (a_i' - a_0 - bx_i)^2/(n-2), \tag{A15}$$

where b and a_0 are given by (A11) and (A12), respectively.

The variance of b and a_0 are given by

$$V(b) = V(a'/x) / \sum n_i w_i (x_i - \bar{x})^2 \tag{A16}$$

$$V(a_0) = V(a'/x)[(1/n) + \bar{x}^2 / \sum n_i w_i (x_i - \bar{x})^2]. \tag{A17}$$

The standard errors are then

$$\sigma_b = [V(b)]^{\frac{1}{2}}, \tag{A18}$$

$$\sigma_{a_0} = [V(a_0)]^{\frac{1}{2}}. \tag{A19}$$

APPENDIX B

Computation of *d* Spacings from Incomplete Ellipses

Referring to Fig. 1 it will be seen that

$$NP = (a+b)\cot(\theta+\beta) + b\cot(\theta-\beta)$$
$$= a\cot(\theta+\beta) + b[\cot(\theta+\beta) + \cot(\theta-\beta)] \tag{B1}$$

$$NR = b\cot(\theta+\beta) + (a+b)\cot(\theta-\beta)$$
$$= a\cot(\theta-\beta) + b[\cot(\theta+\beta) + \cot(\theta-\beta)]. \tag{B2}$$

Let $NR = l$, for brevity, and suppose that two patterns are superimposed on the same film by making two exposures and changing the distance a from the film to the target between the exposures. Then, for example, Eq. (B2) gives

$$l_1 = a_1 \cot(\theta-\beta) + b[\cot(\theta+\beta) + \cot(\theta-\beta)], \tag{B3}$$

$$l_2 = a_2 \cot(\theta-\beta) + b[\cot(\theta+\beta) + \cot(\theta-\beta)], \tag{B4}$$

where the subscripts refer to the film position.

Subtracting (B4) from (B3),

$$l_1 - l_2 = (a_1 - a_2)\cot(\theta-\beta) = c\cot(\theta-\beta)$$
$$\cot(\theta-\beta) = (l_1 - l_2)/c = \Delta/c. \tag{B5}$$

Here c is the distance through which the film has been shifted between exposures and $l_1 - l_2$ is the distance between corresponding ellipses measured on the film along their common major axis.

Let us now assume that the incident radiation consists of two components of wavelength λ_1 and λ_2, respectively, each giving rise to a pattern. We have then from (B5)

$$\theta_1 - \beta = \operatorname{arccot}(\Delta_1/c), \tag{B6}$$

$$\theta_2 - \beta = \operatorname{arccot}(\Delta_2/c), \tag{B7}$$

where the subscripts now refer to different wavelengths. Subtracting (B7) from (B6),

$$\theta_1 - \theta_2 = \operatorname{arccot}(\Delta_1/c) - \operatorname{arccot}(\Delta_2/c)$$
$$= \operatorname{arccot}[(c^2 + \Delta_1\Delta_2)/c(\Delta_1 - \Delta_2)] = \mu. \tag{B8}$$

Let

$$\lambda_1/\lambda_2 = \sin\theta_1/\sin\theta_2 = K,$$

then

$$\sin\theta_1 = \sin(\mu + \theta_2) = K\sin\theta_2. \tag{B9}$$

The second of Eq. (B9) gives finally,

$$\cot\theta_2 = (K - \cos\mu)/\sin\mu, \tag{B10}$$

where μ is given by (B8).

The last expression gives the value of the Bragg angle (and therefore of the interplanar spacing) of a given set of planes in terms of the known x-ray wavelengths, of the film shift between exposures c, and of two quantities Δ_1 and Δ_2 measured on the film (Figs. 1 and 5).

Equation (B10) may be written in a form which gives directly the d spacings, obviates the need for trigonometric tables, and is convenient for computation on a desk calculator. Using the identity $\sin\theta = (1+\cot^2\theta)^{-\frac{1}{2}}$ and the value of $\cot\theta_2$ given by (B10),