THE ROTATION FACTOR FOR EQUI-INCLINATION WEISSENBERG PHOTOGRAPHS

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In the analysis of crystal structures by means of x-rays it is well known that when the reflecting plane does not contain the axis of rotation of the crystal (in other words, when the diffraction spot does not lie on the equatorial line of the photograph), the angular velocity of the plane is effectively decreased. This results in reflection by such a plane during a longer interval of time in each rotation than by planes producing spots on the equatorial or zero layer-line. Cox and Shaw[1] have shown that the effect is purely geometrical, depending only on the angle of reflection and the orientation of the reflecting plane with respect to the axis of rotation of the crystal, and they have calculated the magnitude of this effect for rotation photographs taken with the x-ray beam perpendicular to the rotation axis of the crystal. In view of the fact that it is advantageous[2] to take Weissenberg layer-line photographs with the rotation axis of the crystal inclined to the incident x-ray beam at an angle equal to that made by the rotation axis with the reflected x-ray beams for the layer-line that is being analyzed, the author has derived the relationship for the rotation factor D_e appropriate under such conditions. As Cox and Shaw have stated, the intensity of the spot produced by a reflecting plane is inversely proportional to ω/Ω, where ω is the angular velocity of the crystal about an axis perpendicular to the plane containing the incident and reflected x-ray beams, and Ω is the angular velocity of the crystal about its actual rotation axis.

The value of D_e is obtained by the following construction, which is similar to that used by Cox and Shaw in deriving the value of the rotation factor in the case of an x-ray beam perpendicular to the rotation axis of the crystal. Figure 1 shows the geometrical relations of the crystal, incident x-ray beam, and reflected x-ray beam in stereographic projection. O is the point of emergence of the rotation axis of the crystal; this rotation axis passes through the center of the sphere of projection. The incident x-ray beam passes through A to the center of the sphere of projection. B is the pole of the reflecting plane. The reflected x-ray beam passes from the center of the sphere of projection to C. Let ϕ denote the angle AB, and μ denote the angle DA. The essential feature of the equi-inclination method is that for each layer-line the rotation axis of the

[1] *Proc. Roy. Soc. London*, **127A**, 71–88 (1930).
[2] Buerger, M. J., *Zeits. Krist.*, **88**, 356–380 (1934).

crystal is set at an angle AO to the incident x-ray beam such that the reflected x-ray beam for each spot on the layer-line makes an angle OC with the rotation axis of the crystal equal to AO. Then, since the angle of incidence equals the angle of reflection, we have

$$AB = BC,$$

and since

$$AO = OC = 90° - \mu,$$

therefore

$$OBC = OBA = 90°.$$

Let ν denote the angle AOB. The angular velocity of the crystal is $d\nu/dt$, where t denotes the time, and $d\nu/dt$ is a constant during the in-

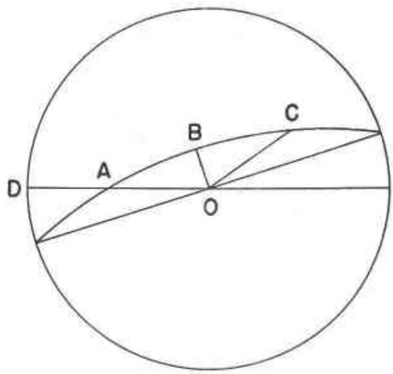

FIG. 1. Stereographic projection showing crystal rotation axis (passing through O and center of sphere), normal to crystal reflecting plane (pole of crystal reflecting plane is point B), incident x-ray beam (passing through A and center of sphere), and reflected x-ray beam (passing through center of sphere and C).

vestigation of the crystal by the Weissenberg method. The angular velocity of the normal to the reflecting crystal plane about the normal to the plane ABC is $d\phi/dt$. Then

$$D_e = \frac{\omega}{\Omega} = \frac{\dfrac{d\phi}{dt}}{\dfrac{d\nu}{dt}} = \frac{d\phi}{d\nu}.$$

Since the spherical triangle OBC has a right angle at B, we have

$$\sin\phi = \sin\nu \cdot \sin(90° - \mu).$$

Thus

$$\frac{d\phi}{d\nu} = \frac{\cos\nu \cdot \cos\mu}{\cos\phi}.$$

But $\phi = 90° - \theta$, where θ is the angle made by the reflected beam with the reflecting crystal plane. Hence

$$D_e = \frac{d\phi}{d\nu} = \frac{\sqrt{\cos^2\mu - \cos^2\theta}}{\sin\theta}. \tag{A}$$

TABLE 1. DATA FOR PLOTTING CURVES OF CONSTANT D_e. VALUES OF $\mu°$ CORRESPONDING TO DIFFERENT VALUES OF SIN θ AND D_e.

$D_e \rightarrow$	.99	.975	.95	.925	.90	.85	.80	.70	.60	.50	.40	.30	.20	.10	.00
Sin θ ↓	$\mu°$														
0.1	0°.81	1°.28	1°.79	2°.18	2°.50	3°.02	3°.44	4°.10	4°.59	4°.97	5°.26	5°.47	5°.62	5°.71	5°.74
0.2	1.62	2.55	3.58	4.36	5.00	6.05	6.89	8.21	9.21	9.97	10.56	11.00	11.30	11.48	11.54
0.3	2.43	3.82	5.38	6.54	7.51	9.09	10.37	12.37	13.89	15.06	15.96	16.63	17.09	17.37	17.46
0.4	3.23	5.10	7.18	8.74	10.04	12.16	13.89	16.60	18.66	20.27	21.51	22.43	23.07	23.45	23.58
0.5	4.04	6.38	8.98	10.95	12.59	15.27	17.46	20.92	23.58	25.66	27.28	28.49	29.33	29.83	30.00
0.6	4.86	7.66	10.80	13.18	15.16	18.42	21.10	25.37	28.69	31.31	33.36	34.92	36.01	36.66	
0.7	5.67	8.95	12.62	15.42	17.77	21.64	24.84	29.99	34.06						
0.8	6.48	10.24	14.47	17.70	20.41	24.92	28.68	34.84							
0.9	7.29	11.54	16.32	20.00	23.10	28.30	32.68								
1.0	8.11	12.84	18.20	22.33	25.84	31.79									

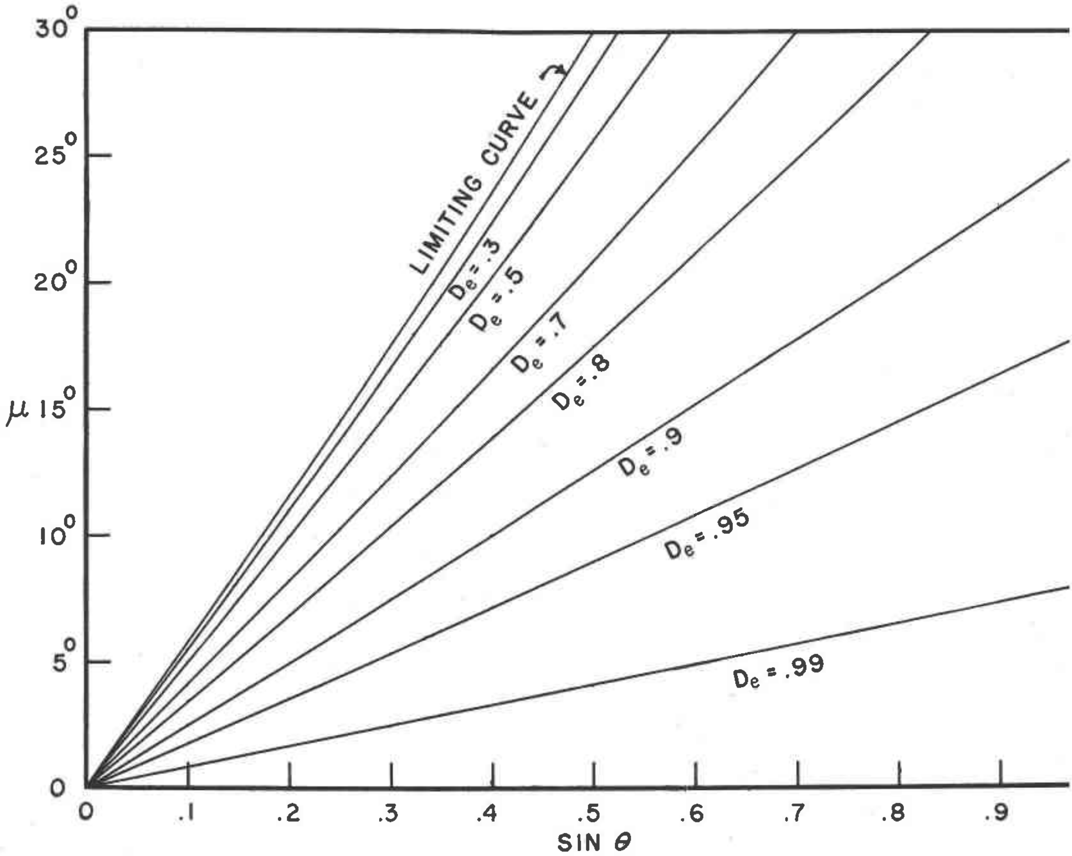

FIG. 2. Rotation factor D_e for equi-inclination Weissenberg photographs.

The variation of D_e with μ and $\sin\theta$ as arguments is shown graphically in Figure 2. Table 1 is intended for the convenience of users of the equi-inclination method in plotting the curves of constant D_e on a larger scale necessary for the graphical determination of the values of D_e corresponding to the reflections on the equi-inclination layer-line films. The value of the rotation factor for any given reflection will always be nearer one in the equi-inclination method than in the method of perpendicular incidence (the crystal being assumed to rotate around the same zone-axis in both cases). Moreover, it is to be noted that in the equi-inclination method the factor D_e approaches $\cos\mu$ for diffraction spots near the incident beam (back reflection), whereas in the method of perpendicular incidence it approaches zero for such spots on all layer-lines except the equator. This constitutes a further advantage of the equi-inclination method. The factor D_e is plotted for values of μ up to 30° only, but this is equivalent to a μ-value of 90° in the method of perpendicular incidence. A μ-value greater than 30° will seldom be required with the equi-inclination method. If such a case is encountered the necessary values of D_e can be computed from equation (A).