d_{hkl} = interplanar spacing (Å)

K = constant (Å^{-1})

q_j = charge on the jth ion

r_{ij} = distance from the ith to the jth ion (Å)

ERFC = complement of the error function

The magnitude of the arbitrary constant K determines the relative convergences of the two parts of the formula. The larger the numerical value chosen for K the worse is the convergence of the first sum, and the better is the convergence of the second sum, and *vice versa*. In practice one has to choose a value of K which makes the combined number of terms in both sums a minimum. In order to check the results for their accuracy and for possible errors the same calculation can be repeated with different values of K. Such check runs showed that the rounding errors and the neglected outer terms of the sums never accumulated to more than 1 unit of the sixth digit, *i.e.* the error was 10^{-6} at most.

The program can be requested from the author by interested persons.

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On the Curves in the Greninger and Leonhardt Nets

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The algebraic equations for the lines in both the Greninger and Leonhardt charts are derived, in order to complete or correct the statements found in the current literature. The meridians are conics and the parallels are quartics. Also, parametric equations are given for computational purposes.

In the X-ray orientation of single crystals, two charts are widely used: The Greninger chart (Greninger, 1935) for the back-reflection Laue method and the Leonhardt chart (Leonhardt, 1924; Dunn & Martin, 1949) for the transmission Laue method. The meaning and the use of both nets are quite well explained in the standard X-ray books, but, especially in the case of the Greninger net, some incomplete (Barrett, 1952; Guinier, 1956; Wood, 1963) or even wrong (Terpstra & Codd, 1961; Cullity, 1956; *International Tables for X-Ray Crystallography*, 1959) statements on the geometrical nature of the curves of the chart are frequently made. The pur-

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pose of this note is to set up the correct characterization of the curves in both charts in a unified description.

The geometry of the Laue method is easily described in terms of the Bragg picture (Fig. 1). OC is the incident X-ray, NN' is the normal to the reflecting plane and CP is the reflected ray, such that $\theta \equiv \pi/2 - \varphi$ is the usual Bragg angle.

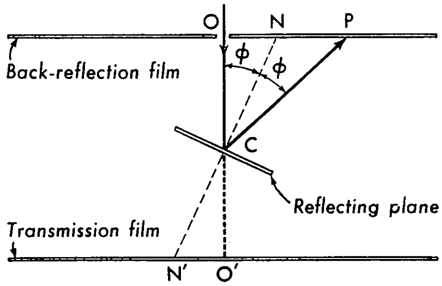

Fig. 1. The geometry of the Laue method in the plane of incidence: The back-reflection situation ($\varphi < 45°$). The plane responsible for the spot P on the film can be identified by its gnomonic projection N.

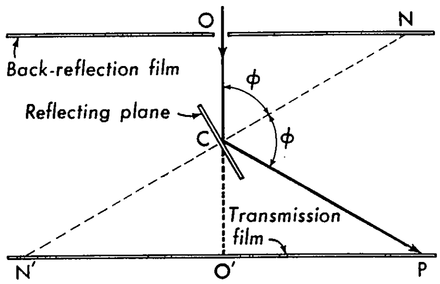

Fig. 2. The transmission situation ($\varphi > 45°$).

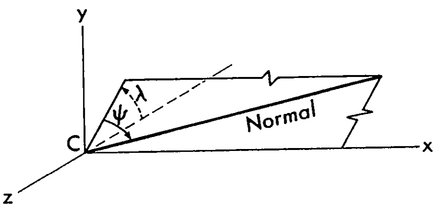

Fig. 3. The direction of a normal as defined by two angles: λ (longitude) and ψ (latitude).

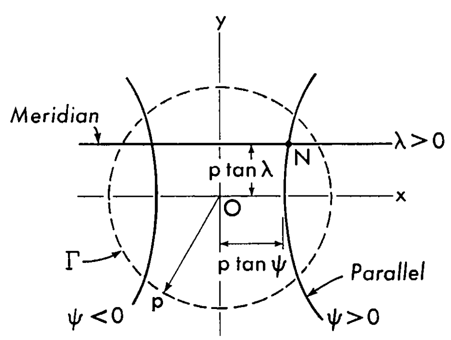

Fig. 4. The gnomonic net for the normals to the planes. Only planes with normals represented inside of the circle Γ, can give spots in the back-reflection film.

CN being the bisector of an interior angle of the triangle COP we may write, taking the segments in absolute value: $NP/ON = CP/OC$ or $OP/ON = (OC + CP)/OC$. This last relation is valid only if the normal makes with the incident beam an angle $\varphi < \pi/4$. If $\pi/4 < \varphi < \pi/2$ the situation changes, since then P will be on the transmission film as shown in Fig. 2. NN' is now the bisector of an exterior angle of the triangle $CO'P$ and the second relation should be $O'P/O'N' = (CP - O'C)/O'C$.

A Cartesian coordinate frame is selected with the z axis along the direction of the incident X-ray, vertical y axis and origin in the crystal C. The coordinates (x, y) of a spot P in the film and those (x_N, y_N) of the gnomonic projection N of the normal of the reflecting plane are obviously related by

$$\frac{x}{x_N} = \frac{y}{y_N} = \begin{cases} +\dfrac{OP}{ON} & \text{if } \varphi < 45° \\ -\dfrac{O'P}{O'N'} & \text{if } \varphi > 45° \end{cases}$$

Combining these with the previous geometrical relations, we obtain

$$\frac{x}{x_N} = \frac{y}{y_N} = \frac{p \pm \sqrt{x^2+y^2+p^2}}{p} \text{ for } \varphi \lessgtr 45° \tag{1}$$

where p is the distance crystal-film. Note that the relation (1) covers both the back-reflection and the transmission case.

It is found convenient to refer to the orientation of the normal in terms of its co-polar and azimuthal angles ψ and λ (Fig. 3), with respect to the x axis as polar axis. We may call them latitude and longitude respectively. The pencils of normals with λ constant will define a *meridian* and those with ψ constant a *parallel*.

By extension, the gnomonic projection of the normals (poles) of the reflecting planes in the plane of the film will show lines that are simply called meridians and parallels. Elementary geometric considerations lead to the equations

Meridians: $e y_N - p = 0$ (where $e \equiv \cot \lambda$, $s \equiv \cot \psi$) $\quad (2M)$

Parallels: $s^2 x_N^2 - y_N^2 - p^2 = 0 \quad (2P)$

which are, respectively, a straight line and a hyperbola (Fig. 4).

The corresponding spot P on the film produced by the Bragg reflected ray will describe two families of curves that are customarily labeled parallels (or latitude lines), and meridians in the Greninger and in the Leonhardt nets. Their algebraic equations are derived in a straightforward way from $(2M)$ and $(2P)$ using the relations (1).

The meridians are:

$$x^2 - (e^2 - 1)y^2 + 2pey = 0\,. \tag{3M}$$

This is a *conic*: a hyperbola for $\lambda<\pi/4$, a parabola for $\lambda=\pi/4$ and a real ellipse for $\pi/4\lambda<\pi/2$ (Fig. 5). In the Greninger chart only the branches of hyperbolae not passing by the origin are of interest: they correspond to the segments of meridians in Fig. 4 interior to the limiting circle Γ. The other branch and the parabola and ellipses belong to the Leonhardt chart, where, however, they are labeled by the values of $90°-\lambda$.

For the parallels we obtain a more involved algebraic equation:

$$(y^2-m^2x^2)^2+p^2(y^2-s^2x^2)=0 \tag{3P}$$

where $m^2\equiv\frac{1}{2}(s^2-1)=\cot\psi\cot 2\psi$. This *curve of degree four* has three biflecnodes: one at the origin with tangents $y\pm sx=0$ and two others at infinity with asymptotes $y\pm mx\pm(\frac{1}{2}p\sqrt{m^2+1})/m=0$. A sketch for the parallel $\psi=30°$ is shown in Fig. 6. One can immediately identify the parts of the branches that will appear in both the Greninger and the Leonhardt nets.

(3*M*) and (3*P*) are thus the correct algebraic equations for the curves plotted in the Greninger and Leonhardt charts. Since the quartic (3*P*) does not seem to be described in the classical repertory of curves (Loria, 1930; Gomes Teixeira, 1905), I would suggest that it be called the 'Greninger–Leonhardt quartic'.

Finally, and for the convenience of those that could want to draw these curves using a computer, I shall write down their parametric expressions. It is not necessary to repeat them for the meridians, as they can be found in many places (*e.g.* Jenner, 1963).

The Greninger–Leonhardt quartic is unicursal, and thus the coordinates of any point of the curve can be expressed as a rational algebraic function of a parameter (Hilton, 1932).

Put $y=\mu x$ in the equation (3*P*) of the parallels and solve for x. Apart of the abscissae $x^2=0$, which correspond to the starting double point (0,0), we get

$$\frac{x}{p}=\pm\frac{\sqrt{s^2-\mu^2}}{\mu^2-m^2}$$

Two formal consecutive changes of parameter $\mu=s\sin\omega$ and $t=\tan\frac{1}{2}\omega$ (a well-known procedure in the integration of irrational functions) will rationalize this expression to

$$\left\{\begin{array}{l} x/p=2s(1-t^4)\Delta^{-1} \\ y/p=4s^2t(1-t^2)\Delta^{-1} \\ \Delta\equiv t^4(1-s^2)+2t^2(1+3s^2)+(1-s^2) \end{array}\right. \tag{4}$$

where no physical significance is attached to the numerical parameter t.

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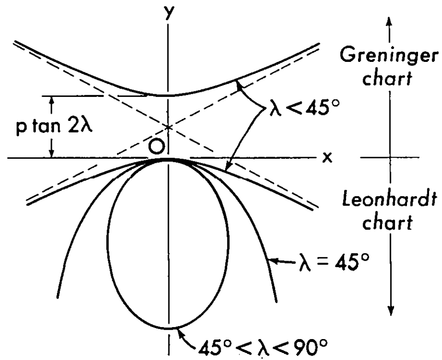

Fig. 5. Meridians (lines of constant longitude λ) in the Greninger and Leonhardt nets.

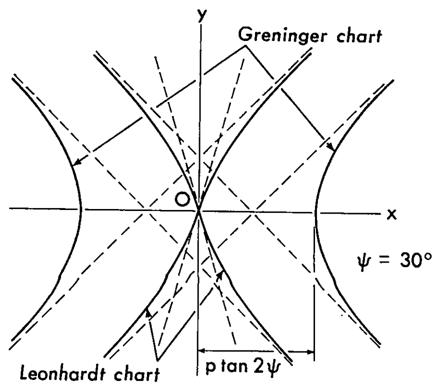

Fig. 6. Parallel $\psi=30°$ in the Greninger and Leonhardt nets.