The Plotting of Laue X-Ray Diffraction Pattern by Computation

by

L.J. Lin and R. Chen

Abstract

Laue x-ray diffraction patterns are generated by computation when the orientation of crystal as referred to incident x-ray beam is known. These plots can serve as standard patterns to index Laue photographs directly.

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Laue diffraction has provided a fundamental and interesting method in x-ray diffraction studies. It is a powerful method in orienting the crystals and in revealing crystal symmetry for crystallographers and mineralogists. Recently Laue diffraction taken with synchrotron radiation[1] offers promising technique in crystal structure determination as compared with the diffractometer data collection. Many methods have been developed to analyze and index the Laue spots on the film. Stereoprojection method linked with the Greninger or Leonhardt chart and the standard projecton of planes is mostly used. However, all of these works are time consuming and are done partially by trial and error to reach the final result. The purpose of this work is to generate, by computer calculation, the Laue x-ray diffraction patterns under the circumstances that one direction of crystal planes is parallel but opposite to the direction of indident x-ray beam. These plots can serve as standard films to index Laue photographs directly.

In preparing Greninger chart, Matthys[2] derived a formula to relate the x and y film coordinates with the α and β, angular coordinate of the crystal poles, as

$$x = -2F \tan \alpha \cos \beta / (\cos^2 \beta - \sin^2 \beta - \tan^2 \alpha) \quad (1)$$

$$y = -2F \sin \beta \cos \beta / (\cos^2 \beta - \sin^2 \beta - \tan^2 \alpha) \quad (2)$$

for arbitrary F, crystal-to-film distance. All parameters x, y, F, α, and β referred to in above equations are shown in Fig. 1, which is commonly used to explain Laue diffraction geometry. All the notations here follow those of Nuffield[3]. Therefore if one pole of the crystal with knowing α and β angles, the position of the diffraction spot can be calculated by (1) and (2).

In order to generate the Laue pattern in cubic crystal system, for example, we let the normal of the plane ($h_1\ k_1\ \ell_1$) be opposite to the incident x-ray beam, CO, and the normal of the plane ($h_2\ k_2\ \ell_2$) along the horizontal of x-ray film, OX'. Therefore the plane ($h_2\ k_2\ \ell_2$) is chosen orthogonal to the plane ($h_1\ k_1\ \ell_1$). The horizontal line OX' is then parallel to CX as shown in Fig. 1. Also ON is the normal of the reflecting plane (HKL). Then the angles between these three normals are identical to the angles between their respective planes and can be calculated by the following equations[4]:

$$\cos\rho = (Hh_1 + Kk_1 + L\ell_1)/[(H^2 + K^2 + L^2)(h_1^2 + k_1^2 + \ell_1^2)]^{1/2} \quad (3)$$

$$\cos\xi = (Hh_2 + Kk_2 + L\ell_2)/[(H^2 + K^2 + L^2)(h_2^2 + k_2^2 + \ell_2^2)]^{1/2} \quad (4)$$

where ρ is the angle NOC and ξ is the angle NOX'.

The angles (ρ, ξ) are related to the angles (α, β). By using trigonometric geometry, we obtain the following equations

$$\tan\beta = (1 - \cos^2\xi - \cos^2\rho)^{1/2}/\cos\rho \quad (5)$$

$$\tan\alpha = \tan\mu\ \sin\beta = \cos\xi\ /(1 - \cos^2\xi) \quad (6)$$

Therefore if the angles ρ and ξ of (KHL) reflection is precalculated through equations (3) and (4), the angular coordinates α and β of the normal ON can be obtained from equations (5) and (6). Consequently, the spot produced by (HKL) reflection on the film can be calculated through equations (1) and (2) as Matthys did for his own Grenninger chart.

Fig. 2 and Fig. 3 are the examples of the backward Laue patterns for the directions of [100] and [111] opposite to the incident x-ray beam respectively from the above computing. In this way one can get any diffraction pattern once the [$h_1\ k_1\ \ell_1$] is decided. The spacing between sample and film, F, is also allowed to change in order to get the desirable Laue patterns. The transmission Laue pattern can be treated by the same algorithm as did for backward diffraction. One example is shown in Fig. 4 as the transmission pattern of [001]. In tetragonal and hexagonal crystal systems, the scheme is similar to that in cubic crystal. The computer program of the above plottings also permits the normal of the plane ($h_1\ k_1\ \ell_1$) misorienting some degrees away from the incident x-ray. The amount of deviation can be measured from film by Greninger net. So the simulated Laue pattern can be generated and compared with the experimental x-ray Laue film directly and would be very helpful in indexing. Fig. 5 is the

Laue pattern of [001] pointing 2 degrees in both α and β measuring directions.

The above calculation and plotting are done on Apple II microcomputer and Graphtec plotter. The listing of these programs is available from the authors for those who are interested.

REFERENCES

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2. D. R. Matthys, Am. J. Phys. *50,* 555 (1982).
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FIGURE CAPTIONS

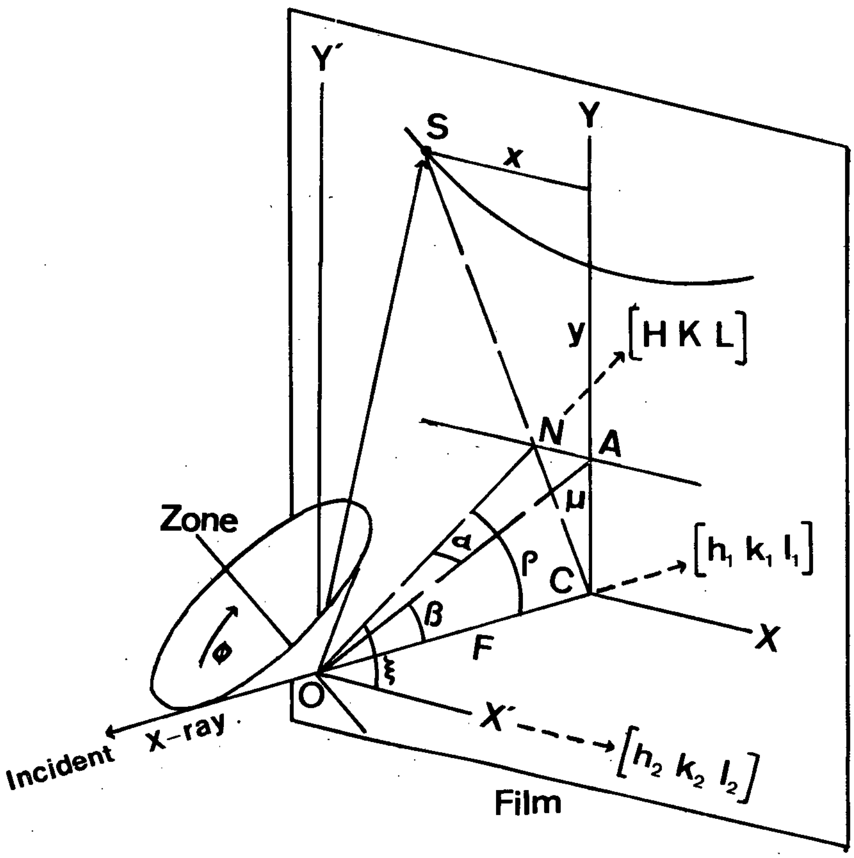
Fige. 1 Schematic view of Laue backward diffraction geometry. [h_1 k_1 ℓ_1] is opposite to incident x-ray. The film is placed at C; the crystal is set at 0 and F cm away from C. The diffraction spot S is recorded on film by reflection plane (HKL) whose normal is specified by angles α and β.

Fig. 2 Laue backward diffraction pattern for [001] pointing to the center of the film, F=7 cm.

Fig. 3 Laue backward diffraction pattern for [111] pointing to the center of the film, F=7 cm.

Fig. 4 Laue transmission diffraction pattern for [001], F=7 cm.

Fig. 5 Laue backward diffraction pattern for [001] tilts 2 degrees both in α and β away from incident x-ray beam. C is the center of the film, F=7 cm.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Incident X-ray
Film

Figure 1

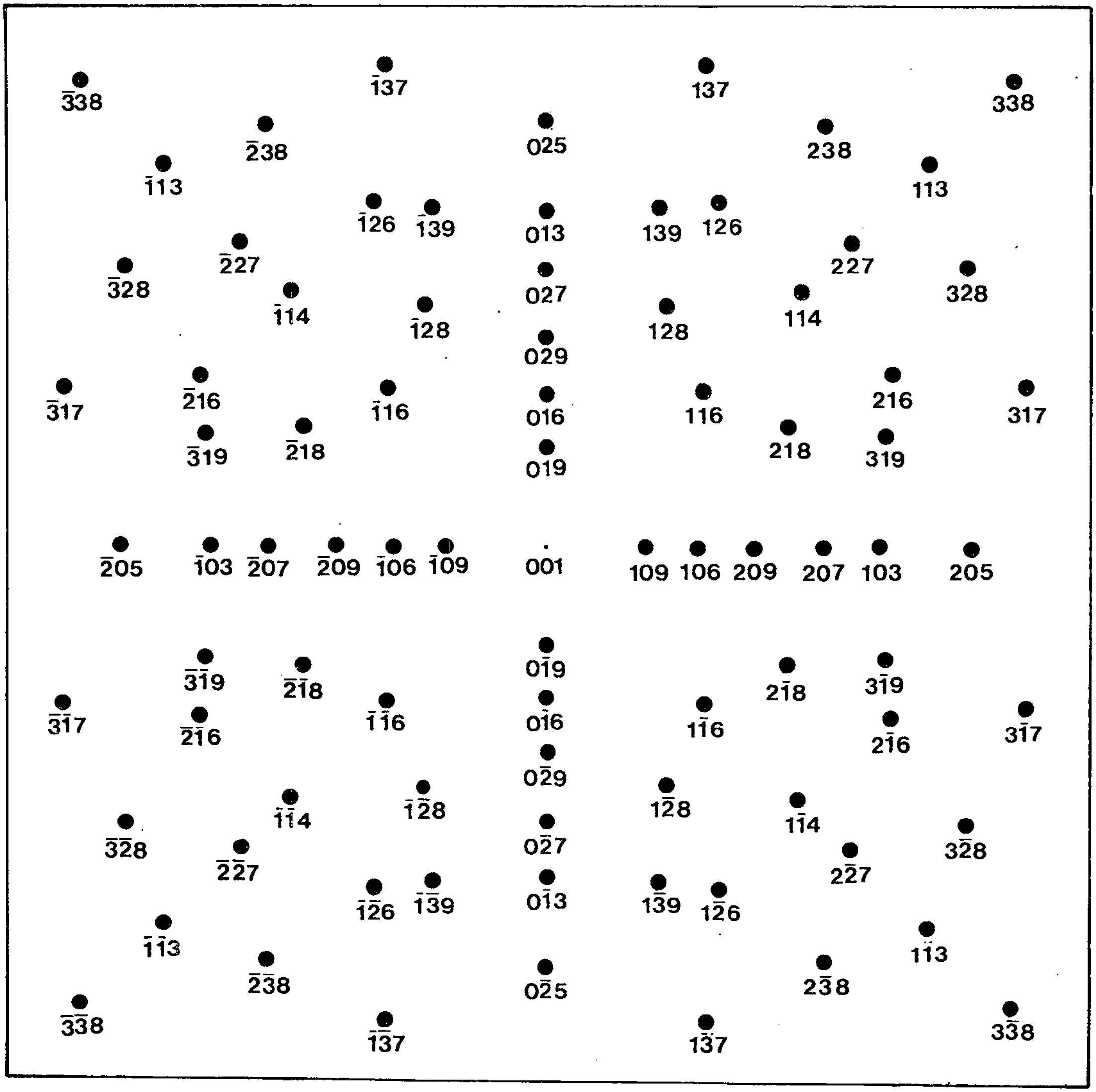
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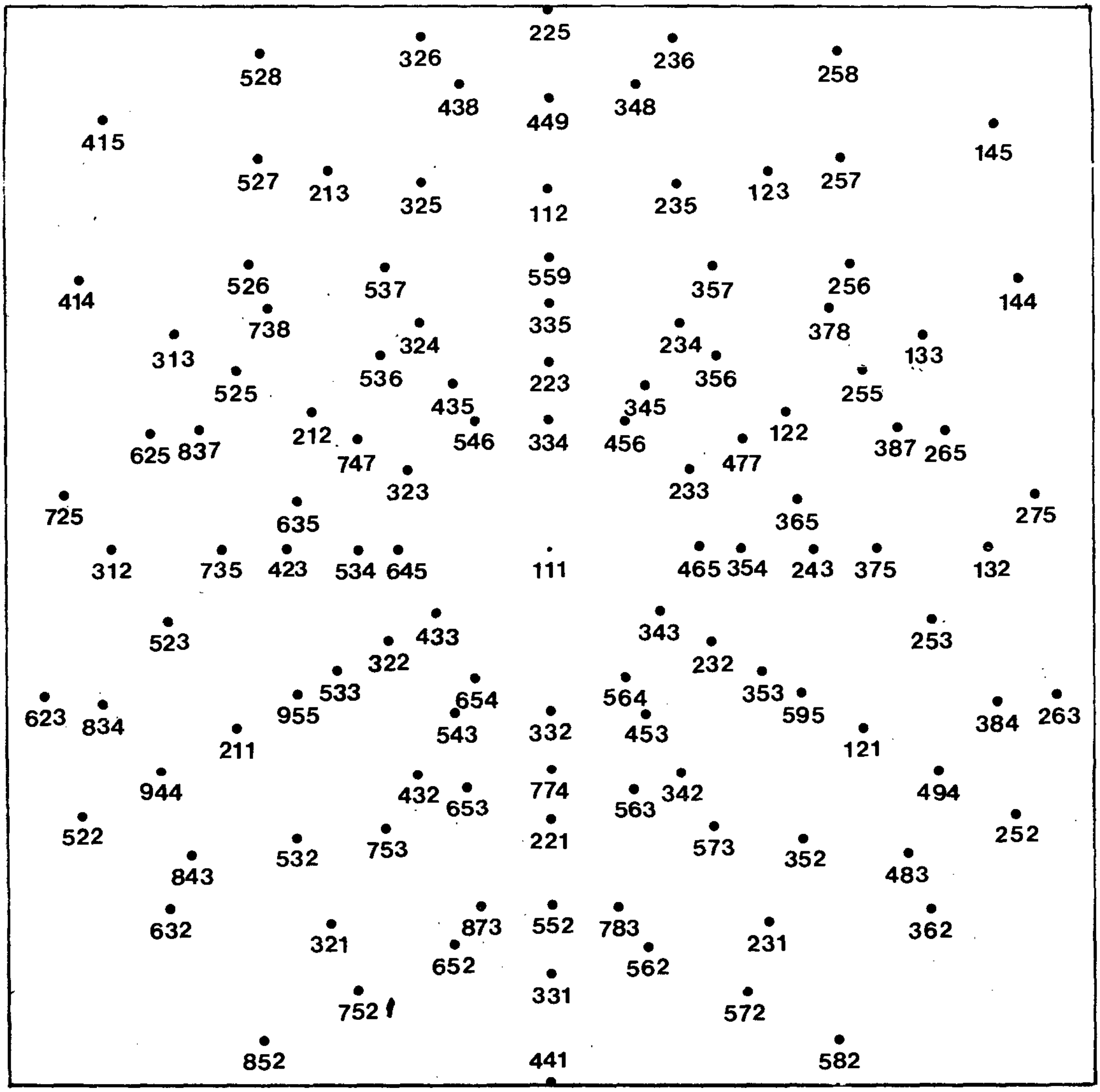
Figure 2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211 543 332 453 121
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Figure 3

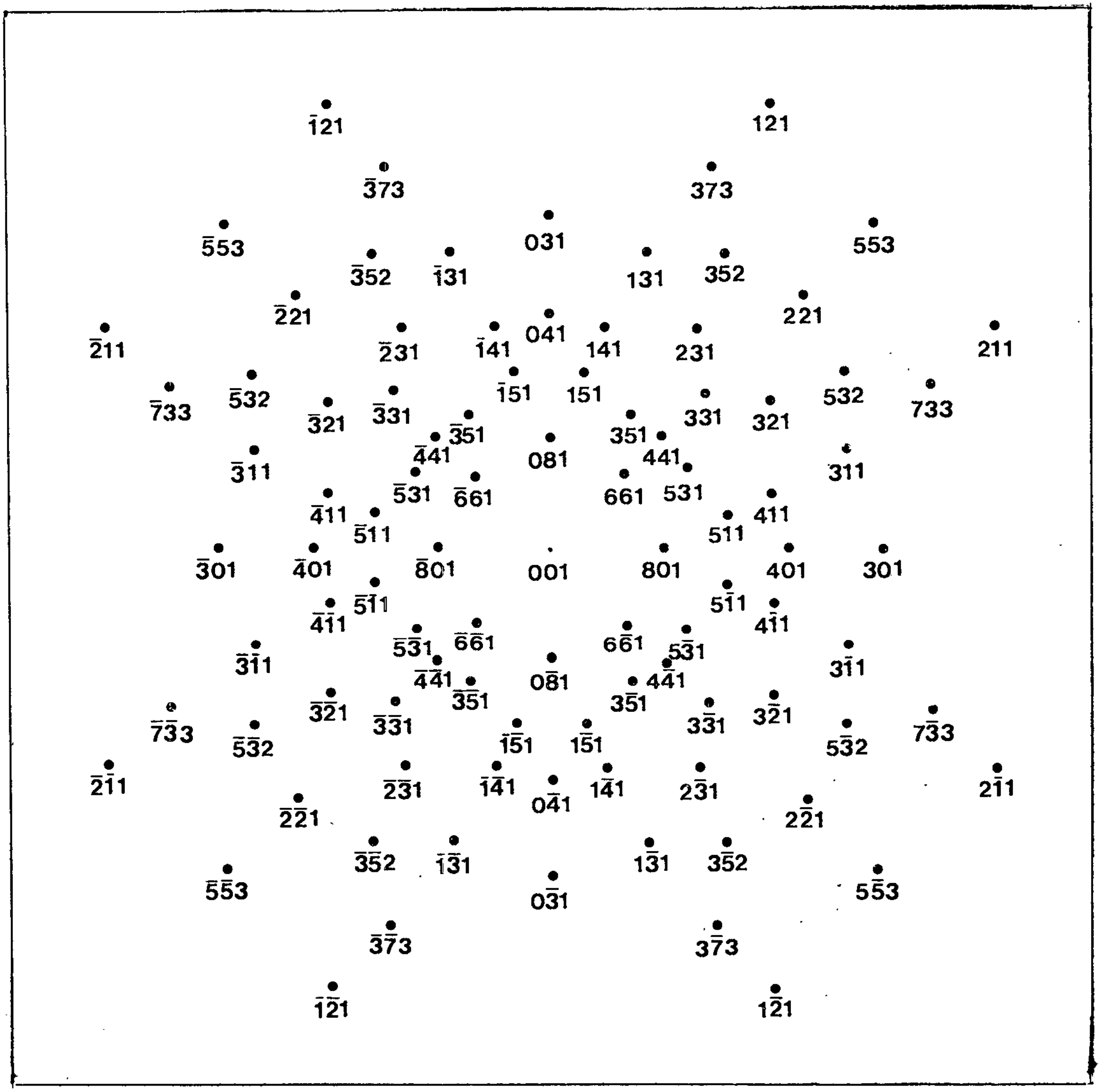

Figure 4

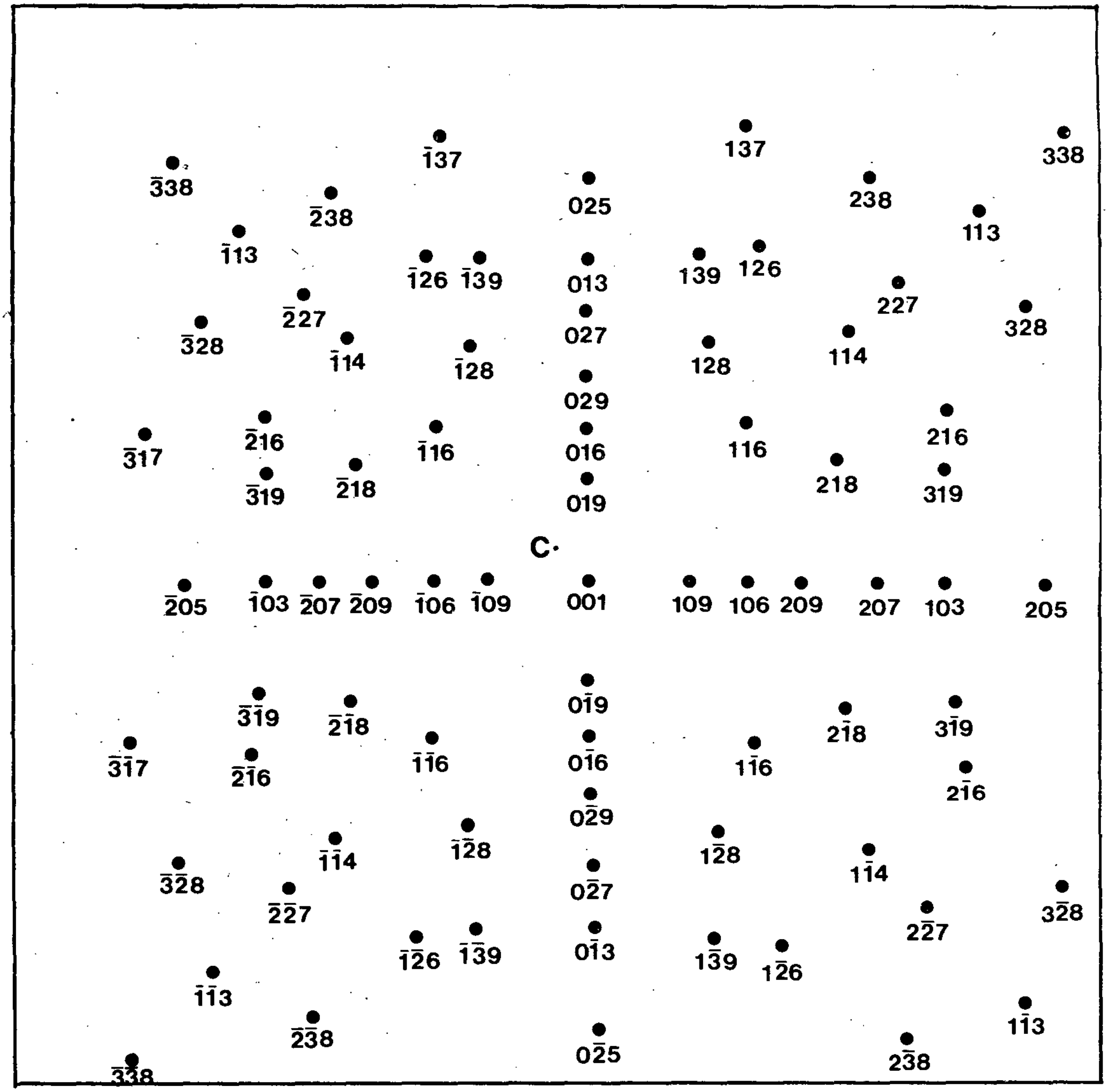
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Figure 5

勞伊X一光繞射圖形之微電腦計算及繪製

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摘　　要

以入射X光方向爲準，若晶體的方向爲已知，則其勞伊X一光繞射圖形可以微電腦計算繪製。這些圖形可當做標準圖形，直接和相同情況下實驗的圖形比較而定出實驗時各繞射面之指數。