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A dynamical theory of the simultaneous reflexion by two lattice planes. II. The effect of the phase factor of the structure amplitude.

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One of the most important tasks to be solved in crystallography is to obtain a method which can furnish the phase factor of the structure amplitude. In this short note it will be shown, by applying the result of the preceding paper (Kambe & Miyake, 1954; which will be referred to as Part I), that the relative phase angle of the structure amplitudes for the lattice planes $h(h_1h_2h_3)$ and $h'(h_1'h_2'h_3')$ may be obtained from the observation of the simultaneous reflexion by these planes.

Let a plane wave with wave number vector **K** be incident on the upper surface of a parallel crystal slab infinitely wide and of finite thickness. For simplicity, we assume that the planes h and h' have an equal spacing and their normals are oriented symmetrically with respect to the plane of incidence so that **K**, in reciprocal space, is considered to be contained always in the c-plane (as defined in Part I) for $c = 1$. The Bragg reflexions h and h' may then appear simultaneously for a certain glancing angle of **K** to the surface.

The wave points to be used in the solution of the diffraction problems are obtained as the points of intersection of the dispersion surface and a line which is perpendicular to the incident surface and lies at a distance from the reciprocal origin equal to the tangential component of **K**. This line, which will be called the ν-normal hereafter, is contained, in the present problem, in the c-plane ($c = 1$), and moves in it when the direction of **K** is changed.

The form of the cross-section of the dispersion surface in the present case is similar to that given by Fig. 1 in Part I, but it should be noticed that, this time, the lines S_h and $S_{h'}$ coalesce into a single line. Now, let us consider the case in which $V_{h'-h}$ is much larger than $|V_h|$ and $|V_{h'}|$. The centres A_+ and A_- are then sufficiently separated from each other, and the approximation of cross-section of the dispersion surface by the hyperbolae for the regions near A_+ and A_- becomes fairly accurate; the distances between the vertices for the hyperbolae around A_+ and A_- are proportional to $|V_h+V_{h'}|$ and $|V_h-V_{h'}|$ respectively. u_+ and u_-, representing the amplitudes of the ψ_+ and ψ_- wave respectively, are calculated for every wave point from (9) of Part I, and we can see readily that, when the wave point lies near A_+, then $u_+ \gg u_-$ in the present condition, so that the ψ_--wave is negligible compared with the ψ_+-wave. When the wave point lies near A_-, the relation is reversed. In either case $|u_h| \risingdotseq |u_{h'}|$, as seen from (10) of Part I. For other wave points, ψ_0 is the only wave having an appreciable amplitude.

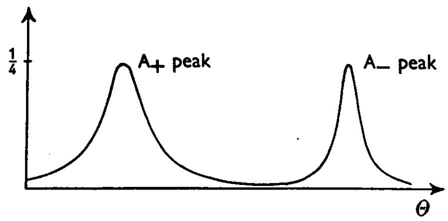

Fig. 1. The ordinate indicates i_h/i_0 or $i_{h'}/i_0$, where i_0, i_h, and $i_{h'}$ are the intensities of the incident wave and the reflexions h and h' respectively.

The intensities of the h and h' reflexions can be calculated by using (10) of Part I and the given boundary condition. The result of the calculation reveals the fact that with the change of the glancing angle of the incident wave the intensities vary in the same way for both reflexions, and have two peaks, each corresponding to the condition that the ν-normal passes A_+ or A_-. The integrated intensities for these two peaks, I_+ and I_- respectively, are proportional to the distances between the vertices of the corresponding hyperbolae, namely to $|V_h+V_{h'}|$ and $|V_h-V_{h'}|$ respectively. When the intensity expressed as the function of the glancing angle Θ of the incident wave *with respect to the h (or h′) plane*, the A_+-peak appears always at a smaller Θ than the A_--peak. Fig. 1 shows schematically the intensity variation of the h (or h') reflexion for the condition where the reflexions h and h' appear behind the crystal, that is, the Laue case; the rapid oscillation of the intensity (*Pendellösung*) is smoothed out.

The above result gives the information of the relative phase of V_h and $V_{h'}$. For example, when both the Fourier coefficients are known to be real, as for centrosymmetrical crystals, their relative signs can be determined at once in the following way: If the area of the peak at the smaller Θ is larger than the other (namely $I_+ > I_-$), then the signs of V_h and $V_{h'}$ are the same; if contrary, they are opposite. When V_h and $V_{h'}$ are complex, put $V_h = |V_h| \exp\{i\delta_h\}$ and $|V_{h'}| = |V_{h'}| \exp\{i\delta_{h'}\}$, then, since

$$\frac{I_+^2-I_-^2}{I_+^2+I_-^2} = \frac{4|V_h|\,|V_{h'}| \cos(\delta_h-\delta_{h'})}{|V_h|^2 + |V_{h'}|^2},$$

the relative phase angle $|\delta_h-\delta_{h'}|$ can be uniquely determined when the ratio of $|V_h|$ and $|V_{h'}|$ is known; this ratio may be obtained by observing the ordinary single reflexions by these lattice planes.

When $V_{h'-h}$ is of comparable order of magnitude to $|V_h|$ and $|V_{h'}|$, it is to be expected that the two peaks corresponding to A_+ and A_- overlap with a certain phase relation, and, besides, the intensity distributions for the h and h' reflexions will not be equal in general. For all that, this case may also, in principle, furnish the information of the relative phase because the intensity distribution depends in general only upon $V_{h'-h}$, $|V_h|$, $|V_{h'}|$ and $|\delta_h-\delta_{h'}|$.

We have assumed so far equal spacing and symmetrical orientation of the h and h' planes, but a similar treatment to that above is possible even when these restrictions are removed, provided that the c-planes are perpendicular to the crystal surface. In principle then, the relative phase angles for all pairs of lattice planes can be determined for the purpose of crystal-structure analysis. The same conclusion holds in the case of X-ray diffraction.

Reference

Kambe, K. & Miyake, S. (1954). *Acta Cryst.* **7**, 218.