structures. For this comparison we have reported in Table 5 the $\mathscr{S}$ values of several structures. We note that the level of distortion of DIF is greater only than naphthalene; while that of DINO is near to anthracene and pyrene.

Table 5. *Comparison of the level of significance of the distortion among different structures*

| Structure | $\mathscr{R}_{obs}$ | $\mathscr{R}$ (0·01) | $\mathscr{S}$ |
|---|---|---|---|
| DIF | 1·142 | 1·083 | 1·7 |
| DINO | 1·149 | 1·042 | 3·5 |
| $S_8$ | 1·154 | 1·015 | 10·3 |
| Anthracene | 1·092 | 1·023 | 4·0 |
| Naphthalene | 1·079 | 1·062 | 1·3 |
| Pyrene | 1·184 | 1·047 | 3·9 |
| Ovalene | 1·141 | 1·021 | 6·7 |
| 1,2,3-trichlorobenzene | 1·070 | 1·038 | 1·8 |

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# The Number of Permitted Modes of Propagation in $N$-Beam Dynamical Diffraction of X-rays

BY SHIH-LIN CHANG

*Instituto de Física 'Gleb Wataghin', Universidade Estadual de Campinas, 13100 Campinas, São Paulo, Brasil*

## Abstract

It is shown that the real part of the root of the dispersion equation for the permitted modes of propagation is always positive for two-beam Laue and Bragg reflections at the exact diffraction position. Based on this, a general rule is proposed to determine the number, $N_p$, of permitted modes of propagation for $N$-beam dynamical diffraction, where no extremely asymmetric reflections are involved. In other words, for both $\sigma$- and $\pi$-polarized wavefields,

$$N_p = 2(N - N_{Bragg}),$$

where $N_{Bragg}$ is the number of Bragg reflections involved. This conclusion is supported by calculations for three-, four-, six- and eight-beam cases.

## I. Introduction

In the dynamical theory of diffraction, the dispersion surfaces, amplitude ratios of wavefields and absorption coefficients are determined from the equation of dispersion. Each dispersion surface specifies a type of wave propagating through a crystal, the so-called mode of propagation. The wavefield and absorption coefficient are associated with their corresponding mode of propagation. The number of modes equals the number of existing wavefields. Other quantities such as the excitation of mode and diffracted intensities are obtained by combining the number of wavefields with the appropriate boundary conditions. Therefore, it is necessary to take the number of wavefields, namely, the number of permitted modes into account in dynamical calculations and only then comparison of the calculations with experiments can be made.

It has been well established that there are four permitted modes of propagation for two-beam (Laue) transmission of X-rays if both $\sigma$- and $\pi$-polarized wavefields are considered. However, according to Kohler (1933) and Authier (1962), there are only two modes allowed in two-beam symmetric Bragg reflection for a thick crystal, *i.e.* $\mu t > 10$, where $\mu$ and $t$ are the linear absorption coefficient and the crystal thickness, respectively. These two modes, which have the direction of energy flow towards the crystal, are associated with

negative Riemann sheets which give positive absorption coefficients (Kato, Katagawa & Saka, 1971). Due to these positive absorption coefficients, the wavefield amplitudes are always attenuated within the crystal. The requirement of the conservation of total energy is hence fulfilled. For extremely asymmetric reflection, for which the angle between the incident (or diffracted) beam and the crystal surface is less than 2°, more than two modes are permitted (Kishino & Kohra, 1971; Bedynska, 1974). For $N$-beam ($N > 2$) Borrmann diffraction, there are $2N$ permitted modes since only transmissions are involved and the characteristics of two-beam (Laue) transmission can be applied. This has been reported by many authors including Ewald & Héno (1968); Héno & Ewald (1968); Uebach & Hildebrandt (1969); Huang, Tillinger & Post (1973); Umeno & Hildebrandt (1975); Post, Chang & Huang (1977). If Bragg reflections are introduced in $N$-beam diffraction, the determination of the number of permitted modes is complicated. Some modes which have negative absorption coefficients should not be considered as permitted modes. In this paper, by considering some characteristics of two-beam Bragg reflection and Laue transmission, we propose a general rule to determine the number of permitted modes for $N$-beam dynamical diffraction.

## II. Theoretical considerations

The number of dispersion sheets is a constant quantity which does not vary as the crystal setting changes. The corresponding number of modes of propagation is then the same throughout all crystal settings. For simplicity, let us consider the number of modes at the exact diffracting position for a singly-polarized wavefield.

### (A) Two-beam cases

The equation of dispersion for a singly polarized wavefield can be written in the following form:

$$y^2 + K\chi_0(1/\gamma_O + 1/\gamma_G)/2y$$
$$+ K^2(\chi_0^2 - C^2\chi_G\chi_{-G})/(4\gamma_O\gamma_G) = 0, \qquad (1)$$

where $y$ ($= K\delta_e$), the accommodation (Ewald, 1917), is the distance between the Laue point and the tie point on the corresponding dispersion surface. Positive $y$ corresponds to the direction towards the interior of the crystal. $\gamma_O$ and $\gamma_G$ are the direction cosines of the direct reflection $O$ and the diffraction $G$ with respect to the inward surface normal, $n_e$, of the crystal, namely,

$$\gamma_O = K_O \cdot n_e \quad \text{and} \quad \gamma_G = K_G \cdot n_e. \qquad (2)$$

$K_O$ and $K_G$ are the unit vectors of the direct and diffracted beams in vacuum. $K$ has the magnitude $1/\lambda$, where $\lambda$ is the wavelength of X-rays in vacuum. $C$ is the polarization factor with $-1 < C < 1$. $\chi_0$ and $\chi_G$ are the complex dielectric susceptibilities for $O$ and $G$

reflections, respectively. Because of the difference in the geometric relationship between the incident and diffracted beams with respect to the crystal surface of Laue transmission and Bragg reflection, the two cases are considered separately.

(i) *Laue case* ($\gamma_O > 0$, $\gamma_G > 0$). Referring to Kato (1974, p. 241), the solutions of (1) are

$$y^r = \text{Re}\,(y) = \begin{cases} y^r(1) \\ y^r(2) \end{cases} = -K\chi_0^r/(2\gamma_O)$$
$$+ [w \mp (w^2 + W^2)^{1/2}]/(2\gamma_G) \quad (3)$$

and

$$y^i = \text{Im}(y) = \begin{cases} y^i(1) \\ y^i(2) \end{cases} = -K\chi_0^i(1/\gamma_O + 1/\gamma_G)/4$$
$$\mp (wv + WV)/(w^2 + W^2)^{1/2}/(2\gamma_G), \quad (4)$$

where $w$; $v$ and $W$; $V$ are the real and imaginary parts of $K\chi_0(1 - \gamma_G/\gamma_O)/2$ and $KC(\chi_G\chi_{-G})^{1/2}(\gamma_O\gamma_G)^{1/2}$, respectively. $\text{Re}(y)$ and $\text{Im}(y)$ are the real and imaginary parts of the argument ($y$). The linear absorption coefficients which are proportional to $y^i$ are

$$\begin{cases} \mu(1) \\ \mu(2) \end{cases} = -4\pi \begin{cases} y^i(1) \\ y^i(2) \end{cases}. \qquad (5)$$

Since $\chi_0^r < 0$ and $\chi_0^i > 0$ (Kato, 1974, p. 182), both $y^r$ and $\mu$ are positive. As stated before, permitted modes always have positive absorption coefficients. Both modes with positive $\mu$ and $y^r$ are permitted. This corresponds to the physical situation that the dispersion sheets always lie below the Laue point at the exact diffracting position for transmission cases and each sheet has a Poynting vector perpendicular to it towards the crystal side. For this case, positive $\mu$ always associates with positive $y^r$. Therefore, the number of permitted modes equals the number of positive $y^r$ at the exact two-beam diffracting position.

(ii) *Bragg case* ($\gamma_O > 0$, $\gamma_G < 0$). Equation (1) still holds for Bragg cases. At the exact two-beam diffraction position, the solutions, $y^r$ and $y^i$, are

$$\begin{matrix} y^r(1) \\ y^r(2) \end{matrix} \Bigg\} = -K\chi_0^r/(2\gamma_O) + [w \pm (w^2 - W^2)^{1/2}]/(2|\gamma_G|),$$

$$\qquad (6)$$

$$\begin{matrix} y^i(1) \\ y^i(2) \end{matrix} \Bigg\} = -K\chi_0^i/(2\gamma_O)$$
$$+ [v \pm (wv - WV)/(w^2 - W^2)^{1/2}]/(2|\gamma_G|). \quad (7)$$

The corresponding absorption coefficients, $\mu$, have the same expression as (5). It can be easily shown that $y^r(1) > 0$ and $y^r(2) < 0$; $\mu(1) > 0$ and $\mu(2) < 0$ (Kato, Katagawa & Saka, 1971; Kato, 1974, p. 343). The

detailed relation between the sign of absorption coefficient and the dispersion surfaces at other angular settings for two-beam Bragg reflection has been given by Chang (1978). Since no waves arrive from the crystal side, the modes associated with negative absorption coefficients are not allowed in Bragg reflection. The only permitted mode corresponds to $y^r(1)$ which is positive. Again positive $\mu$ associates with positive $y^r$. The number of permitted modes is equal to the number of positive $y^r$.

Actually, the number of positive $y^r$ can be easily determined based on Descartes' rule of signs or the properties of the eigenvalue equation. Since the location of tie points only depends on the real part $y^r$ (if the approximation of small imaginary part is employed), the dispersion equation can be expressed, in terms of $y^r$, in a matrix form as

$$\begin{vmatrix} K\chi_0^r/2 - y^r\gamma_0 & C\chi_{-G}^r/2 \\ C\chi_G^r/2 & K\chi_0^r/2 - y^r\gamma_G \end{vmatrix} = 0. \qquad (8)$$

As the susceptibility of the incident reflection is always greater than the diffracted one, i.e. $|\chi_0^r| > |\chi_G^r|$, the signs of the eigenvalues $y^r$ are independent of the off-diagonal elements of the secular determinant of (8). By ignoring $\chi_G^r$ and $\chi_{-G}^r$, (8) becomes

$$(y^r - a_1^r)(y^r - a_2^r) = 0,$$

where

$$a_1^r = -K\chi_0^r/(2\gamma_0)$$

and

$$a_2^r = -K\chi_0^r/(2\gamma_G).$$

Evidently, the signs of $y^r$ depend solely on $\gamma_0$ and $\gamma_G$. The number of permitted modes is then two for Laue $(\gamma_0 > 0, \gamma_G > 0)$ and one for Bragg $(\gamma_0 > 0, \gamma_G < 0)$.

From above considerations, the following conclusion can be made; at the exact diffraction point, permitted modes with positive absorption always have positive values of $y^r$. This is consistent with the fact that, for both Laue and Bragg reflections at the exact two-beam diffracting point, the corresponding tie-points are always situated below the Laue point so that the directions of energy flow are towards the crystal side. However, it should be noted that the permitted modes may have negative $y^r$ at some other settings. It is for this reason that the situation at the exact diffracting position is considered, besides its simplicity in mathematics. At this particular setting, the number of permitted modes is equal to the number of positive $y^r$ of the dispersion equation. This conclusion can be treated as a criterion for determining the number of permitted modes for $N$-beam diffractions at the exact $N$-beam diffraction position.

## (B) Three-beam and N-beam ($N > 3$) cases

The equation of dispersion for a general three-beam diffraction, $O$, $G$ and $H$, can be written as

$$\begin{vmatrix} k^2 - k_O^2 & C_1 k^2 \chi_{-G} & C_2 k_O^2 \chi_{-H} \\ C_3 k_G^2 \chi_G & k^2 - k_G^2 & C_4 k_G^2 \chi_{G-H} \\ C_5 k_H^2 \chi_H & C_6 k_H^2 \chi_{H-G} & k^2 - k_H^2 \end{vmatrix} = 0, \qquad (9)$$

where $C_1$, $C_2$,..., $C_6$ are the polarization factors. Referring to Fig. 1, $\mathbf{k}_O$, $\mathbf{k}_G$ and $\mathbf{k}_H$, starting from the tie point, $T$, are the wave vectors of $O$, $G$ and $H$ reflections inside the crystal. $\mathbf{k}_O'$, $\mathbf{k}_G'$ and $\mathbf{k}_H'$ are the wave vectors from the Lorentz point, Lo, to the corresponding reciprocal-lattice points, $O$, $G$ and $H$, of magnitude $k$. The relations among $k$, $k_O$, $k_G$, $k_H$, to first order in $\Delta k$ can be written as

$$k^2 - k_O^2 \simeq -2K(\mathbf{K}_O.\Delta\mathbf{k}),$$
$$k^2 - k_G^2 \simeq -2K(\mathbf{K}_G.\Delta\mathbf{k}), \qquad (10)$$
$$k^2 - k_H^2 \simeq -2K(\mathbf{K}_H.\Delta\mathbf{k}).$$

$\Delta k$ is a function of $K$ such that

$$\Delta\mathbf{k} = -(\Delta\mathbf{K} + K\delta_e \mathbf{n}_e),$$

where

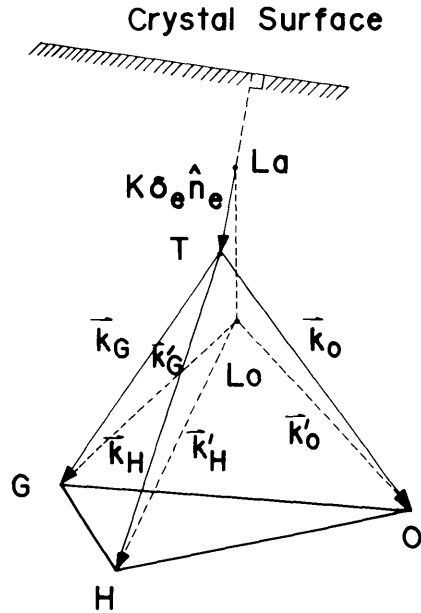$$\Delta\mathbf{K} = \overrightarrow{\text{LaLo}}. \qquad (11)$$

Fig. 1. Geometric relations between the wave vectors and reciprocal-lattice points for a three-beam diffraction case in reciprocal space. La, Lo, and $T$ are the Laue, Lorentz and tie points, respectively. The distance LaLo has been exaggerated in comparison with the wave vectors.

Using (10) and (11) and neglecting the off-diagonal terms and the imaginary parts, (9) becomes

$$(y^r - a_1^r)(y^r - a_2^r)(y^r - a_3^r) = 0, \qquad (12)$$

where

$$a_1^r = -K\chi_0^r/(2\gamma_O),$$

$$a_2^r = -K\chi_0^r/(2\gamma_G),$$

and

$$a_3^r = -K\chi_0^r/(2\gamma_H).$$

For three-beam Borrmann reflection ($\gamma_O > 0$, $\gamma_G > 0$, $\gamma_H > 0$), there are three permitted modes because of three positive $y^r$. For three-beam Bragg–Bragg ($\gamma_O > 0$, $\gamma_G < 0$, $\gamma_H < 0$) and three-beam Bragg–Laue ($\gamma_O > 0$, $\gamma_G > 0$, $\gamma_H < 0$), there are one and two permitted modes, respectively.

Similarly, (12) can be generalized for $N$-beam ($N > 3$) diffraction as

$$(y^r - a_1^r)(y^r - a_2^r)\ldots(y^r - a_j^r)\ldots$$

$$(y^r - a_{N-1}^r)(y^r - a_N^r) = 0, \qquad (13)$$

where

$$a_j^r = -K\chi_0^r/(2\gamma_j) \quad \text{for } j = 1, 2, \ldots, N.$$

It is clear that $y^r$ are always negative for Bragg reflections since the corresponding direction cosines are negative. The number of permitted modes is then equal to $N - N_{\text{Bragg}}$, where $N_{\text{Bragg}}$ is the number of Bragg reflections involved.

More rigorously, the exact eigenvalues, $y^r$ and $y^i$, of (9) (including their signs) can be determined by numerical calculation. The calculation procedure is similar to that given by Post, Chang & Huang (1977) for $N$-beam Borrmann diffraction, where polarization, absorption and crystallographic phases were taken into account. The following cases were subjected to the calculation: (i) three-beam germanium 000, 111, $\bar{1}\bar{1}\bar{1}$, (ii) three-beam Ge 000, 111, 220, (iii) four-beam Ge 000, 004, $\bar{1}\bar{1}3$, $\bar{1}\bar{1}\bar{1}$, (iv) six-beam Ge 000, $20\bar{2}$, $0\bar{2}2$, $\bar{4}2\bar{2}$, $\bar{2}\bar{4}2$, $\bar{4}\bar{4}0$, (v) six-beam GaAs 000, 002, $2\bar{2}4$, $2\bar{2}\bar{2}$, $4\bar{4}2$, $4\bar{4}0$ and (vi) eight-beam GaAs 000, 002, 204, 404, 602, 600, $40\bar{2}$, $20\bar{2}$. Cu $K\alpha_1$ radiation was used. In Table 1, the type of reflection, linear absorption coefficients, $\mu$, the roots, $y^r$, and the number of per-

Table 1. *Calculated results for the accommodations, $y^r$, the linear absorption coefficients, $\mu$, the type of diffraction and the number of permitted modes, $N_p$, for 3, 4, 6, and 8-beam cases*

| Case | | $N$-beam | $N_{\text{Bragg}}$ | Bragg | Laue | $y^r$ (mm$^{-1}$) | | $\mu$ (mm$^{-1}$) | | $N_p$ |
|---|---|---|---|---|---|---|---|---|---|---|
| Ge | 000 | | | | | −310·32 | 132·35 | −100·19 | 382·41 | |
| | 111 | 3 | 1 | 111* | $\bar{1}\bar{1}\bar{1}$ | −263·70 | 382·62 | −67·88 | 130·24 | $2 \times (3 - 1) = 4$ |
| | $\bar{1}\bar{1}\bar{1}$ | | | | | 108·86 | 426·97 | 233·69 | 155·40 | |
| Ge | 000 | | | 111* | | −426·97 | −108·86 | −155·40 | −233·69 | |
| | 111 | 3 | 2 | 220 | | −382·62 | 263·70 | −130·24 | 67·88 | $2 \times (3 - 2) = 2$ |
| | 220 | | | | | −132·35 | 310·32 | −382·41 | 100·19 | |
| Ge | 000 | | | 004* | $\bar{1}\bar{1}\bar{1}$ | −412·44 | 67·95 | −158·57 | 9·01 | |
| | 004 | | | $\bar{1}\bar{1}3$ | | −376·78 | 89·18 | −134·55 | 20·90 | $2 \times (4 - 2) = 4$ |
| | $\bar{1}\bar{1}3$ | 4 | 2 | | | −89·18 | 376·78 | −20·90 | 134·55 | |
| | $\bar{1}\bar{1}\bar{1}$ | | | | | −67·95 | 412·44 | −9·01 | 158·57 | |
| Ge | 000 | | | $20\bar{2}$* | $\bar{2}\bar{4}2$ | −371·71 | 31·52 | −153·18 | 0·37 | |
| | $20\bar{2}$ | | | $\bar{4}2\bar{2}$ | $0\bar{2}2$ | −252·48 | 40·37 | −77·04 | 1·34 | |
| | $\bar{4}2\bar{2}$ | | | $\bar{4}\bar{4}0$ | | −157·20 | 111·86 | −27·60 | 8·45 | |
| | $\bar{4}\bar{4}0$ | 6 | 3 | | | −111·86 | 157·20 | −8·45 | 27·60 | $2 \times (6 - 3) = 6$ |
| | $\bar{2}\bar{4}2$ | | | | | −40·37 | 252·48 | −1·34 | 77·04 | |
| | $0\bar{2}2$ | | | | | −31·52 | 371·71 | −0·37 | 153·18 | |
| GaAs | 000 | | | 002* | $4\bar{4}0$ | −447·07 | 79·04 | −259·65 | 24·18 | |
| | 002 | | | $2\bar{2}4$ | $2\bar{2}\bar{2}$ | −312·47 | 84·86 | −144·38 | 29·29 | |
| | $2\bar{2}4$ | 6 | 3 | $4\bar{4}2$ | | −265·85 | 172·65 | −106·77 | 35·07 | $2 \times (6 - 3) = 6$ |
| | $4\bar{4}2$ | | | | | −172·65 | 265·85 | −35·07 | 106·77 | |
| | $4\bar{4}0$ | | | | | −84·86 | 312·47 | −29·29 | 144·38 | |
| | $2\bar{2}\bar{2}$ | | | | | −79·04 | 447·07 | −24·18 | 259·65 | |
| GaAs | 000 | | | 002* | 600 | −382·47 | 34·22 | −202·36 | 5·10 | |
| | 002 | | | 204 | $40\bar{2}$ | −361·41 | 36·78 | −168·79 | 6·42 | |
| | 204 | | | 404 | $20\bar{2}$ | −351·00 | 58·68 | −174·65 | 16·25 | |
| | 404 | 8 | 4 | 602 | | −310·43 | 60·85 | −125·46 | 19·52 | $2 \times (8 - 4) = 8$ |
| | 602 | | | | | −60·85 | 310·43 | −19·52 | 125·46 | |
| | 600 | | | | | −58·68 | 351·00 | −16·25 | 174·65 | |
| | $40\bar{2}$ | | | | | −36·78 | 361·41 | −6·42 | 168·79 | |
| | $20\bar{2}$ | | | | | −34·22 | 382·47 | −5·10 | 202·36 | |

* Indicates the reflection is symmetric.

mitted modes $N_p$, are listed. The permitted modes are those with positive $\mu$ or positive $y^r$. Clearly, the number of permitted modes satisfies the relation, $N_p = 2(N - N_{Bragg})$.

### III. Discussion and conclusion

With the above considerations, it has been shown that at the exact $N$-beam diffraction position $y^r$ and $\mu$ always have the same sign. As mentioned above, the absorption coefficient of a permitted mode must be positive. The permitted mode should always have positive $y^r$ associated with it. For both $\sigma$- and $\pi$-polarized wavefields, the number of modes having negative absorption coefficients, according to (13) and Table 1, is equal to $2N_{Bragg}$. The number of permitted modes is then the number of the rest of the modes, i.e. $2N - 2N_{Bragg}$. In other words, it is twice the number of transmitted beams, including the incident one. This is exactly consistent with the characteristics of two-beam cases discussed above. Apparently, this relation also holds for $N$-beam Borrmann diffraction, in which no Bragg reflections are involved. The number of permitted modes equals the number of total possible modes, $2N$.

Although this relation is quite general, it is not applicable to those cases which involve extremely asymmetric reflections. For such cases, higher-order terms of $(\Delta k)$ need to be considered. This leads to more permitted modes since the equation of dispersion has the form of a high-order polynomial. Besides, extra modes may be introduced by some related physical phenomenon, such as the specular reflection of X-rays from the crystal surface where the glancing angle of the incident beam is less than 1 or 2° (Kishino & Kohra, 1971).

Nevertheless, without extremely asymmetric reflection in $N$-beam dynamical diffraction, the relation $N_p = 2(N - N_{Bragg})$ holds as a general rule for determining the number of permitted modes of wave propagation. As stated before, the diffracted intensities can be calculated by solving the equations obtaining from the boundary conditions for these $N_p$ wavefields. Based on this, the interpretation of *Aufhellung* (Wagner, 1923; also quoted by Mayer, 1928) and *Umwegangregung* (Renninger, 1937) effects in terms of the dynamical theory of diffraction is possible.

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# Derivation of Possible Framework Structures Formed from Parallel Four- and Eight-Membered Rings

By Mitsuo Sato

*Applied Chemistry, Department of Technology, Gunma University, Kiryu, Japan*

## Abstract

The number of possible combinations of parallel four-membered rings, of the same kind, forming an eight-membered ring is systematically derived by a different method from that of Smith & Rinaldi [*Mineral. Mag.* (1962). **33**, 202–211]. 17 different configurations (including six enantiomorphic) in the *UUDD* ring (*U* and *D* represent upward- and downward-pointing tetrahedra respectively), four different ones (two enantiomorphic) in the *UDUD* ring, and sixteen different ones (seven enantiomorphic) in the *UUDD* ring are shown