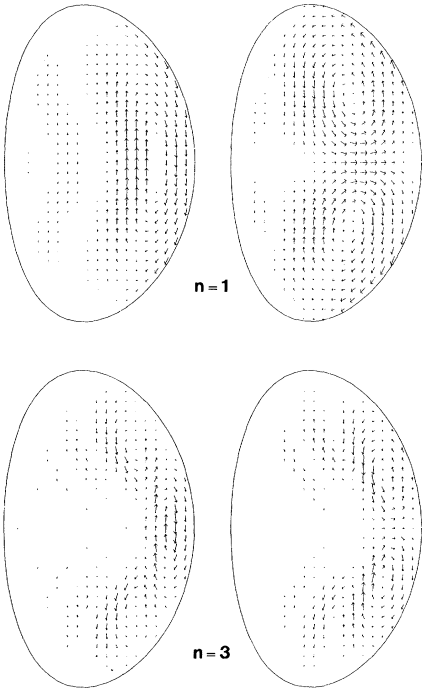


FIG. 3. Eigenfunctions showing the poloidal velocity for the $n = 1$ and $n = 3$ modes for case B ($\beta = 12\%$) for $q_0 = 1.55$. The left- and right-hand diagrams are for φ planes separated by an angle $\pi/2n$.

about 75% of the plasma "radius."

In summary, then, we have shown how a wide range of high-β tokamak equilibria can be calculated using stardard procedures. The model allows independent variation of β, β_p, and q_0, the method of increasing q_0 being similar to the process which occurs in experimental tokamaks. The stability to low-n internal modes has been calculated for a number of these equilibria and stability has been demonstrated for an equilibrium with $\beta = 12\%$.

The authors would like to thank Dr. F. A. Haas for helpful discussions and Mr. C. Ll. Thomas for the use of his equilibrium code.

---

[1] J. F. Clarke, Oak Ridge National Laboratory Report No. ORNL/TM 5429, 1976 (unpublished).

[2] V. S. Mukhovatov and V. D. Shafranov, Nucl. Fusion 11, 605 (1971), esp. p. 630.

[3] J. A. Wesson and A. Sykes, in *Proceedings of the Fifth International Conference on Plasma Physics and Controlled Nuclear Fusion Research, Tokyo, Japan* (International Atomic Energy Agency, Vienna, Austria, 1975), Vol. 1, pp. 449 and 473.

[4] A. M. M. Todd, M. S. Chance, J. M. Greene, R. C. Grimm, J. L. Johnson, and J. Manickam, Phys. Rev. Lett. 38, 826 (1977).

[5] G. Bateman and Y.-K. M. Peng, Phys. Rev. Lett. 38, 829 (1977).

[6] B. J. Green, J. Jacquinot, K. Lackner, and A. Gibson, Nucl. Fusion 16, 521 (1976).

[7] K. Kakishima, T. Tominaya, H. Tohyama, and S. Yoshikawa, Phys. Rev. Lett. 36, 142 (1976).

[8] A. Sykes and J. A. Wesson, Phys. Rev. Lett. 37, 140 (1976).

[9] The JET Project (design proposal for the Joint European Torus), Commission of the European Community Report No. EUR-5516E, 1976 (unpublished).

[10] J. A. Wesson, in *Proceedings of the Seventh European Conference on Controlled Fusion and Plasma Physics, Lausanne, Switzerland, 1975* (European Physical Society, Geneva, 1975), Vol. II, p. 102.

Solution of the X-Ray "Phase Problem"

Ben Post
Physics Department, Polytechnic Institute of New York, Brooklyn, New York 11201

(Received 22 July 1977)

A procedure is described for the experimental determination of phase relationships among x-ray reflections from single crystals. It is shown that when three or more sets of planes diffract simultaneously, the spatial distribution of reflection intensities becomes a sensitive function of the reflection phases. The dynamical theory of diffraction accounts satisfactorily for the intensity variations and is used to establish phase relationships directly from the intensity data.

The direct determination of the phases of x-ray reflections from single-crystal intensity data constitutes one of the oldest and most challenging problems of x-ray physics. It is of particular interest to crystallographers since its solution could make possible the determination of the crystal structures of all substances from which suitable single-crystal data can be obtained.

It has been suspected for some time that coherent interactions among diffracted beams, which take place when several sets of planes diffract simultaneously, may provide clues to the solution

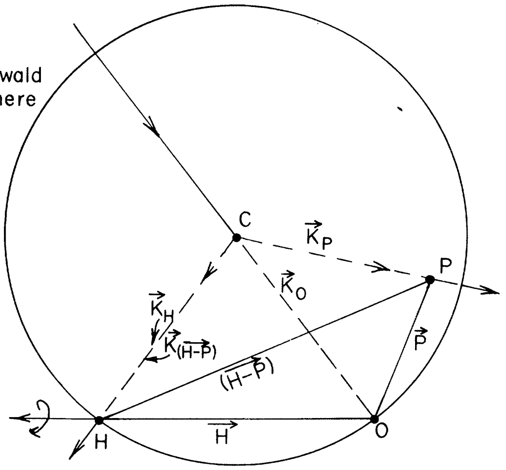


FIG. 1. Schematic representation of three-beam simultaneous diffraction involving rlp's O, H, and P.

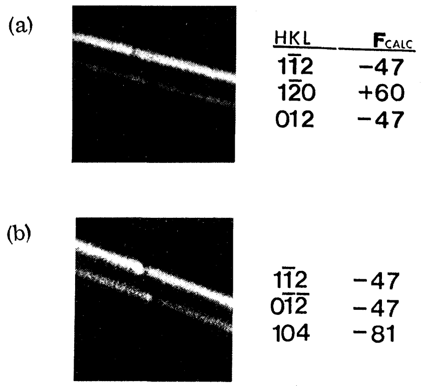


FIG. 2. Intensity distributions along two-beam Cu$K\alpha_1$ and $K\alpha_2$ lines near three-beam points in Al_2O_3, for (a) negative and (b) positive phase products.

of the "phase problem." Lipscomb,[1] Fankuchen,[2a] Eckstein,[2b] Miyake and Kambe,[3] Hart and Lang,[4] and others have investigated the problem from that point of view, with only limited success.

In general, the phases of individual reflections vary with choice of the unit cell origin. The phases of the *products* of groups of structure factors, the sums of whose indices equal zero, are however, invariant to choice of origin, and *their* determination has physical significance. Our discussion is limited to such phase products.

A procedure for generating n-beam simultaneous diffraction is illustrated schematically in Fig. 1. When reciprocal-lattice point (rlp) H is brought to its diffracting position on the surface of the Ewald sphere, conventional two-beam diffraction takes place, and diffracted beams are directed to O and H. When the crystal is rotated about OH without disturbing the setting of H, additional rlp's are brought to their diffracting positions and n-beam diffraction ($n > 2$) occurs. Under such conditions parallel, overlapping, coherent beams are simultaneously directed to the rlp's in diffracting positions. It is evident that simultaneous n-beam diffraction can provide the necessary conditions for interference among discrete coherent beams in simple, controllable form.

Experimental intensitites along two-beam diffraction lines, in the immediate vicinity of three-beam diffractions, are shown in Figs. 2(a) and 2(b) for triplet phase products of ±1, respectively. The techniques used to record the photographs have been described previously.[5] The specimen investigated was a single crystal of aluminum oxide (corundum). Its structure-factor phases are well known. The indices, phases, and magnitudes of the structure factors involved in the three-beam interactions are listed in the figure captions.

The distinctive feature of Fig. 2 is that in (a) the intensity is essentially symmetric, and in (b) it is asymmetric about the three-beam point. I show below that this is a general characteristic of the intensity distributions for the two opposite-phase products, provided that all three structure factors are nonzero. The observed symmetry differences are implict in the dynamical theory of diffraction.[6] They make available a tool for the experimental determination of structure-factor phase products.

The x-ray wave fields in n-beam diffraction obey Maxwell's equations for a medium with a complex, periodic, dielectric constant, under conditions which satisfy Bragg's Law.

The amplitudes are solutions of the linear homogeneous equations:

$$\vec{D}_H = (2\mathcal{E}_H)^{-1} \sum_P \varphi_{(H-P)} \vec{D}_{P[H]}, \tag{1}$$

where $\mathcal{E}_H$, defined by $\mathcal{E}_H = |\vec{K}_H|/k - 1 = \lambda_{vac}/\lambda_{cryst} - 1$, is an unknown to be chosen such that Eq. (1) has a nontrivial solution. $\varphi_{(H-P)}$ is a coefficient in the expansion of the electric susceptibility in a Fourier series. It is proportional to the negative of the structure factor $(-F_{(H-P)})$. $\vec{D}_{P[H]}$ is the vector component of $\vec{D}_P$ perpendicular to $\vec{K}_H$. The summation is over all rlp's, but is limited, in practice, to terms for which the $\mathcal{E}$'s are very small, i.e., to the rlp's very near their diffracting positions.

For a three-beam case, Eq. (1) yields three closely similar pairs of solutions. Without significant loss of generality, I will limit discussion to one member of each such pair. I will discuss centrosymmetric crystals whose origins are at symmetry centers. In such crystals, $\varphi_H = \varphi_{-H}$ and the phase angles of the structure factors are either 0 or π. It is readily shown that the conclusions reached for three beams apply, with only minor modifications, to four-beam and higher-order cases.

The allowed values of $\mathscr{E}_H$ are the solutions of the secular determinant of Eq. (1). They are strongly phase dependent, as can be seen from an examination of the expansion of the determinant at the exact three-beam point:

$$(\varphi_0 - 2\mathscr{E}_0)^3 - (\varphi_H{}^2 + \varphi_P{}^2 + \varphi_{(H-P)}{}^2(\varphi_0 - 2\mathscr{E}_0) + 2\varphi_H\varphi_P\varphi_{(H-P} = 0. \qquad (2)$$

Equation (2) has three unequal real roots summing to zero. The distribution of the signs of the roots is determined by the sign of the last term, i.e., *by the sign of the invariant phase of the structure-factor triplet.* The two possible distributions of the roots ($-++$ or $--+$) lead to propagating modes which differ significantly with respect to excitation and absorption.

The general solution for the $\mathscr{E}_H$ near a three-beam point is usually represented by surfaces in reciprocal space defining the wave-vector sets ($\vec{K}_O$, $\vec{K}_H$, $\vec{K}_P$), one for each mode (Fig. 3). The collection of surfaces representing all the modes is referred to as the "dispersion surface." A calculated section through the dispersion surface, parallel to a two-beam line passing through a three-beam point near the center, is shown in Fig. 3, for both signs of the triplet phase. The points La (Laue) and Lo (Lorentz) are the three-beam diffraction points for reciprocal distances of $1/\lambda_{\text{vac}}$ and $1/\lambda_{\text{cryst}}$ (nondiffracting) from each of the three rlp's.

In general, the modes whose surfaces are closest to the Laue point have the lowest absorption coefficients and are responsible for most of the transmitted intensities.[7] The corresponding modes in Fig. 3 are 1,2 on the left-hand side and 3,4 on the right-hand side. Note that when the triplet phase is positive (dashed lines), the curves corresponding to those modes are approximately symmetrical about the three-beam region (near the center). For negative phase, however, the curves (solid lines) show a large discontinuity just to the right of the three-beam region, and the 3,4 curve on the right-hand side reaches positions equivalent to those of 1,2 on the left-hand side only at large angular distances from the center.

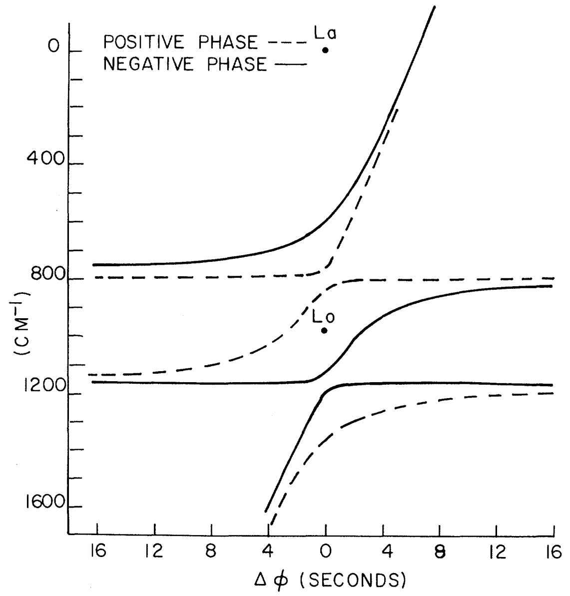


FIG. 3. Section through dispersion surface near three-beam point. Calculated for positive and negative phase products.

The calculated effects of the above on the excitation of modes of propagation are shown in Fig. 4. The effects on the absorption coefficients are very similar. Polarizations of the diffracted beams have been taken into account in these calculations. To reduce confusion I show the two-mode averages for only two pairs of modes (1,2 and 3,4) in the figures. For the positive-phase product the excitations (and the absorption coefficients) undergo only minor changes in passing through the three-beam regions. The corresponding changes are much greater for the negative-phase product.

The intensity of a diffracted beam is given by

$$I_H = \{\textstyle\sum_m [\vec{D}_H(m) \exp 2\pi i \vec{K}_H{}'(m) \cdot \vec{r}\,](\exp - 2\pi \vec{K}_m{}'' \cdot \vec{r})\}^2, \qquad (3)$$

i.e., by the product of terms representing excitation and absorption. The summation is over the m modes. $\vec{K}_H{}'$ and $\vec{K}_H{}''$ are the real and imaginary parts of the propagation vector $\vec{K}_H$. $|4\pi\vec{K}''|_m$ equals u_m, the linear absorption coefficient of mode m. It is evident from Eq. (3) and Fig. 4, that positive and

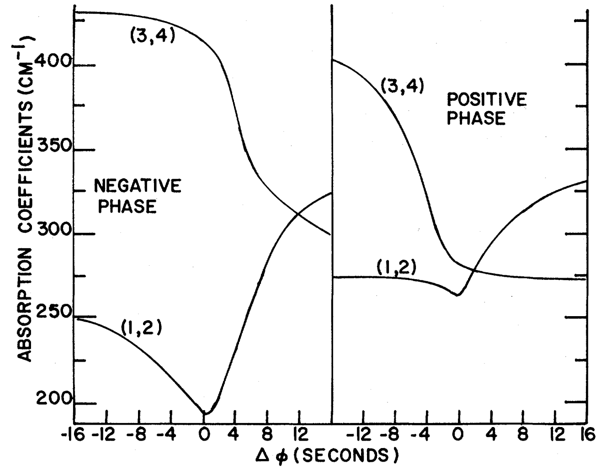


FIG. 4. Relative excitations of modes of propagation. Calculated for negative and positive phase products.

negative structure-factor phase triplets should yield different spatial distributions of diffracted intensity in n-beam diffraction. I have observed such phase effects repeatedly in perfect crystals of germanium and ammonium dihydrogen phosphate as well as in the relatively imperfect crystal of aluminum oxide discussed above. Analysis of Eq. (2) shows that the effects of a change of the phase product on the diffraction process are maximized when all three structure factors are equal to one another, and vanish if one of the structure factors equals zero. The phase effects should therefore be detected as readily when all three structure factors are "weak," as when all are "strong." The extent to which these effects can be detected in imperfect crystals, such as are usually used for crystal-structure analysis, or in noncentrosymmetric crystals remains to be determined.

The author acknowledges with thanks many stimulating and helpful discussions of the problem with Professor H. J. Juretschke. This work was supported by the National Science Foundation and in part by the Joint Services Electronics Program.

---

[1] W. N. Lipscomb, Acta. Crystallogr. 2, 193 (1949).

[2a] I. Fankuchen, private communications, quoted in Ref. 1.

[2b] H. Eckstein, private communication, quoted in Ref. 1.

[3] S. Miyake and K. Kambe, Acta Crystallogr. 7, 218 (1954).

[4] M. Hart and A. P. Lang, Phys. Rev. Lett. 7, 120 (1961).

[5] B. Post, S. L. Chang, and T. C. Huang, Acta Crystallogr., Sect. A 33, 95 (1977).

[6] P. P. Ewald, Ann. Phys. (Leipzig) 49, 1, 117 (1916), and 54, 519 (1917).

[7] P. P. Ewald and Y. Heno, Acta Crystallogr., Sect. A 24, 5 (1968).

Orientational Order in Biaxial Liquid Crystals: The Smectic-VI and -*H* Phases

F. Volino
Groupe de Dynamique des Phases Condensées, Laboratoire de Cristallographie, Université des Sciences et Techniques de Languedoc, Place E. Bataillon, 34060 Montpellier Cedex, France

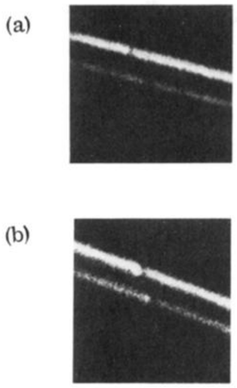
and

A. J. Dianoux
Institut Laue-Langevin, Centre de Tri, 38042 Grenoble Cedex, France

(Received 9 May 1977)

The ^{14}N nuclear-quadrupole resonance (NQR) data of Seliger *et al.* on the smectic-VI and -H phases of terephtal-*bis*-butylaniline are reanalyzed and compared to neutron results. For the smectic-VI phase, both methods lead to remarkably consistent conclusions, but do not differentiate between possible models. For the H phase, the NQR results are consistent both with a model permitting weak orientational order around the long axis and with a model permitting uniform rotation around the long axis plus (anisotropic) fluctuations of this axis. The latter is more realistic since it agrees with the neutron results while the former does not.

In a recent Letter,[1] ^{14}N nuclear-quadrupole resonance (NQR) data on terephtal-*bis*-butylaniline (TBBA) have been presented and analyzed in terms of rotational models for the molecular motions. Concerning the smectic-H phase, it is concluded that the results may be interpreted within the Meyer-McMillan theory[2] which predicts the existence of a polar orientational ordering around



HKL	F_{CALC}
$1\bar{1}2$	−47
$1\bar{2}0$	+60
012	−47

$1\bar{1}2$	−47
$0\overline{12}$	−47
104	−81

FIG. 2. Intensity distributions along two-beam Cu$K\alpha_1$ and $K\alpha_2$ lines near three-beam points in Al_2O_3, for (a) negative and (b) positive phase products.