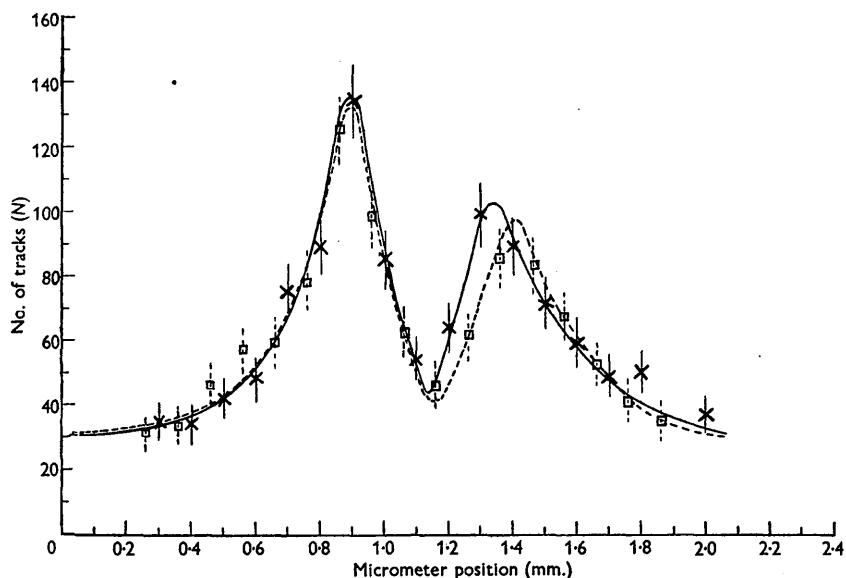


reflected from a single crystal, and a plot of N against distance was made across the centre of an $\alpha_1\alpha_2$ doublet occurring on the first layer line above and below the centre line of the film. These may be assumed to have

number of tracks in the spot, a feature of great potential value in microtechniques or where the intensity of reflexion is so small as to require the film to be placed very close to the crystal in order to obtain a record in a



Crosses and full lines: doublet 1. Squares and broken lines: doublet 2. Vertical lines indicate expected statistical error ($=\sqrt{N}$).

the same shape and to be of equal intensity. The diagram shows the experimental curves to be in agreement within the statistical expectation, and indicates that this and similar emulsions are suitable for the comparison of X-ray intensities.

The advantage of this over existing methods, e.g. photometry, is that the area examined may be very small, of the order of 100μ in diameter, when the integrated intensity can be obtained directly by counting the total

reasonable time. A further application is to the study of low-angle scattering.

The use of short wave-length radiation is preferable as the tracks are longer and more easily identified.

The author is indebted to Miss C. Dilworth (now at the Centre de Physique Nucléaire, Brussels) for assistance during preliminary experiments, and to Prof. C. F. Powell for valuable discussion and encouragement.

Acta Cryst. (1949). 2, 339

An alternative interpretation for vector maps. By A. L. PATTERSON.* *Bryn Mawr College, Bryn Mawr, Pennsylvania, U.S.A.*

(Received 20 May 1949)

The $|F|^2$ series (Patterson, 1934, 1935) which is used in the construction of vector maps can be defined for any number of dimensions by the three equivalent expressions

$$\int f(x_i)f(x_i+u_i) dx_i = \int f(x_i-\frac{1}{2}u_i)f(x_i+\frac{1}{2}u_i) dx_i \\ = \sum |F(h_i)|^2 \exp[-2\pi i \sum h_i u_i] \quad (1)$$

in an obvious notation. The physical interpretation of these expressions in terms of interatomic vectors is well known. The vector map for a given set of points can be generated by inverting the set in the origin and then superposing a series of images of the original set (appropriately weighted) using each point of the inverted set as origin.

There is a second series closely related to (1) which can be defined by the three equivalent expressions

$$\int f(x_i)f(u_i-x_i) dx_i = \int f(\frac{1}{2}u_i-x_i)f(\frac{1}{2}u_i+x_i) dx_i \\ = \sum F^2(h_i) \exp[-2\pi i \sum h_i u_i]. \quad (2)$$

* Now at Institute for Cancer Research, Fox Chase, Philadelphia, Pennsylvania, U.S.A.

The series (2), which involves $F^2(h_i)$ instead of the $|F(h_i)|^2$ of series (1), can now be given a physical interpretation. For a fixed u_i , the integrals (2) calculate the product of the values of the function f at the two points $\frac{1}{2}u_i-x_i$ and $\frac{1}{2}u_i+x_i$ and then integrate this product over the whole cell. The value of the expression (2) at the point u_i is thus a measure of the degree to which the crystal structure approximates to centrosymmetry about $\frac{1}{2}u_i$. If an atom at $\frac{1}{2}u_i-x_i$ has a counterpart at $\frac{1}{2}u_i+x_i$, there will be a contribution to the integral. If not, there will be little or no contribution. If the vector $\frac{1}{2}u_i$ coincides with the vector X_i which locates an atom center there will of course be a contribution since the atom itself always approximates centrosymmetry. The map of the function (2) for a set of points will thus consist of two types of points: (i) points of weight Z^2 at $2X_i$, where X_i is the atomic position co-ordinate, and (ii) points of weight $2Z_1Z_2$ at U_i , where $\frac{1}{2}U_i$ is the co-ordinate of the mid-point of the line joining the atoms Z_1 and Z_2 (the factor 2 appears because each pair makes a contribution for $+x_i$ and for $-x_i$). This map can be constructed for a given set

by using each point of the original set as origin for a weighted image of the set.

It is obvious that the series (2) cannot be calculated for an acentral crystal without a knowledge of the phase angles, although a few of the coefficients $F(h_i)$ may be fixed as positive or negative reals by the space-group criteria. Such cases may well repay investigation, but the purpose of the present note is to point out that, for centrosymmetrical crystals, the series (1) and (2) become identical. This fact suggests a second interpretation for the vector-distance map of a centrosymmetrical crystal. In addition to the usual interpretation in terms of interatomic vectors such a diagram can be looked on as an enlarged mapping of the centrosymmetric properties of the crystal. Whenever a peak appears at a point U_i in the vector map, the crystal will possess 'some centrosymmetry' at the point $\frac{1}{2}U_i$.

This property should be of value in locating centrosymmetrical groups such as benzene or other ring struc-

tures which occur within larger molecules. Two such rings which occur in a centrosymmetric relation would give rise to a peak at a point corresponding to the distance apart of their centers. The content of an intergroup peak for a pair of benzene rings would be about $2 \times 3 \times 6^2 (= 216)$ electrons squared, and would thus be about as large as a peak generated by two atoms of atomic number 15. A peak of such size might well be recognizable above the background of vector maps of this type. In a structure such as coronene or pyrene, which consists entirely of benzene rings, the largest peaks form the distance map of the centers of the rings. It is, of course, recognized that the interpretation of the intergroup maps will be subject to the usual difficulties which accompany the interpretation of the interatomic distance maps.

References

- PATTERSON, A. L. (1934). *Phys. Rev.* **46**, 372.
 PATTERSON, A. L. (1935). *Z. Kristallogr.* **90**, 517.

Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. Copy should be sent direct to the British Co-editor (R. C. Evans, Crystallographic Laboratory, Cavendish Laboratory, Cambridge, England).

Structure Reports Commission

The *Structure Reports* Commission of the International Union of Crystallography (see *Acta Cryst.* (1948), **1**, 340) has co-opted J. M. BIJVOET (Netherlands) and has

appointed him Sub-editor of Section 1 (Inorganic Materials). Preparation of all three sections of the *Reports* for the years 1947-8 is now actively in progress.

Book Reviews

Works intended for notice in this column should be sent direct to the Editor (P. P. Ewald, Polytechnic Institute of Brooklyn, 99 Livingston Street, Brooklyn 2, N.Y., U.S.A.). As far as practicable books will be reviewed in a country different from that of publication.

X-ray Optics. The Diffraction of X-rays by Finite and Imperfect Crystals. Von A. J. C. WILSON. S. 127 mit 33 Fig. London: Methuen and Co. 1949. Preis 6s.

Dieser Band, der zur Buchreihe *Methuen's Monographs on Physical Subjects* gehört, vermittelt einen ausgezeichneten Überblick darüber, wie man diffuse Röntgenreflexe, die durch Teilchengrösse, Unordnungserscheinungen, Gitterverzerrungen und thermische Schwingungen hervorgerufen werden, interpretieren kann. Das Bestreben des Autors, die notwendigen mathematischen Berechnungen auf möglichst einfache Weise darzustellen, kennzeichnet alle Kapitel. Er beginnt mit der Bragg'schen Gleichung und der Einführung des reziproken Gitters. Obwohl der Verfasser absichtlich auf die Verwendung von Vektoren aus Gründen der Einfachheit verzichtet hat, hätte er unter Voranstellung einfacher Vektorenbeziehungen eine einfachere und ebenso verständliche Darstellung des reziproken Raumes erreichen können. Der Einfluss der Teilchengrösse und Form auf die Verbreiterung der reziproken Gitterpunkte und der Debye-Scherrer-Linien auf Pulveraufnahmen wird ausführlich berechnet. Den grössten Raum des Bandes nimmt das Studium der Unordnungserscheinungen nebst ihrem Einfluss auf die rönt-

genographischen Interferenzen ein. Neben allgemeinen Formeln werden die speziellen Fälle Kobalt, Glimmer und Graphit als Beispiele für eindimensionale Fehlordnung und AuCu_3 als Beispiel für dreidimensionale Fehlordnung angeführt. Der Einfluss von Gitterverzerrungen auf das Röntgenbild wird ausgearbeitet und eingehend diskutiert. Das letzte Kapitel bringt einen kurzen Überblick über den Einfluss der thermischen Schwingungen besonders in bezug auf die Abschwächung der Intensitäten der Röntgenreflexe. Auf den wichtigen Einfluss der Elastizitätskonstanten auf die Bildung der diffusen Zonen in unmittelbarer Umgebung der reziproken Gitterpunkte geht der Autor nicht ein.

Der Leser findet in diesem Buch diejenigen Teile der Röntgenoptik, die bisher nur in nicht einfach zu lesenden Originalarbeiten zu finden waren, in zusammengefasster Form dargestellt. Er kann sich deshalb in kurzer Zeit einen guten Überblick über das Gebiet verschaffen. Die einfache und elegante mathematische Darstellung der meisten Teile des Buches werden dazu beitragen, den Stoff einem breiten Leserkreis zugänglich zu machen.

H. JAGODZINSKI

*Mineralogisches Institut der Universität
Marburg/Lahn, Deutschland*