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Multiplicity of solutions of crystal-structure equations.

By H. HAUPTMAN and J. KARLE. *U.S. Naval Research Laboratory, Washington, D.C., U.S.A.*

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In a previous note (Hauptman & Karle, 1950), it was stated that $3(N-1)$ independent magnitudes were sufficient to determine the solution of the crystal-structure problem, and that for the case of three atoms in one dimension the solution is unique. The former statement is ambiguous and the latter incorrect. In general, $3(N-1)$ independent magnitudes are sufficient to determine a finite number of solutions of the crystal-structure problem (Karle & Hauptman, 1951). Since, as a general rule, many more than $3(N-1)$ magnitudes are available from experiment, a unique solution (except, of course, for ambiguities of the Patterson (1944) type) is determined by the data. The following example exhibits four solutions determined by the method described by Karle & Hauptman (1951) for the case of three atoms in one dimension when the minimum amount of algebraic data is used (two magnitudes).

	Co-ordinates of the atoms			
	Solution I	Solution II	Solution III	Solution IV
x_1	0·000 000	0·000 000	0·000 000	0·000 000
x_2	0·159 155	0·386 169	0·320 276	0·159 931
x_3	0·477 465	0·100 825	0·899 699	0·658 078
or, if $\phi_j = 2\pi x_j$				
ϕ_1 =	0·000°	0·000°	0·000°	0·000°
ϕ_2 =	57·296°	139·021°	115·299°	57·575°
ϕ_3 =	171·887°	36·297°	323·892°	236·908°

The atomic scattering factors are given by:

	Plane (100)	Plane (200)	Plane (300)
Atom 1	$f_{11}=0{\cdot}40$	$f_{21}=0{\cdot}30$	$f_{31}=0{\cdot}25$
Atom 2	$f_{12}=0{\cdot}30$	$f_{22}=0{\cdot}25$	$f_{32}=0{\cdot}23$
Atom 3	$f_{13}=0{\cdot}20$	$f_{23}=0{\cdot}16$	$f_{33}=0{\cdot}14$

If $$F_h = \sum_{j=1}^{3} f_{hj}\, e^{-2\pi i h x_j} \quad (h=1,2,3)$$

it is readily verified that

$$|F_1|^2 = 0{\cdot}211\,336 \quad |F_2|^2 = 0{\cdot}155\,563$$

for each of the four solutions. However,

$$|F_3|^2 = 0{\cdot}01921,\quad 0{\cdot}21466,\quad 0{\cdot}21978,\quad 0{\cdot}02565$$

for the respective solutions, so that the specification of $|F_3|^2$ (in addition to $|F_1|^2$ and $|F_2|^2$) would be sufficient to determine a unique solution.

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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 for 1947–1948

The first volume of *Structure Reports* to be prepared under the auspices of the International Union of Crystallography is now ready. It is the aim of these *Reports* to give a critical account of crystal-structure investigations so complete that only those in need of minute detail will find it necessary to consult the original papers.

The volume now published has been prepared under the general editorship of A. J. C. Wilson with C. S. Barrett (Metals), J. M. Bijvoet (Inorganic Compounds) and J. M. Robertson (Organic Compounds) as section editors. It describes some 800 structures published in the years 1947–1948, and contains extensive name, formula and author indexes.

Orders should be placed direct with the publisher:

N.V. A. OOSTHOEK'S UITGEVERS MIJ.
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or with any bookseller. The price is 55 Dutch guilders, post free. A remittance should accompany all orders.

Further volumes covering the years 1940–1946 and 1949 onwards are in course of preparation. The next two volumes to appear will be for the years 1949 and 1945–1946.

International Union of Crystallography

A generous contribution of $5000 towards the publishing activities of the Union has been received from the U.S.A. National Research Council.

Tables for Conversion of X-ray Diffraction Angles to Interplanar Spacing

The National Bureau of Standards announces the publication of *Tables for Conversion of X-ray Diffraction Angles to Interplanar Spacing*. The first six tables give the spacing values for the angles θ from 0 to 90° at intervals of 0·01°. These tables were calculated by using the $K\alpha_1$ wave-

lengths adopted in 1946 for X-ray targets of molybdenum, copper, nickel, cobalt, iron and chromium. The last two tables contain a rearrangement of the data for copper and iron so that the argument is 2θ in intervals of 0·02° from 0 to 180°. The publication is cloth bound and contains 159 pages. It is listed as AMS 10 at $1·75. Order from the Superintendent of Documents, Government Printing Office, Washington 25, D.C., U.S.A.

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.

Das Polarisationsmikroskop, eine Einführung in die mikroskopische Untersuchungsmethodik durchsichtiger kristalliner Stoffe für Mineralogen, Petrographen, Chemiker und Naturwissenschafter im Allgemeinen. By CONRAD BURRI. Pp. 308, with 168 figs. Basel: Birkhäuser. 1950. Price unbound 28·80 Swiss francs, bound in cloth 32·80 Swiss francs.

The several chapters of this text-book of optical crystallography deal thoroughly with crystal optics, the microscope (including theory and ray diagrams as well as hints for the care of the instrument and of the operator's eyes), observations in ordinary light, pleochroism, orthoscopic and conoscopic methods, immersion methods, and the universal stage. In each section the student is first introduced to theoretical aspects of the problem. Practical methods for the application of the new concepts are then described. The treatment throughout the book is accurate and modern, including sufficient analytical formulation to permit quantitative derivation of results. Undue emphasis on the mathematics is avoided by the inclusion of good qualitative explanations of the phenomena. Excellent illustrations, mostly line drawings, are provided; their unusually long and informative legends constitute an uncommon and valuable feature of the book.

An elementary student in crystal optics would obviously need the advice and guidance of an instructor, who would supply specific examples and exercises. A moderately experienced student could easily use this book for further independent work towards an understanding of the subject, and advanced workers will find it a valuable reference work on methods and theories, to be used when the very extended references such as the works of Johannsen and of Rosenbusch are more detailed than necessary. It is a fine addition to its publisher's well-known series of science texts, and a great credit to its author.

Yale University HORACE WINCHELL
New Haven, Connecticut, U.S.A.

Plasticity of Crystals. By E. SCHMID and W. BOAS. Pp. 353 + xvi, with 222 figs. and 42 tables. Translated from the German. London: F. A. Hughes and Co. 1950. Price 35*s*.

It is regrettable that this excellent English translation did not appear many years earlier, when its value would have been much greater. No revisions or additions have been made to the original 1935 German text. To the metallurgist or physicist with active experience in crystal plasticity, the value of the work is already established and no review is necessary. Also the value of the English translation will vary considerably with the individual, his interests and reading knowledge of German. It is safe to say that *Kristallplastizität* is more of a standard reference in current metallurgical literature than in solid-state physics. The experienced worker in the mechanics of crystals is thus the best judge of the value of this book to himself, and the number of references to the original in current literature shows that this translation fills a definite need.

On the other hand, it seems safe to say that this translation was not intended for the student or for the specialist in another field who desires a well-rounded introductory survey of crystal plasticity. For the most part the present work is of value for its comprehensive survey of experimental work prior to 1935 and for the lucid treatment of the geometry of deformation and rotation in a single crystal.

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Books Received

The undermentioned works have been received by the Editors. Mention here does not preclude review at a later date.

Crystal Growth. By H. E. BUCKLEY. Pp. xv + 571, with 357 figs. New York: Wiley; London: Chapman and Hall. 1951.

Structure of Molecules and the Chemical Bond. By Y. K. SYRKIN and M. E. DYATKINA, translated and revised by M. A. PARTRIDGE and D. O. JORDAN. Pp. ix. + 509, with 87 figs. and 174 tables. New York: Interscience Publishers; London: Butterworths Scientific Publications. 1950. Price $8·75.

Selected Topics in X-ray Crystallography from the Delft X-ray Institutes. Edited by J. BOUMAN. Pp. 391, with 192 figs. and 25 tables. Amsterdam: North-Holland Publishing Co. 1951. Price f. 38; 76*s*; $11·00.