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SHORT COMMUNICATIONS

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.

On the atomic scattering factor for O²⁻.

By E. HOVESTREYDT, *Laboratoire de Cristallographie aux Rayons X, Université de Genève, 24 quai Ernest Answermet, CH-1211 Genève 4, Switzerland*

Abstract

The $\sin \theta/\lambda$ dependence of the scattering factor for O²⁻ is approximated by the generally used exponential expression using nine coefficients. The corresponding fit is better than either of the two based upon the functions proposed by Tokonami.

A comparison of the theoretical O²⁻ form factor with experimental measurement by Raccah & Arnott (1967) indicates that the atomic scattering factor for O²⁻ given by Tokonami (1965) is a reasonable one.* The factor is based on calculations by Yamashita [1964, cited by Tokonami (1965)] who used the $1s$ and $2s$ wave functions of Watson (1958) for oxygen in a +1 well and derived the $2p$ function by a variational principle.

The analytical expressions (one for the Cu $K\alpha$ range and one for the Mo $K\alpha$ range) suggested by Tokonami (1965) yield, however, a poor fit. It was therefore decided to develop a better analytical expression based on the generally used fitting curve with nine coefficients.

Results

The nine coefficients for the expression

$$\sum_{i=1}^{4} a_i e^{-b_i \sin^2\theta/\lambda^2} + c$$

were obtained by a least-squares routine. Use was made of the E04HFE program of the *NAG Library* (1978) which is based on a Gauss–Newton algorithm for finding a minimum

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* Various other calculations are known (Schwarz & Schulz, 1978; Schmidt & Weiss, 1979; Schmidt, Sen & Weiss, 1980), but it is beyond the scope of this paper to compare them.

of a sum of squares of non-linear functions. As starting values the coefficients for O, tabulated in *International Tables for X-ray Crystallography* (1974), were supplied.

Table 1 contains the coefficients, calculated by the program, and Table 2 gives a comparison between (*a*)

Table 1. *The nine coefficients of the analytical expression* $\sum_{i=1}^{4} e^{-b_i \sin^2\theta/\lambda^2} + c$ *for the O²⁻ form factor*

a_1	3·75040	b_1	16·5151	c	0·242060
a_2	2·84294	b_2	6·59203		
a_3	1·54298	b_3	0·319201		
a_4	1·62091	b_4	43·3486		

Table 2. *Comparison between the different fitting curves and the scattering factor (f) of O²⁻*

$\sin\theta/\lambda$	f	Fit (present work)	Fit Cu $K\alpha$ range (Tokonami)	Fit Mo $K\alpha$ range (Tokonami)
0·00	10·000	9·999	9·99	9·93
0·05	9·633	9·633	9·63	9·61
0·10	8·671	8·672	8·69	8·72
0·15	7·423	7·423	7·43	7·50
0·20	6·174	6·173	6·17	6·21
0·25	5·081	5·081	5·07	5·05
0·30	4·192	4·193	4·19	4·12
0·35	3·498	3·498	3·51	3·44
0·40	2·968	2·967	2·98	2·95
0·50	2·274	2·274	2·27	2·33
0·60	1·891	1·892	1·88	1·94
0·70	1·676	1·675	–	1·67
0·80	1·543	1·542	–	1·49
0·90	1·447	1·447	–	1·38
1·00	1·367	1·367	–	1·32
1·10	1·291	1·292	–	1·29
1·20	1·216	1·217	–	1·28
1·30	1·142	1·142	–	1·27
1·50	0·995	0·994	–	–
1·70	0·856	0·855	–	–
1·90	0·729	0·729	–	–

Tokonami's form factor, (b) values calculated with the fitting curve presented in this note and (c) those calculated using the functions proposed by Tokonami for the Cu $K\alpha$ and Mo $K\alpha$ ranges, respectively.

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X-ray diffraction from nonstoichiometric titanium sulfide containing stacking faults: errata.

By M. ONODA and I. KAWADA, National Institute for Research in Inorganic Materials, Sakura-mura, Niihari-gun, Ibaraki 305, Japan

Abstract

Mis-expressed terms in equations (13) in Onoda & Kawada [Acta Cryst. (1980), A36, 134–139] should be corrected. All $\exp(-i2\pi\zeta)$, $\exp(-i\pi\zeta/2)$, $\exp(-i\pi\zeta)$ and $\exp(-i3\pi\zeta/2)$ on page 137 are to be replaced respectively by $\exp(i2\pi\zeta)$, $\exp(i\pi\zeta/2)$, $\exp(i\pi\zeta)$ and $\exp(i3\pi\zeta/2)$.

All relevant information is given in the Abstract.

Intensity distribution in powder X-ray diffraction from nonstoichiometric titanium sulfide containing stacking faults: errata.

By M. ONODA, M. SAEKI and I. KAWADA, National Institute for Research in Inorganic Materials, Sakura-mura, Niihari-gun, Ibaraki 305, Japan

Abstract

All $\exp(-i2\pi\zeta)$, $\exp(-i\pi\zeta/2)$, $\exp(-i\pi\zeta)$ and $\exp(-i3\pi\zeta/2)$ in equations (21) in Onoda, Saeki & Kawada [Acta Cryst. (1980), A36, 952–957] are mis-expressed and to be replaced respectively by $\exp(i2\pi\zeta)$, $\exp(i\pi\zeta/2)$, $\exp(i\pi\zeta)$ and $\exp(i3\pi\zeta/2)$.

All relevant information is given in the Abstract.

International Union of Crystallography

International Tables for Crystallography

Professor A. J. C. Wilson has been appointed Chairman of the Union's Commission on International Tables, and Editor in charge of a proposed revision of Volumes II, III and IV. Following his recent retirement as Professor of Crystallography at the University of Birmingham he has moved to Cambridge. His new address is Crystallographic Data Centre, University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW, England.

Professor U. Shmueli, Chemistry Department, Tel-Aviv University, has been appointed Editor of a new volume of International Tables on reciprocal space.

Since 1973 the Commission has been preparing the material for a totally revised and extended edition of the tables of symmetry groups. The results of these years of collaborative effort have led to the production of completely new tables on the 17 plane groups and 230 space groups, comprising about 630 pages. This work is complemented by a comprehensive introduction of about 200 pages in which symmetry is discussed and the theory and use of the tables is described in detail. It is edited by Th. Hahn and will be published for the Union by D. Reidel Publishing Company. The publication of this volume was scheduled for the end of 1982 but because of various delays it is not now expected to be available before mid 1983.

Table of Contents: Foreword. Preface. Part I: Tables for Plane Groups and Space Groups. 1. Symbols and Terms Used in this Volume. 2. Guide to the Use of the Space-Group Tables. 3. Space-Group Determination and Diffraction Symbols. 4. Synoptic Tables of Space-Group Symbols. Group-Subgroup Relations. 5. Transformations in Crystallography. 6. The 17 Plane Groups (Two-Dimensional Space