VAYNSHTEYN, B.K.; LEMMLEYN, G.G.

The orientation of silver on silicon carbide. Trudy Inst. Krist. Akad. Nauk S.S.S.R. 6, 203-6 '51. (MLRA 4:10)
(CA 47 no.15:7281 '53)

VAYNSHTEYN, B. K.

184T112

USSR/Physics - Crystallography 21 Jun 51

"Concerning Vector Models of Crystallic Structures," B. K. Vaynshteyn

"Dok Ak Nauk SSSR" Vol LXXVIII, No 6, pp 1137-1140

To describe crystallic structures the coordinates and wts of atoms must be given, which can be described as syst of weighed points by means of set of complex numbers: $S = (z_1, z_2, .., z_n)$ such that the modulus will define the wt and the arguments, the position of atom thus: $z = \rho \cdot e^{2\pi i x}$, $\arg z = \varphi = 2\pi x$, $|z| = \rho$. Considers operation of "multiplication" of atom by atom: $z_1 z_k = \rho_1 \cdot e^{2\pi i x_1} \cdot \rho_k$.

184T112

USSR/Physics Crystallography (Contd) 21 Jun 51

$e^{2\pi i x_k} = \rho_1 \rho_k \cdot e^{2\pi i (x_1 + x_k)}$, result of which is formation of the vector $x_1 + x_k$ of atom of wt $\rho_1 \rho_k$. Cf. Wrinch, "Phil Mag" 27, 98, 1939. Submitted 23 Apr 51 by Acad D. S. Belyankin.

184T112

1. VAYNSHTEYN, B. K.

2. USSR (600)

4. Crystallography, Mathematical

7. Deciphering crystal structures. Trudy Inst.krist., no. 7, 1952.

9. Monthly List of Russian Accessions, Library of Congress, April 1953, Uncl.

VAYNSHTEYN, B.K.

Electronic Optics

Structural electromography. Vest. AN SSSR, 22, No. 3, 1952.

Monthly List of Russian Accessions, Library of Congress, October 1952. UNCLASSIFIED.

VAYNSHTEYN, B.K.

Crystal structure of $MnCl_2.2H_2O$. Doklady Akad. Nauk S.S.S.R. 83, 227-30 '52. (MLRA 5:5)
(CA 47 no.20:10307 '53)

VAYNSHTEYN B. K.

238T96

USSR/Nuclear Physics - Atomic Number 21 Aug 52
Electron Scattering

"Dependence of the Scattering of Electrons Upon the Atomic Number," B. K. Vaynshteyn

"DAN SSSR" Vol 85, No 6, pp 1239-1242

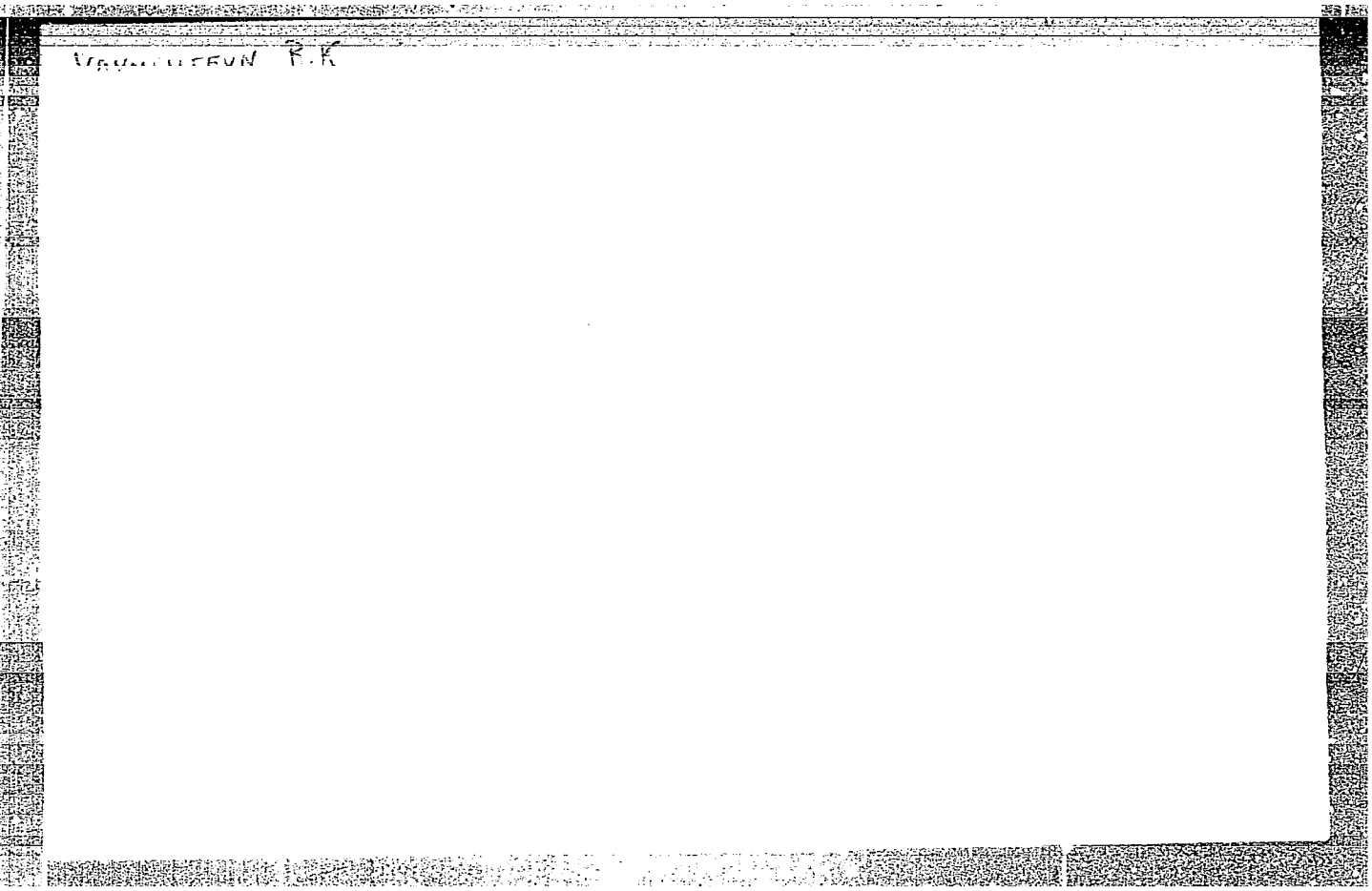
Shows that the mean internal potential is sensitive to the packing density of the atoms in the lattice. Gives a very simple method of computation of the mean internal potential, which gives

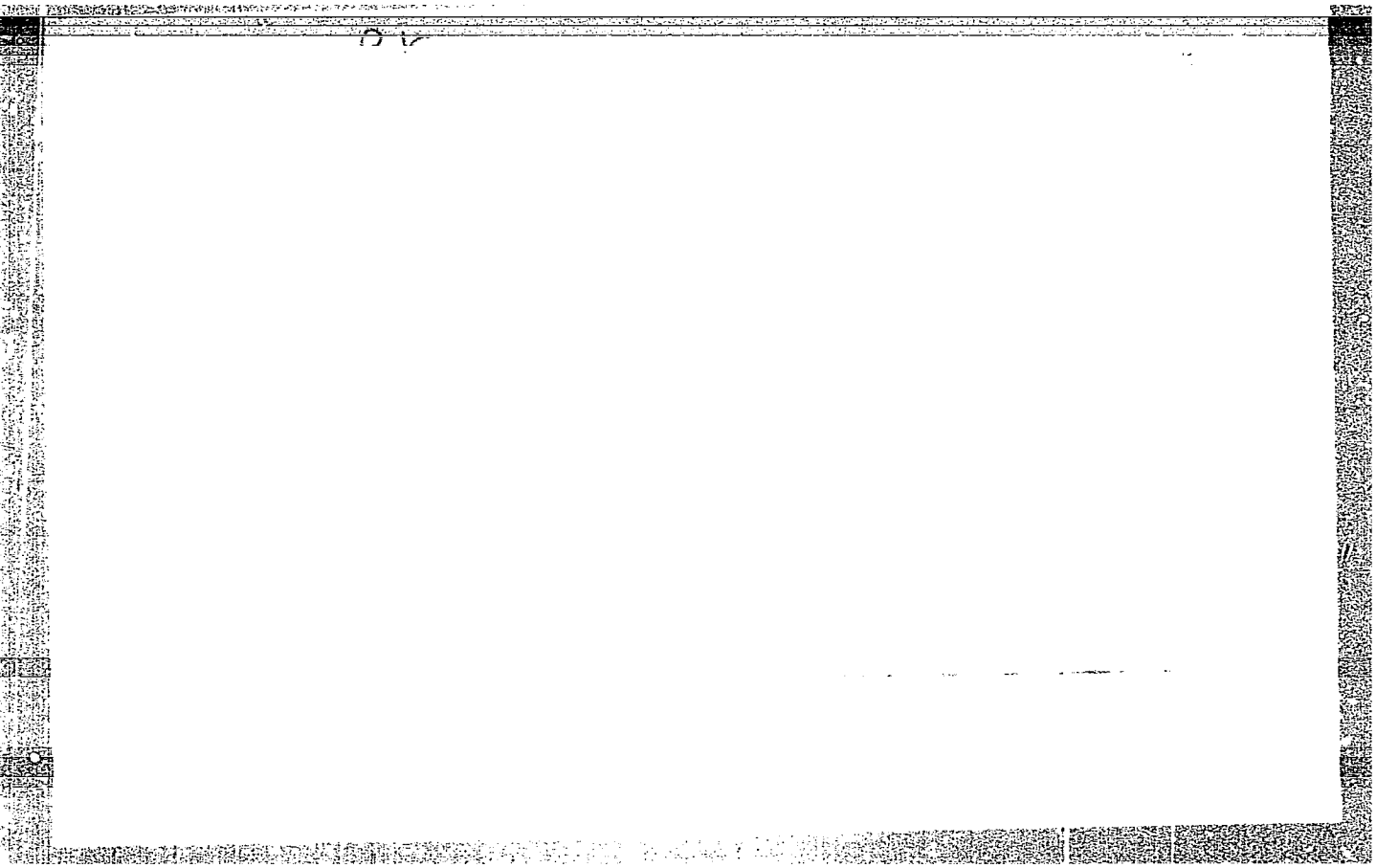
238T96

better results than other more complicated methods such as summation by series. Gives electron scattering coeff f(0) and atomic radii r_a of elements of the first three periods. Submitted by Acad P. L. Kapitsa, 28 Jun 52.

(CA 47 no. 22: 11943 '53)

238T96





APPROVED FOR RELEASE: 08/31/2001 CIA-RDP86-00513R001859110020-4"

VAYNSHTEYN, B.K.

USSR

548.735.44

4015. Normalization of Fourier series for electron density. B. K. Vainshtein. *Dokl. Akad. Nauk SSSR*, 93, No. 5, 821–3 (1953) *In Russian.*

Using Bunyakovskii's theorem the reflected intensities can be expressed as [illegible] where k and x are constants of the type of structure considered, depending on B([illegible]). This can be deduced because g_i, the integral of ρ_i/t over the unit cell has an appreciable magnitude only in the immediate neighbourhood of the ith atom. The radial electron densities round atoms are approximated from unitary f curves and corrected for thermal vibrations. Observed structure amplitudes can thus be put on to an absolute basis.

A. L. MACKAY

Vaynshteyn, B. K.

USSR/Solid State Physics - Structural Crystallography, E-3

Abst Journal: Referat Zhur - Fizika, No 12, 1956, 34599

Author: Vaynshteyn, B. K.

Institution: None

Title: On the Investigation of the Potential of the Crystal Lattice by Electronographic Methods

Original Periodical: T. In-ta kristallografii AN SSSR, 1954, No 9, 259-276

Abstract: Examination of the features of the distribution of the potential in crystals, compared with the distribution of the electron density, and also of the quantitative relationships and dimensionality in the Fourier series of the potential. A new method is proposed for calculating the average internal potential of crystals, based on using the values of $f_{el}(0)$: $\psi_{av}(b) = 114.5 \sum f_{el}(0)/\Omega$. Experimental data related to the phenomenon of electron refraction (splitting of the reflexes on photographs of MgO) are given, for which $\varphi_{av}(MgO) = 10 - 17$ volts, is determined. The electron-diffraction method is applicable to the study of the distribution of the potential in crystals. From the experimental amplitudes Φ_{hkl} normalized to the absolute values, cross sections of the 3 dimensional Fourier series are $\varphi(xoo)$,

USSR/Solid State Physics - Structural Crystallography, E-3

Abst Journal: Referat Zhur - Fizika, No 12, 1956, 34599

Author: Vaynshteyn, B. K.

Institution: None

Title: On the Investigation of the Potential of the Crystal Lattice by Electronographic Methods

Original Periodical: T. In-ta kristallografii AN SSSR, 1954, No 9, 259-276

Abstract: $\varphi(xxo)$, $\varphi(xxx)$ are constructed, and the variation of the potential Al, Ag and Cu is computed. It is established that a distribution of potentials at the maximum is approximately the same for all 3 metals and is independent of the direction of the cross section, i.e., the maxima are spherically symmetrical, but the values of the potentials between the atoms are somewhat different. An examination is made of the effect of the error introduced by terminating the series on the variation of the potential and on the accuracy of the results obtained.

VAYNSHTEYN, B. K.

"A Method of Deciphering F^2 -Series".
Tr. In-ta Kristallogr. AN SSSR, No. 9, pp 287-290, 1954.

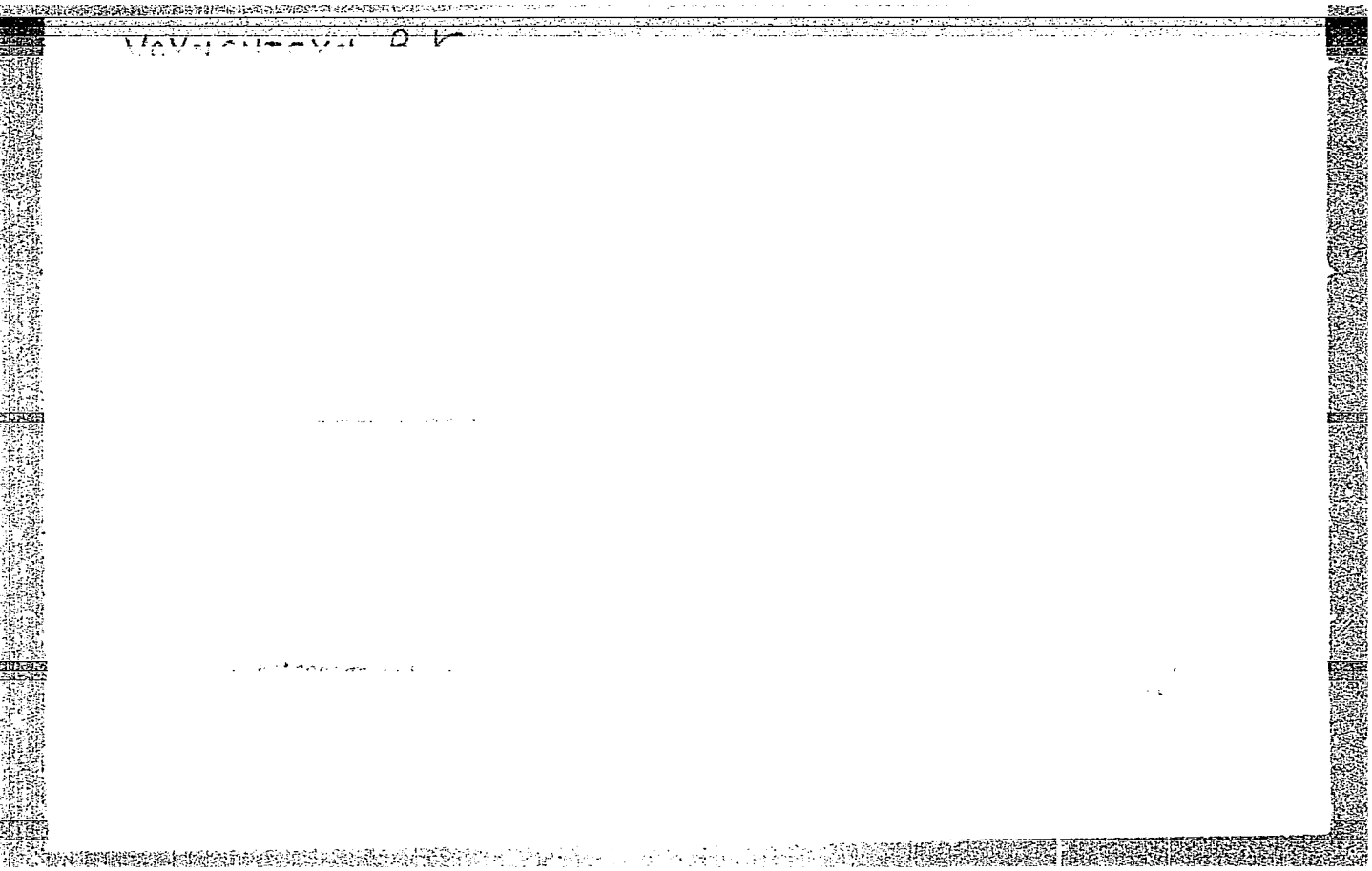
Deciphering two-dimensional distributions of interatomic function by vector convergence ("superimposing and shifting") can be readily accomplished by using a photographic method. Three identical photographic negatives are prepared on which the transparent places correspond to maxima of interatomic functions, and the dark places correspond to back-ground. When the negatives are superimposed on the corresponding shifts, only those maxima which coincide with one another are distinguished, which inturn distinguishes the structure. Only two negatives are required in the case of centrosymmetrical structure. The application of the method is illustrated using the structure of $K[PtCl_3(NH_3)]$ as an example. (RZhKhim, No 4, 1955)

SO: Sum No 884, 9 Apr 1956

VAYNSHTEYN B.K.

PINSKER, Z.G.; VAYNSHTEYN, B.K.

Precision measurements of lattice periods in electronography. (MLRA 7:11)
Trudy Inst.krist. no.9:291-304 '54.
(Electronograph) (Crystallography)



APPROVED FOR RELEASE: 08/31/2001 CIA-RDP86-00513R001859110020-4"

VAYNSHTEYN B.K.

USSR / Physical Chemistry. Crystals B-5

Abs J_0ur : Ref Zhur - Khimiya, No 8, 1957, 25872

Author : B.K. Vaynshteyn, Z.G. Pinsker.
Title : Determination of H Atom in Crystalline Lattices (of Paraffin) by Electron Diffraction Study.

Orig Pub : Tr. In-ta kristallografii AN SSSR, 1954, vyp. 10, 143-163.

Abstract : No abstract.

Card : 1/1

VAYNSHTEYN, B.K.

FD-736

USSR/Physics-Electron density in crystals

Card 1/1 : Pub 146-6/22

Author : Vaynshteyn, B. K.

Title : Quantitative relations in Fourier series of electron density in crystals

Periodical : Zhur. eksp. i teor. fiz., 27, 44-61, Jul 1954

Abstract : A Fourier synthesis according to X-ray data gives the distribtuion of the electron density in a crystalline lattice with peaks corresponding to atoms. The dependence of values characterizing the electron density on atomic numbers is found, taking into account the thermal motion. Problems of normalization and accuracy of F- and F^2- series are analyzed. 12 references including 9 foreign.

Institution : Institute of Crystallography, Acad. Sci. USSR

Submitted : August 19, 1953

VAYNSHTEYN, B.K.

USSR/Chemistry - Crystallography

Card 1/1 Pub. 22 - 22/47

Authors : Vaynshteyn, B. K.

Title : Localization of hydrogen atoms in the crystalline structure of diketopiperazine by the electronographic method

Periodical : Dok. AN SSSR 99/1, 81-84, Nov 1, 1954

Abstract : The application of the Fourier series in the electronographic method of localizing hydrogen atoms in the crystalline structure of diketopiperazine is explained. The role of diketopiperazine groupings in the structure of albumin is discussed. The presence of hydrogen atoms, which form H-bonds and atoms forming no H-bonds in the albumin structure, was established. The spaces between H-atoms were found to be close to the standard values of C - H and N - H spaces. The electron density in the hydrogen atom maximum was calculated. Ten references: 6-USSR and 4-USA (1931-1953). Table; drawing.

Institution : Academy of Sciences USSR, Institute of Crystallography

Presented by: Academician N. V. Belov, June 17, 1954

VAYNSHTEYN, Boris Konstantinovich

VAYNSHTEYN, Boris Konstantinovich - Academic degree of Doctor of Physico-Mathematical Sciences, based on his defense, 6 April 1955, in the Council of the Inst of Crystallography Acad Sci USSR, of his dissertation entitled: "Electron-Diffraction Structure Study." for the Academic Degrees of Doctor of Sciences.

SO: Byulleten' Ministerstva Vysshego Obrazovaniya SSR, List No. 3, 4 February 1956 Decisions of the Higher Certification Commission Concerning Academic Degrees and Titles.

JPRS/NY 554

VAYNSHTEYN, B.K.

USSR/Physical Chemistry - Crystals, B-5

Abst Journal: Referat Zhur - Khimiya, No 19, 1956, 60841

Author: Vaynshteyn, B. K., Tishchenko, G. N.

Institution: None

Title: Conventional Projections in F- and F^2-Series of Fourier

Original Periodical: Tr. in-ta kristallogr. AN SSSR, 1955, No 11, 68-74

Abstract: Analogously to the fact that evolvement of F-series in accordance with the zone of reflections hk0 yields the projection of the structure, the evolvement of series in accordance with F_{hkl} with fixed l, will yield a conventional projection $\sigma_l(xy) = \int_0^c \rho(xyz)\exp(2\pi ilz/c)dz$. Peaks σ_l due to the presence of exponential factor, which assumes depending upon the concrete symmetry of the structure the form cos or sin, can have a positive as well as a negative sign (or vanish altogether) depending upon z-coordinate

Card 1/2

USSR/Physical Chemistry - Crystals, B-5

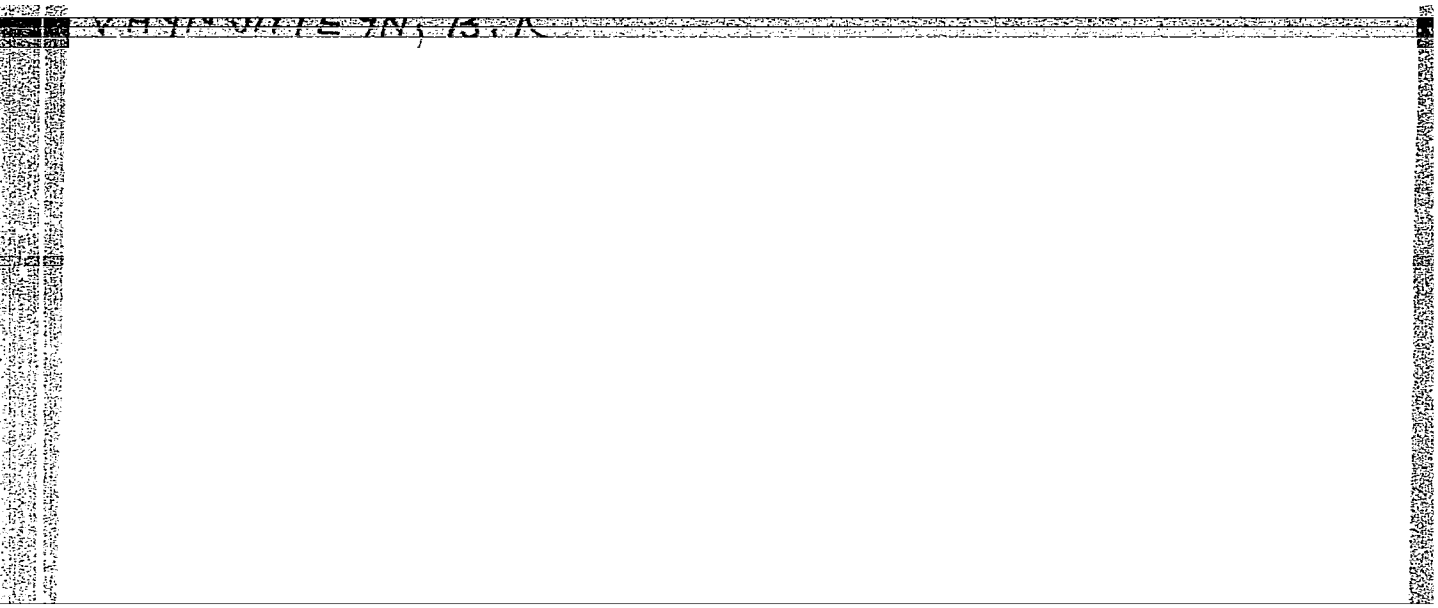
Abst Journal: Referat Zhur - Khimiya, No 19, 1956, 60841

Abstract: of the atom and corresponding value of cos or sin ($2\pi lz/c$). Characteristics of these projections are illustrated by examples of evolvement of σ_1 and σ_2 for the structure CS_2CoCl_4. Characteristics of conventional projections in F_2-series are analogous.

Card 2/2

LOBACHEV, A.N.; PINSKER, Z.G.; VAYNSHTEYN, B.K.

Rotation method in electronography. Trudy Inst.krist.no.11: 75-77 '55. (Electronography) (MLRA 9:6)



APPROVED FOR RELEASE: 08/31/2001 CIA-RDP86-00513R001859110020-4"

KUL'VARSKAYA, B.S.; VAYNSHTEYN, B.K.

Electronographic study of the structure of silver-magnesium and copper-magnesium alloys. Trudy Inst.krist.no.11:97-100 '55.
(MLRA 9:6)
(Silver-magnesium alloys) (Copper-magnesium alloys)

VAYNSHTEYN, B.K., kandidat fiziko-matematicheskikh nauk.

Use of X rays in the study of materials; Fifth all-Union conference.
Vest. AN SSSR 25 no.10:87-90 O '55. (MLRA 9:3)
(X rays--Industrial applications)

VAINSHTEYN, B.K.

Electronography of diketopiperazine. Zhur.fiz.khim. 29 no.2:327-344 F '55. (MLRA 8:7)

1. Akademiya nauk SSSR, Institut kristallografii, Moscow
(Piperazine) (Electronography)

VAYNSHTEYN, B. K

V 1597

62 KINEMATIC SCATTERING OF ELECTRONS BY IDEAL MONOCRYSTALS. B. K. Vainshtein. (Inst. of Crystallography). Doklady Akad. Nauk S.S.S.R. 104, 537-9(1955) Oct. 1. (In Russian)

Reflection intensity of monochromatic waves in electron diffraction from a single, ideally formed, kinematically scattering crystal was analyzed. (R.V.J.)

VAYNSHTEYN, Boris Konstantinovich; PINSKER, Z.G., professor, otvetstvennyy redaktor; RAZUMOVA, L.L., redaktor izdatel'stva; AUZAN, N.P., tekhnicheskiy redaktor

[Structural electronography] Strukturnaia elektronografiia. Moskva, Izd-vo Akademii nauk SSSR, 1956. 313 p. (MIRA 9:11)
(Electronography)

WEISTEIN, B. K.

USSR/Physical Chemistry. Crystals. B-5

Abs Jour: Ref Zhur-Khimiya, No 5, 1957, 14488

Author : B. K. Weistein
Inst :
Title : The Kinematic Theory of Intensity of Reflexes of Electron Diffraction Pictures. I. Pointlike Electron Diffraction Pictures. II. Electron Diffraction Pictures from Textures and Polycrystals

Orig Pub: Kristallografiya, 1956, 1, No 1, 17-26; No 2, 150-158

Abstract: I. The kinematic distribution of electrons by monocrystalline samples was examined. If the crystal is ideal, then the relation of the integral distributed intensity $I_{(hkl)}$ to the initial J_0, occupied by the exposed crystal surface S equals: $I_{(hkl)}/J_0S = \lambda^2 |\phi_{(hkl)}/\Omega|^2 \times (\sin^2 \pi A_3 h_3)/(\pi h_3)^2$. Here λ - wave length, ϕ - structural amplitude, Ω - volume of the nucleus, A_3 - crystal thickness, h_3 - distance, corresponding to A_3 in the rear space

Card 1/4

USSR/Physical Chemistry. Crystals.

Abs Jour: Ref Zhur-Khimiya, No 5, 1957, 14488

B-5

Abstract: function f(∝) were examined and it was shown that for layers from large blocks, dynamically dispersed (when the dispersed intensity is proportional to $|\phi(hkl)|$, and not to the square of this magnitude), a calculation of the mosaic gives the same factor $d(hkl)/\alpha$. II. Formulas for reflex intensities of electronographs of textures and polycrystals were derived on basis of examination of function of crystal distribution along the corners in these compounds. This function for textures is characterized by two components: a constant density of distribution in the full circular interval with a density $n/2\pi$ (n is the number of crystals in the sample) and by the distribution of special axes of the crystals near the axis of the texture f(∝). Expressions were obtained for the neutral intensity of the bows which is independent from f(∝) and for local (in their center) intensity, dependent on f(∝). With the aid of knowing the distribution function the problem of

Card 3/4

USSR/Physical Chemistry. Crystals.

B-5

Abs Jour: Ref Zhur-Khimiya, No 5, 1957, 14488

Abstract: the intensity of the rings of the electron diffraction picture of the polycrystal was examined.

Card 4/4

Vayishteyn, B.K.

Category : USSR/Solid State Physics - Structural Crystallography E-3

Abs Jour : Ref Zhur - Fizika, No 2, 1957 No 3687

Author : Vayishteyn, B.K.
Title : Use of the Convolution Theorem for the Derivation of the Equation for the Temperature Factor

Orig Pub : Kristallografiya, 1956, 1, No 1, 137-138

Abstract : The well known equation, according to which the scattering ability of an atom in thermal motion is the product of the atomic factor f (s) and the temperature factor f_T (s), is obtained more readily by taking into account that the distribution of the scattering substance is described in this case by the convolution ρw (r) of the electron density of the atom and of the function w, describing the thermal motion, and by using the Fourier integral.

Card : 1/1

VAYNSHTEYN, B.K.

USSR / Structural Crystallography. E-3

Abs Jour : Ref Zhur - Fizika, No 4, 1957, No 9193

Author : Vaynshteyn, B.K.
Inst : Institute of Crystallography, Academy of Sciences USSR
Title : Kinematic Theory of Intensity of Reflexes of Electron Diffraction Patterns. II. Electron Diffraction Patterns From Textures and Polycrystals.

Orig Pub : Kristallografiya, 1956, 1, No 2, 150-158

Abstract : Calculation of the intensity of scattering of electrons from textured or polycrystalline compounds requires, as in the case of mosaic single-crystal films (see abstract 9192), the introduction of an angular distribution function for the crystals. For textures, this function is characterized by two components -- with a uniform distribution density over the angles around the axis of the texture over the total angular range of 2π and with the straggling of the axis of the texture in an effective angular

Card : 1/3

USSR / Structural Crystallography. E-3

Abs Jour : Ref Zhur - Fizika, No 4, 1957, No 9193

Abstract : range α . When electron diffraction patterns are made of "oblique textures", when the compound is tilted an angle φ from its initial position perpendicular to the beam, the integral intensity of the small arc satisfies the equation $I_{hkl}/J_0 S = {}^{2} = \lambda^2 |\Phi/\Omega|^2 t L \lambda p/(2\pi R' \sin\varphi)$, where L is the distance between the compound and the screen, p the repetition factor, and R' the horizontal coordinate of the reflex on the electron diffraction pattern (for the remaining symbols see abstract 9192). Thus, for relative values $|\Phi^{rel}_{hkl}| = \sqrt{I^{rel}_{hkl} R'/p}$, if the arcs on the electron diffraction pattern has noticeable angular extent, it is possible and advisable to measure not their integral intensities but their local ones, i.e., the values of I'_{hkl} at the center of the arc. If the length of the small measured section in the center is Δ , then, taking into account the effective angular straggling of the axis of the texture α ,

Card : 2/3

USSR / Structural Crystallography. E-3

Abs Jour - Ref Zhur - Fizika, No 4, 1957, No 9193

Abstract : it is possible to find that $I'_{hkl}/J_0 S = \lambda^2 |\bar{\Phi}|^2 \Omega^2 \varepsilon \Delta d_{hkl} d_{hk0} p/2\pi\alpha L\lambda)$, so that $|\bar{\Phi}^{rel}_{hkl}| = \sqrt{I^{rel}_{hkl}/d_{hkl} d_{hk0} p}$ where d_{hk0} is the interplanar distance of the reflex, corresponding to hkl, but lying on the zero layer line. For electron diffraction patterns of a polycrystal, we have $I'_{hkl} = J_0 \lambda^2 |\bar{\Phi}|^2 \Omega^2 V' d^2_{hkl} \Delta p/(4\pi L\lambda)$, so that

$$|\bar{\Phi}^{rel}_{hkl}| = \sqrt{I'^{rel}_{hkl}/d^2_{hkl} p}.$$

Card : 3/3

POLAND/ Physical Chemistry - Crystals B-5

Abs Jour : Referat Zhur - Khimiya, No 4, 1957, 10978

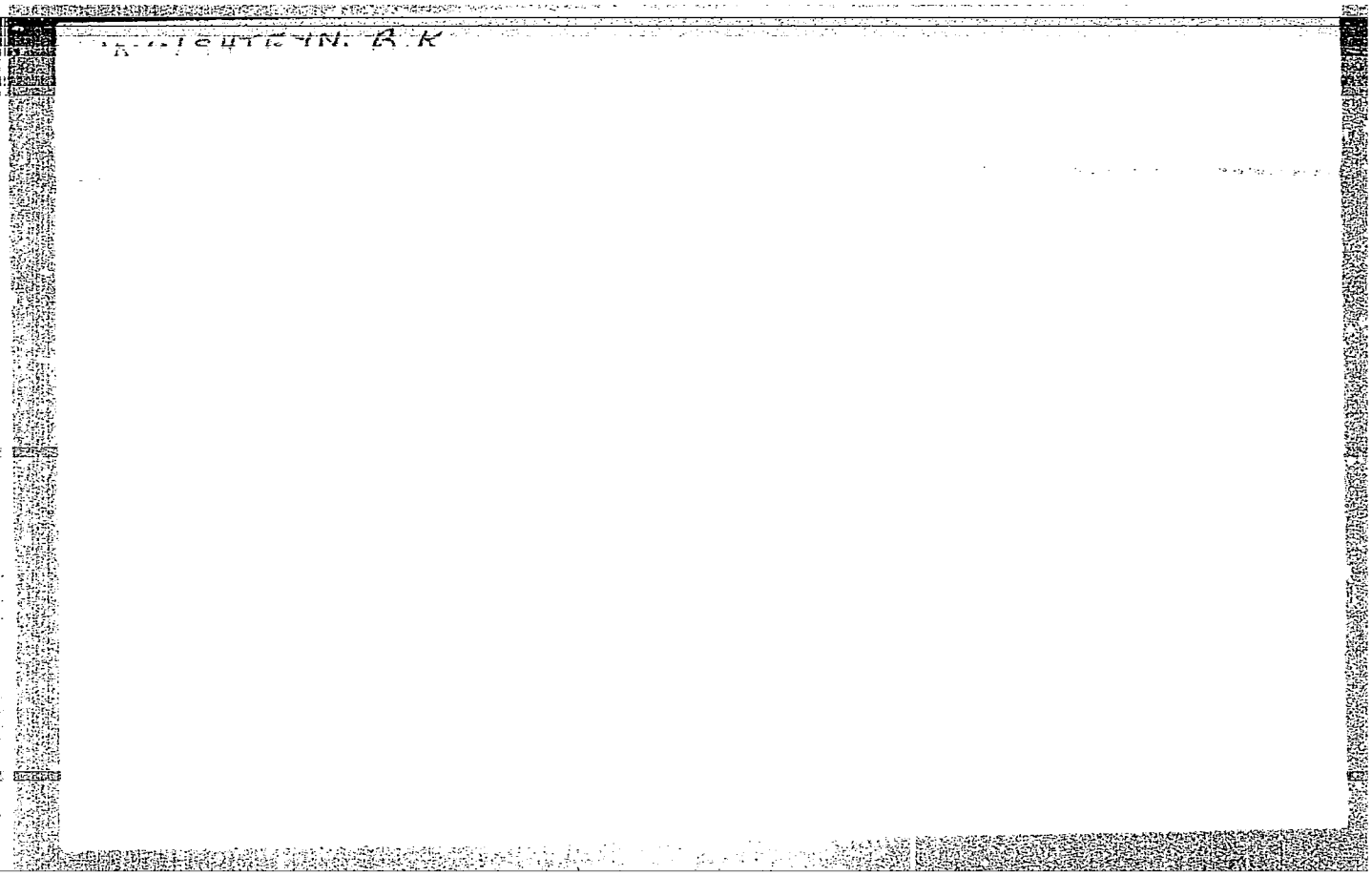
Author : Vaynshteyn, B.K., Stasova, M.M.
Title : Electronographic Investigation of Cryptohalite

Orig Pub : Kristallografiya, 1956, 1, No 3, 311-320

Abstract : Position of H atoms in the structure of cryptohalite $(NH_4)_2$ SiF_6 was investigated by the method of expressing electronographic data as Fourier potential series. Lattice period, a 8.35 kX. Determination of position of Si, F, N atoms has confirmed previous X-ray data. On projections and three-dimensional section of Fourier potential position of H atoms was determined. Tetrahedral NH groups are distributed, statistically, in six positions in each of which apices of tetrahedron, -- H atoms, are directed toward four of the 12 F atoms that surround the NH_4 group. Ph. gr. Fm3m. Analysis of shape and height of peaks of Si and F potentials indicates positive ionization of Si and negative of F.

Card 1/1

Inst. Crystallography



The problem is discussed in terms of lithium and oxygen (ionized and unionized) and lithium oxide. R. F. S. Hearmon

VAYNSHTEYN, B. K

USSR/Physical Chemistry. Crystals. B-5

Abs Jour: Ref Zhur-Khimiya, No 5, 1957, 14494

Author : M. M. Stasova, B. K. Vaynshteyn
Inst : Institute of Crystallography
Title : A More Precise Determination of the NH_4 Group Structure within the Ammonium Chloride Structure

Orig Pub: Tr. In-ta kristallogr. AN SSSR, 1956, vyp. 12, 18-24

Abstract: An electron diffraction study was made of polycrystallic NH_4Cl layers, obtained through sublimation in air on a celluloid base. The electron diffractions were microphotographed on a self-recording microphotometer MF-4. By the method of Fourier-potential (projection of (100) and size of (110)) the position of H atoms in NH_4Cl was determined at room temperature and it was precisely evaluated by the building of a differential synthesis (Fo-Fn). H atoms are located along lines N-Cl, forming a tetrahedron around the N atom and are statistically occupying 8-multiple position in F lim O_h^1. The distance

Card 1/2

USSR/Physical Chemistry. Crystals. B-5

Abs Jour: Ref Zhur-Khimiya, No 5, 1957, 14494

Abstract: N-H is equal to 0.98±0.04 A. The thermal motion of H atoms proceeds principally perpendicularly to line N-H. R = 0.152, taking into account the zero reflexes, $2 > B \gtrsim 1$. The position of the peak potential for H atom falls in the limits of error of the experiment with neutron diffraction data, giving the position of the nucleus (Levy, N. A., Peterson, S. W., Phys. Rev., 1952, 86, 766-770).

Card 2/2

VAYNSHTEYN, B.K., doktor fiziko-matematicheskikh nauk.

Conference on crystallography in Madrid. Vest.AN SSSR 26 no.8: 66-68 Ag '56. (MIRA 9:9)
(Madrid--Crystallography--Congresses)

VAYNSTEYN, B. K. and PINSKER, Z. G.

Institute of Crystallography, Moscow: "Structure Analysis by Electron Diffraction", Symposium 2-1 (Introductory Lecture); "The Investigation of Some Carbines and Nitrides of Crom Iron Tungsten Molybdenum by Electron Diffraction", (Section 5-15) papers submitted at the General Assembly and International Congress of Crystallography, 10-19 Jul 57, Montreal, Canada.

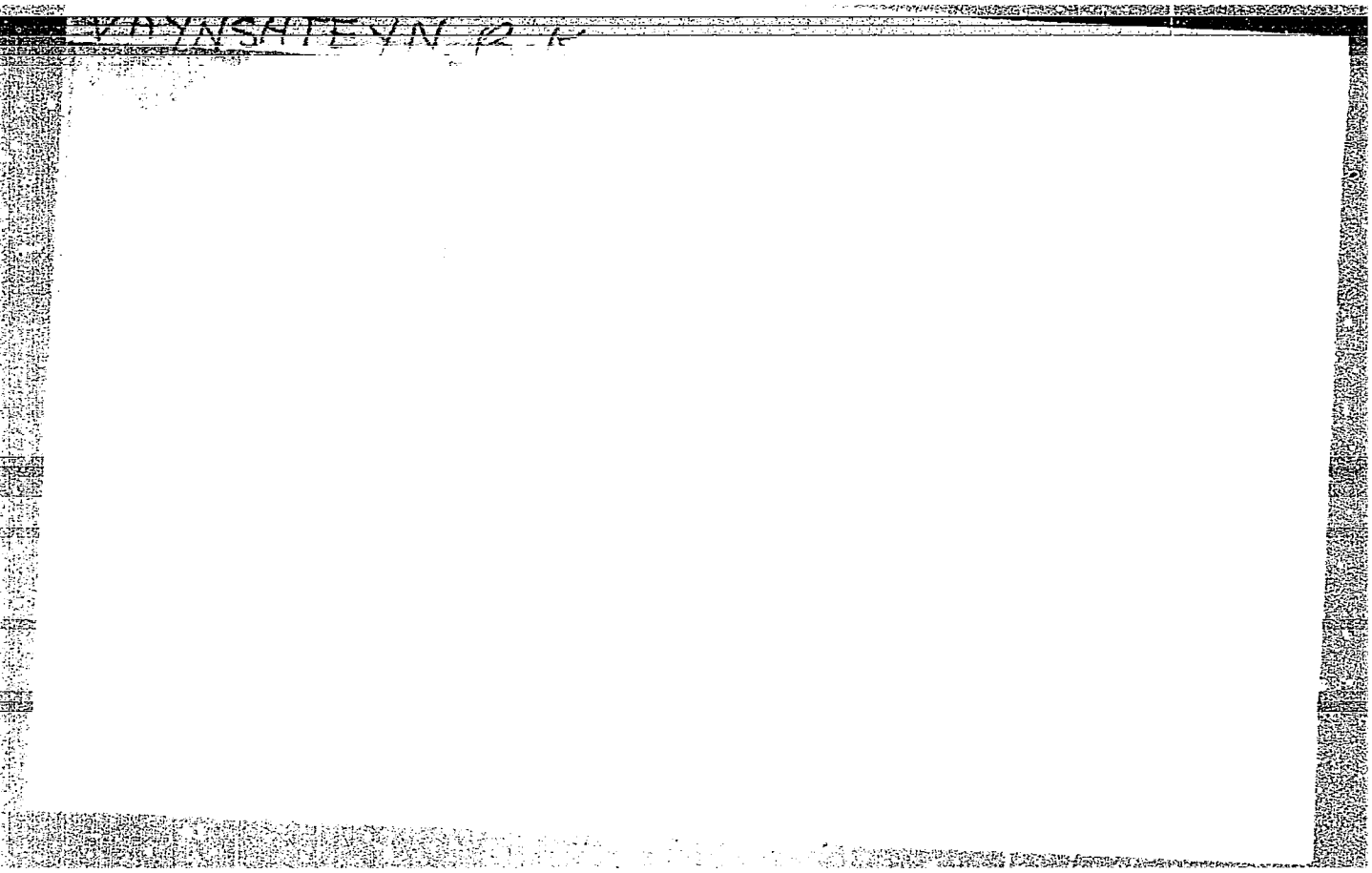
C-3,800,189

VAYNSTEYN, B. K.

Institute of Crystallography, Moscow'

"Refelction Intensities of Electron Difraction Patterns (General Case)" (Symposium 2-13) a paper submitted at the General Assembly and International Congress of Crystallography, 10-19 Jul 57, Montreal, Canada.

C-3,800,189



VAYNSHTEYN, B.K.

AUTHOR: Vaynshteyn, B.K. 70-3-4/20

TITLE: Reflexion intensities of electron diffraction patterns (general case). (Intensivnost' refleksov elektronogramm (Obshchiy sluchay)

PERIODICAL: "Kristallografiya" (Crystallography), 1957, Vol. 2, No.3, pp. 340 - 351 (U.S.S.R.)

ABSTRACT: The specimens to be used for structure analysis by electron diffraction are aggregates of a very large number of single small crystals (blocks). Hence, to compute the intensity one needs to consider, first, the law of scattering in a single block, and second, the structure of a specimen made up by these blocks.

For specimens used in structure analysis by electron diffraction, in most cases such conditions are satisfied when the kinematic theory is applicable, i.e. the blocks are of a small size. There are, however, cases when dynamic scattering is observed. Cases of scattering intermediate between the kinematic and the dynamic are also of interest; these so far have not been explained.

In solving the problem for the general case of the specimen consisting of blocks having any (various) thickness, in the first place the integral intensity of reflexion by a single

Card 1/3

Reflexion intensities of electron diffraction patterns (general case). (Cont.)

crystal is calculated. Subsequently, the structure of the specimen is taken into consideration; it is described by introducing the function of crystal distribution among angles $f(\alpha)$, as well as the function of their distribution according to their dimensions $p(A)$. A concrete consideration of the form $f(\alpha)$ for specimens of different types (mosaic monocrystals, textures, poly-crystals) leads to the introduction into the intensity formulae of L, a factor analogous to the Lorentz factor in X-ray analysis. The form of this factor L has been previously found by the author. The final formula includes also the function $p(A)$. If all the crystals (blocks) in the specimen are small, the general formula is reduced to a purely kinematic case, and the squares of structure factors enter into it. If the size of all the blocks exceeds the critical one, formulae of the dynamic theory are obtained, into which the structure factor enters in the first power. A general case may be also described, when the distribution function $p(A)$ is such that the specimen contains blocks the dimensions of which are both greater and smaller than the critical size. The intensity of reflexion from such specimens can be described in sufficient approximation by a

Reflexion intensities of electron diffraction patterns (general case). Cont.)

formula comprising both the first and the second power of the structure factor.

For the sake of comparison with experiment, precision data of Lennander, a Swedish author, have been used. He measured the intensities of electron scattering from polycrystalline specimens of aluminium, silver and gold. From the line profiles characteristic of each specimen the function p(A) has been obtained, followed by a calculation of the intensities. The values obtained are in good agreement with the experimental ones. In particular, an explanation of the deviations from the kinematic law f^2 for gold and silver is given. The scattering in aluminium is practically completely kinematic, which fact is quite natural since aluminium is the lightest of the elements investigated.

There are 9 figures, 2 tables and 21 references, of which 11 are Slavic.

ASSOCIATION: Institute of Crystallography, Ac.Sc. U.S.S.R. (Institut Kristallografii AN SSSR)

SUBMITTED: February 26, 1957.
AVAILABLE: Library of Congress

70-4-16/16

AUTHOR: Pinsker, Z.G. and Vaynshteyn, B.K.

TITLE: Structure analysis by electron diffraction (Elektronograficheskiy strukturnyy analiz)

PERIODICAL: "Kristallografiya" (Crystallography), 1957, Vol.2, No.4, pp. 552-572 (U.S.S.R.)

ABSTRACT: The progress of studies in the field of electron diffraction during the last thirty years is reviewed. The development of structure analysis by electron diffraction has been the most important trend of investigation, promoting the advance of the theory of electron scattering and of the experimental technique.

In establishing the limit of applicability of the kinematic theory, it is necessary to consider in addition to the crystal dimensions and ordinal numbers of components forming a given phase, also the degree of complexity of the structure and its symmetry. Various experimental data are considered which refer to revealing dynamic effects in examining experimental scattering curves, in measuring the banded structure on patterns obtained in a divergent beam and in measuring the effects of dynamic birefringence. The possibility of using the Kikuchi lines and Kikuchi bands for structure analysis is considered.

The general course of structure determination by the

70-4-16/16

Structure analysis by electron diffraction. (Cont.)

electron-diffraction method is given. A discussion is presented of the Fourier synthesis as well as of the advantages and peculiar features of the electron-diffraction structure analysis as compared to the X-ray and the neutron-diffraction method.

A description is given of the camera used in electron-diffraction analysis at the Institute of Crystallography. This is followed by a brief presentation of the results of the electron-diffraction studies carried out on hydrates of chlorides of some metals, clay minerals (seladonite); of the investigations of the position of hydrogen atoms in some inorganic and organic structures; of the studies of semi-conducting alloys of Bi, Cd, Tl, Sb, Se, Te and some other elements, including investigations of the amorphous structure of some phases of this kind. In connection with the discussion of the studies enumerated, many important peculiar features and possibilities of the electron-diffraction method are indicated, namely: precision of locating light atoms, study of the ionisation state of some atoms, a more precise determination of the composition of phases by the structure method, etc. There are 23 figures and 84 references, 58 of which are Slavic.

ASSOCIATION: Institute of Crystallography, Ac.Sc. USSR (Institut Kristallografii AN SSSR)

SUBMITTED: March 11, 1957.

AVAILABLE: Library of Congress.

Card 2/2

WAYNSHTEYN, B.K.

USSR/Solid State Physics - Structural Crystallography E-3

Abs Jour : Ref Zhur - Fizika, No 1, 1958, 882

Author : Vaynshteyn, B.K.
Inst :
Title : Normalization of the Intensity Curve in the Radial-Distribution Method.

Orig Pub : Dokl. AN SSSR, 1957, 112, No 4, 640-643

Abstract : The author considers the problem of the inversion of the intensity curve I(s) (where $s = 4\pi \sin \nu/\lambda$), which makes it possible to find the distribution functions in the investigated object and the number of nearest neighbors of a given atom. The ordinary method of normalization, based on the use of the damping of the oscillations of the functions I(s) at large values of s, involves a definite absolute and substantial relative normalization error. The author proposes that the entire curve I(s) as a whole be used for the normalization. The normalization

Card 1/2

VAYNSHTEYN, B. K., (Dr. of Physical-Mathematical Sciences)

"Structural Electronography"

for this work author received award by the Academy of Sciences of the USSR, 1957. Priroda, No. 2, 1958. pp. 113-114.

30-58-3-12/45

AUTHOR: Belov, N. V., Member, AS USSR
Vaynshteyn, B. K., Doctor of Physical and Mathematical Sciences

TITLE: The Congress of Crystallographers Held at Montreal (Kongress kristallografov v Monreale)

PERIODICAL: Vestnik Akademii Nauk SSSR, 1958, Nr 3, pp. 64-67 (USSR)

ABSTRACT: The fourth congress took place in the summer of last year and was attended by more than 700 scientists from 21 countries. The Soviet delegation consisted of N. V. Belov, L. M. Belyayev, G. B. Bokiy, Ye. G. Bronnikova, B. K. Vaynshteyn, G. S. Zhdanov, V. I. Iveronova, A. I. Kitaygorodskiy, Z. G. Pinsker and S. I. Shchetinin. They had a special number of the periodical "Crystallography" taken with them, which contained all reports delivered by the delegation on this congress, as well as a collection of scientific investigations "The Growth of Growth of Crystals". The work of this congress was carried out by 18 sections. In the plenary sessions lectures were delivered on topical problems of modern crystallography.

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The Congress of Crystallographers Held at Montreal 30-58-3-12/45

On the last two days special symposia on electronography and on the physical research methods of crystallography were held. Great importance was attached to consultations held outside the official sessions on various scientific problems. A large group of reports dealt with the theory, the method, and the new results obtained by investigations on the atomic structure of crystals. In the section "Progress in Structural Determination", A. I. Kitaygorodskiy among other things, dealt with the correlation theory among structural factors. Much attention was paid to electronic computors. Also new types of apparatus were on show in special exhibitions of this congress. N. V. Belov reported on new silicate structures. The authors regretted the fact that, in the field of structural determination, mainly only such structures were precisely dealt with as are already known. A report on general problems of crystal chemistry was delivered by G. Shdanov. The report by G. B. Bokiy and G. A. Kukina dealt upon the crystal chemistry of the complex compounds of bivalent platinums. A. I. Kitaygoroskiy spoke about several results achieved in the

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investigation of organic structures at the Institute for Organoelementary Compounds of the AS USSR. Z. G. Pinsker spoke about the results obtained by electronographic investigations of some carbides and nitrites. Radiographic investigations of displacements were dealt with by V. I. Iveronova. L. M. Belyayev delivered a report on the investigation of a distribution of activators in halide-crystals of alkaline metals. Ye. G. Bronnikovs gave a survey of the methods of breeding piezo-electric crystals in the USSR. On a plenary session the Soviet delegation showed the film. "The crystallization of two-teased diphenylamine (dvulistnikov difenilamine). In the section dealing with the symmetry theory N. V. Belov, reported on the 1651 group of the spatial black- and white, as well as on groups of colored symmetry. In a symposium Z. G. Pinsker and B. K. Vaynshteyn delivered a lecture on problems of structural electronography and its development in the USSR. B. K. Vaynshteyn gave a report on electron dispersion by means of crystalline polydispersion preparations. Parallel to the congress a full session of the

The Congress of Crystallographers Held at Montreal 30-58-3-12/45

Society of Crystallographers was held, on which occasion new elections were finally carried out as the result of which N. V. Belov was elected vice-president for 6 years and other Soviet scientists were elected members of various commissions. The Soviet delegation was able to visit scientific research laboratories of the universities of Montreal and in the vicinity of this town, as well as the National Research Center in Ottawa. They were able to convince themselves of the high level of these institutions. The congress showed that crystallography is developing according to plan.

Card 4/4

SOV/70-3-1-5/26

AUTHORS: Vaynshteyn, B.K. and Kurdyumova, R.N..

TITLE: Cubic Modification of $(NH_4)_2GeF_6$ (Kubicheskaya modifikatsiya $(NH_4)_2GeF_6$)

PERIODICAL: Kristallografiya, 1958, Vol 3, Nr 1, pp 29 - 31 + 1 plate (USSR)

ABSTRACT: According to Hoard and Vincent (Ref 1), $(NH_4)_2GeF_6$ has a hexagonal structure with a = 5.85, c = 4.775 Å ; space group D_{3d}^3 . The present authors have established by means of electron diffraction the existence of a cubic modification of $(NH_4)_2GeF_6$. The cubic structure is assumed to be that shown in Figure 3. The Ge atom is at 4(a)000 , the N atoms are at 8(c)1/4 1/4 1/4 , the F atoms are at 24(e) x 00 , and the space group is O_h^5 . From experimental structure amplitudes, the one-dimensional potential distribution was found and hence a value was obtained for the parameter x which was found to be equal to 0.203 . This gives the Ge-F distance

Card1/2

Cubic Modification of $(NH_4)_2GeF_6$

equal to 1.72 ± 0.01 kX . The position of the H atoms was not determined but it seems likely that it is the same as in cryptohalite (Ref 3).
There are 3 figures, 1 table and 7 references, 3 of which are English and 4 Soviet.

ASSOCIATION: Institut kristallografii AN SSSR (Institute of Crystallography of the Ac.Sc.USSR)

SUBMITTED: April 25, 1957

AUTHORS: Stasova, M.M. and ~~Vaynshteyn, B.K.~~ 70-3-2-2/26

TITLE: The Electronographic Determination of the Structure of Tl_2Se (Elektronograficheskoye opredeleniye struktury Tl_2Se)

PERIODICAL: Kristallografiya, 1958, Vol 3, Nr 2, pp 141 - 147 (USSR).

ABSTRACT: The crystal structure of Tl_2Se has been determined. The unit cell is tetragonal with a = 8.52 ± .02 and c = 12.68 ± .03 Å and space group $C_{4h}^3 = P4/n$. Z = 10. The structure consists of empty tetrahedra of Tl atoms joined by layers of Se atoms. Linear groups Tl_2Se lie on the lines (0, 1/2, z) and (1/2, 0, z) and between them there is room for the introduction of extra interstitial Se atoms making the composition non-stoichmetric.
As well as powder electronograms, texture diagrams were obtained from the specimens, the texture axis being c. The space group is pseudo $D_{4h}^8 = P4/ncc$ and only the very weak reflections 101 and 111 indicate the less symmetrical groups $C_{4h}^3 = P4/n$ or $C_{4h}^4 = P4_2/n$. The specific gravity

Cardl/2

The Electronographic Determination of the Structure of Tl_2Se 70-3-2-2/26

was found pyknometrically to be 8.62. 107 reflections were recorded and from them Patterson sections were calculated. In terms of the P4/ncc group, the atomic parameters were found to be:

Tl (16); x y z with x=0.140, y=0.148, z=0.081,
Se (8) ; x x 1/4 with x = 0.340,
Se (4) ; 0 1/2 z with z=0 (having weighting 1/2)
Tl (4) ; 0 1/2 z with z = 1/4.

108 observed and calculated structure amplitudes are tabulated. There are 7 figures, 2 tables and 6 references, 2 of which are Soviet, 3 German and 1 English.

ASSOCIATION: Institut kristallografii AN SSSR
(Institute of Crystallography of the Ac.Sc.USSR)

SUBMITTED: September 23, 1957.

Card 2/2

AUTHOR: Vaynshteyn, B.K. 70-3-3-6/36

TITLE: Certain Data on the Crystal Chemistry of Hydrogen (Nekotoryye dannyye po kristallokhimii vodoroda)

PERIODICAL: Kristallografiya, 1958, Vol 3, Nr 3, pp 293 - 297 (USSR).

ABSTRACT: From published data by many authors values of the effective radius of the hydrogen atom in crystals of various kinds are collected. For ionic structures, the effective radius is 1.5 A, for metallic 0.41 and for covalent, 0.30 - 0.35. Deviations from additivity, particularly in covalent C-H bonds, where for the usual organic case of tetrahedral carbon atoms the appropriate value is about 1.12 A are noted. Bond lengths are reviewed under the headings: hydrides, molecular compounds or groups (C-H bonds, H-N and O-H bonds), hydrogen bonds. Particular reference is made to Bernal (Usp. Khim. Vol 25, pp 643-661, 1956) and to Sokolov (Usp.Fiz.Nauk, 1955, Vol 57, pp.206-278). There are 28 references, 13 of which are Soviet and 15 English.

ASSOCIATION: Institut kristallografii AN SSSR (Institute of Crystallography, Ac.Sc.USSR)

SUBMITTED: January 15, 1958

Card 1/1

AUTHORS: Vaynshteyn, B.K. and Pinsker, Z.G. 70-3-3-19/36

TITLE: The Horizontal EG Electronograph (Gorizontal'nyy elektronograf EG)

PERIODICAL: Kristallografiya, 1958, Vol 3, Nr 3, pp 358 - 361 (USSR).

ABSTRACT: The latest model of electronograph designed by the authors at the Institute of Crystallography is described. The beam runs horizontally and the maximum accelerating voltage is 75K. The plate size is 13 x 18 cm and the specimen-film distance is 700 mm. The line broadening to instrument inaccuracies is about 0.05 mm; for λ = 0.05 A and line radius r = 50 mm this corresponds to a spacing error of 0.001 A. The multiplet structure of the 111, 222 and 422 line of MgO are resolved. There is a small secondary gun for keeping the specimen discharged. The table size is 150 x 60 cm and the stabilised HT supplies are housed in a cabinet 73 x 60 x height 150 cm. A hairpin filament sending a beam through a 0.1 mm aperture in the Wehnelt cylinder is used and it can be displaced, while operating, in two mutually perpendicular directions. The magnetic lens has 20 000 turns of 0.51 mm dia. wire. The specimen chamber is fitted with windows, a universal specimen mount and internal illumination. A central valve divides the

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apparatus into two independent vacuum chambers, film box + camera body and specimen chamber + gun installation. The apparatus uses a mechanical forevacuum pump (RVN-20) and an oil diffusion pump (TsVL-100). With the oil pump hot, working pressure can be reached in 4 min. Safety devices cut off the HT if the cupboard is opened. The apparatus is in production. (It is to be seen working at the Brussels Fair .)
There are 2 figures and 7 Soviet references.

ASSOCIATION: Institut kristallografii AN SSSR (Institute of Crystallography, Ac.Sc. USSR)

SUBMITTED: February 22, 1958

SOV/70-3-4-3/26

AUTHORS: Vaynshteyn, B.K. and Aybers, Dzh.A.(J.A. Ibers)

TITLE: The Atomic Scattering Factors for Electron Scattering of Elements of the Third Period (Atomnyye amplitudy rasseyaniya elektronov dlya elementov tret'yego perioda)

PERIODICAL: Kristallografiya, 1958, Vol 3, Nr 4, pp 416-419 (USSR)

ABSTRACT: The authors were appointed by the Electron Diffraction Commission of the International Union of Crystallography to prepare tables of the atomic scattering factors for the third volume of the International Tables. Values of the factors (f_e) for the elements 1 to 18 are presented here for criticism. They are quoted to two places of decimals at intervals of $(\sin\theta / \lambda) \times 10^{-8}$ of 0.05. f_e is calculated from f_x (the X-ray scattering amplitude) by $f_e = (Z - f_x)(\sin\theta / \lambda)^{-2}$ and f_x is taken from values calculated by the Hartree-Fock

Card 1/2

The Atomic Scattering Factors for Electron Scattering of Elements of the Third Period

method principally, but also by the method of assuming a hydrogen-like atom (He and Si) and by interpolation (F, Al, Cl).
There are 1 figure, 2 tables and 7 references, 1 of which is Soviet, 1 German and 5 Swedish.

ASSOCIATION: Institut kristallografii AN SSSR, Moskva
(Institute of Crystallography of the Ac.Sc.USSR, Moscow) - B.K.Vaynshteyn.
(J.A. Ibers of California)

SUBMITTED: April 22, 1958

AUTHORS: Voronova, A.A. and ~~Zaynshteyn, B.K.~~ SOV/70-3-4-7/26

TITLE: The Electronographic Investigation of the Crystal Structure of $CuCl_2.3Cu(OH)_2$ (Elektronograficheskoye issledovaniye $CuCl_2.3Cu(OH)_2$)

PERIODICAL: Kristallografiya, 1958, Vol 3, Nr 4, pp 444-451 (USSR)

ABSTRACT: $CuCl_2.3Cu(OH)_2$ was found to be monoclinic with space group $C_{2h}^2 = P2_1/m$ and cell dimensions $a = 5.73$, $b = 6.12$, $c = 5.63$ A and $\beta = 93^\circ 45'$ with $Z = 1$. It is isomorphous with the more stable compound $CuBr_2 3Cu(OH)_2$. The minerals atakamite and para-atakamite have the same formula but the former is orthorhombic and the latter hexagonal. For electronographic investigation, the specimen was deposited on a celluloid film and covered with a second film. Patterns of several other phases were also obtained. From texture pictures, the cell dimensions were obtained and the intensities were measured. From these, by means of Patterson projections, potential projections on Oyz and xOz were calculated. The known

Card 1/3

The Electronographic Investigation of the Crystal Structure of $CuCl_2 \cdot 3Cu(OH)_2$

structure of the Br compound was used as a guide and the parameters of the Cl compound were found to be very similar: Cu_I 2(a) positions with (x,y,z) = (0,0,0); Cu_{II} 2(e) with (0, 0.25, 0.50); Cl 2(e) with (0.392, 0.25, 0.210); OH_I 2(e) with (0.85, 0.25, 0.883); OH_{II} 4(f) with (0.857, 0, 0.324). The compound has a layer structure with the Cu atoms distributed pseudo-hexagonally in the Oyz plane, the Cl and OH ions lying on both sides of this plane forming a close-packed layer. The cations are at the centres of deformed octahedra, Cu_I surrounded by 2 OH_I, 2 OH_{II} and 2 Cl, and Cu_{II} surrounded by 4 OH_{II}, 1 OH_I and 1 Cl.

SOV/70-3-4-7/26

The Electronographic Investigation of the Crystal Structure of $CuCl_2 \cdot 3Cu(OH)_2$

There are 8 figures, 4 tables and 15 references, 5 of which are Soviet, 3 English and 7 Swedish.

ASSOCIATION: Institut kristallografii AN SSSR
(Institute of Crystallography, Ac.Sc.USSR)

SUBMITTED: April 16, 1958

Card 3/3

SOV/70-3-4-8/26

AUTHORS: Vaynshteyn, B.K., Lobachev, A.N. and Stasova, M.M.

TITLE: Electronographic Determination of the C-H Distance in Certain Paraffins (Elektronograficheskoye opredeleniye rasstoyaniya C-H v nekotorykh parafinakh)

PERIODICAL: Kristallografiya, 1958, Vol 3, Nr 4, pp 452-460 (USSR)

ABSTRACT: The distance C-H in paraffins was found to be 1.123 ± 0.015 KX which greatly exceeds the usually assumed value of 1.09 KX . The paraffins $C_{18}H_{38}$(I), $C_{30}H_{62}$(II) and a mixture (III) of composition about $C_{28}H_{58}$ with melting points 28°, 66.2° and 53.5°, respectively, were re-examined by electron diffraction. Their orthorhombic pseudocells were almost the same (a = 7.458, b = 4.977. c = 2.534 (I) KX) . The hk0 zones of reflections were carefully recorded and photometered giving tables of $\emptyset_{hko.obs.}$ up to 260. As the structure, except for the exact position of the hydrogen atoms, was known the scattering curve for carbon could be recalculated. The appropriate temperature factor was B = 4 . Difference syntheses for the H positions were finally calculated

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Electronographic Determination of the C-H Distance in Certain Paraffins

SOV/70-3-4-8/26

giving distances in KX of:
C-C (I) 1.538, (II) 1.527, (III) 1.510
$C-H_I$ (I) 1.140, (II) 1.121, (III) 1.102
$C-H_{II}$ (I) 1.127 (II) 1.140, (III) 1.112
and angles H_I-C-H_{II} of (I) 114°, (II) 107.5°, (III) 102°.

There are 5 figures, 3 tables and 23 references, 14 of which are Soviet, 1 Italian, 5 English and 3 Swedish.

ASSOCIATION: Institut kristallografii AN SSSR
(Institute of Crystallography, Ac.Sc.USSR)

SUBMITTED: March 11, 1958

Card 2/2

SOV/70-3-4-20/26

AUTHORS: Dvoryankin, V.F. and Vaynshteyn, B.K.

TITLE: A Low-temperature Crystal Holder for the Electronograph EG (Nizkotemperaturnyy kristalloderzhatel' dlya elektronografa EG)

PERIODICAL: Kristallografiya, 1958, Vol 3, Nr 4, pp 504-506 (USSR)

ABSTRACT: A crystal holder attachment for the standard EG horizontal-beam electronograph of the Institute of Crystallography is described which can enable a specimen grid to be cooled to liquid N_2 temperature (with drawing). The grid holder is at the end of a tube, which can be filled with liquid N_2, protruding into the specimen space. The channel through which the beam passes along the axis of the instrument can be rotated about the cooling tube to cut off the beam which may heat the specimen very noticeably. The cooling tube entering the camera is surrounded by a double-walled screen also entering the camera which can also be filled with liquid N_2 to act as a guard tube. The copper crystal holder is itself surrounded, except for entrance and outlet apertures, with a copper box connected to the cooled guard tube. Operation without a guard tube proved

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A Low-temperature Crystal Holder for the Electronograph EG

unsatisfactory. A Cu-constantan thermocouple is provided to measure the specimen temperature. The mechanism by which the specimen carrier can be moved is, except for rotation about the tube, mentioned but not described. It is recommended that a cold trap immediately above the pump should also be fitted as otherwise any condensible vapours will contaminate the specimen slightly in spite of the guard chamber. Specimen pictures from NH_4Br phases (II) and (III) are reproduced.
There are 7 references, 3 of which are Soviet, 1 in English and 3 Scandinavian.

ASSOCIATION: Institut kristallografii AN SSSR
(Institute of Crystallography of the Ac.Sc.USSR)

SUBMITTED: May 12, 1958

SOV/70-3-5-1/24

AUTHOR: Vaynshteyn, B.K.

TITLE: Quantitative Relations in Conditioned (Generalised) Fourier Projections of the Electron Density in Crystals (Kolichestvennyye sootnosheniya v uslovnykh proyektsiyakh Fur'ye elektronnoy plotnosti kristallov)

PERIODICAL: Kristallografiya, 1958, Vol 3, Nr 5, pp 527-538 (USSR)

ABSTRACT: The form of the peaks in conditioned (generalised) projections of the electron density in crystals is discussed mathematically. Formulae are given for calculating the heights of these peaks, for finding the accuracy of the values of the electron density and for the horizontal and vertical co-ordinates of the atoms in such projections. Modulus projections are also considered.
The paper is a detailed analysis of the properties of generalised Fourier projections in unspecific mathematical terms. Various theorems concerning the functions used are developed and formulae for the parameters of the projection are deduced. The references collect most of the previously published material on such projections.

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SOV/70-3-5-1/24

Quantitative Relations in Conditioned (Generalised) Fourier Projections

There are 7 figures and 16 references, 9 of which are Soviet and 7 English, and 1 table.

ASSOCIATION: Institut kristallografii AN SSSR
(Institute of Crystallography of the Ac.Sc.USSR)

SUBMITTED: July 11, 1958

Card 2/2

AM4008921 BOOK EXPLOITATION S/

Vaynshteyn, Boris Konstantinovich

Diffraction of X-rays on chain molecules (Difraktsiya rentgenovy*kh luchey na tsepny*kh molekulakh) Moscow, Izd-vo AN SSSR, 63. 0371 p. illus., biblio., index. Errata slip inserted. 4,000 copies printed. At head of title: Akademiya nauk SSSR. Institut kristallografii.

TOPIC TAGS: chain molecule, polymer, polymer chain, x-ray diffraction, chain molecule aggregate, chain molecule structure, molecule arrangement in polymer, diffraction pattern analysis, diffraction pattern synthesis, parallel chain molecules, nonparallel chain molecules, amorphous polymer

PURPOSE AND COVERAGE: The monograph is devoted to the theory of diffraction of x-rays by chain molecules and their aggregates (polymers). It treats the prediction of the diffraction pattern of

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a chain molecule whose structure is specified and in which the mutual arrangement of the molecule aggregate is defined by means of certain functions. It also treats the inverse problem, namely the deductions that can be drawn from an observed diffraction pattern regarding the structure of a given polymer and its component molecules, and under what conditions these deductions are valid. Various examples from the field x-ray diffraction of molecules are presented frequently to illustrate the different models or effects. A complete classification of possible types of structures of chain molecules and their mutual arrangement in polymers is included for completeness.

TABLE OF CONTENTS [abridged]:

AM4008921

SUB CODE: CH, PH SUBMITTED: 14Apr63 NR REF SOV: 048

OTHER: 138 DATE ACQ: 07Oct63

Card 3/3

VAYNSHTEYN, Boris Konstantinovich, doktor fiz.-mat. nauk; PINSKER, Zinoviy Grigor'yevich, doktor khim. nauk; LYUSTIBERG, V.F., inzh., ved. red.; KHIMCHENKO, N.V., kand.tekhn. nauk; SOROKIN, T.M., tekhn. red.

[Electron diffraction camera for structural studies]Elektronograf dlia strukturnykh issledovanii. Moskva, Filial Vses. inta nauchn. i tekhn. informatsii, 1958. 13 p. (Peredovoi nauchno-tekhn. i proizvodstvennyi opyt. Tema 33. No.P-58-100/5) (MIRA 16:3)

(Electron diffraction apparatus)

SOV/70-3-6-2/25

AUTHOR: Vaynshteyn, B.K.

TITLE: Functional Projections in the Structural Analysis of Crystals (Funktsional'nyye proyektsii v strukturnom analize kristallov)

PERIODICAL: Kristallografiya, 1958, Vol 3, Nr 6, pp 659-663 (USSR)

ABSTRACT: A function projection is a projection derived from the electron density distribution by multiplication with an arbitrary projecting function $f(x,y,z)$. This projection can be calculated by combining a conditioned projection and the Fourier coefficients of the expansion of $f(x,y,z)$. All known and proposed new forms of projection can be regarded as variant functional projections. The functional projection is:

$$\sigma_f(xy) = c\int_0^1 \rho\,(xyz)\; f\,(xyz)\; dz \qquad (1)\,.$$

It can be decomposed by expanding $f(x,y,z)$ as:

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Functional Projections in the Structural Analysis of Crystals

$$f(xyz) = A_c(xy) + \sum_{L=1}^{\infty} A_L(xy) \cos\left[2\pi Lz\right] + \sum_{L=1}^{\infty} B_L(xy) \sin\left[2\pi Lz\right] \quad (5),$$

$$A_o = \int_0^1 f(xyz)\, dz \quad (6a),$$

$$A_L = 2\int_0^1 f(xyz) \cos\left[2\pi Lz\right] dz \quad (6б),$$

$$B_L = 2\int_0^1 f(xyz) \sin\left[2\pi Lz\right] dz \quad (6B)$$

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and hence:

$$\sigma_f(xy) = A_0(xy)\sigma_0(xy) + \sum_{L=1}^{\infty} A_L(xy)\sigma_{\cos L}(xy) + \sum_{L=1}^{\infty} B_L(xy)\sigma_{\sin L}(xy) \quad (8).$$

1) If $f(x,y,z) \geq 1$ we have the ordinary Fourier projection but there are further variants if $f = 1$ in the region $z_1(xy) \leq z \leq z_2(xy)$ and $f = 0$ otherwise. This gives - 2)

$$A_L = \frac{2}{L}(\sin [2\pi Lz_2] - \sin [2\pi Lz_1]) \quad (11)$$

$$B_L = \frac{2}{L}(\cos[2\pi Lz_1] - \cos [2\pi Lz_2])$$

- Booth's bounded projection.

Functional Projections in the Structural Analysis of Crystals

3) $f(xyz) = \delta(z - z_1)$ and $A_o = 1$, $A_L = 2\cos[2\pi L z_1]$, $B_L = 2 \sin [2\pi L z_1]$. This is a plane section at height z_1 - the usual three-dimensional section.

4) Inclined plane parallel-sided bounded projection and various bounded projections of non-uniform thickness are generated by using arbitrary functions for $z_1(xy)$ and $z_2(xy)$. The expressions for A_L and B_L are as in 2).

5) Various inclined and curved plane sections are as for the ordinary section but z_1 is a function of x and y.

6) Generalised projection - $f(xyz) = \cos 2\pi L_1 z$ or $\sin 2\pi L_1 z$, all A_L and $B_L = 0$ except for $L = L_1$ when $A_{L_1} = B_{L_1} = 1$.

7) Generalised projection displaced along z so that $f(xyz) = \cos [2\pi L_1 (z - z_1)]$.

Functional Projections in the Structural Analysis of Crystals

8) Modular projection where

$$|\sigma_L(xy)| = \sqrt{\sigma^2_{\cos\ L}(xy) + \sigma^2_{\sin\ L}(xy)} \qquad (16)$$

9) Generalised projection with curved planes where

$$f(xyz) = \cos\left[2\pi L(z - z_1(xy))\right] .$$

10) Linear combination of generalised projections where the coefficients are sums of the coefficients in the individual projections.

11) "Perspective function ", for example $f(xyz) = z$.

Here:

$$A_o = 1, \quad A_L = 0, \quad B_L = -1/\pi L \qquad (17) .$$

Elaborations of this are also possible.

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Functional Projections in the Structural Analysis of Crystals

12) Weighted projection. f(xyz) is related to some density distribution - for example - of all the heavy atoms A_L and B_L must be calculated from the general formula. There are 6 figures and 13 references, 9 of which are Soviet and 4 English.

ASSOCIATION: Institut kristallografii AN SSSR (Institute of Crystallography of the Ac.Sc.USSR)

SUBMITTED: September 8, 1958.

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SOV/20-120-3-24/67

AUTHORS: Vaynshteyn, B. K., Lobachev, A. N.

TITLE: The C - H Distance in the Crystal Structure of Paraffins (Rasstoyaniye C - H v kristallicheskoy strukture parafinov)

PERIODICAL: Doklady Akademii nauk SSSR, 1958, Vol. 120, Nr 3, pp. 523-525 (USSR)

ABSTRACT: The paraffins C_nH_{2n+2} are a useful object in electric diffraction analysis. The present paper investigates the paraffins $C_{18}H_{38}$ (I), $C_{30}H_{62}$ (II) as well as a paraffin with the melting point 53,5° (III). The latter has already been investigated on an earlier occasion (Ref 3). The elementary cells of all these thin paraffins in thin layers are practically equal to one another. The authors here investigate only projections (with respect to the reflections hk0), because the C - H distance occurs in an undistorted form in this case. The following operations were carried out in the course of the investigation:
1) Taking of electron diffraction pictures obtained by electron transmission.
2) Determination of elementary cells, 3) Microphotometrization

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of the rings hk0 of the electronographs taken vertically to the beam. 4) Transition from intensities to amplitudes. 5) Construction of Fourier (Fur'ye) syntheses of a certain potential $\varphi'(x,y)$ on a certain plane. 6) Determination of an experimental curve of the elementary scattering of carbon. - A further number of operations is then enumerated. Also the estimation of accuracy is discussed in short. A diagram illustrates by way of an example the total synthesis and the difference-n-synthesis for $C_{30}H_{62}$. The values obtained for the C - H distances are shown in form of a table. There is no reason to believe in the existence of any real difference between $C - H_1$ and $C - H_2$, nor of the existence of any such difference in the paraffins under investigation. Other bonds may influence the C - H distance considerably. There are 1 figure, 1 table, and 9 references, 6 of which are Soviet.

ASSOCIATION: Institut kristallografii Akademii nauk SSSR (Institute of Crystallography, AS USSR)

SOV/2o-12o-3-24/67

The C - H Distance in the Crystal Structure of Paraffins

PRESENTED: February 5, 1958, by N. V. Belov, Member, Academy of Sciences, USSR

SUBMITTED: January 31, 1958

1. Methanes--Crystal structure 2. Methanes--Synthesis
3. Methanes--Electron diffraction analysis

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VAINSHTEIN, B.K.

"New Determinations of Hydrogen Atoms Positions and the Accuracy of the Electron Diffraction Structure Analysis"

a report presented at Symposium of the International Union of Crystallography Leningrad, 21-27 May 1959

24(2) SOV/26-59-10-9/51

AUTHOR: Vaynshteyn, B.K., Doctor of Physical and Mathematical Sciences

TITLE: Advances in Crystallography (The International Fedorov Conference)

PERIODICAL: Priroda, 1959, Nr 10, pp 55-57 (USSR)

ABSTRACT: The 230 ways of arranging asymmetric objects in space were discovered independently during the last decade of the 19th century by Ye.S. Fedorov, A. Schoenflies and W. Barlow. From 21 to 27 May 1959, the crystallographers of the USSR carried out an International Crystallographic Conference which was held at Leningrad and timed for the 40th anniversary of the death of Soviet crystallographer Ye.S. Fedorov. It has been organized by the Akademiya nauk SSSR (AS USSR) and the MSK, i.e. Mezhdunarodnyy Soyuz kristallografov (International Union of Crystallographers). The 600 participants came from the USSR, USA, France, Great Britain, Czechoslovakia and other countries. The audience heard

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Advances in Crystallography (The International Fedorov Conference)

the lecture of Academician N.V. Belov from the Institut kristallografii AN SSSR (Institute of Crystallography of the AS USSR) on the importance of Fedorov's research work and a new conclusion of the so-called "Fedorov Groups". American crystallographer W.H. Zachariasen who investigated the structure of uranium compounds and transuranium elements, reported on the results of investigating the uranyl compounds. In these compounds, one atom of uranium usually forms two linear short bonds with the atom of oxygen. According to G.B. Bokiy from the MGU, analogic linear groups are found in the osmium and ruthenium compounds. N.P. Trifonov (USSR), St. Novák (CSR) and some other scientists reported on the use of electronic computing devices analyzing crystallographic information. In this connection R. Pepinsky (USA) mentioned that the computer IBM-707 has been established at the "P. Groth Institute" of the University of Pennsylvania. It is planned to establish a similar center in the USSR. Some new results of electronographic analysis were given in the

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Advances in Crystallography (The International Fedorov Conference)

lectures of Z.G. Pinsker, S.A. Semiletov, B.B. Zvyagin and the author. N.M. Popov reported on a new electronograph with a capacity of 400 kilowatts. The participants of the conference also saw the Soviet motion picture "Obrazovaniye kristallov" (The Formation of Crystals) by A.V. Shubnikov and V.F. Parvov. Besides numerous foreign scientists, the article mentions Soviet scientists G.S. Zhdanov, Professor A.I. Kitaygorodskiy, B.N. Delone, I.S. Zheludev, V.L. Indenbom and P.A. Akishin.

ASSOCIATION: Institut kristallografii Akademii nauk SSSR/Moskva (Crystallographic Institute of the AS USSR/Moscow)

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SOV/70-4-1-1/26

AUTHOR: Vaynshteyn, B. K.

TITLE: A New Type of Relation Between Structural Factors (Novyy tip svyazey mezhdu strukturnymi faktorami)

PERIODICAL: Kristallografiya, 1959, Vol 4, Nr 1, pp 3-12 (USSR)

ABSTRACT: Exact equations are deduced, which, under certain conditions, relate structural factors belonging to mutually parallel layers of the reciprocal lattice. These equalities are valid in the general case of the absence of a centre of symmetry and in structures with several kinds of atoms. In the most general case the equalities pass into inequalities and a quantitative estimate of this situation is given. The type of equations discussed are distinctly different from those of Harker and Kasper, of Zachariasen and of Sayre. They derive from the conditioned projection

$$\sigma_L(x,y) = \frac{1}{A}\sum_{L=\text{const.}} F(hkL)\exp\left[-2\pi i(hx + ky)\right]$$

The molecular projection is derived from the L^{th} layer and

$$\sigma_L(x,y) = \left(\sigma^2_{\cos L}(x,y) + \sigma^2_{\sin L}(x,y)\right)^{1/2}.$$

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A New Type of Relation Between Structure Factors

Also $s = 4\pi \sin\vartheta/\lambda$, $s_{min} = 2\pi L/c$ and $s_L^2 = s^2 - s_{min}^2$,

$$\varkappa_L(s) = \left(\sum_i f_i^2 (s_{hk0})\right)^{1/2} \Big/ \left(\sum_i f_i^2 (s_{hkL})\right)^{1/2} \quad \text{and}$$

$$\dot{F}(hkL) = F(hkL)\, \varkappa_L(s)$$

$|\dot{\sigma}_L|$ denotes a modular projection and if there is overlapping $\sigma_o(x,y) \geqslant |\dot{\sigma}_L(s,y)|$. If overlapping is inappreciable $|\dot{\sigma}_L(x,y)|^2 = \sigma_o^2(x,y)$, σ_L is, in general, complex.

$$F_{\underline{H}}(|\sigma|^2) = \frac{1}{A} \sum_{\underline{H}} F_{\underline{H}}(\sigma)\, F^*_{\underline{H} - \underline{H}'}(\sigma),$$

hence $\sum_{hk} F(hk0) F^*(h - h', k - k', 0) =$

$$= \sum_{hk, L_1 = \text{const}} \dot{F}(hkL_1)\, \dot{F}^*(h - h', k - k', L_1) =$$

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A New Type of Relation Between Structure Factors

$$= \sum_{hk, L_2 = \text{const}} \dot{F}(hkL_2)\, \dot{F}(h - h', k - k', L_2) = \ldots\ldots$$

This is the basic equation. If $h', k' = 0$ Parsival's equations are obtained

$$\sum_{hk} |F(hk0)|^2 = \sum_{hk, L_1 = \text{const}} |\dot{F}(hkL_1)|^2 = \sum_{hk, L_2 = \text{const}} |\dot{F}(hkL_2)|^2 = \ldots$$

which are used for normalisation. If they are not fulfilled, overlapping is indicated and the basic equation is inapplicable. Using unitary structure factors $\hat{F}$,

$$\sum_{hk} \hat{F}(hk0)\, \hat{F}^{*}(h - h', k - k', 0) = \sum_{hk, L_1 = \text{const}} \hat{F}(hkL_1) \hat{F}^{*}(h-h', k-k', L_1), \quad \text{etc.}$$

The variable index k can be suppressed giving

$$\sum_{h} F(h00) F^{*}(h-h', 00) = \sum_{h, K_1, L_1 = \text{const}} \dot{F}(hK_1, L_1) \dot{F}^{*}(h - h', K_1, L_1)$$

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A New Type of Relation Between Structure Factors

The basic equation was verified for a hypothetical two-dimensional model with different kinds of atoms for both centro- and non-centro-symmetrical cases. For further verification the hk0 and hkl layers of $(CH_2CONH)_2$, diketopiperazine, were used. Possible ways of using the equations are discussed, the use of modern computing techniques being suggested. A possible use is the experimental measurement of structure factors too far inside or outside the sphere of reflexion. If there is overlapping, the basic equation becomes an inequality. The basic equation is compared with other relationships (Sayre, Zachariasen) and is shown to be connected with them. There are 5 figures, 2 tables and 9 references, 5 of which are Soviet.

ASSOCIATION: Institut kristallografii AN SSSR
(Institute of Crystallography, Academy of Sciences, USSR)

SUBMITTED: December 12, 1958

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SOV/70-4-4-7/34

AUTHORS: Simonov, V.I. and Vaynshteyn, B.K.

TITLE: The Use of Functions Isolating a Structure From Among the Interatomic Vectors for Finding the Phases of the Structure Amplitudes

PERIODICAL: Kristallografiya, 1959, Vol 4, Nr 4, pp 505-509 (USSR)

ABSTRACT: On the basis of the superposition method, formulae are proposed for determining the phases of the structure amplitudes. The efficacity of one of the formulae is verified on the h0l zone of the known structure of seidozerite.
If there is no overlapping and no parasitic peaks the functions $\sum(\bar{r})$, $\Pi(\bar{r})$ and $M(\bar{r})$ give maxima which approximate to $\rho(\bar{r})$, the electron-density distribution. In as much as these functions are equal, their Fourier coefficients are like each other. So knowing the phases of one of these isolating functions, they could be attached to observed values of $|F_{hkl}|$ for a Fourier synthesis. If there is no centre the process would require more care.

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The Use of Functions Isolating a Structure From Among the Interatomic Vectors for Finding the Phases of the Structure Amplitudes

For a centrosymmetric structure, $2\bar{r}_o$, the vector between centre-related atoms can be found by Mamedov's method (Ref 19). The origin is chosen to be at a centre of symmetry and the Patterson function can be written as:

$$P(\bar{r}) = 1/V \sum_{\bar{H}} F_H^2 \exp\left[-2\pi i \bar{H}(\bar{r} \pm \bar{r}_o)\right] .$$

The $\sum$-function is:

$$\sum(\bar{r}) = 2/V \sum_{H} (F_{\bar{H}}^2 \cdot \cos 2\pi \bar{H}\bar{r}_o) \exp\left[-2\pi i \bar{H}\bar{r}\right] ,$$

which, when compared with:

$$P(\bar{r}) = 1/V \sum_{H} F_H \exp\left[-2\pi i \bar{H}\bar{r}\right]$$

gives the Fourier coefficients. $\Pi(\bar{r})$ and $M(\bar{r})$ are treated similarly. The formula actually used is from

The Use of Functions Isolating a Structure From Among the Interatomic Vectors for Finding the Phases of the Structure Amplitudes

$\Pi(\bar{r})$ and relates the signs by:

$$S(F_{\bar{H}}) = S\sum_{\bar{H}'} \left\{ (F^2_{\bar{H}'} \cos 2\pi \bar{H}'\bar{r}_o)\left[F^2_{\bar{H}-\bar{H}'} \cos 2\pi(\bar{H} - \bar{H}')\bar{r}_o\right] + \right.$$

$$\left. + (F^2_{\bar{H}} \sin 2\ \bar{H}'\bar{r}_o)\left[F^2_{\bar{H}-\bar{H}'} \sin 2\pi(\bar{H} - \bar{H}')\bar{r}_o\right] \right\} .$$

This was applied to the $h0\ell$ zone of seidozerite which has the symmetry $p2$. Out of 378 non-zero reflexions the heavy atoms, $(Zr + Na_I)$, determined 68 incorrectly. Calculation with the above formula is most laborious and pairs were selected from the 102 strongest reflexions. A table of $|F|$ on transparent material which could be superimposed on another table was used. The signs of all 378 reflexions were calculated from the formula given and all but 36 (9.5%) were correct. Using the heavy atom calculation, 19% were wrong. This method uses the

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The Use of Functions Isolating a Structure From Among the Interatomic Vectors for Finding the Phases of the Structure Amplitudes

minimum information about the structure, only the position $\bar{r}_o$ of one atom and a wide selection of F^2_{exp}. Putting the intensities on an absolute scale to include F^2_{000} introduces some error. Various other deficiencies are discussed but the method is considered promising. The function $M(\bar{r})$ would be better but more difficult to handle mathematically. Acknowledgments are made to Academician N.V. Belov and to V.D. Andreyev.
There are 1 figure and 22 references, of which 15 are Soviet, 1 English, 1 German and 5 international.

ASSOCIATION: Institut kristallografii AN SSSR (Institute of Crystallography of the Ac.Sc. USSR)

SUBMITTED: May 4, 1959

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SOV/70-4-5-2/36

AUTHORS: Ibers, J. A., Vaynshteyn, B. K.

TITLE: Expanded Tables of the Atomic Electron Scattering Power According to a Statistical Theory Consistent With Electron Exchanges

PERIODICAL: Kristallografiya, 1959, Vol 4, Nr 5, pp 641-645 (USSR)

ABSTRACT: The authors present a newly computed three-page table of the electron scattering power of the atoms whose atomic numbers range from 20 to 104 and sin ϑ/λ varies from 0 to 1.5 · 10^{-8}. The table is prepared for the third volume of the scheduled new edition of the "International Tables" for crystallography. An unpublished table of the atomic X-ray scattering power, prepared for the same publication by Thomas, L. H., Umeda, K., and King, K., was made available to the authors of this article. The statistical electron scattering power values are computed according to the Thomas-Fermi-Dirac model consistent with the electron exchange within a static atom. The values for Tl and heavier atoms are attained by extrapolation and the values at sin ϑ/λ =

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