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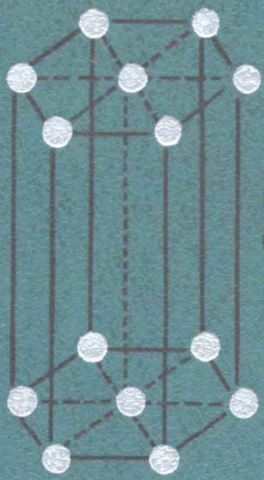

FUNDAMENTALS OF CRYSTAL PHYSICS

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Ю. И. Сиротин
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ОСНОВЫ КРИСТАЛЛОФИЗИКИ

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CONTENTS

PREFACE TO THE SECOND RUSSIAN EDITION

The principal author of this book, Yuri Isakovich Sirotin (1923-1974), had untimely passed away before the first edition came off the press. Many of his creative ideas remained unrealized. The final preparations of the manuscript for the first edition and the revision of the work for the second edition had to be done without him. The responsibility for all the possible faults and failures of the book is all mine.

Numerous minor corrections, changes and some abridgements have been made for the second edition, but on the whole the construction of chapters and sections, the numeration of equations and tables remain unchanged. The need to curtail the size of the book called for the elimination of the tables of numerical experimental data defining various physical properties of crystals.

A subject index has been added. Some additions to the list of references have not made it exhaustive; it contains only the principal monographs and papers mentioned in the book.

The manuscript has been reviewed by the Department of Crystal Physics of the Moscow State University (Head of Department—prof. I. A. Yakovlev) and the Department of Crystallography of the Leningrad State University (Head of Department—prof. V. A. Frank-Kamenetsky) and has been recommended as a textbook for physics specializations at the higher educational institutions.

I am grateful to the reviewers and all persons who have sent their comments on the first edition, especially to T. N. Tarkhova.

M. P. Shaskolskaya

EXCERPTS FROM THE PREFACE TO THE FIRST RUSSIAN EDITION

Within the last 15-20 years experimental crystal physics has emerged from the academic boundaries of a few research laboratories into the wide world of practice. The new, rapidly developing branches of science and technology, such as quantum electronics, quantum and non-linear optics, production of semiconductor instruments, piezotechnology, acoustics, etc., all involve the use of monocrystals and their singular peculiarities, as well as the use of new crystal-physical phenomena which are being discovered in rapid succession. Books on crystal physics have become an imperative necessity. The success of Nye's textbook (1967), whose two Russian editions soon went through, was not accidental. However, there appears to be necessary, along with Nye's book, a fuller and more detailed work, even though it may be less suitable for those becoming initially acquainted with the subject.

It was the authors' intention that the present monograph should satisfy this need. In preparing the book, the authors wished to combine the general physical with the symmetric approach, this being the distinctive feature of the Soviet school of crystal physics, founded by A. V. Shubnikov. The authors tried their best to utilize and promote A. V. Shubnikov's ideas throughout the whole book.

This book has developed from the lectures and practical courses on crystallography and crystal physics delivered by the authors at the Moscow Institute of Steel and Alloys and at the Department of Crystal Physics of the Moscow State University.

Structural crystallography and crystal chemistry, structure-sensitive properties, defects and the growth of crystals were deliberately omitted from the book. Moreover, the size of the book and the manner of presentation prevented the inclusion of experimental measurement methods and of the examples of the practical application of the described physical properties of crystals. The recent publication of a book on problems in crystal physics (by Perelomova and Tagieva, 1972), edited by one of the present authors, partly compensates for the lack of problems in our book which were left out for reasons of space.

Only those essentials of geometric crystallography have been included here which are necessary in crystal physics; the well-known comments of academician N. V. Belov (1957, 1958) on the crystallography course for physicists have been taken into account.

Only those topics of the extensive material on tensor calculus have been chosen which are important for crystal physics, some of them are barely mentioned in the existing books. Along with the coordinate (index) representation of tensor relations, non-coordinate representation is also used in our book, thus allowing the reader to decide which of the representations is more convenient in each particular case. Notation used by different authors for non-coordinate representation is of two types: the first one is used, for instance, in monographs by F. I. Fedorov (1958, 1965), the second one, derived from Gibbs, is applied in the course by Borisenko and Tarapov (1966) and in monographs by Lurie (1955, 1970). The notation of the second type is used in this book, since it is suitable for tensors not only of the second but also of the higher ranks. The theory of group representations is not described in our book, because it is used in those rare cases when it would be difficult to do without it.

In the course on crystal physics the influence of the symmetry and dissymmetry of crystals on their basic physical properties is emphasized, especially the anisotropy of these properties. In this respect there turns out to be a similarity of properties that are essentially different in other respects, such as diffusion and dielectric permittivity, magnetostriction and piezooptical effect. A description of the anisotropy of one of these properties can be applied to a considerable extent to another property, at least qualitatively. The quantitative characteristics of anisotropy greatly change, however, from property to property and from substance to substance. Such data can be found in handbooks, e.g. Landolt-Boernstein (1966, 1969, 1971), Krishnan (1958), Voronkov, Grechushnikov, Distler, Petrov (1965) and in reviews, which served as a basis for the compilation of illustrative tables of material constants of crystals, permitting the reader to obtain an idea of the magnitude of an effect and its anisotropy.

For giving a lucid idea of the anisotropy of physical properties of crystals our book contains illustrations that characterize it: representation surfaces, their sections and stereographic projections. Some of them have been taken from literature, while others were calculated and drawn, under the guidance of one of the present authors, by Sh. M. Butabayev and L. G. Yanusova in cooperation with P. L. Rubin*. The authors are deeply grateful to them for their great and difficult work which has contributed considerably to the improvement of our book.

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* Sh. M. Butabayev drew Figs. 24.2, 24.11, 47.5*a*, 54.3, 54.10, 58.2, 58.3, 81.2; L. G. Yanusova, Figs. 44.1, 47.2, 47.3, 47.4, 47.5*b*, 47.6, 54.4, 54.5, 54.6, 54.7, 54.8, 56.3.

Elastic properties were chosen as the principal object for demonstrating the anisotropy of the physical properties of crystals, since they are comparatively simple and well known. Strain tensor and not the displacement vector was chosen as the basic characteristic of strain, this allowing brevity of description and demonstration of the similarity between the basic equations of electro- and elastostatics. A comprehensive description of various phase transitions with a double change of symmetry (Ch. VII, Sec. 65) is a methodological novelty; it shows that within the boundaries of the applicability of the theory, all changes of the properties of crystals in phase transition depend on the groups of the symmetry of the phases connected by the given transition.

The appendices mainly contain reference data related simultaneously to several sections of our book.

The authors together drew up the plan and discussed the contents of all sections of the book, and in many cases it is difficult to determine the extent of the contribution of each of them. Chapters I, III and IV were written mainly by M. P. Shaskolskaya, and the rest largely by Yu. I. Sirotin.

The authors are grateful to S. A. Akhmanov, L. K. Zarembo, V. A. Koptsik, V. K. Semenchenko, M. M. Umansky, with whom they discussed individual sections of the book, as well as to V. A. Frank-Kamenetsky, V. A. Bokov, and V. N. Rozhansky who took the trouble of reviewing the book. The authors thank their former students E. Bartenev, N. Voropayeva, S. Orlov, G. Titova and V. Shcherbakov.

Yu. I. Sirotin, M. P. Shaskolskaya

LIST OF NOTATION

For the notation of the symmetry elements see Sections 3 and 8, Tables 3.1 and 8.1, for those of the symmetry classes (point groups) see Secs. 5, 6, 8, Tables 6.1, 6.2, 6.3, 8.1; for notation of the antisymmetry elements see Sec. 67; for those of space groups see Sec. 10; for those of the point groups of magnetic symmetry see Sec. 69; for those of Shubnikov's group see Sec. 69.

For Miller and Bravais symbols see Secs. 12 and 13, Table 13.1. Miller and Bravais symbols for planes and faces are given in parentheses (...), symbols of directions or edges are given in brackets [...], of a simple form or a set of symmetrically equivalent directions are given in braces {...}, of a bundle of symmetrically equivalent directions are in French quotes ⟨...⟩. The minus sign in a symbol is over a digit.

Vector notation is in semi-bold type italics of the Latin alphabet, for instance ***p***, ***n***, ***V***.

Tensor notation is in semi-bold type ordinary letters of the Latin alphabet and semi-bold type letters of the Greek alphabet, for instance **s**, **T**, $\boldsymbol{\varkappa}$.

Scalar (dot) product is denoted by a dot ($\cdot$), vector product by an oblique cross ($\times$).

Two dots (:) denote a double-dot product of tensors, three dots ($\vdots$) are a component product of tensors.

Two identical vector notations together (e.g., **kk**, **mm**) signify a tensor product of a vector multiplied by itself (see Sec. 18). [V], [V^2], etc. are Jahn symbols (see Sec. 42). Operators within a group are listed in braces.

$\subset$—symbol of the inclusion of a subgroup into a group

$\in$—symbol of belonging to a group, of inclusion into a set

$\cap$—symbol of the group intersection

$\subseteq$—symbol of a non-strict inclusion into a group

I—unit tensor

δ^{α}_{β}, δ_{ij}—Kronecker's tensor

$\delta^{\alpha\beta\gamma}$, $\delta_{\alpha\beta\gamma}$, δ_{ijk}—Levi-Civita pseudo-tensor

$\boldsymbol{a}_1$, $\boldsymbol{a}_2$, $\boldsymbol{a}_3$—base vectors of a lattice

$\boldsymbol{a}^1$, $\boldsymbol{a}^2$, $\boldsymbol{a}^3$—base vectors of a reciprocal lattice

$\boldsymbol{e}_1$, $\boldsymbol{e}_2$, $\boldsymbol{e}_3$—mutually orthogonal unit vectors of the Cartesian coordinate (usually crystal-physical) system

X, Y, Z—crystallographic axes

X_1, X_2, X_3—axes of the Cartesian coordinate (usually crystal-physical) system

$P^{\beta}_{\alpha'}$, $Q^{\alpha'}_{\beta}$, $P^{\mu}_{\lambda'}$, $Q^{\lambda'}_{\mu}$—transformation matrices of common rectilinear coordinates

$c_{i'j}$—matrix of the transformation of Cartesian coordinates (matrix of cosines)

$r_{i'j}$—matrix of rotation of Cartesian coordinates

$\boldsymbol{E}$—electric-field vector

$\boldsymbol{H}$—magnetic-field vector

$\boldsymbol{D}$—electric-field induction vector

$\boldsymbol{P}$—polarization vector

$\boldsymbol{\varkappa}$, $\varkappa_{ij}$—tensor of dielectric permittivity

$\boldsymbol{\eta}$, η_{ij}—tensor of dielectric impermeability

$\boldsymbol{\lambda}$, λ_{ij}—tensor of thermal conductivity coefficients

$\mathbf{k}$, k_{ij}—tensor of thermal diffusivity coefficients

$\boldsymbol{\rho}$, ρ_{ij}—tensor of specific resistance

$\boldsymbol{m}$—wave normal unit vector

$\boldsymbol{s}$—ray unit vector

N_o, N_e—principal refractive indices of uniaxial crystals

N_1, N_2, N_3 or N_g, N_m, N_p—principal refractive indices of biaxial crystals

n_1, n_2 and n_o, n_e—refractive indices for an arbitrary direction of light propagation

χ—character of representation (Secs. 47 and 66)

$\boldsymbol{u}$—displacement vector

$\boldsymbol{\varepsilon}$, ε_{ij}, ε_{λ}—small strain tensor

$\boldsymbol{\omega}$, ω_{ij}—small rotation tensor

$\mathring{\boldsymbol{\varphi}}$, $\mathring{\varphi}_i$—small rotation axial vector

$\boldsymbol{\sigma}$, σ_{ij}, σ_{λ}—stress tensor (in Secs. 32 and 76—electric conductivity tensor)

α, α_{ij}—thermal expansion tensor (in Secs. 26, 27 and 80—tensor of dielectric susceptibility, in Sec. 76—tensor of thermoelectric coefficients)
$\mathbf{s}$, s_{ijkl}, $s_{\lambda\mu}$—tensor of elastic compliance coefficients
$\mathbf{c}$, c_{ijkl}, $c_{\lambda\mu}$—tensor of elasticity coefficients
U—internal energy per unit volume
Φ—thermodynamic potential per unit volume
S—entropy per unit volume
T—temperature
C—heat capacity per unit volume
$\mathbf{d}$, d_{ijkl}, $d_{i\mu}$—tensor of piezoelectric coefficients
x_A, x_a—generalized thermodynamic coordinates
X_A, X_a—generalized thermodynamic forces
$\mathbf{\Pi}$, Π_{ijkl}, $\Pi_{\lambda\mu}$—tensor of piezoresistive coefficients
$\mathbf{m}$, m_{ijkl}, $m_{\lambda\mu}$—tensor of elastoresistive coefficients
J_a—generalized fluxes in thermodynamics of irreversible processes
K_a—forces conjugate to fluxes in the thermodynamics of irreversible processes
L_{ab}—kinetic coefficients
$\boldsymbol{\pi}$, π_{ijkl}, $\pi_{\lambda\mu}$—tensor of piezooptical coefficients
$\mathbf{p}$, p_{ijkl}, $p_{\lambda\mu}$—tensor of elastooptical coefficients
$\mathbf{r}$, r_{ijkl}, $r_{\lambda\mu}$—tensor of electrooptical coefficients
$\mathbf{K}$, K_{ijkl}, $K_{\lambda\mu}$—tensor of Kerr coefficients
χ, χ_{ijk}—tensor of quadratic dielectric susceptibility
θ, θ_{ijkl}—tensor of cubic dielectric susceptibility
$\mathbf{G}$, G_{ij}—pseudotensor of gyration

Indices:
α, β, $\gamma = 1, 2, 3$ correspond to the axes of the crystallographic system of coordinates, they can be written as superscripts or as subscripts
i, j, k, $l = 1, 2, 3$ correspond to the Cartesian (usually crystal-physical) system of coordinates
λ, μ, ν, $\varkappa = 1, \ldots, 6$ allow the replacement of two tensor indices by one; in the main part of the text (beginning with Ch. VI) they are written as subscripts, while in the Appendix both as superscripts and subscripts
A, B, C, $D = 0, 1, \ldots, 9$—in the notation of generalized thermodynamic forces and coordinates, including temperature and entropy, and in the corresponding thermodynamic matrices (Ch. VII)

$a, b, c, d = 1, 2, \ldots, 9$—in the notation of generalized thermodynamic forces and coordinates, excluding temperature and entropy, and in the corresponding thermodynamic matrices (Ch. VII and Sec. 74)
$a, b, c, d = 1, 2, \ldots, 9$—in the notation of generalized fluxes, forces conjugate to them, and matrices of kinetic coefficients (Sec. 76)

Cases when the indices are used in a different sense or have other meanings are specified in the text.