

International tables for crystallography,
Vol. D: **Physical properties of crystals.**

Edited by André Authier. Dordrecht/
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Crystal physics or physical crystallography has become a promising field in solid-state technology and materials science for the prediction of new properties. However, to handle the tools for doing crystal physics efficiently, a sound knowledge of tensor calculus as well as of symmetry-group theory is required. Frequently, this represents a considerable threshold to this subject. Therefore, I consider it good news that the main aim of this volume is bringing together tensors and crystal symmetry (including quasiperiodic symmetry) so that the mathematically minded reader may understand how crystal anisotropy may be set on a quantitative basis and how to get some experience with practising that. On the other hand, this implies that non-directional properties as well as those considered by some authors as being not at all accessible to a tensorial description have been left out though being physical.

This Volume D of an impressive series of reference books in the field of crystallography [eight volumes of *International Tables for Crystallography* (IT) are currently available: A, A1, B–G and, in addition, a Teaching Edition of Vol. A] divides into three parts. The focus of the entire volume ITD, and of the first part in particular, is on the description of physical properties from the point of view of an anisotropic continuum covering more than 50% of the total volume. The contents remind me of J. F. Nye's widespread classic on *Physical properties of crystals*. Part 2 is taking a quantum-mechanical point of view when describing lattice vibrations and electrons including their interactions with photons. Then, dealing with structural phase transitions, the third part emphasizes the issue of a domain substructure (the catchword 'domain' is the most frequent substantive in the index).

book reviews

Works intended for this column should be sent direct to the Book-Review Editor, whose address appears in this issue. All reviews are also available from **Crystallography Journals Online**, supplemented where possible with direct links to the publisher's information.

A closer look at the book reveals a number of special features of this volume. The 'groundwork of crystal physics' as J. F. Nye called it, *i.e.* fundamentals of tensor algebra and analysis as well as the reduction of tensor components due to symmetry properties of both the medium and the fields have been summarized in chapter 1.1 by A. Authier in a concise manner, taking as examples special cases of a property (up to the fourth rank) and ending up with coefficient schemes for all 32 point symmetries. During the past decades, the representation theory of groups has become a widespread tool for an efficient treatment of tensor components. Therefore, chapter 1.2 by T. Janssen on this topic should facilitate working with irreducible representations and characters. These are also displayed nicely in tables for the 32 crystallographic point groups. Moreover, a valuable achievement of this volume should be mentioned here deserving special acknowledgement: Given the point group, the accompanying software package *TenChar* on a CD-ROM (by M. Ephraïm, T. Janssen, A. Janner, A. Thiers) enables firstly the number of independent elements and the relations between the elements of a tensor to be calculated and secondly the characters of the irreducible representations (including various related features) to be determined.

While the tensor calculus of the majority of textbooks published so far is restricted to the point symmetries of periodic structures, the present book, in a special chapter (1.10) by T. Janssen, takes into account quasiperiodic structures too. Since the phason as an additional degree of freedom does not occur in periodic crystals, a treatment in a separate chapter is appropriate. Along with the concept of tensors and symmetry in n -dimensional space, examples of selected properties of quasicrystals like piezoelectricity and elasticity will be of great help for the reader.

The macroscopic properties of crystals have been arranged in Part 1 according to the conventional subdivision of physical properties (mechanical, magnetic, optical, transport). Since a certain property may be defined as a connector between two fields or products of fields, a comprehensive treatment of all properties would turn out an

open-end job. Hence, a selection of properties has been presented, illustrating the way this subject should be dealt with. Their relevance for technology, however, might require amendments in the near future.

Elastic properties have become a well established subject in crystal physics because of their multivalent involvement in this matter. Stress and strain have to be introduced at the beginning as the only fields represented by tensors of second rank. Moreover, even linear elastic constants are already of fourth rank which gives the opportunity to demonstrate how anisotropy depends on both the symmetry of the material and the property considered. Therefore they are treated in chapter 1.3 as a first example of a property by A. Authier and A. Zarembowitch including the non-linear static and dynamic case. This is followed (chapter 1.4) by a description of thermal expansion by H. Küppers connecting mechanical and thermal variables. Elasticity and thermal expansion are brought together *via* the Grüneisen formula anticipating phonons which are the subject of Part 2. In both chapters, experimental methods have been reviewed. The treatment of magnetic properties (chapter 1.5) by A. S. Borovik-Romanov and H. Grimmer demands more space since magnetic symmetry is being introduced, while for the non-magnetic point and space groups the reader may refer to symmetry groups given in ITA. Tables of the 90 magnetic point groups and figures of the magnetic lattices are provided. The authors then selected as cross effects piezomagnetism, magnetoelectricity and magnetostriction to break general symmetry arguments down to particular crystals and tensors. The traditional hard core of crystal physics, (linear) crystal optics, follows in chapter 1.6 written by A. M. Glazer and K. G. Cox. The term 'linear' includes optical rotation as well as the linear electro-optic and photoelastic effects. A subchapter on practical polarizing microscopy, decorated with coloured images, gives a brief introduction to this important method. It is chapter 1.7 on non-linear optics by B. Boulanger and J. Zyss that is the most extensive of Part 1. This will certainly be acknowledged by the reader in view of the actuality and complexity of this subject,

which is rarely treated properly in common textbooks. Susceptibility tensors are presented up to the third order for all crystalline point symmetries. The more sophisticated problem of phase matching is considered in some detail. Tables of suitable refractive-index conditions will facilitate exploiting the non-linear properties. Transport properties are the subject of chapter 1.8 by G. D. Mahan, where by definition the flow of electric charge and heat is regarded as transport. The treatment differs from that of previous chapters by taking an atomistic view, based on Ziman's approach, connecting scalar conductivities with scattering rates or lifetimes of electrons and phonons. Though the placement of a chapter on atomic displacement parameters (1.9 by W. F. Kuhs) within Part 1 (*Physical properties*) seems somewhat arbitrary, it is in any case a helpful addendum for crystallographers. Given the site symmetry of an atom, extensive tables enable the constraints to be obtained that are imposed on displacement tensor coefficients up to sixth rank. Coloured graphical representations of the density modulation due to Gram-Charlier series expansions are displayed.

Part 2 is on electrons and phonons as elementary single particles or collective excitations, which are commonly the subject of texts in solid-state physics. It is the emphasis on the impact of symmetry that gives this part a special crystallographic flavour. Taking a tetragonal crystal as an example, in chapter 2.1 on phonons, G. Eckold has worked out the symmetry constraints for lattice vibrations in some detail. Electrons as another type of fundamental unit behind the physical properties of crystals are then considered by K. Schwarz in chapter 2.2 from the viewpoint of the energy band structure they are forming. Relevant crystallographic ingredients to this quantum-mechanical stuff are the impact of symmetry and the tensor character of the electric field gradient. Chapters 2.3 and 2.4 that follow may be considered more in-depth treatments of experimental methods to determine either higher-order dielectric susceptibilities by Raman scattering (chapter 2.3 by I. Gregora) or elastic coefficients by Brillouin scattering (chapter 2.4 by R. Vacher and E. Courtens). Both are referring to phonons.

Symmetry constraints and the tensor character of properties also govern Part 3 of this volume, where ferroic materials form the predominating thread. In chapter 3.1 on structural phase transitions, J.-C. Tolédano, V. Janovec, V. Kopský, J. F. Scott and P. Boček introduce the Landau theory and

work out the behaviour of property tensors at ferroic phase transitions. An extensive list of point-group-symmetry descents associated with irreducible representations provides a quick survey of the ferroic symmetry expected for a given parent group. Again, microscopic models of the phase transition as well as concrete sample structures are discussed. At this point, a second software package supplied on CD (*GI★KoBo-1*) by V. Kopský and P. Boček should be mentioned that will be of great help: Importantly, the reader may find for each symmetry descent the form of tensors up to rank 4 for the parent group. Moreover, it provides information that is not yet available in textbooks, e.g. tables of the fine structures of domain states. As the important counterpart to the concept of ferroic domains, twinning appears in Part 3. Both have in common the occurrence of two or more orientation states. This conceptual relationship is dealt with in three chapters or stages: 3.2 *Twinning and domain structures* by V. Janovec, Th. Hahn and H. Klapper, 3.3 *Twinning of crystals* by Th. Hahn and H. Klapper, and 3.4 *Domain structures* by V. Janovec and J. Přivratská. This is certainly one of the most thorough recent treatments of this subject. If the interface between domains or twins is taken as the principal common feature, grain boundaries may be included as well, which leads to the more general concept of bicystallography. This view is outlined in chapter 3.2. Since some associated notions of group action appear in chapters 3.3 and 3.4, the necessary mathematical tools of group theory are additionally introduced in this chapter. The following chapter 3.3 is an almost encyclopedic article on twinning in direct space that is explicitly aimed at clarifying the terminology first and then putting the description of morphology, genetics, lattice geometry and interface onto a systematic ground. A number of illuminating figures and carefully chosen examples facilitate the read. Authors pay attention to the distinction of twins due to growth, phase transition or mechanical stress. Finally, knowing that physical properties of crystals are significantly influenced by their domain structure, the reader of chapter 3.4 will appreciate an introduction to the basic concepts and tools to handle the domain states quantitatively. Useful synoptic tables are provided, displaying domain pairs and twin laws for non-ferroelastic as well as for ferroelastic domain pairs.

In total, 28 authors from 9 different countries contributed to this volume. The authors are renowned specialists in their field so that an in-depth treatment could be

realized. On the other hand, a certain inhomogeneity seems inevitable in those cases. I just mention some examples. In the chapter on transport properties of crystals (chapter 1.8), crystal anisotropy is neglected throughout. Hence, the reader is left only with the remark of section 1.1.3.5.2 that a melting drop of wax on a plate of gypsum forms an elliptical halo, *i.e.* this chapter does not go beyond introductory solid-state physics. Another point refers to the use of the Gaussian system in chapter 1.5. A conversion table of units is inadequate to resolve this inconsistency. In a few cases, different symbols for the same entity or group have been used (*e.g.* the axes of order infinity on pages 17 and 100; stress and strain in chapters 1.1, 2.1, 3.4). A list of terms and symbols at the end of the volume would certainly be useful even if not complete. Subsequent extensive author and subject indices facilitate access to all chapters.

One may, of course, readily find properties missing in any book on this subject because there are so many of them hitherto known. In the present case it is probably inadequate because of the scope of this book. Nevertheless, I would recommend some of them should be taken into consideration for a future edition, like atomic diffusion (connecting a property with atomic defects directly), thermoelectricity (because of its technological relevance) and plastic deformation by slip (contrasting mechanisms of mechanical twinning in sections 3.3.10.2 and 3.3.10.8). Also, more experimental data of materials properties would be helpful to understand the order of magnitude of an effect.

Like with other volumes in this series, the standard of production of ITD is excellent. Only a few figures stand out (1.5.2.3–1.5.2.7, 1.5.3.4). Fig. 1.7.3.4 and others in chapter 1.7 suffer from a poor feedback of the printer which gives rise to unphysical progression of the curves. The readability of ITD could be improved because the glossiness of the printed letters hinders reading under bright illumination.

It took me quite a time to get through the 500 large-sized pages, which is approximately equivalent to twice the number in commonly formatted textbooks, including the software. Having done that with great pleasure, I may testify that Volume D contains a vast wealth of experience from crystallographers in the broadest sense. With its wealth of concrete detail, the book can serve well as a reference work, whose study will be rewarding both to beginners and to experts in various branches of solid-state and materials sciences. Full references both

to original work and for further study are provided at the end of each chapter. The series title *International tables for crystallography* for Volume D is justified thanks to the combination of many useful tables with comprehensive explanatory parts and due to setting standards of the basic concepts in this field for the international community. It fills a gap in that it provides an up-to-date reference enriched by useful software. The book addresses tools and subjects that are of special interest to researcher and post-graduate students who want a better quantitative understanding of known materials and the development of new materials. This may concern not only the traditional readers of *International tables for crystallography*, but also solid-state physicists, chemists and materials scientists. Thus, people who want to be guided in their study or research by a sound and comprehensive reference to crystal physics should have access to ITD.

Finally, special thanks are expressed to the editor, André Authier, to all contributing authors, and to the Technical editors, Nicola Ashcroft and Amanda Berry, for their tremendous work.

P. Paufler

Department of Physics
Dresden University of Technology
D-01062 Dresden
Germany
E-mail: paufler@tu-dresden.de

books received

The following books have been received by the Editor. Brief and generally uncritical notices are given of works of marginal crystallographic interest; occasionally, a book of fundamental interest is included under this heading because of difficulty in finding a suitable reviewer without great delay.

Cristallographie. Deuxième édition revue et augmentée. Par Dieter Schwarzenbach et Gervais Chapuis. Paris: Presses Polytechniques et Universitaires Romandes, 2006. Pp. xii + 344. Prix broché EUR 55.45. ISBN 2-88074-672-8.

Utilisant des connaissances d'algèbre linéaire et la transformation de Fourier, la présentation de la matière est néanmoins essentiellement géométrique. La nécessité de se familiariser avec la vision tridimensionnelle d'objets étant probablement la difficulté la plus importante rencontrée par les étudiants, un soin particulier a été apporté à la réalisation des figures. Ce livre comporte en outre toute une série d'exercices et leur solution. *Sommaire:* 1. Cristallographie géométrique, 2. Symétrie, 3. Diffraction des rayons X par les cristaux, 4. Résolution de structures cristallines, 5. Éléments de structures cristallines, 6. Propriétés tensorielles des cristaux, 7. Exercices.

Franz Ernst Neumann (1798–1895). Zum 200. Geburtstag des Mathematikers, Physikers und Kristallographen. Herausgeber R. Fritsch, E. Neumann-Redlin-von Neumann und T. J. Schenck. (Bilingual German/Russian.) Kaliningrad und München: Terra Baltica und Ludwig-Maximilians-Universität, 2005. 252 Seiten. Broschiert Preis: EUR 10. ISBN 5-98777-005-X, 3-922480-17-9.

Aus Anlass des 200. Geburtstages von Franz Neumann fand 1998 sowohl ein Seminar im Deutsch-Russischen Haus von Kaliningrad (früher: Königsberg) als auch ein Dies Academicus an der LMU München statt. Der vorliegende Band enthält die Ansprachen und wissenschaftlichen Beiträge in deutscher und russischer Fassung. *Inhalt:* K. K. Lavrinovič: Eröffnung; E. Neumann-Redlin-von Meding: Franz Ernst Neumann (11.9.1798–23.5.1895); E. F. Kondrat'ev: Franz Ernst Neumann – ein Vektor, in die Zukunft weisend; P. Paufler: Tensoreigenschaften trikliner Kristalle: Eine Hommage auf Franz Ernst Neumann; J. Batt: Die Bedeutung Franz Ernst Neumanns für die Mathematik; K. K. Lavrinovič: F. E. Neumann und F. W. Bessel; P. Roquette: Königsberger Mathematiker im 19. Jahrhundert; R. Fritsch: Mathematiker unter Franz Ernst Neumanns Nachkommen; O. M. Badmaeva: Plastische Portraits von Franz Ernst Neumann. Anhang.