International Union of Crystallography

Acta Cryst. (1979). A35, 508

Commission on Journals

Decisions taken at meetings in Warsaw, August 1978

The attention of authors planning to submit papers to *Acta Crystallographica* or *Journal of Applied Crystallography* is drawn to the following actions taken by the Commission on Journals at meetings held in Warsaw, 1–3 August 1978.

Estimated standard deviations

All measured or derived quantities which are of importance either to the conclusions or understanding of the paper, or to use by others, are required to be accompanied by their estimated standard deviations. The value of such quantities without estimated standard deviations is regarded as being sufficiently ill-defined as not to warrant publication.

International symbols for units

The system of units known as SI is to be used, except that the ångström (symbol Å, defined as 10^{-10} m) is preferred to the nanometer (nm) or picometer (pm). When there is good reason for using other units (for example, when a dimension is determined by a standard machine tool or commercial practice) the SI equivalent should follow in parentheses [see *Notes for Authors. Acta Cryst.* (1978), A34, 143–157]. A useful publication on the SI system is *A Guide to International Recommendations on Names and Symbols for Quantities and on the Units of Measurement* (1975) by D. Armstrong Lowe (Geneva: World Health Organization).

Structural data

Routine checking of papers containing structural data, for consistency between the atomic coordinates and lattice constants and the quoted bond lengths, bond angles and torsion angles, is now being introduced by all Co-editors. Since the detection of inconsistency will result in a paper being returned to its authors, care should be taken to ensure that the final tables and results presented in the manuscript correspond accurately to the primary data.

Anisotropic thermal parameters

Anisotropic thermal parameters are to be published only if the table of values is very short, or they are necessary for understanding the paper, or they possess unusual features or cast doubt on the structure but do not lead to rejection of the paper. In all other cases, the table of values is to be deposited: a brief discussion of deposited values should instead be presented, including the maximum and minimum values found and the presence of any nonpositive-definite coefficients determined. In addition, the equivalent values of the Debye–Waller factor should be given for publishing with the list of atomic coordinates.

Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (J. H. Robertson, School of Chemistry, University of Leeds, Leeds LS2 9JT, England). As far as practicable books will be reviewed in a country different from that of publication.

Acta Cryst. (1979). A35, 508–509

Quantum chemistry of solids: The chemical bond and energy bands in tetrahedral semiconductors. By A. LEVIN. Pp. xii + 249. Moscow: Khimiya Press, 1974 (in Russian); New York: McGraw-Hill, 1977 (in English). Price £14·10, US $24.00.

'All matter is made of atoms'. Richard Feynman, in his famous lectures on physics, regards this statement as the most important and informative piece of present scientific knowledge. If just one sentence could be passed to the next generation, this should be the one, he says. The previous generation still disputed seriously about the real existence of the atom. Now it is a well established fact. We have many means, well known by all crystallographers, that make the detailed atomic structure of matter concretely visible. Still, the quantitative significance of this statement poses some problems.

The idea of atomic constituents of matter involves identification of the basic structural units of matter with free atoms. Of course, we get free atoms when we decompose matter, and matter when we put free atoms together; we can even recognize the atomic species in our density maps. However, a conclusive physical proof of the idea requires derivation or at least understanding of the measurable properties of matter on the basis of the measurable properties of free atoms and of their mutual interactions. This is easy for many mechanical and thermal properties, but as soon as we turn to phenomena, where basic electronic properties enter the scene, difficulties arise.

The band calculations, on which our understanding of electronic properties are based, preferably ignore the atoms. Many attempts to derive band structures from the properties of constituent atoms by tight binding or LCAO methods have sadly failed. There has grown the general belief that reasonable results can be reached by some plane-wave methods only, where the atomic properties have no role. This is the situation where this book enters the game.

This book is the first extensive and quantitative apology of the chemical or atomic view on band theory. It boldly opposes the general opinion of solid-state physics. True, dating from 1974, it is no longer quite up to date in its details. However, it still deserves attention today. In the present hasty times one seldom meets books which are so carefully considered in their structure and all details. The book starts with an introduction to the basic theory at a level which brings it within the reach of a newcomer. It proceeds logically, explains every step clearly and thoroughly and displays honestly the physical argumentation, motivation and consequences of the assumptions and approximations, which are so often omitted and left to the headache of the reader.

The book is concentrated merely on elements with diamond structure and on the related partially covalent crystals with ZnS structure. In spite of this restriction it is instructive in a general sense. It gives a coherent presentation of the methods and ideas followed and may thus give impulses to new applications and developments.

The main approach is the 'equivalent orbital' or EO LCAO method. The bonds are described in terms of symmetry-related local orbitals, and the band structure resulting from the corresponding Bloch functions is discussed. Band widths, gaps and other critical measures of the band structure are expressed in terms of several Coulomb and resonance integrals, which – on the assumption that 'matter is made of atoms' – are related to spectroscopic and thermodynamic data on the atoms and structurally-related molecules. This makes the treatment both semiempirical and semiquantitative, but, on the other hand, it gives a simple and astonishingly consistent explanation of many known properties of the crystals. It is able to produce, in a simple parametric form, plausible explanations for both the systematic behaviour and the lack of it, either horizontally as a function of ionicity or vertically as a function of the atomic masses.

As minor points of criticism, one may note some unconventional use of terms *e.g.* 'self consistent' instead of 'self adjoint' or 'Hermitian' and 'associated' instead of 'augmented' plane waves for APW; also some non-standard notations are used. The list of references is impressive. It gives a good view also of the Russian literature in the field. It is also interesting to see how many western books are available in Russian translation, although in case of real need a western reader might prefer a reference to the original.

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Acta Cryst. (1979). A**35**, 509–510

Neutron diffraction. Edited by H. DACHS. Pp. xiii + 357. Berlin-Heidelberg-New York: Springer-Verlag, 1978. Price DM 65·00, $32.50.

The reviewer [*Acta Cryst.* (1976). A**32**, 749] of a new edition of another volume of this same title discussed the advantages and disadvantages of employing a single author or an edited group to write on what is now such an extensive topic as 'neutron diffraction'. At first sight the appearance of this volume edited by Professor Dachs might suggest that students of the subject will now be able to make their own detailed comparison of the two approaches. However, this is not really the case, predominantly for two reasons. First, the present book has taken a stricter view of the word 'diffraction' and does not, for example, stray into incoherent inelastic-scattering studies. Secondly, the point of view is very close to the Institut Laue–Langevin and its highly-developed modern practices and it is rather a far cry from the beginner with no more than a medium-flux reactor and possibly ageing instruments. Indeed, as the editor says, there is a specific intention 'to stress the technical aspects of the subject'.

The book has nine chapters, each by a separate author, and the coverage may be gleaned from the following shortened titles: *Principles*; *Polarized neutrons*; *Combination of X-ray and neutron data*; *Magnetic structures*; *Disordered structures*; *Phase transitions and critical phenomena*; *Biological problems*; *Liquid structure*; *Dynamical neutron diffraction.* All of these are fields in which rapid progress is being made at the present time. Each chapter is a competent review and contains an immense amount of information: they are all well-furnished with up-to-date references, totalling over seven hundred in the book as a whole. Inevitably some of the chapters are better than others and the reviewer is particularly impressed by Hayter's review of polarized neutron techniques, Coppens's meticulous and extremely clear account of X–N methods and the final chapter by Rauch & Petrascheck on dynamical neutron diffraction. These chapters seem especially valuable for the way in which they gather together diverging strands of scattered publications in the best tradition of a review article. Quite apart from their technical content, the nine chapters differ immensely in style, ranging from a high literary standard to a presentation which sometimes verges on the colloquial. It is difficult to accept that the term 'neutron scatterer' can include not only atoms and magnetic moments but also the experimenter himself.

For a scientific publication the book, which is in offset printing, has an exceptionally large number of errors and misprints. In some of the chapters no checking of the text seems to have taken place and it is a great pity that authors who so valiantly write in a tongue other than their native one should suffer in this way. Spelling mistakes are not uncommon, pairs of letters are reversed, singulars and plurals are confused, prepositions are wrongly used, authors' names are mis-spelt. At best, these blemishes merely irritate the reader but it is difficult not to wonder whether there may not also be errors in factual data. Here a reviewer can only note what offends his memory as he reads – but certainly the