

mented by balloon help messages, contain intuitive symbols to indicate their function, and more advanced operations can be accomplished through a variety of pull-down menus. The structure and data-sheet windows are coupled, and selections or adjustments made in one are immediately reflected in the other.

Data can be input manually, but the program also reads a variety of standard formats. Expansion of this list, for example to all commercially available packages that are typically used, would be a welcome addition, but availability of a free format read allows for adequate interaction with most. Structure development is accomplished through functions to expand molecular fragments, fill unit cells, display multiple unit cells, complete user-defined coordination spheres and delete nonbonded atoms or whole fragments.

Structure representation can be toggled between a stick diagram, stick and ball, space-filling spheres and thermal ellipsoids. Presentation can be made in either a draft-quality flat mode or a more realistic render mode. Rotation and orientation of the structure are easily accomplished with menu buttons for 'X/Y rotation', 'Z rotation', 'center of rotation definition', and 'shift' for structure repositioning within the window. Analysis of structural detail is facilitated by a 'zoom' function. On the very low-end Pentium system used for this review (120 MHz), rotation function on all but the stick diagram was rather slow and jerky; however, dramatic improvement would be expected with even moderate system enhancement.

*DIAMOND* was specifically written for inorganic structures and its features for displaying these in polyhedral format are a strength of the program. Various polyhedron formats are available, and the definition and design of these, based on the central atom, is straightforward and easy. The definition and inclusion of 'dummy atoms' provides a particularly useful tool for many of these types of structures. Combined with the structure-development features described above, nice quality packing diagrams of even very complicated inorganic structures can be produced with a minimum of input. Once constructed, the structure can be examined from various directions through a pull-down menu for this purpose.

Although written for inorganic structures, *DIAMOND* is equally useful for viewing molecular compounds or even proteins, and is especially good for those involving significant intermolecular interactions, such as hydrogen bonding. Connectivities can be defined for a variety of criteria, in order to distinguish between types of interactions present in a structure. A fragment

selection feature is especially useful, as whole supramolecular features can be highlighted.

The wide variety of functions available in *DIAMOND* make it a powerful tool for both teaching and research. Its modest price and substantial academic discount warrant its consideration for any crystallographic teaching laboratory, and the planned release of a 'student' edition will make it even more attractive.

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## Book Reviews

*Works intended for notice in this column should be sent direct to the Book-Review Editor, whose address appears on the inside front cover of the journal. As far as practicable, books will be reviewed in a country different from that of publication.*

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**Materials crystal chemistry.** By RELVA C. BUCHANAN and TAEUN PARK. Pp. vii + 462. New York: Marcel Dekker, Inc., 1998. Price US \$175. ISBN 0-8247-9798-1

This book is 'intended primarily for engineers, advanced undergraduates and graduate students in materials engineering, materials science and allied scientific disciplines'. It contains four chapters, entitled: *Fundamentals of Atoms, Molecules and Solids* (130 pp.); *Fundamentals of Crystallography* (94 pp.); *Crystal Structures* (84 pp.) and *Structure Changes in Crystals* (112 pp.). Two appendices, special functions in quantum mechanics and quantum mechanical background for the simple expression of the lattice energy of ionic crystals, a bibliography and an index make up the rest of the work.

When I began to leaf through the first two chapters, with their large numbers of detailed subtopics, I had high hopes that I was looking at a new genre of texts for teaching this subject. Usually, texts on crystal chemistry treat atomic theory and bonding at the level of freshman chemistry and crystallography receives only a cursory overview. The primary emphasis in most texts is on crystal structures and the crystallography section needs to be supplemented with a second text. It seemed that this text covered these topics in

sufficient depth to be used alone. Alas, my hopes were quickly dashed, and I was forced to conclude that this book fails on two levels, both at the level of scientific detail and at the level of basic communication.

My disappointment began on p. 9 of chapter 1, where the authors define potential energy 'as the work done by the electron in moving from infinity (zero energy) to  $r$ '. The equation appears, however, as

$$|V| = \left| \int_0^r F dr \right|,$$

instead of with a lower limit of  $\infty$  and, with the absolute signs removed in the next lines, there are inconsistencies in the signs of the resultant work and force terms. Misprints or misconceptions? It is difficult to say, as both abound throughout the text. Bad editing and poor proofreading are evident in the misplacement or omission of definite and indefinite articles, misspellings and different spellings for the same word in the same line ('micelle' and 'miscelle', etc.) and downright confusion of language. What, for example, is one to make of this sentence on p. 104? 'The metallic radii are defined in the same way as ionic crystals except for no difference between atoms as cation and anion.', or the particularly egregious error on p. 132 where, in a section headed '3. Block (*sic*) Equation', a paragraph begins 'The base of band theory in solid state physics is Block theory which describes (*sic*) the wave function of an electron in a periodic potential. In crystal, the position...'. After these experiences, I admit that I did not go carefully through the remaining mathematical equations, either in the chapter or in the appendices.

I had higher hopes for chapter 2, *Fundamentals of Crystallography*, but here too problems quickly emerged. The first page of the chapter discusses stacking directions of points to form a lattice and introduces the concept of the unit cell, but then a statement appears that when the 'atomic arrangement is taken into account, the stacking direction is no longer arbitrary' as if one could not always select a triclinic unit cell as long as it contains the asymmetric unit. Confusion between the metric of a unit cell and the dimensional requirements imposed by symmetry is present throughout the chapter. Thus the circular 'lattice provides the basis for crystal symmetry' where later the authors state that the geometry of the unit cell is determined by the symmetry. They also state that 'Any solid exists in one of three states: single-crystal, poly-

crystal and non-crystalline (amorphous). All have periodicity ranging from perfect for a single-crystal to essentially non-existent (*sic*) for the amorphous state.' Why a polycrystalline material is a separate state is not clarified. 'Parallelepiped' is used in a discussion of what the authors refer to as 'planar lattices' that is so involved as to obscure their significance, though it is eventually defined correctly. There is a good discussion of Miller indices, with many examples, but there is recurring confusion between lattice points and atom site occupancy, *e.g.* 'The motif placed on (*sic*) each lattice point...'; a 'symmorphic space group exists when only a single atom or ion exists at the Bravais lattice points...'. Finally, to gladden the heart of every crystallographer, 'The actual atomic positions are obtainable from the analysis of the lattice of a crystal.' and 'Knowing the space group and equipoints ... one can readily determine the crystal structure and arrangement of the atoms or ions in the unit cell or crystal.'. X-ray diffraction intensities and structure factors are never mentioned and although *International Tables for Crystallography* are mentioned once in a parenthesis in the text, there is no reference to them in the Reference section or in the index.

Ch. 3 deals with crystal structures and contains sections on space filling by atoms, simple binary ionic crystals, more complex structures with closest packing such as perovskites and spi-

nels, and covalent crystals. It is a standard treatment of topics found in all books dealing with solid-state chemistry.

The concluding chapter deals extensively with polymorphism, thermodynamic discussion of phase changes, and various types of transformation with illustrative examples such as in quartz. There are also discussions of defects, substitution and silicate structures. But even here the very first equation of the chapter has 'The free energy change with temperature and pressure is given by:

$$\Delta G = \Delta E + P\Delta V - T\Delta S$$

...', correct only when temperature and pressure are constant.

In summary, I cannot recommend this book in its present state. The large number of errors and misstatements disqualify it as a textbook and its price puts it totally out of reach of most students. The choice of topics for a course in materials engineering is a good one, however, and I hope that the authors will eventually revise their work so that it meets the goals they set themselves.

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## New Commercial Products

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## Oxford Cryosystems North America

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