

smoother when 64 Mbytes are available.

Documentation: Documentation is provided in the form of HTML documents. There is also an on-line version of this documentation available at <http://www.nirim.go.jp/~weber/JAVA/JSV/jsv.html>.

Availability: JSV1.07 can be downloaded from <http://www.nirim.go.jp/~weber/JAVA/JSV/jsv.html>.

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J. Appl. Cryst. (1999). **32**, 1028

JMap3D – VRML isosurface generator

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(Received 25 June 1999;
accepted 2 July 1999)

The crystallographic problem: This program was written specifically for the purpose of rendering electron density data into three-dimensional isosurfaces, utilizing the VRML2.0 format (virtual reality modelling language). The user's electron density data have to be provided in a simple ASCII format or in binary format. The file format is described in the documentation included in the distribution. *JMap3D* can create up to five isosurfaces, whereby for each isosurface a different electron-density file may be specified. In this way it is possible to show, for example, Fourier data together with difference Fourier data or MEM data. For each isosurface an isodensity value can be specified, as well

as colour and transparency of the isosurface. Additionally, the unit-cell box, transparent cell walls and cell grid lines may be added to the VRML file.

Method of solution: After reading the electron density data (or any other volumetric data), the polygonization of the isosurface is performed by means of a so-called marching cubes algorithm. The number of generated polygons can be very high (>50000). *JMap3D* allows a coarser grid of the input data to be used, thus reducing the polygon count as well as the size of the VRML file. When displayed with Gouraud shading, generally no loss of quality is observed as a result of choosing a subset of the full data set. In addition to that, *JMap3D* has a built-in feature for performing a polygon count reduction, based on a so-called progressive meshes algorithm. Depending on the isosurface topology, the polygon count can thus be reduced to about 10% of the original number without seriously affecting the truthfulness of the isosurface. This algorithm basically removes many small and nearly coplanar triangles by transforming them into fewer but larger triangles.

Program specification: The program is written in Java™ using the JDK1.2™ (Java Development Kit) from Sun Microsystems (Sun Microsystems, 1999). It therefore can be executed under Windows, as well as under Linux, which is gaining popularity in the scientific community.

Software environment: For executing *JMap3D* a Java virtual machine, such as the Java interpreter, which is included in JDK1.2, must be installed on your computer. A VRML viewer from the Java3D–VRML working group is included in the distribution. This, however, requires Java3D to be installed on your computer in addition to JDK1.2. This viewer is mainly provided for Linux users, since other VRML viewers running under Linux may not be readily available. For Windows users, the stand-alone VRML viewer *GLVIEW3.6* (Grahn, 1999) is recommended, which is far better than any VRML browser plug-in tested by the author.

Availability: A public version of *JMap3D* can be downloaded from <http://www.nirim.go.jp/~weber/JAVA/JMAP3D/JMAP3D.html>.

Keywords: *JMap3D*; VRML; 3D electron-density maps.

References

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Software Reviews

Software for review in this section should be sent direct to the Software-Review Editor, whose address appears on the inside front cover of the journal.

J. Appl. Cryst. (1999). **32**, 1028–1029

DIAMOND – Visual Crystal Structure Information System

Available from: Crystal Impact, K. Brandenburg & M. Berndt GbR, Postfach 1251, D-53002 Bonn, Germany (tel. +49 228 73 5825; e-mail: sales@crystalimpact.com; WWW: <http://www.crystalimpact.com>). Current version: 2.1b. Price: Single license €998.00 or US \$1100.00. Additional users: €498.00 or US \$550.00. Site licence (per department): €1998.00 or US \$2200.00. In all cases there is a 50% academic discount.

DIAMOND – Visual Crystal Structure Information System is a Windows-based graphics program (Windows 95 or higher required) for drawing crystal structures. Installation of the program is simple and straightforward. Although no written manual is provided in either hard-copy or electronic form (a minor drawback), a tutorial is available that is quite helpful in getting started. An online manual is also available, and provides ready answers to most questions that arise. Additional support is provided through the Internet (<http://www.crystalimpact.com/diamond/support.htm>) or through direct electronic correspondence (support@crystalimpact.com). A database of 40 mineral structures provides numerous examples of the capabilities of the program.

DIAMOND features a split-screen format with the left portion of the screen serving as the structure window and the right portion being a 'data sheet' containing useful crystallographic information such as crystal system and space group, lattice dimensions, atomic coordinates, vibrational displacement parameters and selected geometric parameters. The relative sizes of these two windows can be readily adjusted through mouse repositioning of a 'splitter'. Numerous options for structure construction and manipulation are available. On-screen buttons, supple-

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.

J. Appl. Cryst. (1999). **32**, 1029

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 ∞ 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-