Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (R. F. Bryan, Department of Chemistry, University of Virginia, McCormick Road, Charlottesville, Virginia 22901, USA). As far as practicable, books will be reviewed in a country different from that of publication.

Acta Cryst. (1998). A**54**, 516

Simulations for solid state physics. An interactive teaching resource for students and teachers. Edited by ROBERT H. SILSBEE and JÖRG DRÄGER. Pp. xvii + 348 + CD-ROM. Cambridge: Cambridge University Press, 1997. Price £60.00, US $80.00. ISBN 0-521-59094-9.

The authors, physicists at Cornell University, have produced a remarkable work, a combination of computer simulations of basic physical processes at the atomic level, contained on a CD-ROM, and associated tutorials and exercises presented in the book. The simulations are of generally high quality, allowing control over all required parameters, and may be used to help develop understanding at all levels from the purely introductory to the very advanced. They may be run on Windows based computers, Power Macintosh systems, or on UNIX workstations with 1024 × 768 pixel (or better) 256 color displays. Given the required hardware, installation is straightforward and quick. The quality and speed of execution are, of course, platform dependent.

There are 14 simulation packages, covering diffraction, lattice dynamics and related phenomena, dynamics of classical and quantum free electrons, electron energy bands and states, dynamics and transport in single and in partially filled bands, carrier densities and band bending in semiconductors, ferro- and antiferromagnetism and magnetic domains, and dislocations and plastic flow. All are well tried and tested and function smoothly.

The authors' approach throughout, understandably, is very much physics oriented, but crystallographers will find the first three simulations useful in their own teaching, while steering students away from such statements as 'there is no direct way to deduce a crystal structure from the diffraction pattern' (p. 27); in this review, I concentrate on them.

Simulation package *Bravais* covers the fundamentals of crystal lattices and X-ray diffraction, using two-dimensional examples; *Laue* deals with diffraction in perfect and imperfect one-dimensional crystals; and *Born* treats the properties of plane waves and lattice dynamics in one dimension.

Bravais offers nine preset simulations, which allow for a wide range of options and exercises, from simple presentation of the basic geometrical ideas to the ability to solve a simple two-atom structure from its diffraction pattern. An attractive feature is the instant side-by-side presentation of structure and diffraction pattern as lattice size and shape and basis position and content are varied.

Laue's nine preset simulations explore the Bragg condition, atomic form factors, the structure factor, order–disorder, atomic displacements and thermal disorder, and even quasi-crystals. The immediate effectiveness of these simulations is reduced somewhat by annoying changes of scale in the calculated diffraction patterns that visually obscure the important reciprocal relationships between the sizes of the objects and their diffraction patterns. However, patterns can be copied and stored for later detailed examination.

Born's simulations explore the properties of plane waves, both standing and travelling, the normal modes of a finite chain, wave packets, pulse propagation, the effect of impurities, and anharmonicity. Again, the wide range of available options within each preset lets one use these simulations at all levels of understanding.

The authors do their best to remove any 'blackbox' connotations from the simulations by carefully describing the mechanics of each program, the assumptions made, algorithms used, and the actual and potential bugs and problems that may be encountered. They have provided teachers and students of diffraction and solid-state physics, at all levels, with a sophisticated and highly useful tool to help understand fundamental concepts and the often elusive link between algebraic function and physical form. The license agreement included with the hardcover edition allows for network installation of the programs at an educational institution and a paperback edition of the book (ISBN 0-521-59911-3) without CD-ROM is available for student use.

ROBERT BRYAN

Department of Chemistry
University of Virginia
Charlottesville
VA 22901
USA

Acta Cryst. (1998). A**54**, 516

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.

Quantum dynamics of simple systems. Edited by G.-L. OPPO, S. M. BARNETT, E. RIIS and M. WILKINSON. Pp. x + 373. Bristol: Institute of Physics Publishing, 1997. Price £27.00, US $50.00. ISBN 0-7503-0490-1 (paper). The book is a paperback reprint of the hardcover (ISBN 0-7503-0-351-4) collected proceedings of the 44th Scottish Universities Summer School in Physics, held in Stirling in August 1994 (a NATO Advanced Study Institute). Eleven lectures and 61 poster abstracts are included, together with a list of participants and a subject index.

Dynamics of crystal surfaces and interfaces. Edited by P. M. DUXBURY and T. J. PENCE. Pp. x + 247. New York: Plenum Publishing Corporation, 1997. Price US $95.00. ISBN 0-306-45619-2. This book contains papers presented at the Traverse City, Michigan, conference on the title topic, held 4–8 August 1996. The book focuses on 'atomic processes, step structure and dynamics; and their effect on surface and interface structures and on the relaxation kinetics of larger length-scale non-equilibrium morphologies'.