Byron DeLaBarre's studies focus on 'Determining the Phases for a Difficult Protein Structure.' Shannon Farrell's research involves 'Sulphur *K*- and *L*-Edge XANES of 3d Transition Metal Sulphides and Silicate and Germanate Glasses.' The exploration of 'New Negative Thermal Expansion Materials Related to Cubic ZrW_2O_8', will be conducted by Cora Lind. Oshrit Navon's thesis research concerns the 'Polymorphism and the Influence of Crystal Forces on Molecular Conformation.' K. Scott Weil will continue his 'Investigation of the Formation, Structure, and Magnetic Behavior of Compounds in the Nickel–Molybdenum–Nitride System.'

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.

J. Appl. Cryst. (1999). **32**, 378–379

Advanced computing in electron microscopy. By Earl J. Kirkland. Pp. ix + 250 (CD-ROM included). New York: Plenum Press, 1998. Price: US $72.50. ISBN 0-306-45936-1.

Because of significant improvements in instrument optics, electron sources, and detection systems, high-resolution electron microscopy has become an increasingly powerful tool for the study of microcrystalline materials. Theoretical descriptions of image production, including the transfer function of the objective lens and the multiple scattering interactions as the electron beam traverses the specimen, have been available for at least a quarter century. Why, then, should there be yet another book on high-resolution electron microscopy, a subject that has been already treated in many sophisticated monographs? The answer is implicit in the book's title.

This book, written by an expert on computer simulations in electron microscopy, shows how the greatly expanded and cheap computer power available nowadays can be used effectively for the interpretation of electron microscope experiments. It discusses how computational methods are optimally designed, a practical approach not encountered in many other texts. Several programs written by the author (*e.g.* the fast Fourier transform) are included in the text and a number of others commonly encountered in simulations are conveniently included in a compact disc to be used on a Macintosh, or PC with Windows 95 or NT. C source code is also provided for Unix-based systems. Although various possible roles of computers in modern electron microscopy are mentioned in the short introductory first chapter, the book is primarily concerned with applications to image simulation.

The second chapter is a brief introduction to the electron microscope as an optical instrument. While much of the discussion treats the conventional transmission electron microscope (CTEM), the author demonstrates quite effectively how the optics of bright-field and dark-field scanning transmission electron microscopes (STEM) are closely related to the CTEM *via* a principle known as reciprocity. Obviously, a major component of the microscope is its objective lens. After a discussion of the relativistic electron wavelength and its dependence on electron accelerating voltage, the spherical aberration of the objective lens and its partial correction by focal changes are encountered. In the third chapter, idealized electron scattering by a weak phase object is introduced to expand the discussion of the objective lens transfer function. Various optimized lens defocus conditions that allow the maximum bandpass of information at the same contrast sign are discussed, including the well known Scherzer focus. The effects of partial coherence or total incoherence of the electron source on the imaging experiment are then introduced in terms of this transfer function.

The very interesting fourth chapter deals with image simulation, particularly the pixel detail needed to visualize various specimen details but also the optimal sampling of the image for transformation to its diffraction pattern or *vice versa*. The concept of the Nyquist limit is introduced, but not specifically in the context of the Shannon sampling theorem. Practical aspects of carrying out discrete Fourier transforms, avoiding artifacts due to image wrap-around, are mentioned, as is the most efficient way to display diffraction patterns as their power spectra. Thin specimen images are then simulated in Chapter 5, again in terms of the weak phase object. The derivation of accurate electron scattering factors is then presented in great detail, including the need for an imaginary form factor for heavier atoms. Steps in the computation of bright-field phase-contrast images are then given with examples for single atoms and a thin crystalline object (silicon). Coherence effects on these images are then reintroduced.

Chapter 6 was of particular value to this reviewer since it discusses multiple-beam dynamical scattering and its influence on images. There are two approaches to modeling multiple beam scattering, the Bloch wave solution (usually in matrix form) and the multislice calculation. Although these methods are physically equivalent, the former is shown to be computationally much more costly than the latter so that the multislice method is most often employed nowadays. Various aspects of these calculations that can lead to error are introduced including the (noncommutative) properties of some operators. Advice for slicing the crystalline specimen into optimal thin layers is given as are tests for validity of the calculation (repeat of slightly different boundary conditions for consistency) and its convergence. The problem of aliasing and bandwith on convolution operations is mentioned. Experimental design for simulating defect-containing crystals is given (the notion of periodic continuation as a superlattice). The next chapter examines a number of crystalline examples. Not only are image simulations shown here but also the production of convergent-beam electron-diffraction patterns, the most reliable way of determining space-group symmetry in crystallography (although that aspect is not mentioned). Finally the problem of quantitative matching of simulated images to experiment is discussed, with several figures of merit recommended.

The final chapter is a user's guide to the programs included in the CD-ROM. One can carry out multislice calculations of dynamical scattering and then simulate images at various degrees of beam coherence. STEM simulations are also included as is the possibility for computing convergent-beam diffraction patterns. Appendices discuss the 'shareware' included on the CD for plotting various functions such as the lens transfer function, a list of files on the CD-ROM, a nice demonstration of the central section theorem in diffraction, available sources of electron scattering factors and their parameterization for programs on the CD-ROM, bilinear interpolation and a program giving a perspective view of three dimensions.

In general, I have a very favorable impression of this book. Most of the material is presented reasonably well for someone who is already familiar with the field. (Indeed the preface suggests that the reader might have some previous familiarity with quantum mechanics, Fourier transforms and diffraction.) Again, the major recommendation for the volume is its very practical approach to computational problems, with a voice of experience pointing out where one can easily go astray. I do, however, have a few minor criticisms, even though the scientific presentation is generally first-rate. First, I think that the background section is somewhat uneven. There are some topics, including the Shannon sampling theorem, the resultant limits to transforming accurately to a diffraction pattern of a given resolution, and the issue of wrap-around effects, that could have been discussed in much greater detail, particularly since this book is devoted to image simulation. Certainly much of this information can be found in works cited in the excellent reference list, but it would be more efficient if it were included in this one volume. Since some X-ray crystallographers are becoming interested in high-resolution electron microscopy, it would have been helpful if the relationship between the back focal plane (where the diffraction pattern is found) and the image plane of a lens could have been stated more explicitly, even though the current presentation is not confusing to those already familiar with electron microscopy. Several images and diffraction patterns are poorly reproduced. Details of the convergent-beam patterns on p. 148, for example, are quite badly obscured, as is an illustration of the intensity distribution of an electron probe on p. 141, to name just two of several examples. On a nonscientific level, better editing would have tidied up occasionally appalling grammar and the far too abundant typographical errors. It needs more than a spell-checker to distinguish between 'incite' and 'insight'! None of the reservations mentioned, however, should obscure the great usefulness of this volume and the software provided with it. It should be on the shelf of any serious electron microscopist interested in the experimental study of crystalline objects at high resolution.

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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.

J. Appl. Cryst. (1999). **32**, 379

Group III nitride semiconductor compounds. Physics and applications. Edited by Bernard Gill. New York: Oxford University Press, 1998. Pp. xvii + 470. Price US $145.00. ISBN 0-19-850159-5. The book contains 11 contributions on the preparation, properties and applications of nitride semiconductors. It is intended as a tutorial introduction to the field for graduate students and young researchers.

Scanning probe microscopy of polymers. (ACS Symposium Series 694). Edited by B. D. Ratner and V. V. Tsukruk. New York: Oxford University Press, 1998. Pp. xii + 367. Price US $125.00. ISBN 0-8412-3562-7. This volume is 'developed from a symposium sponsored by the Division of Polymer Chemistry, at the 212th National Meeting of the American Chemical Society, Orlando, FL, August 25–29 1996'. It contains an Introduction, 13 papers on polymer morphology and structure, three on studies of local surface properties and four on current trends in SPM techniques.

Disperse systems. By Makoto Takeo, Pp. xi + 317. Weinheim: Wiley-VCH Verlag GmbH, 1999. Price £85.00. ISBN 3-527-29458-9. The book discusses the nature and physical properties of disperse systems, including colloids, sols, micelles, vesicles, bilayers, emulsions, gels and aerosols. It is intended for use in 'graduate courses in physics, physical chemistry, and chemical engineering and as a reference for those doing academic or industrial research'.

New Commercial Products

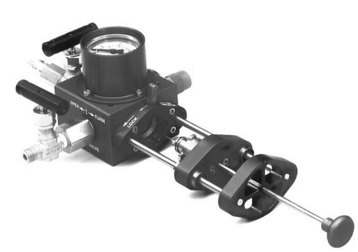
Announcements of new commercial products are published by the Journal of Applied Crystallography free of charge. The descriptions, up to 300 words or the equivalent if a figure is included, should give the price and manufacturer's full address. Full or partial inclusion is subject to the Editor's approval and to the space available. All correspondence should be sent to the Editor, Professor A. M. Glazer, Editor Journal of Applied Crystallography, Clarendon Laboratory, University of Oxford, Parks Road, Oxford OX1 3PU, England.

The International Union of Crystallography can assume no responsibility for the accuracy of the claims made. A copy of the version sent to the printer is sent to the company concerned.

J. Appl. Cryst. (1999). **32**, 379

Portable xenon pressure chamber

Oxford Cryosystems has teamed up with the University of Oxford to design and manufacture a portable xenon pressure chamber, the Xcell. This device is designed to easily produce heavy-atom derivatives for macromolecular X-ray crystallography.



The Xcell encloses the crystal sample in a small chamber. The chamber can then be pressurized with xenon from a cylinder to a maximum of 25 bar. A quick-release connector allows the Xcell to be isolated from the gas supply whilst still under pressure, making the device both highly portable and highly usable. Other benefits of the Xcell include:

a small pressure chamber to minimize the consumption of expensive xenon;

various safety features such as a preset relief valve allowing a maximum pressure of 25 bar inside the cell;

carefully controlled inlet and vent valves to enable the chamber to be pressurized and vented without damage to the crystal sample;

compatibility with common sample-mounting systems.

For further information on the Xcell, pricing and delivery, please contact Oxford Cryosystems.

Oxford Cryosystems, 3 Blenheim Office Park, Lower Road, Long Hanborough, Oxford OX8 8LN, England (e-mail: info@oxfordcryosystems.co.uk)

J. Appl. Cryst. (1999). **32**, 379–380

Crystallographica Search-Match

Oxford Cryosystems has announced the launch of *Crystallographica Search-Match* (CSM), an all-new search-match program for use with the Powder Diffraction File (PDF). CSM is suitable for any materials scientist whose work involves identification or quality control using powder diffraction samples.

CSM takes advantage of the latest 32-bit technology and modern search techniques to allow fast, automatic