PEKPIK and *MODEL*. *GENEV* provides for the special treatment of weak reflection data, a general index-rescaling scheme, the application of inflexion-point least-squares to the Wilson plot, and the estimation of errors for the normalized structure factors. *GENSIN* generates both triplet and quartet relationships with a range of user controls. *GENTAN* provides for automatic starting set selection, permuted and random phase assignments, block and cascade phase refinement and different weighting schemes. The phase set having the best chance to yield the structure is selected using an absolute-measure-of-success (AMOS) parameter based on psi-zero triplets, negative quartets, *R*(Karle) and a combined figure of merit.

Software environment: The direct-methods programs are an integral part of the *XTAL* system, and are not intended for use as stand-alone routines. The distributed source code is in the pre-processor language RATMAC (Munn & Stewart, 1979) which is translated on site into the locally available Fortran (66 or 77). Programs are adapted to the local operating system and linking environment through the MACRO feature within RATMAC. The software currently runs on a wide range of machine types. For larger structures, *GENTAN* requires either a VMS operating system or a random-access I/O facility.

Hardware environment: The current version of the *XTAL* system requires a minimum hardware configuration of 128 kbytes of memory; 32-bit integer and floating-point words and 20 Mbytes of offline memory (*e.g.* disk storage). *GENEV, GENSIN* and *GENTAN* have been implemented and tested on Control Data, Digital Equipment, IBM, Perkin Elmer and Univac computers.

Program specification: Reflection data are input *via* an *XTAL* binary file, and control parameters as free-format line data. Run times vary according to structure size and machine type. A typical example involving 120 non-H atoms/cell, 228 *E* values, 3121 triplets, 1497 quartets and 8 phase sets runs in 0·21, 4·58 and 3·56 CPU minutes on a DEC VAX 780, and 0·25, 6·40 and 4·80 minutes on a CDC Cyber 750/175. *GENEV, GENSIN* and *GENTAN* are 2010, 2490 and 4520 lines of RATMAC code, respectively.

Documentation: *GENEV, GENSIN* and *GENTAN* are documented as separate chapters in the *XTAL Users Manual* (Stewart & Hall, 1983). The program description and input instructions are detailed therein. The source code is fully commented.

Availability: These programs are distributed as part of the *XTAL* Crystallographic System. An information brochure on this system is available from Professor J. M. Stewart, Computer Science Center, University of Maryland, College Park, MD 20742, USA.

Keywords: Direct-methods software; Structure-invariant methods; Normalized structure factors; Tangent refinement; *XTAL* system.

References

Munn, R. & Stewart, J. M. (1979). Tech. Rep. TR-804. Computer Science Center, Univ. of Maryland, College Park, Maryland.

Stewart, J. M. & Hall, S. R. (1983) Tech. Rep. TR-1364. Computer Science Center, Univ. of Maryland, College Park, Maryland.

Stewart, J. M. & Hall, S. R. (1985). *J. Appl. Cryst.* **18**, 263.

Crystallographers

J. Appl. Cryst. (1985). **18**, 264

This section is intended to be a series of short paragraphs dealing with the activities of crystallographers, such as their changes of position, promotions, assumption of significant new duties, honours, etc. Items for inclusion, subject to the approval of the Editorial Board, should be sent to the Executive Secretary of the International Union of Crystallography (J. N. King, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England).

Dr **V. Cody**, an associate research scientist at the Medical Foundation of Buffalo, New York, USA, has been awarded the Faculty Research Award of the American Cancer Society for her study of the relationship between molecular structure and biological activity of drugs which inhibit tumour growth.

Dr **C. J. Humphreys**, of the Department of Metallurgy and Science of Materials at the University of Oxford, has been appointed to the Henry Bell Wortley Chair of Materials Engineering at the University of Liverpool. He is the Chairman of the Union's Commission on Electron Diffraction.

Gloria B. Lubkin has been appointed Editor of *Physics Today*, the monthly magazine of the American Institute of Physics which has a circulation of 80 000 and is written for physicists and those interested in the physical sciences. She has been on the staff of *Physics Today* for more than 21 years. She was elected a Fellow of the American Physical Society in 1973 and was a founding member of the APS Committee on Women in Physics in 1971.

Dr **D. Ringe**, Department of Chemistry, Maryland Institute of Technology, and Dr **B. Wallace**, Department of Biochemistry, Columbia University, have been named by the Biophysical Society as the first recipients of the Margaret Oakley Dayhoff Award. The award honours the memory of Dr Dayhoff, former President of the Biophysical Society, Professor of Biophysics at Georgetown University and Director of Research at the National Biomedical Research Foundation, and will be awarded each year to a junior woman scientist working in a field within the range of interest of the Biophysical Society.

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.

J. Appl. Cryst. (1985). **18**, 264–265

Industrial crystallization. By *S. J. Jančić* and *P. A. M. Grootscholten*. Pp. xvi + 434. Delft University Press and D. Reidel Publishing Co., Dordrecht, 1984. Price US $ 64.

The information explosion that has occurred over the past decade in virtually all of the areas relating to nucleation and crystal-growth kinetics, and in the analysis of particulate systems, is invoked by the authors to justify the comment that no single book can now offer a comprehensive text on the broad subject of industrial crystallization. They are probably right.

Accordingly, they have taken a slightly restricted view of the subject by confining their attention to crystallization from solution, which is still by far the major field of industrial activity. Their objective has been to exploit the links that are slowly being forged between theory and practice in order to be able to design, build and operate better crystallizers at all scales of operation. They have done a commendable job.

The first part of the book (nine chapters) entitled *Fundamentals of crystallization from solutions* deals with primary and secondary nucleation, crystal-growth kinetics, the population balance concept and its application to the MSMPR crystallizer. Methods of characterizing particulate systems, the laboratory measurement of crystallization kinetics and the assessment of transport phenomena in solid–liquid systems all get thorough treatment.

The second part (six chapters) entitled *Crystallizer design* covers the use of

crystallization kinetics in the design of basic modes of batch and continuous crystallization. Some of the problems associated with slurry handling and certain aspects of down-stream processing (pre-thickening, dewatering and drying) are also briefly considered.

The book is well written, a good number of worked examples offer useful guidelines for research workers, designers and industrial users. By today's standards it offers good value for money.

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Industrial crystallization 84. Edited by *S. J. Jančić* and *E. J. de Jong*. Pp. xii + 498. Amsterdam: Elsevier, 1984. Price US $ 113.

The 105 papers presented at this 9th symposium, held under the auspices of the European Federation of Chemical Engineering Working Party on Crystallization in The Hague, are grouped into four main sections: *Fundamentals; Additives and impurities; Precipitation and melt crystallization; Design and operation.*

A keen interest is developing in the solid–liquid interfacial regions and in the bulk-solution phase. A variety of techniques is now being exploited, the most promising of which seems to be Raman spectroscopy, to gather evidence of the semiordered layer near the surface of a growing crystal. The existence of such a layer, which could serve as a growth unit reservoir or as a source of secondary nuclei, has been postulated by many authors for more than half a century, but it is only now that we appear to have the means of verifying it.

The metastable zone continues to attract attention and so do the problems of small crystal and size-dependent growth. The role of impurities in the crystallization process remains an active area of investigation and the industrial importance of this branch of study cannot be overemphasized. Slowly but surely we are approaching the point where we should be able not only to explain why certain effects operate, but also how to select the best habit modifier for a specific job. Theoretical studies from the worlds of crystallography and statistical mechanics are now being integrated to give a better understanding of the problems of crystal morphology.

Although inorganic systems substantially predominate over the organic as working substances in the papers presented at this symposium, it is in connection with the latter that some of the most interesting industrial developments are found, particularly related to crystallization from the melt. One such process, pressure-melt crystallization using pressures up to 3000 bar (1 bar = 10^5 Pa), appears to have considerable potential from an energy-saving point of view. Precipitation also looms large in the list of topics covered, and several papers dealing with alumina, sodium bicarbonate and calcium carbonate are of industrial relevance.

Mathematical modelling featured in several papers, usually with the object of providing better routes to crystallizer design and control. A step change in this branch of activity would be made if only the problem of on-line or *in situ* measurement and assessment of crystallization kinetics could be solved. This goal may not be far away.

The book is photolithographically reproduced, but it is very expensive.

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Current topics in materials science, Vol 10. Edited by *E. Kaldis*. Pp. vi + 515. Amsterdam: North Holland, 1982. Price US $ 106.50, Dfl 250.00.

Five stimulating reviews of considerable interest are contained in this book.

In chapter 1, E. I. Givargizov, N. N. Sheftal and V. I. Klykov face the topic, crucial for solar cell research, of *Diataxy (graphoepitaxy) and other approaches to oriented crystallization on amorphous substrates*. The economic relevance of the subject is related to the fact that conventional methods of deposition of epitaxial layers on single-crystal substrates increase the price of solar cells. Perhaps diataxy could reach the goal of satisfactory oriented layer growth on amorphous substrates. Many problems remain unsolved in this field. Both fundamental phenomena in nucleation and growth of crystals and technical improvements in crystallization processes were used and were found to be important in overcoming the difficulties. 'Artificial epitaxy' or diataxy is discussed in detail together with more conventional techniques. It turns out that the role, for oriented crystallization, of close-packed crystallographic planes is understood, whereas that of the presence of a liquid phase (melt or solution) remains unclear as far as its mechanism is concerned. The experimental data and speculative analysis refer mainly to semiconductor materials as the most relevant in modern technology.

Chapter 2 (by E. I. Gerzanich, V. A. Lyakhovitskaya, V. M. Fridkin and B. A. Popovkin) is devoted to SbSI *and other ferroelectric A(V)B(VI)C(VII) materials*. The monograph widely treats the physical, chemical and structural properties of these ferroelectric, piezoelectric and semiconducting materials. For a long time crystal growth of such materials was not possible. Apart from the fundamental physics of these materials, their applications are also discussed: particularly in relation to the development of optical memory systems, electrooptics, non-linear optics and related disciplines. The list of references (more than 300) will be useful to any researcher in the field.

Chapter 3, by W. Albers, reviews the problem of *Non-stoichiometry of inorganic solids*. This is a fundamental topic both for chemistry and condensed-matter physics and finds its origin in the occurrence of native defects in compounds. The approach is from the point of view of thermodynamics. The subject is so wide that only the most important aspects of the problem are treated and the review is not, as declared by the author, exhaustive with respect to the enormous amount of experimental data published during the past decades.

In chapter 4, G. N. Papatheodorou discusses the *Spectroscopy, structure and bonding of high-temperature metal halide vapor complexes*. Emphasis is on the new techniques using high-temperature Raman spectroscopy (vibrational spectra) and absorption spectroscopy (electronic excitation spectra). Conclusions regarding molecular structures and the correlation of structure with thermodynamic properties are also reviewed. An outline of the importance of vapor complexes in current technology is given in the last section.

Gem materials, natural and artificial is the subject of the last review, by I. Sunagawa. In this excellent synthesis the author shows how gem research is a very active field of modern material science and how some techniques (*e.g.* high-pressure synthesis of diamonds) have now become traditional for other materials as well. With the exception of pearl, coral and a few organic gem materials, gemstones are principally natural minerals or mineral assemblages that have been used since prehistoric times. About 70 mineral