and does not give a full-matrix solution in the strictest sense. Here, a simple procedure is outlined whereby twin data may be refined by inclusion of the volume fraction in the normal equations, using least-squares programs that are generally available.

If $[x_i]$ are the positional coordinates of one part of the twin and the twinning operation is represented by the matrix $[T_{ij}]$, the coordinates of the twinned fraction of the crystal (with reference to the axes of the untwinned fraction) are given by

$$[x_i'] = [T_{ij}][x_i].$$

Similarly, the anisotropic temperature factors β_{ij}' of the twinned fraction are given by

$$\beta_{ij}' = \sum_{k=1}^{3}\sum_{l=1}^{3}[T_{ik}][T_{jl}]\beta_{ij}.$$

The above equations are used to generate the parameters of the twinned fraction for each twin law and are subsequently applied as linear constraints in the refinement cycles. If n is the number of atoms in the asymmetric unit and p is the number of twinned fractions, the site occupancies (s) of one twin-equivalent atom in $p-1$ fractions are refined with the following constraints operative

$$s_{ij} = s_{1j} \qquad i=2,n;\ j=1,p-1$$
$$s_{ip} = 1 - \sum_{j=1}^{p-1} s_{1j} \qquad i=1,n.$$

No manual manipulation is required once the refinement is in progress. All reflexions are used and there is only one additional variable per twin law. Several least-squares programs (*RFINE*: Finger, 1968; *CRYLSQ*: Stewart, Kruger, Ammon, Dickinson & Hall, 1972) are currently available that incorporate linear constraints of the necessary form.

References

FINGER, L. W. (1969). *RFINE*. A Fortran IV Computer Program for Structure Factor Calculation and Least-Squares Refinement of Crystal Structures. Geophys. Lab., Carnegie Inst., Washington. (Unpublished manuscript).

GRAINGER, C. T. (1969). *Acta Cryst.* A**25**, 427–434.

STEWART, J. M., KRUGER, G., AMMON, H., DICKINSON, C. H. & HALL, S. R. (1972). Univ. of Maryland Computer Sciences Tech. Report TR-192.

SUDARSANAN, K., YOUNG, R. A. & DONNAY, J. D. H. (1973). *Acta Cryst.* B**29**, 808–814.

International Union of Crystallography

Commission on Crystallographic Apparatus

Abstracts of Papers for the Madrid Conference on Anomalous Scattering

The Inter-Congress Conference on Anomalous Scattering, organized by the Commission on Crystallographic Apparatus, was held 22–26 April 1974 in Madrid, Spain for the purpose of stimulating new and current use of anomalous scattering and for improving the present theoretical and experimental approaches to the interpretation and measurement of anomalous scattering. Invited papers were presented in the following sessions: 1. Theoretical calculation of dispersion corrections. 2. Experimental determination of dispersion corrections. 3. Absolute intensity measurement including anomalous scattering. 4. Effects of dispersion on atomic parameters. 5. Use of anomalous scattering in protein structure analysis. 7. Absolute configuration and tensorial properties. 8. Novel methods for using anomalous scattering.

Abstracts of 35 papers have been printed and are available, price £1 postaid, from the Executive Secretary International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

The proceedings of the Conference will be published in book form at a date to be announced later.

Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (M. M. Woolfson, Physics Department, University of York, Heslington, York YO1 5DD, England). As far as practicable books will be reviewed in a country different from that of publication.

The dynamics of atoms in crystals. By W. COCHRAN. Pp. 145, Figs. 85. London: Arnold, 1973. Price £4.60; (paperback) £2.30.

As Professor Cochran points out in an excellent introductory chapter, the study of the vibrations of atoms in crystals has a long history, the initial papers being published more than 60 years ago. However, the number of papers on this subject remained quite small until the late 1950's, and the enormous volume of literature existing today has been published only in recent years. The aim of Professor Cochran's monograph is to expound as simply as possible the basic principles of the subject and to guide the student, by means of selected references for further reading, through the morass of published material.

The topics covered in the first five chapters are real and reciprocal-space lattices, dynamics of one-dimensional chains, simple three-dimensional crystals, interatomic force constants, the determination of phonon frequencies, particularly by means of neutron coherent inelastic scattering, and the interpretation of these data in terms of force models for various solids. Following this introduction to the basic concept of harmonic phonons, there are chapters on various related physical properties such as heat capacity, thermal conductivity, dielectric and optical properties (infrared absorption, Raman and Brillouin scattering) and thermal ex-

pansion. Many of these properties depend upon the non-harmonic character of atomic vibrations, and Professor Cochran provides brief but adequate discussions of phonon scattering by other phonons, by defects and crystal boundaries, so that the basic physics of each property can be readily appreciated. The similarities and differences between electrons and phonons and between neutron scattering and electron scattering are nicely brought out, as is the importance of the electron–phonon interaction. Finally, the connexion between lattice dynamics and phase transitions ('soft' modes) is very well described in relation to the general problem of phase transitions.

The treatment throughout the book is at a reasonably uniform and elementary level, though perhaps a little too condensed in some places. The newcomer to the subject might appreciate some expansion of the sections dealing, for example, with the reciprocal-lattice concept, anharmonicity and thermal conductivity. There are no explicit exercises for the student, but he is encouraged to work through some of the derivations and perhaps find a few 'deliberate mistakes'! (*e.g.* Fig. 3.4). This leads me to a relatively minor but general criticism of the book: the typesetting, alignment of margins and the overall appearance of some of the pages are somewhat below the average standards for scientific textbooks. There are also, inevitably, a few typographical errors which should be corrected in future editions. Nevertheless, at £2·30 for the paper-back version, this little book is an absolute 'must' for anyone starting to learn about the motions of atoms in crystals. Highly recommended.

G. DOLLING

Atomic Energy of Canada Ltd.
Neutron and Solid State
Physics Branch
Chalk River Nuclear Laboratories
Chalk River
Ontario
Canada K0J 1J0

Computed electron micrographs and defect identification. By A. K. HEAD, P. HUMBLE, L. M. CLAREBROUGH, A. J. MORTON and C. T. FORWOOD. Pp. x + 400. Figs. 133, Tables 22. Amsterdam: North Holland, 1973. Price U.S. $40.00.

For those who have followed the work of this Australian school the book holds few surprises. It is a review of their considerable contribution to the subject in recent years. However the book is in no sense a stringing together of published material, nor is it evident that the work is produced by several authors. In fact the presentation of the book has been very carefully thought out, with some excellent introductory chapters which will be particularly valuable for those coming to the subject for the first time. Computer programs, some of which have been freely distributed in the past, are here thoroughly introduced and explained and listings of the programs are given for cubic, hexagonal and tetragonal crystals. The text is illustrated with a rich variety of examples, although they are largely drawn from work on f.c.c. and b.c.c. metals and alloys with relatively little work on other crystal systems or on ceramic materials. Impressive agreement between experiment and theory is demonstrated. The authors are careful to emphasize the limitations of their technique though there is very little discussion of many-beam diffraction effects and no reference to weak-beam work. Moreover, the approach is essentially limited to straight dislocations, not too close to crystal surfaces, with distortions calculated from linear anisotropic elasticity theory.

As far as the identification of perfect dislocations is concerned some may feel that the philosophy of the Australian school is misguided. They deliberately examine situations of extreme pattern detail, using relatively thin foils, inclined dislocations and close reflecting planes. Apart from the fact that this approach is not applicable to layer structures many experimentalists will prefer to work with thicker crystals, mid-foil dislocations and widely separated diffracting planes where the problem is altogether simpler, and analytic expressions for elastic distortions can unambiguously provide the required information without recourse to elaborate calculations. However there can be little doubt about the value of the computed micrograph technique for studying the partial dislocations bounding stacking-fault configurations, and this problem is thoroughly discussed.

In view of its price this book will not be purchased without good reason but it must surely be available in the library of any laboratory regularly studying defects in materials and it will certainly prove most valuable in the training of research students.

J. W. STEEDS

H. H. Wills Physics, Laboratory
University of Bristol
Tyndall Avenue
Bristol BS8 1TL
England

Crystal structures - a working approach. By HELEN D. MEGAW. Pp. xviii + 563. Figs. 208, Tables 42. London: Saunders, 1973. Price £8.30

The results of a crystal structure analysis can be summarized in a set of data (space group, lattice parameters, atomic coordinates, *etc.*) which usually constitute an essential part of an original paper. The data are given together with a discussion of the methods used, of the reliability of the results and with a description of the structure as seen from the point of view of the author in its relation to the particular chemical, physical or purely crystallographic problem which led to the research. But it is possible to obtain a variety of views of a crystal structure, starting from the same fundamental data. To do this it is necessary to know how to interpret the conventional symbols and to be trained in dealing with crystal geometry. That is what the author of the book wants to teach and that is what the subtitle 'a working approach' means. Indeed the purpose of the book is to show how crystal structures ought to be looked at in order to obtain from them the particular information in which one is interested. The importance of this is self-evident since a knowledge of crystal structure is fundamental in interpreting many aspects of modern solid-state physics and chemistry.

The plan of the book is developed for that purpose. The first three chapters are introductory in character and deal with general concepts of crystal-structure building, interatomic forces in crystals and the lattice nature of crystals. In the third chapter a number of simple fundamental struc-