

there is an obvious relationship between surface band structure and LEED calculations and hence that the programs provided could be used for either. The methods used are based on a dynamical formulation of the scattering problem and use approaches due to J. B. Pendry.

The set of programs provided comprise almost 200 of the 278 pages of the volume. They are most complete and an offer is made to send a magnetic-tape copy of these programs to interested parties. In fact, one of the members of our laboratory (Dr A. Smith) has made use of this offer and has used such a tape. This experience has shown that the programs work quite well to the extent that the authors claim although, as stated in the book, since there are so many different types of problems, exhaustive tests of the programs have not been carried out.

The book cannot be used without reference to the work of J. B. Pendry, *Low energy electron diffraction* (Academic Press, 1974). This is acknowledged by Van Hove and Tong. Pendry's book contained a set of programs that could deal with simple substances. In the volume under review a significant new method has been introduced, the 'combined space method', which, together with further developments, allows a much wider range of real crystals to be dealt with. It is a pity that the detailed formulation of symmetry lacks contact with the treatments of symmetry in dynamic diffraction that have occurred in other areas of diffraction and crystallography such as electron diffraction and X-ray diffraction. It is clear from reported work in the literature, as well as the many results displayed in this volume, that surface structure analysis, using the methods described in this text, is now a common activity. In addition to the coordinates of atoms at real surfaces, the thermal vibration amplitudes of these atoms are also being estimated. At present this is done at the level of a simple Debye-Waller factor.

This book is an invaluable tool for those research groups which are involved in the study of atomic and electronic surface structure. There is a useful summary of results in these areas which is reasonably complete to the year 1978. The book is not truly a book in the traditional sense but rather a brief review of LEED theory combined with a detailed instruction manual for the use of a set of computer programs for the calculation of LEED intensities and some other surface properties.

D. LYNCH

CSIRO  
Division of Chemical Physics  
Bayview Ave  
Clayton  
Victoria 3168  
Australia

*Acta Cryst.* (1982). A38, 878

**Superionic solids: principles and applications.** By S. CHANDRA. Pp. xi + 404. Amsterdam: North Holland, 1981. Price US \$78.00, Dfl 160.00.

Although the field of superionic conductors, preferably referred to as solid electrolytes or fast ion conductors, has attracted an intense research effort over the last decade or so,

a good teaching text was hitherto unavailable. Chandra's book represents, in the first place, a welcome effort to take the reader with little knowledge of solids through a descriptive and well illustrated course to a well rounded understanding of this area. Even for the specialist, the description extends to include comprehensive compilations of up to date data digested in a very satisfying fashion.

In the second place, the chapters on *Experimental probes* and *Applications* provide a uniquely wide-ranging coverage ideal for those entering the field or diversifying their interests within the field.

Finally, there are two chapters which more formally and extensively develop the theoretical description of *Ion transport in point defect type ionic and superionic solids* and *Ion transport in molten sublattice type superionic solids*.

The book will be valued by teachers, students and research workers alike for its unified yet detailed approach which only a single author could bring to a work such as this.

A. T. HOWE

Amoco Research Center  
PO Box 400  
Naperville  
Illinois 60566  
USA

*Acta Cryst.* (1982). A38, 878-879

**Crystal cohesion and conformational energies.** Part 26 of **Topics in current physics.** Edited by R. M. METZGER. Pp. ix + 154. Berlin-Heidelberg-New York: Springer Verlag, 1981. Price DM 54.00, US \$23.00.

This book contains four chapters devoted to the calculation of cohesive energies in organic crystals and dimers and of energies in larger biomolecules.

In the first chapter D. E. Williams reviews his approach to the calculation of lattice energies of organic crystals by means of the empirical atom-atom potential method, using transferable parameters. He discusses various types of interaction-energy contributions and amply describes methods for the derivation of the parameters and point charges needed for the potentials. Detailed results are shown and discussed for 18 hydrocarbon crystals. Special attention is paid to the tedious formulation of the analytical expressions for the matrix elements used in the least-squares formalism for the refinements of the parameters.

F. A. Momany shows in the second article how conformational analysis can aid in polypeptide drug design. After a brief introduction of the method used for the calculation of the conformational energy of a polypeptide (*viz* using empirical potentials and the computer program *ECEPP*) he illustrates it with a number of examples. These include peptide backbones and modifications of these [*e.g.* *N*-methyl analogs, depsiptides, carbazic acid ( $\alpha$ -aza) analogs], aspects of bond types, chain reversal and direction reversal, disulfide bonds and modification of side chains (*e.g.*  $\alpha,\beta$  dehydro analogs). For these examples a number of iso-energetic contour diagrams is given, from which favorable conformations can be deduced. The author also discusses