Chemical Fortran

Fortran IV in Chemistry: An Introduction to Computer-assisted Methods. By G. Beech. Pp. x+303 (Wiley: London and New York, October 1975.) £8.75.

UNDERGRADUATE chemistry courses have so far not shown as much response to the advent of the computer as engineering courses, and they do not reflect its importance as a research tool. It is still possible to teach both theory and laboratory techniques without reference to the computer; the main impetus towards Fortran programming and computer-assisted techniques lies in the knowledge that nearly every chemistry graduate soon becomes involved with computers. Dr Beech's book will be invaluable to those responsible for the introduction of these methods at undergraduate level, and essential reading to undergraduates and research students meeting them for the first time. Perhaps the most striking feature of the book is the care with which the chemistry and the underlying mathematics are developed as well as the computing. The operation of the programs listed is always fully described in the text.

An elementary knowledge of Fortran is assumed. The first chapter gives those elements not met on a first programming course, and those which may depend on the particular machine used. Next, normal numerical and statistical methods are given, including non-linear equations and a particularly clear account of matrix operations and eigenvalues. Practical examples of the application to experimental data are taken from chemical kinetics, electrochemistry, thermal analysis, multicomponent spectroscopic data and mass spectroscopy. The next chapter covers a very wide range of computer simulations of experimental observables: modelling simple kinetic and radiochemical systems (including Monte Carlo techniques), thermodynamics and equilibria, crystal lattice energies, statistical mechanics, spectroscopic data (including curve addition and reduction), crystal field simulations and nuclear magnetic resonance line splitting and intensity. Theoretical topics treated include particle-in-a-box (one dimensional with bond length alteration, and two dimensional) and atomic and molecular orbitals (LCAO and Huckel calculations). In this section, emphasis is rightly placed on plotting out the results.

Data acquisition by analogue to digital instruments is described, followed by data processing (including convolution smoothing and baseline corrections), illustrated by application to nuclear magnetic resonance spectra. Complex data systems are described for mass spectrometry, gas chromatography and γ-ray spectrometry. The book closes with a useful review of the literature, including handling chemical information on the computer. Each chapter is followed by problems and a bibliography. The book is well produced, and in view of its extensive coverage, good value. It is warmly recommended for both undergraduate and postgraduate use. **B. P. Levitt**

Changing role of ion beams

New Uses of Ion Accelerators. Edited by J. F. Ziegler. Pp. xii+482. (Plenum: New York and London, 1975.) $33.60.

THE current state of world economics demands that equipment, manpower and money are used as efficiently as possible. Nuclear physics has long been singled out as one of the 'big science' areas and more than a generation of expansion has provided a legacy of ion accelerators of which the low energy machines (that is about 5 MV and below) are used increasingly today in fields far removed from the compilation of nuclear structure data. But the story now is not merely one of keeping highly specialised machinery occupied. So interesting and valuable have the applications of ion beams to materials science and solid-state physics turned out to be that many Van de Graaff accelerators, for example, are now used exclusively in analytical experiments complementing (or replacing) more well established techniques. An analogous situation exists in the new field of ion implantation where exciting property changes are induced with ions usually below 500 keV in a variety of materials. The result is that nuclear physics laboratories are undergoing a metamorphosis towards solid-state applications which encompass physics, chemistry, materials science and metallurgy.

This book covers new developments in analytical methods, such as Rutherford backscattering, channelling, nuclear reactions and characteristic X rays for composition analysis, as well as ion implantation and ion-induced X rays. The editor deserves praise for welding the wide-ranging subject matter so satisfactorily; and it is perhaps significant that nearly four-fifths of the book relates to analytical techniques since this is the area in which ion accelerators are making immediate impact. The previous volume—which had a similar title—appeared eight years ago. It was an excellent monograph which should have been more widely disseminated and its publication set the stage for constructive interaction between accelerator users and other physicists. It is encouraging to see how much ground has been covered in the intervening period and it is interesting to note the change of emphasis. In the present volume, for example, nuclear astrophysics and beam foil spectroscopy give way to superconductivity, corrosion studies and pollution species detection.

The principal value of this book is the bringing together of the detailed procedures for backscattering and X-ray data collection and analysis, as well as up-to-date overviews of current developments in ion implantation and X-ray excitation theory. It is a rare thing to find accounts written from what is clearly first-hand experience of the systematics of establishing a first-class analytical service using an accelerated beam of protons or helium ions. Inevitably in a book consisting of contributed chapters there is duplication but the essentials are there, and numerous real-life examples are included. Surprisingly there is very little reference to the ion implantation of semiconductors. Perhaps it was felt that this important field (virtually synonymous now with advance in device technology) receives adequate cover elsewhere. As semiconductor implantation, however, has provided the bread and butter of the industrial side of ion implantation for many years, and is likely to continue doing so, an omission of this sort is regrettable. It is unfortunately made all the more obvious since the contributed chapter on superconductors is wrongly labelled 'semiconductors' in the text! Rutherford backscattering should be referred to as such to distinguish elastic Coulomb interactions from inelastic reactions arising within the nucleus (nuclear backscattering). Although they receive attention in separate chapters, the two are referred to a little indiscriminately elsewhere. Having said that, the treatment and power of such methods of analysis (and the two chapters on ion-induced X-ray physics) are excellently covered.

Accelerator users, present and intending, should reach for this volume. No-one contemplating an integrated analytical programme or materials project with solids should be ignorant of the applications of ion beam machines and the growing expertise which surrounds them. It is a pity that oversights in production and a lack of standardisation of diagrams detract slightly from an otherwise well conceived book.

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