BOOK REVIEWS

Dove, M. T. *Introduction to Lattice Dynamics* Cambridge, (Cambridge University Press), 1993. xvii + 258 pp., Price £35. ISBN 0 521 39293 4.

This book provides an excellent introduction to the theory of lattice dynamics as currently applied in mineral physics where the two main areas of application comprise computer modelling of crystal structures and their properties, and the study of polymorphic phase transformations. The author is clearly aware of the fact that, in many cases, practising mineral physicists lack an advanced training in theoretical physics and the book is designed to provide a carefully thought out and graded introduction to the necessary theory. The book contains twelve chapters of text and the most advanced aspects of the subject are contained in chapters 6 and 11. Specific mathematical techniques are relegated to a suite of eight appendices which contain such items as the Ewald sum, the mathematical basis of Landau theory and an up-to-date compilation of existing references to phonon dispersion data. The book ends with a very comprehensive list of references, and a good subject index.

Chapter 1 discusses the need for a dynamical treatment of the structure of the crystal and reviews the conventional treatment of interatomic interactions in terms of coulombic, van der Waals and other forces. Lattice energy is defined in terms of the sum over pairwise interactions between atoms throughout the single crystal and the concept of modelling is introduced through the use of empirical interaction potentials. The chapter ends with a brief account of the wave description of atomic displacements through the introduction of the wave and displacement vectors.

The limitations on vibration of the atoms in a single crystal imposed by translational symmetry are used in Chapter 2 to define the concept of the Brillouin zone. The origin of dispersion curves is discussed for a simple monatomic crystal and an example of the dispersion curves for the rare gas structures is included. The origin of optical modes of vibration associated with the presence of several atoms in the unit cell is dealt with in Chapter 3 which emphasizes the distinction between acoustic and optic modes of vibration. The symmetries of the vibrational modes at both general and special points in the Brillouin zone are discussed as are features of the dispersion curves that are dictated by symmetry conditions.

The amplitudes of lattice vibrations are dealt with in Chapter 4 and at this point quantum theory is used to define the vibrational energy and the separation of the energy levels of the vibration modes at very low temperature where the role of Bose-Einstein statistics on the occupation of energy levels becomes important. A calculation of the actual magnitude of atomic displacements is provided at this stage and reference to the resulting crystallographic temperature factor is included.

The implications of lattice dynamics in the context of the thermodynamic properties of the single crystal are developed in Chapter 5 which begins by defining the partition function, and thus the free energy, for the crystal in terms of the energy of the lattice vibrations considered as quantised harmonic oscillators. The Einstein and Debye approximation models for the heat capacity of the crystal are described. The relationship between calculations at constant volume and at constant pressure is discussed and an actual example of the calculated density of states for NaCl is illustrated. The chapter ends with a brief introduction to the discussion of polymorphic phase transformations from this theoretical point of view.

Chapter 6 is by any account a difficult chapter which contains a general theoretical framework for the treatment of lattice dynamics and provides an exact solution of the dynamical behaviour of the single crystal using comprehensive matrix methods. This matrix formalism is necessary since, for atoms in low symmetry positions in complex structures, it is usual to find that the same type of displacement is present in a number of different vibrational modes and solutions to the complete vibrational problem necessarily involves the inclusion of all the relevant atomic coordinates and force constants in a single calculation. The student who wishes to obtain an overview of this topic might well start by studying the simpler case involved in defining the vibration modes and frequencies for a simple molecule under point group symmetry alone.

With the exception of Chapter 11 the chapters that follow deal with practical aspects of the application of the theory of lattice dynamics. Chapter 7 is concerned with the relationship between macroscopic

elasticity and the acoustic modes. Chapter 8 deals with the role of anharmonic vibration in relation to the onset of phase transformations and contains an exact model of a displacive phase transition. Chapter 9 is devoted to a brief account of the theory and practice of neutron diffraction in the determination of mode frequencies and Chapter 10 provides a similar coverage of infrared and Raman spectroscopy.

Chapter 11 makes a further return to theory and comprises a formal quantum mechanical treatment of the vibrations of the single crystal. Creation and annihilation operators are introduced and the corresponding form of the Hamiltonian defined. This formalism is used to provide information on the phonon population of the vibration modes.

The final chapter deals briefly with the application of relevant aspects of lattice dynamical theory to computer simulation studies on crystalline material. In this technique the random dynamic displacements and velocities of individual atoms in a chosen volume of the crystal (usually a simple multiple of the unit cell volume) are followed in real time and subject to chosen anharmonic interaction potentials. Extremely small time steps are used in order to avoid accumulated errors. The results of the extended simulation may be used to study selected features of the dynamic behaviour of the crystal. It is possible to control the temperature of the ensemble, and determine selected thermodynamic properties of the crystal. Anharmonic behaviour associated with simple displacive phase transformations can be reproduced. Of necessity periodic boundary conditions set a limit to the study of the vibrations throughout the whole of the Brillouin zone but by careful choice of the periodic unit of structure it is possible to sample the vibration spectrum at special points within the Brillouin zone. The author discusses the limitaflons of the method in some detail.

Overall this is a very well organised and helpful book on a topic which has very wide applications in mineral physics. It is strongly recommended to readers with a wide range of ability and practical experience in the subject. J. D. C. McCONNELL

Kretz, R. *Metamorphic Crystallization* Chichester and New York, (John Wiley and Sons), 1994. xiv + 507pp., Price £22.50 (paperback). ISBN 0-471-94214-6.

Professor Kretz has long been an important influence in metamorphic petrology for his pioneering work in the 1960s and 70s on textures and segregation processes, and I viewed the announcement of his textbook with considerable interest. It is a fat paperback, abundantly illustrated, and crammed with samplings across the subject. The precise level at which it is aimed is not entirely clear: the opening chapter assumes a high degree of familiarity with much of the subject matter of the remainder, and although terminology is introduced from first principles, it seems more likely that this is intended as a graduate student text.

The work is divided into five large chapters, followed by a range of appendices. The first introduces the basic concepts of metamorphism, and this is followed by chapters on mineral thermodynamics, phase equilibrium, chemical kinetics and granular microstructures and crystallization mechanisms. There is no systematic treatment of specific field areas, rock types or facies series; instead individual topics are illustrated with specific examples, many of them drawn from the high grade rocks of the Grenville province of Canada.

The approach to thermodynamics is classical, but with a strong emphasis on mineralogical examples. However, although a little thermodynamic data is tabulated, there are neither worked examples of calculations, nor problems, so that the treatment is very much theoretical. With everything from Maxwells relationships to Margules models in a single chapter, the main value is likely to be in helping students with an existing thermodynamic background to learn to apply it to petrology: the true beginner is likely to be daunted by the copious equations, impossible to cross reference because they are not numbered except for a small block of about 70 in the middle of the chapter. Furthermore, the book is rather reminiscent of an earlier generation of petrology texts, in providing copious equations that are never subsequently used.

In a similar way, the kinetics chapter provides a detailed introduction to classical chemical kinetics, again without any worked examples, but is remarkably weak in explaining how these ideas apply to metamorphism. On the final page the author notes that in nature factors such as the rate of heat supply may be important in controlling reaction rates, but there is no attempt to amplify this point or introduce the relevant literature. Furthermore there are many new developments in mineralogical kinetics from the material sciences which are not mentioned here.

The sections dealing with metamorphic textures and processes were the ones of which I had the highest expectations, but they consist primarily of a summary of Kretz's own work, as originally published, with no new insights into the subject and precious little attention to what has been done by others. For example corona textures are illustrated with an example from an earlier paper by Kretz and co-workers, which is described in some depth, but there is no mention of the debate in the literature by other workers of whether or not coronas form in a closed system.