of polytypism appears to be the Jagodzinski's disorder theory.

References

BOZORTH, R. M. (1922). *J. Amer. Chem. Soc.* **44**, 2232.

CHADHA, G. K. & TRIGUNAYAT, G. C. (1967a). *Crystal Growth.* Supplement to *J. Phys. Chem. Solids*, p. 313.

CHADHA, G. K. & TRIGUNAYAT, G. C. (1967b). *Acta Cryst.* **22**, 573.

CHADHA, G. K. (1967c). Ph. D. Thesis, Delhi Univ.

FRANK, F. C. (1951). *Phil. Mag.* **42**, 1014.

GOMES DE MESQUITA, A. H. (1968). *Acta Cryst.* B**24**, 1461.

JAGODZINSKI, H. (1954a). *Neues Jb. Miner. Mh.* **3**, 49.

JAGODZINSKI, H. (1954b). *Acta Cryst.* **7**, 300.

JAIN, R. K. & TRIGUNAYAT, G. C. (1968). *Z. Kristallogr.* **126**, 153.

KLEBER, W. & FRICKE, P. (1963). *Z. Phys. Chem.* **224**, 353.

KRISHNA, P. & VERMA, A. R. (1963). *Proc. Roy. Soc.* A**272**, 490.

LUNDQVIST, D. (1948). *Acta Chem. Scand.* **2**, 177.

MITCHELL, R. S. (1956). *Z. Kristallogr.* **108**, 296.

PEIBST, H. (1963). *Z. Phys. Chem.* **223**, 193.

RAMSDELL, L. S. & KOHN, J. A. (1952). *Acta Cryst.* **5**, 215.

SCHNEER, C. J. (1955). *Acta Cryst.* **8**, 279.

SRIVASTAVA, O. N. & VERMA, A. R. (1962). *Z. Kristallogr.* **117**, 450.

SRIVASTAVA, O. N. & VERMA, A. R. (1964). *Acta Cryst.* **17**, 260.

SRIVASTAVA, O. N. & VERMA, A. R. (1965). *Acta Cryst.* **19**, 56.

TRIGUNAYAT, G. C. & VERMA, A. R. (1962). *Acta Cryst.* **15**, 499.

VERMA, A. R. (1957). *Proc. Roy. Soc.* A**240**, 462.

VERMA, A. R. & KRISHNA, P. (1966). *Polymorphism and Polytypism in Crystals.* New York: John Wiley.

YUASA, T. & TOMITA, T. (1966). *J. Phys. Soc. Japan.* **21**, 2084.

YUASA, T. & TOMITA, T. (1967). *J. Phys. Soc. Japan.* **23**, 136.

ZHDANOV, G. S. & MINERVINA, Z. V. (1945). *J. Phys.* **9**, 151

The Geometry of Lattice Planes

BY J. F. NICHOLAS*

School of Physics, University of Warwick, Coventry, England

The advantages are discussed of using a ball model to determine the arrangement of lattice points in a given lattice plane and for determining the stacking properties of such planes. It is shown that the ball model can be considered as a simple analogue computer for solving the Diophantine equations involved. To date, such ball models have been used only for cubic and hexagonal crystals, but they can be constructed for many other structures.

In papers with the above title, Jaswon & Dove (1955) and Bevis (1969) have presented systematic methods for mapping the projection of a lattice on to a plane of given Miller indices (hkl). The aim of this paper is to draw attention to another method, that of constructing a ball model of a crystal divided parallel to (hkl), and to note an error in the earlier papers.

The essential problem is that of finding lattice vectors $\mathbf{u}, \mathbf{v}, \mathbf{w}$ such that $\mathbf{u}, \mathbf{v}$ define a primitive mesh in an (hkl) plane and $\mathbf{u}, \mathbf{v}, \mathbf{w}$ define a primitive unit cell in the lattice. It is usually advantageous if the vectors are as small as possible, *i.e.* if the angles between them approach 90°.

Jaswon & Dove (1955) solve the problem by using

$$\mathbf{a}' = l, 0, \bar{h}$$
$$\mathbf{b}' = 0, l, \bar{k} \tag{1}$$

to define a unit mesh in (hkl) and then searching out all extra lattice points within this mesh in order to determine a primitive mesh. They then look for a suitable $\mathbf{w} = w_1, w_2, w_3$ by solving

$$hw_1 + kw_2 + lw_3 = 1 . \tag{2}$$

On the other hand, Bevis (1969) chooses

$$\mathbf{u} = -\frac{k}{d}, \frac{h}{d}, 0 , \tag{3}$$

where d is the highest common factor of h and k, looks for an integral solution m_1, m_2 of

$$m_1 k - m_2 h = d , \tag{4}$$

and can then write down

$$\mathbf{v} = k(1 + m_3) - lm_2, -h(1 + m_3) + lm_1, -d , \tag{5}$$

where m_3 (or, more simply, $1 + m_3$) is an arbitrary integer. Equation (2) is then solved to give $\mathbf{w}$.

* Permanent address: Division of Tribophysics, C.S.I.R.O., University of Melbourne, Australia.

Both methods calculate the shift vector **t**, which is the projection of **w** onto (*hkl*), as

$$t = w - d, \tag{6}$$

where **d** is a vector perpendicular to (*hkl*) and of magnitude equal to the spacing between (*hkl*) planes. The projections of successive planes are then plotted by calculating the magnitudes of and angles between **u**, **v** and **t**. Since **w** is not uniquely defined by equation (2), there are many possibilities for **t** and Jaswon & Dove specify that **t** shall be as short as possible; even this restriction often leaves **t** ambiguous (see, for example, Fig. 2). It may be noted that Bevis uses **h** to denote the vector **d** in his equations (4) and (14) although in his *Introduction* and in the preamble to equation (14) he has used **h** in the more usual sense as the vector with components (*hkl*) relative to the reciprocal axes, *i.e.* as the vector parallel to **d** but of length equal to the reciprocal of the interplanar spacing.

Equations (2) and (4) can normally be solved very quickly by a trial-and-error process but, since the necessary algorithms exist, it is of course possible to carry out the whole process on a computer (*e.g.* Bacigalupi, 1964). This only gives immediate and complete results for those fortunate enough to have direct access to a terminal with plotting facilities.

A completely different approach is to construct a ball model of a half-crystal which terminates on an (*hkl*) surface. Methods of doing this for a variety of cubic and hexagonal structures are given in Moore & Nicholas (1961) and Nicholas (1961, 1962), while a selection of results appears in Nicholas (1965). From such a model, a plot of the unit mesh and of the stacking of planes can be produced photographically or, if greater accuracy is required, suitable vectors **u**, **v**, **w** can easily be selected and indexed on the model and the plot carried out as in the other methods. Thus, the ball model can be considered as a simple and economical analogue computer for solving Diophantine equations such as (2) and (4) and for producing a plot. As an example, Fig. 1 shows a model of a (5, 8, 11) surface in a body-centred cubic crystal (the example chosen

by Bevis), together with a plot showing the unit mesh in the surface and the stacking vector **w** as derived from the photograph.

The advantages of modelling are that a visual impression of the stacking over several layers is available, a variety of planes can be considered in quick succession, the simplest unit mesh (*e.g.* the rectangular mesh in Fig. 1, which is not described by Bevis) is obvious, and any gross errors in calculating a plot of mesh shape can be eliminated by comparison with the model. The indexing of the vectors depends on prior indexing of a basis such as *OABC* in Fig. 1(*a*), but this is necessarily done when the model is being set up. It is worth noting that the identification of equivalent vectors is always simpler on the model itself than on a photograph.

Although surface models have only been built for cubic and hexagonal structures, the theory in Nicholas (1961) describes a method for their construction in any structure for which a 'ball' model of the bulk crystal can be made. No general rules can be laid down for the construction of such bulk models but a large range of structures can be modelled by using base plates to force the first layer of balls into a predetermined pattern and/or by using balls having a degree of asymmetry.

The error referred to in the opening paragraph arises when the analysis is applied to lattices indexed relative to a centred unit cell and (*hkl*) is such that

$$hw_1 + kw_2 + lw_3 = \tfrac{1}{2} \tag{7}$$

has solutions for w_1, w_2, w_3 equal to a lattice vector (with at least two of the w_i non-integral). This implies that there are other lattice planes between those whose maps are separated by **t**. Bevis (1969) tabulates the conditions when this occurs for various centrings of the cell and then asserts that the extra planes are to be plotted at $\tfrac{1}{2}$**t** from the original ones. Jaswon & Dove (1955) and Jaswon (1965) make equivalent assertions. In fact, as can be seen from Fig. 2, which shows a plot of (111) planes in a body-centred cubic lattice, the displacement need not be $\tfrac{1}{2}$**t**. However, it must be one of $\tfrac{1}{2}$**t**, $\tfrac{1}{2}$(**u** + **t**), $\tfrac{1}{2}$(**v** + **t**), $\tfrac{1}{2}$(**u** + **v** + **t**), the selection depend-
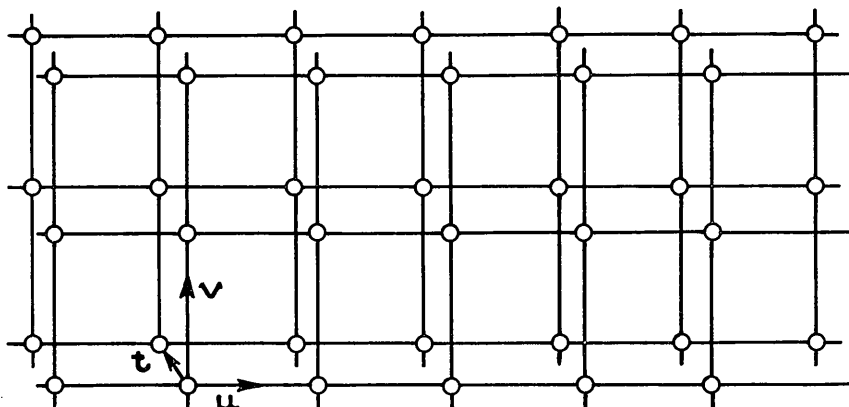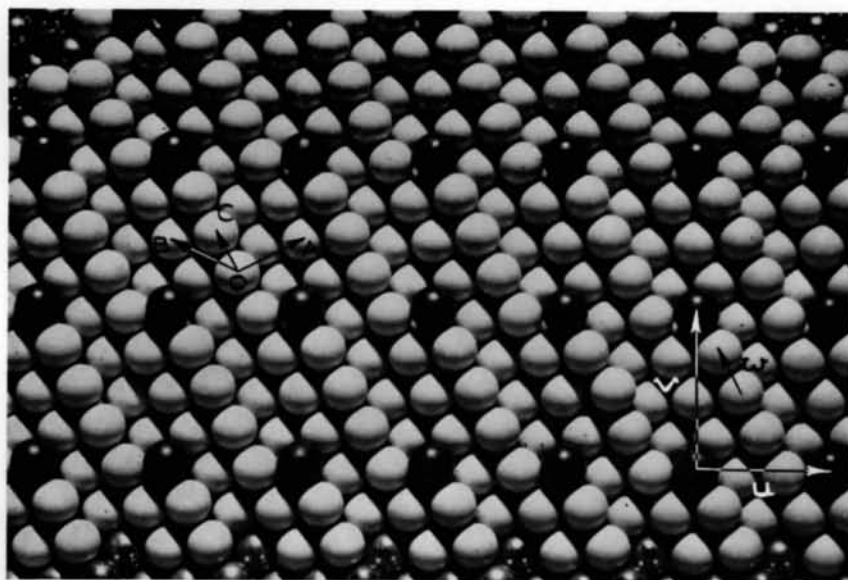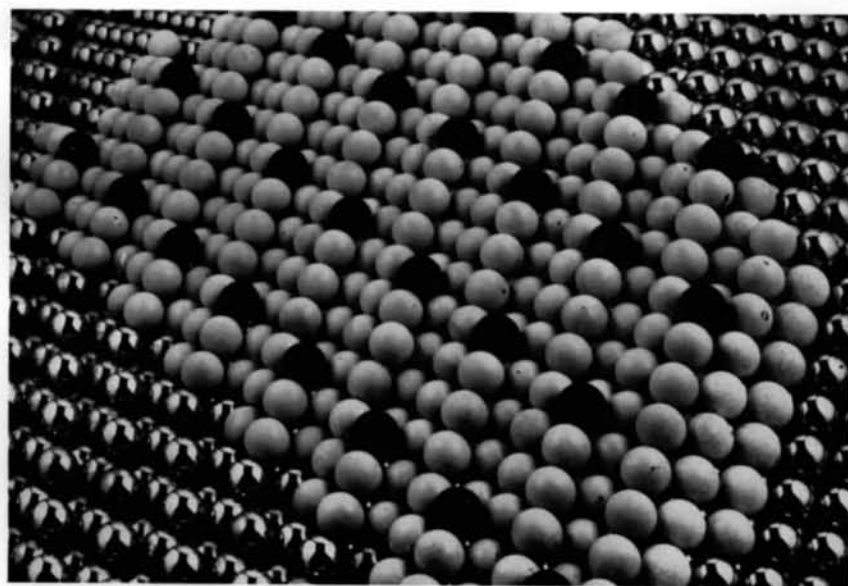

Fig. 1 (*cont.*). (*c*) Two lattice planes as traced from the photograph of the model (see Plate 42).

(a)

(b)

Fig. 1. Model of $(5,8,11)$ surface in a body-centred cubic lattice viewed (a) normal to the surface and (b) obliquely. The dark balls represent lattice points in the outermost plane, the white ones those in lower planes. The vectors $OA = 1,\bar{1},0$; $OB = 0,1,\bar{1}$; $OC = \frac{1}{2},\frac{1}{2},\frac{\bar{1}}{2}$ shown in (a) define a primitive unit cell in the lattice. By tracing ball-to-ball displacements, the rectangular unit mesh can be shown to have edges of $\mathbf{u} = OA + BO = 1,\bar{2},1$ (horizontal) and $\mathbf{v} = OA + 3OC = \frac{5}{2},\frac{1}{2},\frac{\bar{3}}{2}$ (vertical), while the shortest $\mathbf{w}$ is clearly OC. The plot in (c) (p. 471) shows two lattice planes as traced from the photograph.

ing on the original choice of w, with or without Jaswon's restriction on the size of t. The simplest way of plotting centred lattices is temporarily to ignore the centring, choose u,v,w as lattice vectors, with integral components, which define a unit cell of volume equal to that of the centred unit cell, and plot the lattice planes so described. Then, centre each of the seven vectors u,v,w, u+v, v+w, w+u, u+v+w that satisfies the conditions in Table 1. Finally, plot extra nets of points based on each of the centring points.

Table 1. *Conditions under which a lattice vector with integral components* s_1, s_2, s_3 *will be centred*

Lattice	Condition	Number of tested vectors that will be centred
Body-centred	s_1, s_2, s_3 of same parity	1
Face-centred	$s_1 + s_2 + s_3$ even	3
Base (C)-centred	$s_1 + s_2$ and s_3, both even	1

I am indebted to the Association of Commonwealth Universities for the award of a Visiting Professorship, to CSIRO for a grant of leave, and to the University of Warwick for hospitality while this note was prepared.

References

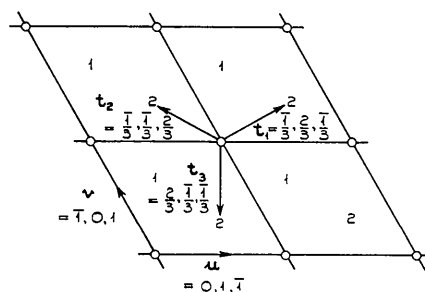BACIGALUPI, R. J. (1964). *NASA Technical Note*, NASA TN D-2275.

Fig. 2. Plot of (111) planes in a body-centred cubic lattice; the numbers show lattice points in successive planes with ones representing body-centre sites. Three possible shift vectors [as defined by equations (2) and (6)] t_1, t_2, t_3 are shown, all being of equal length. The lattice vector joining successive layers is clearly not $\frac{1}{2}u$ but could be $\frac{1}{2}(t_1 + v)$ or $\frac{1}{2}(t_2 + u + v)$ or $\frac{1}{2}(t_3 + u)$.

BEVIS, M. (1969). *Acta Cryst.* A**25**, 370.

JASWON, M. A. (1965). *Mathematical Crystallography.* p. 116. London: Longmans.

JASWON, M. A. & DOVE, D. B. (1955). *Acta Cryst.* **8**, 88.

MOORE, A. J. W. & NICHOLAS, J. F. (1961). *J. Phys. Chem. Solids,* **20**, 222.

NICHOLAS, J. F. (1961). *J. Phys. Chem. Solids,* **20**, 230.

NICHOLAS, J. F. (1962). *J. Phys. Chem. Solids,* **23**, 1007.

NICHOLAS, J. F. (1965). *An Atlas of Models of Crystal Surfaces.* New York: Gordon & Breach.

One-Dimensional Models for Small-Angle X-ray Diffraction from Crystalline Polymers. I. General Model

BY D. J. BLUNDELL

Imperial Chemical Industries Limited, Petrochemical and Polymer Laboratory, P.O. Box 11, The Heath, Runcorn, Cheshire, England

The relationship between a one-dimensional model for predicting small-angle X-ray scattering from crystalline polymers and a three-dimensional structure containing a one-dimensional periodicity is discussed. The basic features of previous models are reviewed. Based on the approach of Hosemann for a simple two-phase system, a model is formulated in which the density variation within the crystalline regions is described by an arbitrary function $\xi(y)$.

Introduction

This article is concerned with the formulation of a general one-dimensional model suitable for describing discrete small-angle X-ray scattering from crystalline polymers. The diffraction occurs at angles around one degree and is generally attributed to a regular alternation in texture every 100–300 Å between crystalline and amorphous-like intercrystalline regions. In most types

of sample, the periodicity within each local scattering sequence is essentially one-dimensional. This is well illustrated by the case of samples made by sedimenting a suspension of solution grown polymer crystals. In their simplest form, the crystals are about 100 Å thick, bordered on their planar surface by thin layers of amorphous-like material (Keller, 1968). Thus on sedimenting, the crystals stack on top of one another to form a periodic crystalline–amorphous structure perpendicular