

maxima of a Fourier series are sound. It is also clear that formula (1) is capable of resolving the maxima corresponding to interatomic vectors.

The statistical procedure in vector space constitutes a direct method for attacking structure problems. The validity of these statistical concepts, coupled with the attractiveness of working directly in coordinate space, indicate the direction of future developments, namely, the search for probability distributions for the phases of the structure factors as well as for the atomic coordinates, rather than the interatomic vectors.

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## A Three-dimensional Coordinate Model for Demonstration of Inorganic Crystal Structures

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A transparent plastic framework is described in which coloured pins may be inserted to show the arrangements of atoms in simple unit cells.

Numerous types of three-dimensional model have been devised to show arrangements of atoms in crystal lattices, but few are quickly adaptable to the study of symmetry or coordination relationships in a wide variety of structures. Most X-ray crystallographers have at some time coveted a three-dimensional black-board.

A model of the type shown in Fig. 1 has proved useful, in both research and teaching, for setting out atom positions in simple inorganic structures, particularly those belonging to the cubic and tetragonal systems. It comprises sheets of clear 'Perspex',  $\frac{1}{8}$  in. in thickness, each having a coordinate 'net' of small holes drilled at suitable intervals. Successive sheets are held at regularly spaced intervals by nuts and washers on threaded brass rods; the rods are conveniently mounted in a heavy base-plate of thick 'Sindanyo' sheet. Atom centres are marked by brightly coloured map-marking pins dropped into the holes; such pins are available in a variety of sizes, shapes, and colours from large stationers. The pins are conveniently dropped into position by means of a long pair of tweezers. The particular model shown in Fig. 1 has a cubic array of holes, and was originally designed to depict a single unit cell of the spinel structure. The holes are drilled to a square pattern at 1 in. intervals, and the upper surfaces of successive sheets are 1 in. apart. Nine sheets, each containing nine rows

of nine holes, provide all the coordinates required to set up the ideal spinel cell, in which all the atom coordinates are multiples of  $\frac{1}{8}$ . Many simpler cubic cells can be shown on the same framework. Tetragonal cells can be accommodated by adjusting the spacing of the sheets to the required  $c/a$  ratio, the  $c$  axis being set perpendicular to the plane of the sheets.

Another similar model has been constructed for hexagonal (including rhombohedral) structures, having the sheets drilled to provide sixfold symmetry; the sheets again contain nine rows of holes in each of two directions  $120^\circ$  apart, allowing atom coordinates to be set off in multiples of  $\frac{1}{3}$  in the conventional hexagonal cell.

The models are particularly convenient in showing coordination relationships clearly. They are proving useful in research in the examination of ionic environments in ferromagnetic solids; possible modes of interaction between ions can be visualized much more clearly from such models than from diagrams or lists of coordinates. In teaching work numerous typical structures can be built up at little expense. Random and ordered replacement in solid solutions are readily contrasted on the lecture bench by interchanging a few coloured pins. By running wires or coloured threads through rows of holes to represent symmetry axes, the operation of the different types of axes (including screw axes) is effectively demonstrated; pins are in-

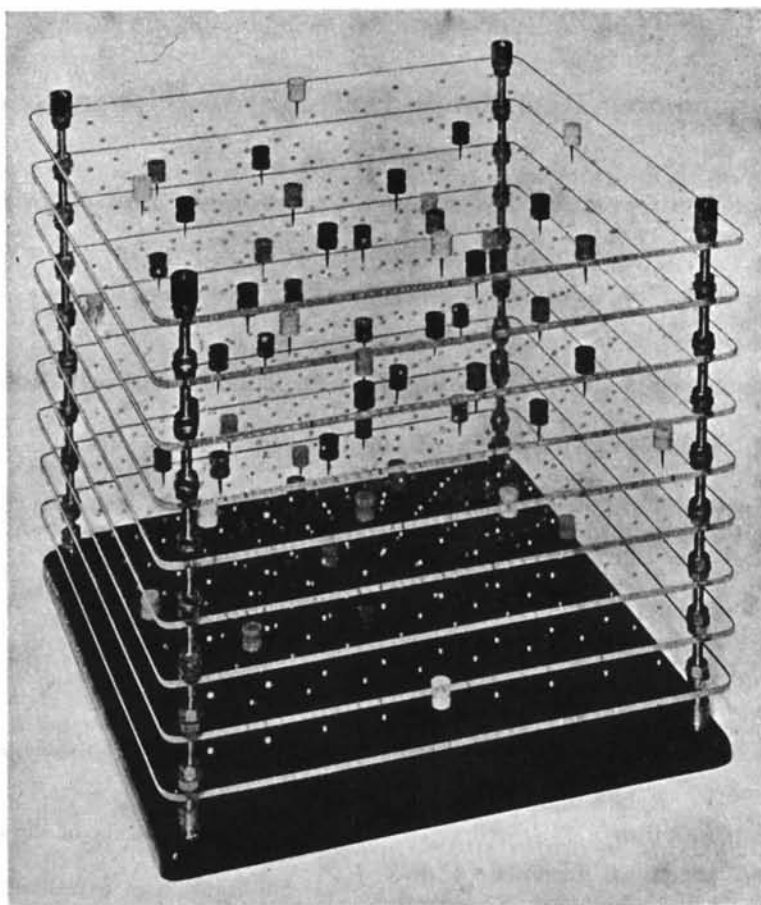


Fig. 1. 'Perspex' model of the ideal spinel structure. The conventional origin of the unit cell is at the centre of the model.

sented successively at the positions reached by successive symmetry operations. Symmetry planes and centres can be represented respectively by coloured threads or ribbons wrapped round the model and by pins with small, distinctively coloured round heads. Apart from demonstration of axes, centres and planes of symmetry severally, their combinations are readily shown. The complete set of symmetry elements corresponding with a space group can be set up on the model, and the repetition of atoms in general or special positions illustrated by inserting pins in succession to show the operation of each element of symmetry.

Models of orthorhombic structures would require specially drilled sheets; monoclinic and triclinic lattices would need special drilling and some arrange-

ment to displace successive sheets in their own plane. Nevertheless, the wide occurrence of the simpler systems among inorganic compounds, and the low cost and adaptability of the models, makes them an attractive addition to most crystallographic laboratories.

The 'Perspex' sheets tend to collect dust quickly. They are conveniently cleaned with a soft mop, warm water, and a detergent; use of a detergent such as 'Sterege' allows free drainage and leaves a sparkling surface after air-drying.

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