

recognition sites. Because of its selectivity for peripheral CCK receptors, L-364, 718 is unlikely to be useful in treating brain disorders, even though it probably penetrates the blood-brain barrier.

What might be therapeutic targets for a peripheral CCK antagonist? CCK itself decreases appetite both in animals and humans¹⁰, and some pharmaceutical companies have looked for CCK-mimicking

drugs as appetite suppressants. Whether L-364,718 and related agents will treat disorders of the stomach, intestine, pancreas, gall bladder or other peripheral organs is an open question. □

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Five-fold symmetry

Disorder among the atoms

from Alan L. Mackay

THE revolution in crystallography following the discovery¹ that textures with icosahedral symmetry can form from rapidly solidified alloys such as Al₃Mn is now at the stage where the new insights are being consolidated (see, for example, ref. 2). Knowles and Stobbs, whose latest work is reported on page 313 of this issue³, and others are trying to allocate positions to the atoms to account quantitatively for the electron, X-ray and neutron diffraction data. The task turns out not to be so easy for various reasons.

About six different alloys have so far been shown to have icosahedral phases, each of which is probably related by slight atomic movements to different crystal structures, so that no single arrangement of atoms can answer all the questions. There is also a phase known as the T-phase, which seems to be a periodic stacking of quasi-crystal sheets. Most models of quasi-crystal structures are based on icosahedral clusters of several layers, on the general lines of those found for the crystalline Mg₃₂(Al,Zn)₉₉ by Bergmann, Waugh and Pauling in 1957 (ref. 4). The problem now is to obtain a detailed proof accounting both for determinate structure and for those statistical departures from it which may account for the present difficulties in allocating atomic positions.

Our understanding of the whole question of 'textures' — the way local order is developed on larger scales — in this context needs re-examination; even the simple case of defining exactly the texture of a drawn metal wire is not clear. Here the structural elements are crystalline grains of certain spread of grain size and orientation. The X-ray diffraction spots are each caused by a number of grains.

As long ago as 1931, Carl Hermann⁵ pointed out that textures could have icosahedral point group symmetry. The geometrical 'Penrose tiling' produces such a texture. In this tiling, the projection of a six-dimensional (hypercubic) lattice into three dimensions gives a tiling of three-dimensional space by two quasi-unit cells, two kinds of rhombohedra, having the same faces but one obtuse and the other

acute⁶. The Penrose tiling is an algorithm for filling space with these two rhombohedral 'quasi-unit cells' such that the resulting array of quasi-lattice points has icosahedral diffraction symmetry if a sufficient volume is considered. It is thus an algorithm for giving a texture with no statistically indeterminate elements.

In orthodox crystallography it is only convenience that leads us to use parallelepipedal unit cells repeating by translation. We could as well use space-filling cells; indeed, this would be more realistic for the hexagonal system, where hexagons correspond better to the physical interactions than the conventional crystallographic parallelepipeds. Correspondingly, in quasi-crystals we could use rhombic triacontahedra, each of which could be made of 10 acute and 10 obtuse rhombohedra, as the physical units, and allow them to overlap in the way prescribed by the Penrose tiling. This is perhaps a more physical way of building in the local icosahedral symmetry.

Unfortunately, the allocation of six-dimensional crystal indices from scattering data involves an ambiguity. Any real number can be expressed (to a prescribed accuracy) as $a + b\tau$, where a and b are integers and τ is irrational, for example the golden number. Thus, as any point in the three-dimensional reciprocal space determined from a diffraction pattern can be given integer indices, two for each dimension, so the allocation of unique indices is not a convincing test for a particular geometrical model. The test of the existence of a particular generation of a quasi-lattice corresponding to a packing of rhombohedra is luckily more stringent and in practice all observed reciprocal lattice points can be attributed to the reciprocal lattice corresponding to a rhombohedral side of length 4.6 Å.

The mathematical theory of how to dispose asymmetrical units in these tiles is not yet properly developed and structure analysis is thus at the pre-space-group stage. Cahn and Gratias⁷ have made a beginning by examining the extinctions produced by projecting centred 6-

dimensional hypercubic lattices. Thus, a potentially complete theory is available for producing a structure which has the required diffraction effects and which has no statistical features at all.

Knowles and Stobbs³ constructed small regions of this kind of structure and calculated diffraction patterns by regarding the structures as large molecules. They find that on the basis of arranging atoms in the two kinds of unit cells no particular structure looks convincing. In agreement with other authors (S. J. Poon, S. Preische & Y. Shen; personal communications) they find that a model with an average atom at the quasi-lattice points gives better agreement than any plausible arrangement of real atoms.

The next question to answer is what kind of disordering is necessary to produce this averaged structure. One possibility is a phase-shift disorder — the staggering of the five lines or columns of atoms in quasi-crystals by half a spacing. High-resolution electron microscopy suggests that the Bragg electron-density waves, which are measured in amplitude and direction (but not in phase) by the sharp diffraction spots, can be phase-modulated (with a range of wavelengths of about 80–100 Å). These dislocations are called phasons. Adjacent grains scatter coherently for the same reflection but with different phases. Anti-phase domains would be an example of a crystal structure broken up by the occurrence of phasons of magnitude π , causing extinctions and variations in spot intensity. A crude summary of the process is the appearance with rapid cooling of many nuclei that are sufficiently mobile to rotate into close angular correspondence with each other over micro-metre ranges. The icosahedral group is optimal as it has the highest order (60).

It looks as if the techniques of X-ray diffraction from a substantial volume may not be sensitive enough to determine both a definite structure and its local disordering and that a model, having passed this hurdle, must also account for electron microscope observations where phase information is also available. Phasons will not be localizable as diffraction methods measure only structure amplitudes and sufficient phasons would perhaps tend to make all reflections much the same intensity, as Knowles and Stobbs observe. □

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