

case in more than one dimension, and holds for those arrays of lattice points which can be derived by bounded projection from a lattice of higher dimensionality (an alternative definition of a quasilattice)⁵. Determination of the atomic arrangement still, as far as we know, waits for the development of a method of calculating structure factors and for the apportionment of statistical and determinate features of the texture.

ALAN L. MACKAY

*Department of Crystallography,
Birkbeck College,
University of London,
Malet Street, London WC1E 7HX, UK*

1. Shechtman, D., Blech, I., Gratias, D. & Cahn, J.W. *Phys. Rev. Lett.* **53**, 1951 (1984).
2. Pauling, L. *Nature* **317**, 512–514 (1985).
3. Nelson, D. & Sachdev, S. *Phys. Rev.* **B32**, 689–695.
4. Bancel, P.A., Heiney, P.A., Stephens, P.W., Goldman, A.I. & Horn, P.M. *Phys. Rev. Lett.* **54**, 2422–2425 (1985).
5. Elser, V. *Acta crystallogr.* (in the press).
6. Mackay, A.L. *Sov. Phys. Cryst.* **26**, 517–522 (1981) *Physica* **114A**, 609–613 (1982).

SIR—We recently presented X-ray and electron diffraction data on the icosahedral phase of rapidly quenched Al-Mn and introduced a simple indexing scheme based on the symmetry of an icosahedron (Bancel *et al.*, ref. 1 and in the press). We used our X-ray diffraction measurements to argue against models for the structure of this material that require multiple scattering from different crystallites to explain the electron diffraction patterns. Linus Pauling has proposed² a new crystalline model for the icosahedral phase, which he compares with X-ray powder diffraction data obtained from Shechtman and Blech³.

In Pauling's model, the icosahedral symmetry observed in the electron diffraction patterns is accommodated by multiple twinning of cubic crystals. Although twinning makes the analysis more complicated, it is still possible to check whether the (hkl) indices given in Table 1 of Pauling's paper can be consistent with the observed electron diffraction patterns. Consider any two of Pauling's cubic vectors, which are separated by some angle ϕ . Upon twinning, each vector is rotated via a set of icosahedral symmetry operations to a new set of positions. The same twinning operations act upon both cubic vectors, so that the angle ϕ is preserved during rotation. If one now calculates the angle that the vectors of one icosahedral set make with the vectors of the other set, the angle ϕ should certainly appear. Pauling's model fails this test on nearly all counts¹. Thus, the icosahedral diffraction spots cannot be attributed to rotations of the cubic structure which Pauling proposes.

Pauling states that the agreement between the X-ray peak positions of Shechtman's data and the d-spacings predicted by his model provides compelling evi-

dence that his structure is the correct one. We are not convinced by this argument because we believe that seven of the peaks he indexes are actually due to a different phase present in the sample. We have measured X-ray powder diffraction patterns from a large number of rapidly quenched icosahedral alloys, and find that reflections 3,4,6,8,10,15, and 16 listed in Pauling's Table are due to a contaminant phase that appears when excess Si is present in the sample. These peaks are not found in the electron diffraction patterns. (Note that Shechtman's sample contained several atomic % Si). We feel that this fortuitous agreement of several spurious peaks is an argument for the hypothesis that any powder diffraction pattern can be indexed via a sufficiently large cubic unit cell.

The question remains as to whether a crystal structure incorporating a large unit cell might still describe the electron and X-ray diffraction data. Based on recent low angle electron and X-ray diffraction data we can specify a minimum size for any proposed cubic unit cell. For any periodic structure the squares of any two d-spacings must be in integer ratios unless the corresponding diffraction spots have the same symmetry (so are collinear) in which case the ratio of the d-spacings is a ratio of integers. We have observed two such spots which lie along the major axes of the 2-, 3-, and 5-fold symmetry planes with d-spacings of 8.85(7) and 5.42(3) Å, the ratio of which is 1.633. The lowest rational approximate, within experimental error, to this number, is 13/8. This implies a minimum cell size of $a_0 = 8(8.85\text{Å}) = 71\text{Å}$. A 27Å cubic unit cell cannot produce two *collinear* spots with these radii even with the inclusion of multiple twinning. Although our arguments are stated in the context of a twinning model, numerous high resolution microscopy measurements vitiate the possibility of twins in these structures. In the absence of twinning our limit of 70Å as a minimum cell size holds and is valid for any crystal symmetry. A crystal structure adhering to this criterion would have to include well over 10,000 atoms in its unit cell.

Finally, we find somewhat curious Pauling's statement that "Crystallographers can now cease to worry that the validity of one of the accepted bases of their science has been questioned". No one has seriously questioned the premise that fivefold or icosahedral symmetry is inconsistent with periodic translational order. Rather, it has been observed that particular arrangements of atoms without simple periodic translational order and with crystallographically disallowed symmetries may nonetheless give rise to sharp diffraction patterns⁴. The study of "quasicrystalline" structures is mathematically intriguing. Furthermore, even if all the phases of Al-Mn should turn out to be crystalline, the

theory of quasicrystalline materials may well provide clues to the properties of materials that have local icosahedral symmetry.

PETER A. BANCEL
PAUL A. HEINEY

*Department of Physics and Laboratory
for Research on the Study of Matter,
University of Pennsylvania,
Philadelphia, Pennsylvania 19104, USA*

PETER W. STEPHENS

*Department of Physics,
State University of New York,
Stony Brook, New York 11794, USA*

ALAN I. GOLDMAN

*Physics Department,
Brookhaven National Laboratory,
Upton, New York 11973, USA*

1. Bancel, P.A., Heiney, P.A., Stephens, P.W., Goldman, A.I. & Horn, P.M. *Phys. Rev. Lett.* **54**, 2422 (1985).
2. Pauling, L. *Nature* **317**, 512 (1985).
3. Shechtman, D. & Blech, I. *Metal Trans.* **16A**, 1005 (1985).
4. Levine, D. & Steinhardt, P.J. *Phys. Rev. Lett.* **53**, 2477 (1984).

SIR—In the analysis of apparent icosahedral symmetry of Al-(Mn-, Fe-) alloys by Pauling¹ one observation remained unaccounted for. Mössbauer data of Swartzendruber *et al.*² indicate the presence of two types of sites for the transition metal. The occurrence ratio was found to be close to the golden mean $(\sqrt{5}+1)/2=1.61803$. In the model of an aperiodic "icosahedral phase" this can be easily explained by two types of differently distorted icosahedra. In order to fill the three-dimensional space in the sense of the 5-fold Penrose tile the occurrence ratio of two different elements should be exactly the golden mean.

On the other hand, in the Pauling's picture of multiple twinning of cubic crystal the growth process can be seen as starting from the 12-vertex icosahedral seed (Fig. 1 of ref. 3), with the next layer being dodecahedral (20 atoms). In any structure based on these two mutually complementary polyhedra the occurrence ratio of 20/12=1.667 could be expected for different types of lattice sites. But this ratio differs from the golden mean by only 3%.

A plausible suggestion is, therefore, that Swartzendruber *et al.*² did, in fact, observe the above ratio (20/12) rather than the golden mean. If this is the case, then the dilemma between the "icosahedral phase" and Pauling's model based on a cubic cell could be resolved by the Mössbauer experiment with the peak intensity resolution greater than 3%.

A.A. BEREZIN

*Department of Engineering Physics,
McMaster University,
Hamilton, Ontario,
Canada L8S 4M1*

1. Pauling, L. *Nature* **317**, 512 (1985).
2. Swartzendruber, L.J., Shechtman, D., Bendersky, L. & Cahn, J.W. *Phys. Rev.* **B32**, 1383 (1985).
3. Bergman, G., Waugh, J.L.T. & Pauling, L. *Acta crystallogr.* **10**, 254 (1957).