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Acta Cryst. (1989). A**45**, *FC33–FC36*

A structural model for a quasicrystalline material

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(Received 12 October 1989; accepted 23 October 1989)

Abstract. A structural model for a quasicrystalline material of approximate composition $Al_{65}Cu_{20}Fe_{15}$ is presented. The validity of the model was tested by comparing the optical diffraction of projections of the model with experimental electron diffraction patterns of crystal fragments.

Introduction. Our approach to a model of a quasicrystalline structure involves the use of high-resolution transmission electron microscopy (HRTEM) images to derive the local structures of the so-called prolate and oblate rhombohedra that fill a space of the restricted, conformal symmetry. We have studied quasicrystals of the alloy $Al_{65}Cu_{20}Fe_{15}$ prepared and characterized by Tsai, Inoue & Masumoto (1987) and we gratefully acknowledge their gift of a sample.

Experimental. The transmission electron microscopes used in order to obtain electron diffraction patterns and high-resolution micrographs were a JEM-2000FX and a JEM-4000EX.

Model structure. From HRTEM images (Fig. 1) along the fivefold axis, an aggregate of 174 atoms was constructed. The centre of the aggregate is an icosahedron. The icosahedron is surrounded by an icosidodecahedron (I) in such a way that the vertices of the icosahedron cap the inside of the pentagonal faces of the icosidodecahedron. The next shell is a small rhombicosidodecahedron (SR). The triangular faces of the SR form octahedra with the triangular faces of the icosidodecahedron, and the pentagonal faces of the two polyhedra I and SR form pentagonal

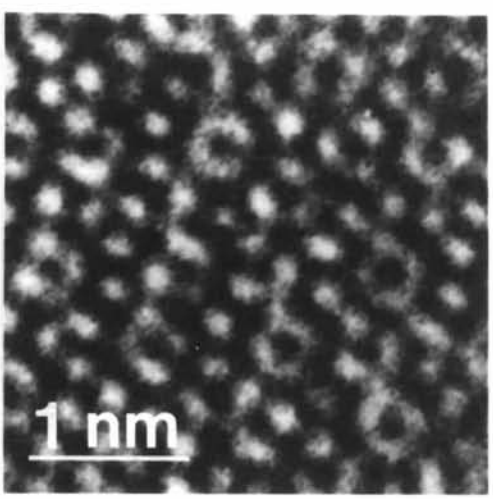

Fig. 1. HRTEM image of an $Al_{65}Cu_{20}Fe_{15}$ crystal recorded along the fivefold axis at an accelerating voltage of 400 kV and a structural resolution of 1.6 Å.

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0108-7673/89/12FC033-04$3.00

antiprisms. The last shell is composed of twelve truncated icosahedra. These share pentagonal faces with the SR. This arrangement of, in all, thirteen icosahedra forms a 'super-icosahedron'. This complete aggregate is shown in Fig. 2.

Using the conformal or dilatation symmetry, discovered in quasicrystal material (Shechtman, Blech, Gratias & Cahn, 1984; Shechtman & Blech, 1985), we show that these super-icosahedra were organized in space, in agreement with HRTEM images, in such a way that parts of this arrangement formed the vertices of an obtuse rhombohedron (oblate form). Together with an acute rhombohedron (prolate form), such polyhedra fill space and also form the triacontahedron (Kowalewski, 1938). It was pointed out by Mackay (1982) that this can be regarded as three-dimensional Penrose tiling. Mackay also showed optically that such tilings gave sharp diffraction spots.

In the oblate and the prolate structures the vertex aggregates (super-icosahedra) are connected in two different ways: along the twofold axis *via* two mutually interpenetrating icosidodecahedra, which form a block of the WAl_{12} structure, and along the fivefold axis *via* icosahedral fusion. The interior structure of the oblate and prolate forms was derived, *via* icosidodecahedral interpenetration and/or expansion of the WAl_{12} block. These were found to be organized as trillings, sixlings or fivelings, meeting along the threefold axis to generate large blocks of pyrochlore structure type. We have found this arrangement in many complex alloy structures with translational symmetry, like $MnAl_4$ [Stenberg (1989) working from Shoemaker, Keszler & Shoemaker (1989)] and several other aluminides. In the centre of the prolate structure a 14-atom unit of b.c.c. arrangement is created. A polyhedral model of the prolate structure is shown in Fig. 3.

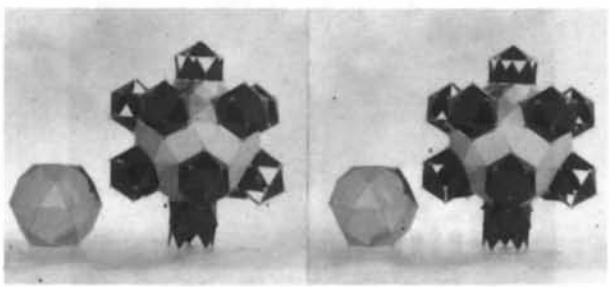

Fig. 2. Stereo pairs of the polyhedra model of the 'super-icosahedron' with its central icosidodecahedron shown to the left.

In the oblate rhombohedral structure the vertex SR interpenetrate somewhat along the short space diagonal in such a way that the SR has one of its triangles in common with a triangle of the icosidodecahedron which is in the inside of the other vertex SR. The oblate structure becomes asymmetric, but again the space between the SR's is filled by twinned units of WAl_{12}. Again a central unit of pyrochlore is formed. A polyhedral model of the oblate is shown in Fig. 4.

The overall picture of the structure is a conformal packing of SR aggregates, glued together by multiple twin units of WAl_{12} or pyrochlore. The WAl_{12} structure is simply related to several other important structure types with its network of atoms that can be described as trigonal prismatic (skutterudite), octahedral [$Sc(OH)_3$], square-planar ($CaCu_3Ge_4O_{12}$) and icosahedral (WAl_{12}).

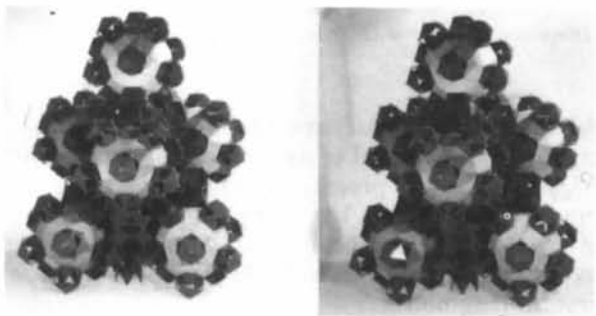

Fig. 3. Stereo pictures of the prolate structure shown with one acute vertex (bottom) missing.

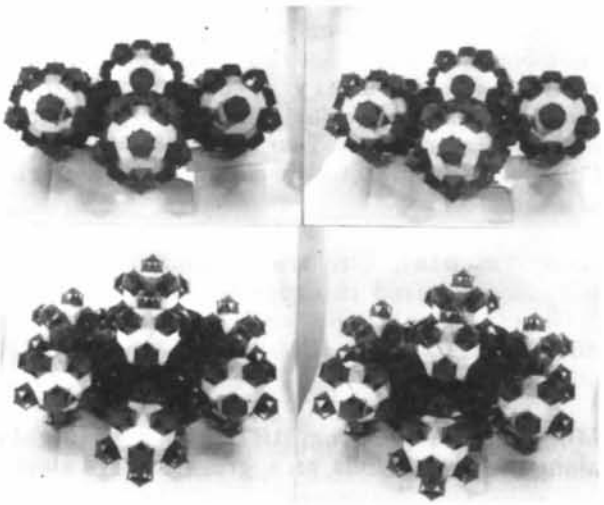

Fig. 4. Stereo pictures of the oblate structure in the fivefold direction (top pair) and in an overview.

Table 1. *Calculated data for the structural model*

	Prolate	Oblate	Weighted average
Volume*	$\iota^{14}/4$	$\iota^{13}/4$	
Number of atoms	305	182	
Z†	10.5	9.7	10.3
Volume/atom‡	15.2	15.7	15.3
Density§	3.96	3.83	3.92

*$\iota=(1+5^{1/2})/2$.
† Average coordination number calculated using only the three interatomic distances of the structure.
‡ For comparison, the corresponding figure for the $CuAl_2$ structure is 14.9.
§ Composition $Al_{65}Cu_{20}Fe_{15}$.

It was obvious during the study of the icosidodecahedron interpenetration principle that this gives rise to alternative positions that could change the structure of the glue. If this occurs locally when a real quasicrystal is formed during the quenching, a disorder is obtained, which can easily be imagined to disappear during heat treatment. With such a mechanism there is no need to violate the matching rules of three-dimensional Penrose tiles to explain order–disorder transitions.

In the proposed structure all atoms follow conformal or dilatation symmetry and only three kinds of nearest-neighbour distances are present, *viz* unity (the Al–Al atom distance of the icosahedral edge, 2.96 Å, which is the average Al–Al distance taken from $CuAl_2$ and WAl_{12}), $(\iota^2+1)^{1/2}/2=0.951$ and $3^{1/2}/2=0.866$, where $\iota=(1+5^{1/2})/2$. The unit edge of the prolate and oblate forms is the same, *viz* $\iota^4(\iota^2+1)^{1/2}/2$. Various data for the structural model are given in Table 1.

From a crystal model of the shape of a triacontahedron, built of ten oblates and ten prolates, consisting of about 6000 atoms, various projections of atoms were calculated and their optical diffraction patterns (ODP) were compared with the corresponding experimental electron diffraction patterns (EDP) (*cf.* Fig. 5). The metric agreement is excellent and the observed deviation of the intensities between the ODP and the EDP, which is most prominent in the twofold symmetry projection (Fig. 5*C*), we believe reflects the one kind of 'atoms' used in the model.

Several models for a quasicrystalline structure have been reported (Shechtman & Blech, 1985; Audier & Guyot, 1988; Janot, de Boissieu, Dubois & Pannetier, 1989). Janot *et al.* have derived a structure using neutron diffraction on quasicrystals of $MnAl_4$ type. Although this structure is different from the one studied by us (dilatation ι^3 instead of ι) there seem to be certain similarities. This, together with a much more elaborate description of our work, will appear in a forthcoming article.

We wish to thank the Swedish Natural Science Research Council for financial support.

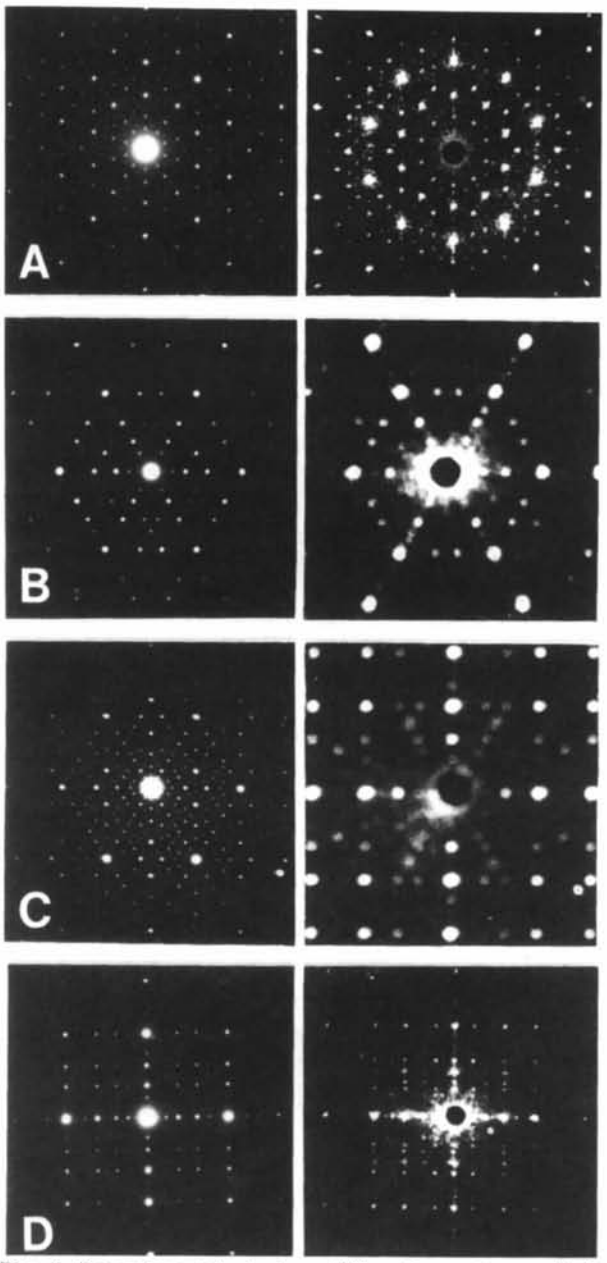

Fig. 5. Experimental electron diffraction patterns (left) compared with optical diffraction patterns of the structure model projected with fivefold symmetry (*A*), threefold symmetry (*B*), twofold symmetry (*C*) and a pseudo-twofold symmetry (*D*).

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