

The γ -brass structure and the Boerdijk–Coxeter helix

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Abstract

The γ -brass structure was for a long time regarded as a modified bcc structure. It is more accurately described in terms of a 26-atom cluster consisting of four interpenetrating icosahedral clusters. An alternative description in terms of a 38-atom cluster is also illuminating. We discuss the γ -brass structure in terms of the packing of spheres and the packing of ‘almost regular’ tetrahedra and demonstrate a close relationship to the helical sphere packings investigated by Boerdijk, who considered the configuration of touching spheres centred at the vertices of a Coxeter helix, and extended it by adding an extra layer of spheres. Adding a further layer of spheres gives a rod-like structure in which every sphere of the original helix is surrounded by twelve others, configured as a somewhat distorted icosahedron. Thus each tetrahedron of the initial structure is then shared by four icosahedra. This 26-sphere cluster is a slightly distorted form of the 26-atom γ -brass cluster.

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1. Introduction

Bradley and Thewlis [1] identified the structure of γ -brass and described it in terms of a cubic unit cell consisting of 27 cubic units – a $3 \times 3 \times 3$ array – of a bcc lattice. The points at the vertices of this block and the one at its centre are removed, so that we get a structure with a unit cell containing $27 \times 2 - 2 = 52$ sites (Fig. 1). The γ -brass structure was identified to be a distorted version of this geometrical model, in which the atoms are shifted from the exact positions. Bradley and Jones [2] described it in terms of a cluster of concentric shells centred around the vacant sites. The first shell is a regular tetrahedron of 4 atoms. This is surrounded by 4 more atoms, over its faces, forming a larger tetrahedron. The third shell is octahedral, 6 sites – one over each edge of the small tetrahedron. The fourth is cuboctahedral, 12 sites. We have a cluster of $8 + 6 + 12 = 26$ atoms. The remaining 26 sites in the unit cell are accounted for by the shells around the vacancies at the vertices of the unit cell.

In *The Nature of the Chemical Bond* [3] Pauling describes the $3 \times 3 \times 3$ model of γ -brass. He then casually

makes the cryptical remark: “the structure is an icosahedral one”.

Nyman and Andersson [4] described the 26-atom cluster as a packing of equal spheres (a convenient idealization – in the γ -alloys, of course, the spheres (atoms) are of more than one kind). Place four spheres in contact. Then place a sphere over each face of the tetrahedral cluster. The centres and bonds then form a ‘stella quadrangula’ built from five regular tetrahedra (Fig. 2(a)). Six more spheres placed over the edges of the original tetrahedron form the octahedral shell. In terms of the network of centres and bonds the cluster can be represented by a structure built from equilateral triangles (Fig. 2(b)) or as a packing of tetrahedra. In this latter description 12 tetrahedra, not quite regular, are packed around a stella quadrangula, giving a ring of five tetrahedra around each edge of the inner tetrahedron. Then 24 more tetrahedra give the 26-vertex structure built from 41 tetrahedra (Fig. 3).

Without increasing the number of vertices, 16 more tetrahedra can be inserted, revealing the structure to be four interpenetrating icosahedra sharing a common tetrahedral building block (Fig. 4). This ‘ γ -brass cluster’ can be augmented by placing three extra spheres over four of the triangular faces of the cuboctahedral shell. We then have a cluster of 38 ‘atoms’, located at the vertices of a packing of 81 tetrahedra (Fig. 5). This

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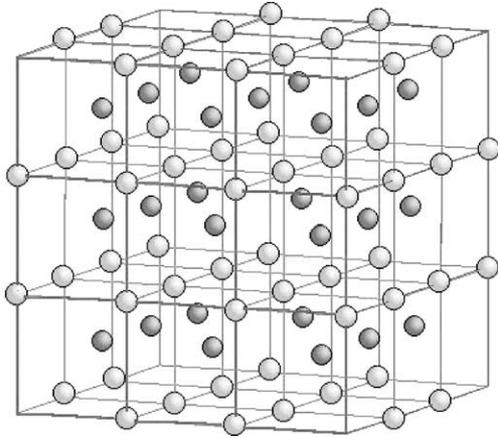


Fig. 1. The bcc structure underlying the description of γ -brass given by Bradley and Thewlis.

cluster can be built from one tetrahedral and three slightly irregular icosahedral building blocks – an interesting geometrical configuration discovered by Pearce [5].

2. The Pearce cluster

The dihedral angle of a regular icosahedron is $\delta_I = 138.19^\circ$ and the dihedral angle of a regular tetrahedron is $\delta_T = 70.53^\circ$. Thus, $2\delta_I + \delta_T = 360^\circ - 14.11^\circ$. An ‘oblate’ icosahedron can be produced from a regular icosahedron by increasing the dihedral angles at the relevant edges to 144.25° . The deformation is slight, and a cluster of four oblate icosahedra can be produced in which each icosahedron is in face contact with the other three, as in Fig. 5 [5]. Thus the network of bonds in gamma brass can be described in terms of structures very similar to the Pearce cluster – four icosahedra in face contact with each other and with a central tetra-

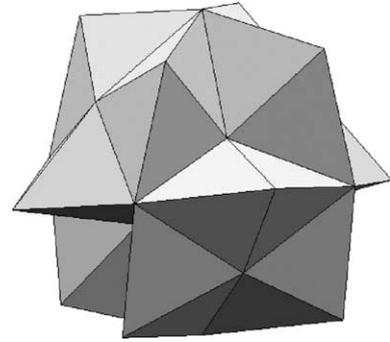


Fig. 3. The γ -brass cluster as a packing of 41 tetrahedra.

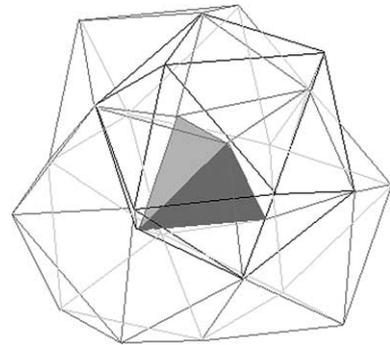


Fig. 4. The γ -brass cluster built from 57 tetrahedra; a configuration of four interpenetrating icosahedra sharing a common tetrahedral building block.

hedron. The icosahedra in γ -brass are distorted, but not ‘oblate’. They each contain a central atom.

The 38-atom clusters can combine by sharing three atoms between a pair of clusters. The structure can be continued along every threefold axis (Fig. 6). Observe how the whole structure can be described in terms of tetrahedral building blocks. This description of a γ -alloy is implicit in the work of Belin and Belin [6].

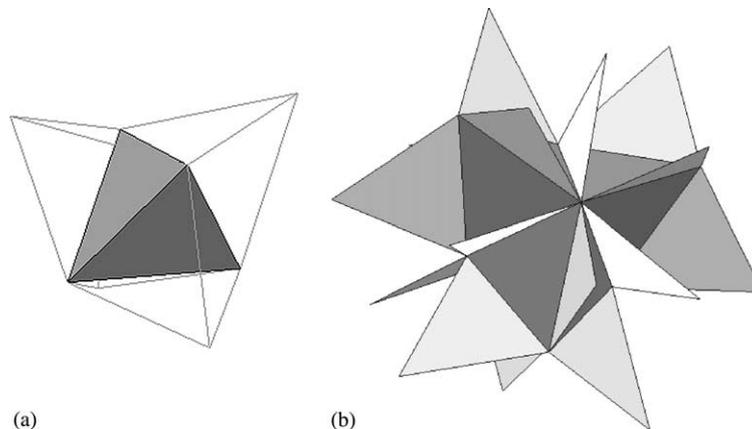


Fig. 2. (a) The stella quadrangula. (b) The construction of γ -brass cluster as described by Nyman and Andersson [4].

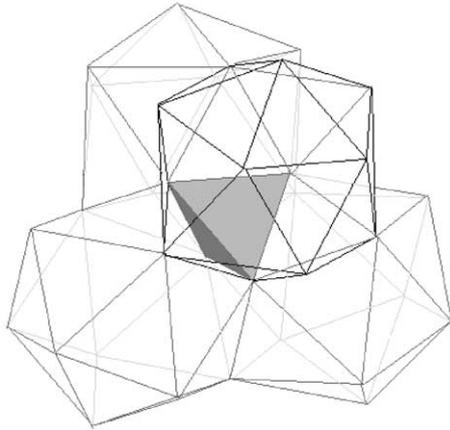


Fig. 5. The 57-tetrahedron cluster augmented to a cluster of 81 tetrahedra with 38 vertices (4 of them constituting the innermost tetrahedron). The final figure is a modified ‘Pearce cluster’ consisting of 81 tetrahedra.

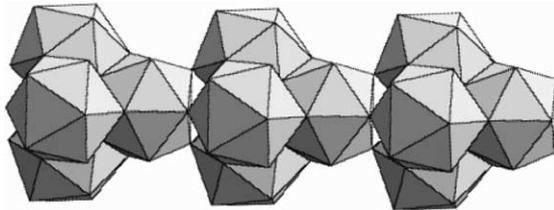


Fig. 6. With only a slight deformation a pair of 38-atom clusters can share three vertices. In γ -brass, this gives rise to the linking of 38-atom clusters to form rod-like structures along the threefold axes.

3. The Boerdijk–Coxeter helix

Coxeter [7] suggested a straightforward extension of the concept of a *regular polygon*. A regular polygon as usually defined is a cycle of vertices ...1, 2, 3, ... and edges ...12, 23, ... obtained from a single point by repeated action of a rotation. Coxeter’s extension replaces ‘rotation’ by the more general ‘isometry’ (distance preserving transformation). A *screw transformation* generates a *helical polygon* (or *polygonal helix*), an infinite sequence of vertices ...-1, 0, 1, 2, ... and edges joining consecutive vertices. A *Coxeter helix* is a polygonal helix such that every set of four consecutive vertices form a regular tetrahedron. This produces a twisted rod of tetrahedra, the *Boerdijk–Coxeter helix* [8,9]. The structure is aperiodic. A model can be produced by folding a strip cut from the tiling of the plane by equilateral triangles. Buckminster Fuller [10] called the helical tower of tetrahedra the *tetrahelix*. It is generated by the repeated action of a screw transformation, which can be determined as follows [9,11,12]:

In matrix notation, an isometry in Euclidean space has the form

$$\mathbf{x} \rightarrow R\mathbf{x} + \mathbf{a}, \quad RR^T = I. \tag{1}$$

If $\mathbf{a} = 0$ we have a pure rotation about the origin. A rotation in E_3 through an angle θ about an axis along the unit vector \mathbf{n} is given by the rotation matrix

$$R = e^{\theta N} = I + N \sin \theta + N^2(1 - \cos \theta), \tag{2}$$

where N is the skewsymmetric matrix

$$N = \begin{pmatrix} 0 & -n_3 & n_2 \\ n_3 & 0 & -n_1 \\ -n_2 & n_1 & 0 \end{pmatrix}. \tag{3}$$

It is convenient to use a 4×4 matrix notation. Defining $\mathbf{X} = \begin{pmatrix} \mathbf{x} \\ 1 \end{pmatrix}$, $S = \begin{pmatrix} R & \mathbf{a} \\ 0 & 1 \end{pmatrix}$, then Eq. (1) is

$$\mathbf{X} \rightarrow S\mathbf{X}. \tag{4}$$

The points in E_3 with coordinates $(-1, -1, -1)$, $(-1, 1, 1)$, $(1, -1, 1)$ and $(1, 1, -1)$ are the vertices of a regular tetrahedron (edge length $\sqrt{8}$); so are $(-1, 1, 1)$, $(1, -1, 1)$, $(1, 1, -1)$ and $(5/3, 5/3, 5/3)$. These can be taken to be two consecutive tetrahedra of a B–C helix. This is sufficient to deduce that

$$S = \begin{pmatrix} -1 & 1 & 1 & 5/3 \\ 1 & -1 & 1 & 5/3 \\ 1 & 1 & -1 & 5/3 \\ 1 & 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} -1 & -1 & 1 & 1 \\ -1 & 1 & -1 & 1 \\ -1 & 1 & 1 & -1 \\ 1 & 1 & 1 & 1 \end{pmatrix}^{-1} \\ = \frac{1}{3} \begin{pmatrix} 2 & 2 & 1 & 2 \\ 2 & -1 & -2 & 2 \\ -1 & 2 & -2 & 2 \\ 0 & 0 & 0 & 3 \end{pmatrix}. \tag{5}$$

Then, from $N \sin \theta = (R - R^T)/2$, $\cos \theta = (1 + \text{trace}R)/2$, we get, for the angle θ of rotation of the B–C helix (per edge of the Coxeter helix) and the direction \mathbf{n} of the screw axis,

$$\cos \theta = -2/3, \quad \mathbf{n} = [2 \ 1 \ 0]\sqrt{5}. \tag{6}$$

The number of edges of the Coxeter helix, per turn, is $2\pi/\theta = 2.73119\dots$. The advance of the helix, per edge, is $\mathbf{n} \cdot \mathbf{d}$, where \mathbf{d} is any edge (e.g. $[0 \ 2 \ 2]$). Since we have chosen tetrahedra with edge length $\sqrt{8}$, we have the advance per edge, for a B–C helix of tetrahedra of unit edge length, $d = 1/\sqrt{10}$.

4. Sphere packing

Boerdijk [8] investigated the tetrahelix in connection with dense packings of equal spheres. The configuration of four spheres in a tetrahedral configuration, each touching the other three, gives the Rogers upper bound for the upper limit of any possible packing fraction for equal spheres. The bound can never be achieved because regular tetrahedra won’t pack together in E_3 . However, sphere packings that fill only a portion of space can

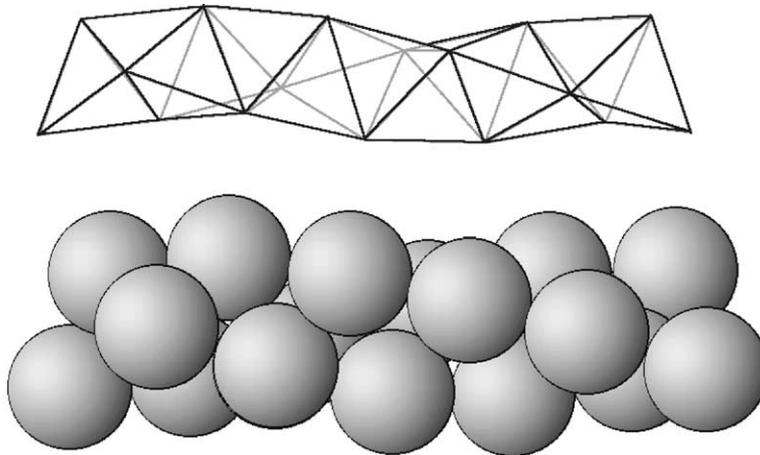


Fig. 7. The tetrahelix or Boerdijk–Coxeter helix and the associated helical packing of spheres.

come much closer to the bound than hexagonal close packing, the densest lattice packing. Boerdijk considered the dense rod shaped packing in which the sphere centres lie on the vertices of the tetrahedra (Fig. 7), and the effect of adding further spheres to this helical structure, over the mid points of edges of the Coxeter helix. This determines additional, only slightly irregular, tetrahedra, so that every edge of the helix is shared by five tetrahedra.

5. Extension of the helical sphere packing

Further extensions of Boerdijk's helical sphere packings may be considered. The next stage gives a rod-like structure in which *every vertex of the original helix of tetrahedra is surrounded by twelve others*, configured as a somewhat distorted *icosahedron* (Fig. 8). Thus each tetrahedron of the initial structure is now shared by four icosahedra. This 26-sphere cluster is a slightly distorted form of the 26-atom γ -brass cluster. Another interesting subset of the tetrahedra in this structure is the triplet of distorted B–C helices twisted around each other as in Fig. 9 [11,13]. One could go on adding more spheres, but

the deviation of the tetrahedra from regularity (corresponding to lower density of the sphere packing) becomes more severe.

6. The polytope $\{3, 3, 5\}$

Regular tetrahedra cannot be packed to fill Euclidean space E_3 , but in E_4 they can. The vertices all lie on a hypersphere, a space of constant curvature S_3 . The polytope $\{3,3,5\}$ [7,13,14] has 120 vertices, 720 edges, 1200 equilateral triangle faces and 600 *regular tetrahedral* cells. Five cells surround each edge and twenty surround each vertex – forming a *regular icosahedron*. Circuits of 30 face-sharing tetrahedra occur in $\{3,3,5\}$. They are each metrically identical to the Boerdijk–Coxeter structure in three dimensional Euclidean space. Sadoc and Mosseri [15] have devised methods of understanding the structures of Frank–Kasper phases [16] in terms of *unfolding* $\{3,3,5\}$ to fit into E_3 , by introducing disclination networks.

All the figures of structures involving tetrahedra that we have discussed exist in E_4 with all the tetrahedra *regular*, as part of the polytope $\{3,3,5\}$.

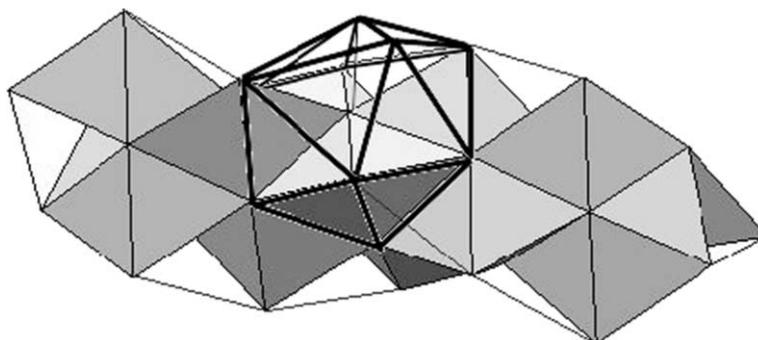


Fig. 8. The augmented helical sphere packing, containing γ -brass type clusters, represented as a polytetrahedral structure.

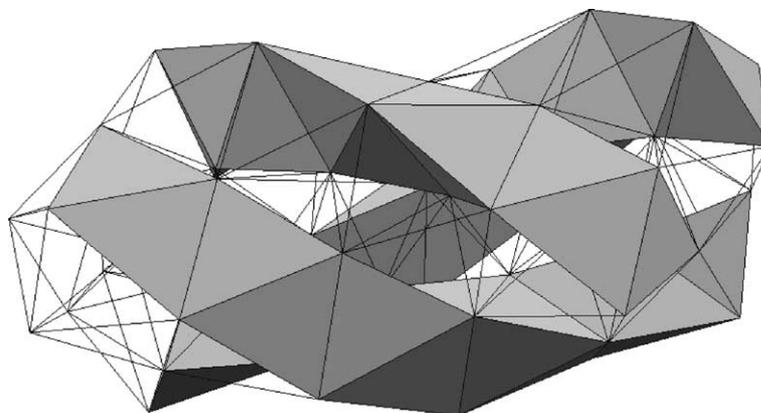


Fig. 9. The augmented Boerdijk–Coxeter helix viewed as three B–C helices twisted around a fourth.

7. Conclusions

Two sphere packing arrangements, the γ -brass structure and a rod-like sphere packings based on an augmented Boerdijk–Coxeter helix, have been considered and shown to be closely related. A 38-atom cluster, with atoms at the vertices of a packing of 81 regular and ‘almost regular’ tetrahedra, can be identified in γ -brass. Each of these shares a triangular face with eight others. Our approach, based on step-by step computation of vertex positions in a packing of tetrahedral building blocks, suggests a promising approach to the modelling of Frank–Kasper phases, and quasicrystalline phases and their approximants.

Acknowledgements

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