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Structural realization of the polytope approach for the geometrical description of the transition of a quasicrystal into a crystalline phase

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Abstract

A geometrical model is proposed for the recently observed transformation under the action of highly localized stresses during the surface scratch test of the icosahedral phase into a body-centred cubic (BCC) phase, the disordered version of the B2 phase with the CsCl structure, which occupies a large portion of the Al–Cu–Fe phase diagram around the $\text{Al}_{50}(\text{Cu}, \text{Fe})_{50}$ concentration. The model is founded on a polytope concept and the concept of the eight-dimensional root lattice E_8 . In accordance with these concepts many crystalline or quasicrystalline structures can be derived from the polytope (the four-dimensional polyhedron) by fulfilling operations of lowering its local curvature with subsequent mapping of decurved polytope fragments onto Euclidian three-dimensional space. The properties of the E_8 lattices give foundation to the possibility of mapping a quasicrystalline structure on a crystalline structure. The structural transformation is effected through intermediate atomic configurations coinciding with both structures, which are determined by a four-dimensional icosahedron (the $\{3, 3, 5\}$ polytope). For the transformation of the icosahedron of the icosahedral phase into a rhombic dodecahedron of the cubic B2 phase, the cubic A15 structure plays the role of an intermediate configuration since it can be represented as a three-dimensional packing of linearly interlaced chains of Frank–Kasper polyhedra with coordination numbers $Z = 12$ (icosahedron) and $Z = 14$. The transition between the rhombic dodecahedron of a B2 structure and the Frank–Kasper polyhedron with $Z = 14$ requires insertion of disclination quadruplets into some facets of the rhombic dodecahedron. The proposed geometrical model can be applied also to the polymorphic BCC–FCC transformation since the Miller indices of

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the Frank–Kasper polyhedron with $Z = 14$ coincide with the observed indices of habit planes of iron martensites.

1. Introduction

The problem of atomic positions in a quasicrystal is still unresolved. It is clear however that the quasicrystal structure represents in itself a certain packing variant of icosahedral atomic clusters in a three-dimensional space. Besides the symmetry of point diffraction patterns, this is confirmed indirectly by several experimental observations:

- (1) the relative easiness of the quasicrystal transformation into the relevant crystalline approximant, in many cases the latter having diffraction patterns quite similar to the diffraction patterns of the quasicrystal;
- (2) the formation of quasicrystals during melt quenching;
- (3) the relative easiness of a transition between quasicrystalline and glassy structures under the action of a stress [1, 2] or during irradiation by accelerated particles [3, 4].

A justification for including in this list points (2) and (3) comes from the icosahedral configuration of the main building units of metallic liquids and an inheritance of these configurations by metallic glasses after rapid quenching. It was shown recently by soft x-ray and photoelectron spectroscopy measurements in the Al–Cu–Fe system that the Al–Cu–Fe icosahedral quasicrystal and its approximants represent a region of specifically enhanced stability in the Al–Cu–Fe phase diagram [5]. Moreover, on the experimental curve of Al 3p densities of states at the Fermi level $n(E_F)$ versus electron to atom ratio e/a , the value $n(E_F)$ of the icosahedral quasicrystal is positioned at the minimum along the sequence FCC Al, crystalline Al–Cu Hume–Rothery phases, crystalline ternary phases ϕ -Al₁₀Cu₁₀Fe, ω -Al₇Cu₂Fe, cubic β -phases with B2 (CsCl) structure, orthorhombic, rhombohedral and pentagonal approximants, icosahedral phase [5]. Bearing in mind this position of the quasicrystal in the $n(E_F)$ versus e/a relationship, the quasicrystal itself can be regarded as an intermediate intermetallic compound having some structural proximity with other phases in this system. Furthermore, the transformation of the icosahedral phase into the disordered, high-temperature variant of the B2 phase has been observed in this system under the action of a sliding WC–Co indenter during a surface scratch test [6]. This result can be rationalized only with some difficulty since the B2 structure does not contain icosahedral coordination polyhedra in its BCC lattice.

In order to overcome this obstacle we must find

- (1) some foundation of the possibility of mapping an icosahedral quasicrystal structure on the crystal structure;
- (2) some mechanism for the reconstruction of the coordination polyhedron itself with the number of vertices of the polyhedron (atoms) being constant.

Point (1) is needed for a global description of the quasicrystal–crystal transition. Point (2) is needed for a local description of the same transition. In the case of success one can obtain the possibility to deal with both types of phase transition, i.e. continuous transformations or nucleation-and-growth transformations.

The foundation for mapping the quasicrystal on the crystal structure (point (1)) is contained in several papers in which icosahedral quasicrystals have been derived from the eight-dimensional root lattice E_8 [7–9]. As has been said in [8], ‘a root lattice E_8 is a “mother”

(i.e. praphase) of all quasicrystalline structures'. The concept of the praphase or the prototype phase was introduced by Aizu [10]. The praphase is the real or hypothetical high symmetrical structure with its substructures corresponding in the three-dimensional space E^3 to structures of real phases participating in the transformation. The E_8 lattice is determined by the maximal exclusive simple Lie algebra [7–9] and contains the six-dimensional sublattice $A_3 \times A_3$ (A_3 is the FCC lattice). This property determines a possibility to obtain crystalline approximates with the FCC lattice from the E_8 lattice by the cut-projection algorithm. The E_8 lattice is its own self-dual, $E_8 = E_8^*$, therefore it contains also the six-dimensional sublattice $A_3^* \times A_3^*$ where A_3^* is also dual to the A_3 lattice, i.e. A_3^* is the BCC lattice. Since a hexagonal lattice A_2 is the sublattice of A_3 , the E_8 lattice determines also the hexagonal close packed structure as the final result.

The foundation of point (2) is contained in the so-called polytope concept [11] since close-packed metallic alloys and intermetallic compounds have a tetrahedron-based structure. The best way to find the description for the reconstruction of the coordination polyhedron is the use of a $\{3, 3, 5\}$ polytope as a joining of 600 tetrahedra. In particular, this concept allows us to analyse different modes of joining tetrahedra. Regarding the melting of metals as some reconstruction of a pentagonal bipyramid, Rivier and Duffy [12] were able to calculate the value of the melting entropy in good accordance with the experimental value of $R \ln 2$ (R is the gaseous constant). The reconstruction of the pentagonal bipyramid in [12] was effected by throwing over between several diagonals. It must be noted that the pentagonal bipyramid represents in itself a joining of five tetrahedra around a common edge, i.e. this is a fragment of the $\{3, 3, 5\}$ polytope [12]. In this paper we present a geometrical model as a possible description of a transition from icosahedral atomic packing (an icosahedral phase) to a packing of rhombic dodecahedra (a crystalline β -phase with the CsCl structure). The observed disorder of the B2 phase after the scratch test, which breaks its symmetry down to a BCC lattice, does not need to be accounted for in the present model.

2. Model

As was said in the introduction, crystalline structures with FCC, BCC and hexagonal lattices can be derived from the E_8 lattice. So, any joining of clusters as fragments of crystalline or quasicrystalline structures can be inserted into the E_8 lattice. These properties of the root lattice E_8 determine firstly a possibility for a continuous transition from a quasicrystalline phase to a crystalline phase, and secondly a possibility of a local transition of some quasicrystalline region into crystalline regions. Bearing in mind the foundation of these two possibilities on the E_8 lattice, we must only find a way to reconstruct different coordination polyhedra into each other.

Only finite clusters can be mapped from the $\{3, 3, 5\}$ polytopes, so the polytope itself cannot serve as the praphase but a construction of a certain infinite crystallographic lattice. The $\{3, 3, 5\}$ polytope is mapping onto itself by the subgroup $Y \times Y'$ of the $SU(2) \times SU(2)$ group in which the particular unitary group $SU(2)$ is isomorphic to a sphere S^3 . It means the eight-dimensionality of the determination of the $SU(2) \times SU(2)$ group and, as the final result it determines an insertion of the $\{3, 3, 5\}$ into the crystallographic root lattice E_8 , which is the densest packing of S^7 spheres in eight-dimensional Euclidian space E^8 [7–9]. Such a lattice is the eight-dimensional root lattice E_8 . The first coordination sphere of E_8 consists of 240 vectors of the E^8 ; this multiplicity is isomorphic to joining of two non-crystallographic (finite) root lattices H_4 and τH_4 ; $\tau = 1.618 \dots$ is the golden number. The H_4 lattice consists of 120 vectors connecting the centre of the S^3 sphere with vertices of the $\{3, 3, 5\}$ polytope. The τH_4 lattice is determined by the $\tau\{3, 3, 5\}$ polytope representing in itself the $\{3, 3, 5\}$ polytope multiplied by τ [9]. The sequence of sections of the $\{3, 3, 5\}$ polytope (starting from a vertex) by hyperplanes E^3 outstanding by distance x_4 from the equator will be as

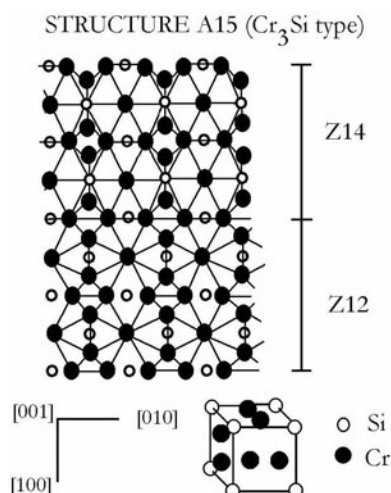


Figure 1. The plan of the A15 structure with filled circles as A atoms and open circles as B atoms. A delineation of a Frank-Kasper polyhedron Z14 is shown in the upper part of the figure; in the lower part of the figure the delineation of an icosahedron Z12 is shown. Two adjacent Z14 polyhedra generate between them an icosahedron Z12, and vice versa: two adjacent icosahedra Z12 generate between them a Frank-Kasper polyhedron Z14. All atoms of the A15 structure belong simultaneously to Z14 and Z12 networks.

follows: a point ($x_4 = 2$), an icosahedron ($x_4 = \tau$), a dodecahedron ($x_4 = 1$), an icosahedron ($x_4 = \tau - 1$), an icosidodecahedron ($x_4 = 0$) [11, 13]. Thus, the section of the join of polytopes $\{3, 3, 5\} \cup \tau\{3, 3, 5\}$ by the E^3 hyperplane ($x_4 = \tau$) represents in itself the $\{5, 3\}$ dodecahedron containing the $\{3, 5\}$ icosahedron in it:

$$(\{3, 3, 5\} \cup \tau\{3, 3, 5\}) \cap E^3(x_4 = \tau) = \{3, 5\} \cup \{5, 3\}, \quad (1)$$

where $\{3, 5\} \subset \{3, 3, 5\}$, $\{5, 3\} \subset \tau\{3, 3, 5\}$. The E^3 hyperplane at $x_4 = \tau$ is the nearest to the north pole $x_4 = 2$ and intersects simultaneously both $\{3, 3, 5\}$ and $\tau\{3, 3, 5\}$, and those are the reasons for the selection of that hyperplane.

Due to the impossibility of subdividing E^3 into tetrahedra, clusters having icosahedral order can achieve to a comparatively small (limited) size only, hence an energetically advantageous limiting size does evidently exist for clusters of the $\{3, 3, 5\}$ polytope which are *mapped* into the E^3 space. Eight out of 20 vertices of the dodecahedra form a cube which is capable already of fulfilling subdivision of the E^3 space, and so the cluster contained in (1) and determined by three sections of the $\{3, 3, 5\}$ polytope ($x_4 = 2$, $x_4 = \tau$, $x_4 = 1$) can be regarded as a limiting one during *mapping* of the $\{3, 3, 5\}$ polytopes into the E^3 space.

This cluster of the $\{3, 3, 5\}$ polytope with 21 vertices corresponds uniquely to the unit cell of the A15 structure, i.e. the certain set of vectors from E_8 determines uniquely the unit cell of the A15 structure:

$$E_8 \supset \{3, 3, 5\} \supset \text{A15 unit cell} \subset \text{A15}. \quad (2)$$

The A15 structure (figure 1) represents a centred cube (Si positions) in which the distorted icosahedron is inscribed (Cr positions). Thus the unit cell of the A15 phase is the energetically admissible limit for *mapping* the cluster from the $\{3, 3, 5\}$ polytope into the E^3 space.

If Y is the rotation group of an icosahedron consisting of 60 elements $u(\vec{k}, 2\pi/n)$, where \vec{k} is the unit vector of the icosahedron axis just about which the rotation on the $2\pi/n$ angle is effected, hence Y' is the group consisting of 120 elements of the form $u'(\vec{k}, 2\pi/n)$ and

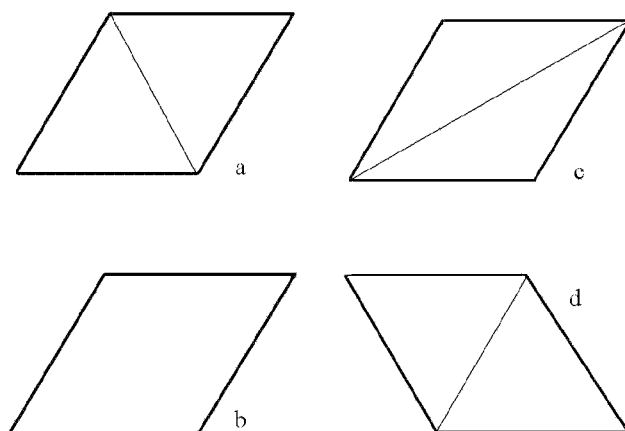


Figure 2. Insertion of the disclination quadruplet into a rhombus. (a) A triangulated rhombus; (b) skipping a diagonal is the operation of two-dimensional enlargement; (c) drawing the new diagonal is the operation of two-dimensional subdivision; (d) equalization of edge lengths, i.e. a relaxation to the new shortest interatomic bond corresponding to the minimum of the interatomic interaction potential. Steps (a)–(b) correspond to the disclination quadruplet k , i.e. to the nontrivial product of the enlargement and subdivision operations. The quadruplet k changes the number of edges meeting in the quadrangle vertices by ± 1 ; this is equivalent to inserting $+2\pi/l, -2\pi/l, +2\pi/l, -2\pi/l$ -disclination through each vertex of the quadrangle. The fulfilment of the operations (a)–(d) did not change topological and metric parameters of this rhombus; only the rhombus orientation in the plane has been changed.

$u'(\vec{k}, 2\pi/n + 2\pi) = -u'(\vec{k}, 2\pi/n)$, these elements are uniquely corresponding to $\pm 2\pi/n$ disclinations which were inserted into the icosahedron along the \vec{k} axis. A disclination changes the space curvature and is characterized by the unit vector of the axis \vec{k} and by the rotation magnitude $\pm 2\pi/n$ about this axis. For example, a $-2\pi/5$ -disclination inserted along the fivefold axis of the icosahedron by substituting two hexagonal caps instead of pentagonal ones transforms it into the Frank–Kasper polyhedron with 14 vertices (Z14). At $n \neq 1$ the disclination changes the vertex number of the icosahedron, in the case $n = 1$ the only action of the 2π -disclination (or disclination quadruplet [12]) corresponding to the element -1 of the Y' group is the permutation between long and short diagonals of the corrugated rhombus consisting of two adjacent faces of the icosahedron (figure 2). By inserting a $-2\pi/5$ -disclination into the $\{3, 3, 5\}$ polytope a rod composed from Frank–Kasper polyhedra⁵ Z14 = $[5^{12}, 6^2]$ will be generated. The crystalline A15 phase can be assembled from these Z14 rods [13]. That phase can be also regarded as assembled from icosahedra Z12 = $[5^{12}]$ joined in rods along the threefold symmetry axis in the face-to-face mode. So, for the A15 structure relations are valid:

$$A15 = \cup[5^{12}] = \cup[5^{12}, 6^2], \quad (3)$$

where the polyhedron Z14 is the result of the action of the $-2\pi/5$ -disclination on the icosahedron.

Skipping six edges of the icosahedron does not change its Euler characteristic $\chi = V - E + F$ (V, E, F denote respectively numbers of vertices, edges and faces) but results in a topological cuboctahedron which is capable of transforming into the ideal cuboctahedron $[4^{12}]$

⁵ The symbol $[5^{12}, 6^2]$ denotes a polyhedron with 12 vertices in which five edges are meeting and two vertices in which six edges are meeting.

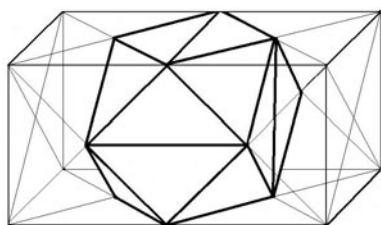


Figure 3. An Archimedean cuboctahedron (thick lines) as the first coordination sphere for any point of an FCC lattice (thin lines) delineated between two adjacent unit cells. Square faces of the cuboctahedron are parallel to cube faces $\{100\}$; triangular faces are parallel to octahedral faces $\{111\}$. The drawing of diagonals (conditional edges) on all square faces of a cuboctahedron transforms the cuboctahedron into a topological icosahedron. Inversely, skipping six edges of the icosahedron transfers it into the topological cuboctahedron.

(figures 3, 4). Similarly, a delineation of corrugated rhombuses from pairs of adjacent faces in the Z14 polyhedron, and the permutation between short and long diagonals in these rhombuses by insertion of 2π -disclinations with the subsequent skipping of edges does not change χ and generates a topological rhombic dodecahedron $[4^6, 3^8]$, which is capable of transforming into the cubic rhombic dodecahedron (figure 5). All these transformations correspond to elements of the $Y' \times Y'$ group. In their turn, inner automorphisms of E_8 correspond to these elements of the $Y' \times Y'$ group, hence the possibility of transformations of clusters forming the A15 structure is determined by the insertion of the A15 unit cell into E_8 (relation (2)). Hence reversible transformations

$$[5^{12}] \leftrightarrow [4^{12}] \quad \text{and} \quad [5^{12}, 6^2] \leftrightarrow [4^6, 3^8] \quad (4)$$

and the A15 unit cell itself are determined by *mapping* of clusters from the $\{3, 3, 5\}$ polytope (or E_8) into E^3 . The transformation indicated above can be regarded as energetically tolerable since

- (i) the number of cluster vertices does not change;
- (ii) lengths of interatomic bonds (edges) and valence angles between them in initial and final configurations are varied by not more than 10%.

The cuboctahedron and rhombic dodecahedron are coordination polyhedra of FCC and BCC lattices respectively; these lattices in their turn are sublattices A_3 and A_3^* of the autodual lattice $E_8 = E_8^*$. The algorithm was proposed in [9] permitting us to obtain icosahedral and tetrahedral quasicrystals and all possible approximants from E_8 . By joining relations (2)–(4) one can obtain a scheme:

$$\begin{array}{ccc} [4^{12}] \subset A_3 \subset E_8 = E_8^* \supset A_3^* \supset [4^6, 3^8] & & \\ \Downarrow & \cup & \Downarrow \\ [5^{12}] \subset A15 \leftarrow \{3, 3, 5\} \rightarrow A15 \supset [5^{12}, 6^2]; & & \end{array} \quad (5)$$

the said scheme together with the algorithm of [9] represents transformations between FCC and BCC structures through E_8 as the praphase both on global and local levels. Naturally, the transformation of the icosahedral phase into the B2 phase with BCC structure is also inside the framework of this scheme. A coordination polyhedron of the HCP structure is the hexacuboctahedron, so this scheme describes also transformations with the participation of the HCP structure (see figure 4(b)).

The experimentally observed habit planes of iron martensite in the coordinate axes of the FCC phase are $\{15.10.3\}$, $\{522\}$, $\{755\}$ [14]. This is in exact coincidence with indices of faces

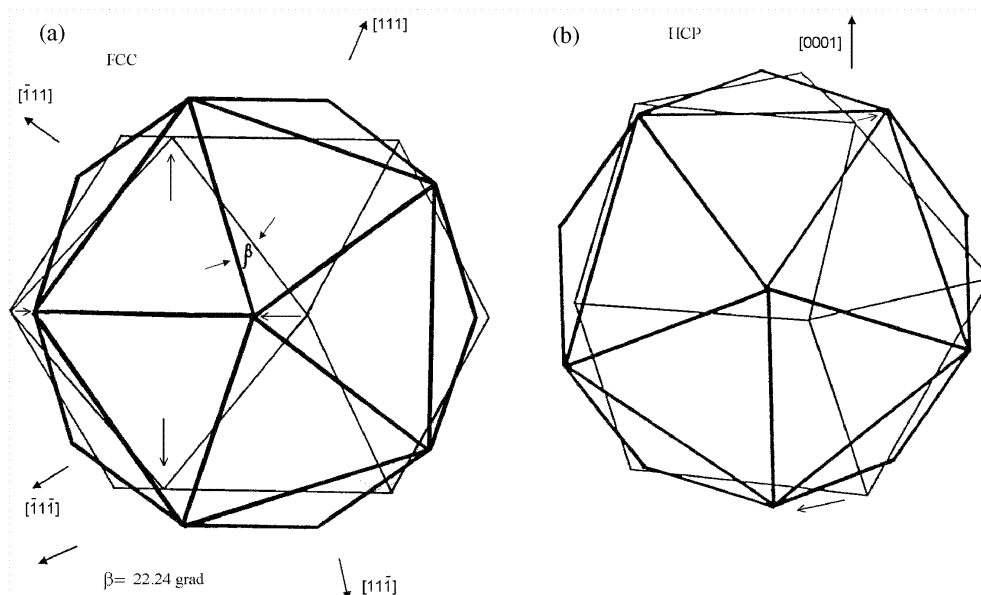


Figure 4. Transformation of a cuboctahedron of the FCC lattice (a) and a hexacuboctahedron of the HCP structure (b) into an icosahedron. Coordination polyhedra of close-packed structures are shown by thin lines; the final icosahedral configuration is shown by thick lines. The simultaneous rotation of triangular faces about their normals switches the cuboctahedron into the icosahedron. The necessary value of the rotation angle is 22.24° . Arrows on square faces of the cuboctahedron indicate directions of atomic displacements during the transformation. A coordination polyhedron of the HCP structure can be obtained from the cuboctahedron of the FCC lattice by the rotation of the upper half of the polyhedron on 60° about the threefold symmetry axis. Square faces of the hexacuboctahedron share a common edge. The hexagonal axis $\langle 0001 \rangle$ is parallel to the figure plane.

of the Frank–Kasper polyhedron Z14 in a cubic coordinate system when the $\langle 111 \rangle$ direction is parallel to the sixfold symmetry axis of the Z14 polyhedron (figure 6). This coincidence can be treated as evidence of the proposed mechanism of the polymorphic transformation through the E_8 lattice as the praphase. Further evidence is the phase transition in the solid molecular O_2 -crystals from the rhombohedral (distorted FCC) β -phase to the γ -phase with the A15 structure [15]. It is interesting that in the structure of the γ - O_2 phase O_2 molecules having a spherical distribution of the electron density are positioned in vertices of the BCC lattice (Si positions) while disc-shaped molecules are positioned in icosahedron vertices (Cr positions) while in the low temperature β -phase O_2 molecules have a linear dumbbell configuration.

Bearing in mind above mentioned connection of the A15 structure with the root lattice E_8 the results of [16] where change of the sequence of operations for decreasing the polytope curvature leads to the polymorphism of the $Mg_{32}(Zn, Al)_{49}$ phase (Bergman phase) seem far from accidental. The existence of an intermediate configuration of this phase between the BCC-modification and the primitive cube modification was found in [16], and this intermediate configuration has the A15 structure. According to the authors of [16], the origin of polymorphism relies upon the existence of equivalent, alternative steps along the different stages of the polytope decurling.

The transformation of the cuboctahedron into the icosahedron has been suggested as a microscopic mechanism for the transition between two space isomers of the carborane

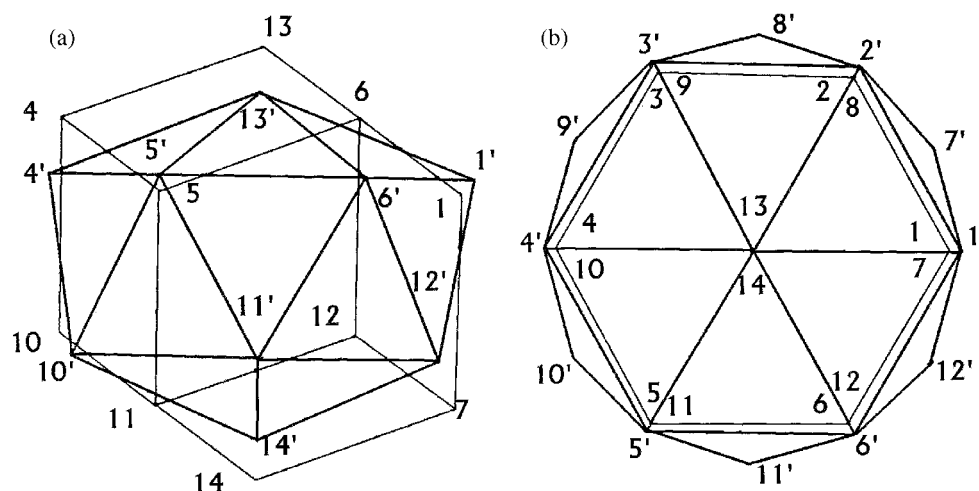


Figure 5. The transformation of a rhombic dodecahedron of a BCC lattice into a Frank–Kasper polyhedron Z14. Thin lines and unprimed numbers designate respectively edges and vertices of the rhombic dodecahedron; thick lines and primed numbers designate edges and vertices of the resulting Frank–Kasper polyhedron Z14. Any vertex of the rhombic dodecahedron with number N becomes the vertex N' of the Z14 polyhedron after the transformation. (a) The figure plane is parallel to $\{110\}$ of the BCC lattice; the threefold symmetry axis is passing through vertices 13 and 14 along $\langle 111 \rangle$ in the plane of the figure. The same axis also is in coincidence with the sixfold symmetry axis of the Z14 polyhedron passing through vertices 13' and 14'. (b) The figure plane is perpendicular to the threefold symmetry axis of the rhombic dodecahedron and at the same time is perpendicular to the sixfold symmetry axis of the Frank–Kasper polyhedron Z14. The projections of vertices 13 and 14 are in coincidence with the projections of vertices 13' and 14'. The projections of edges 13–6, 13–4 and 13–2 of the rhombic dodecahedron are in coincidence with the projections of edges 13'–6', 13'–4' and 13'–2' of the Z14 polyhedron.

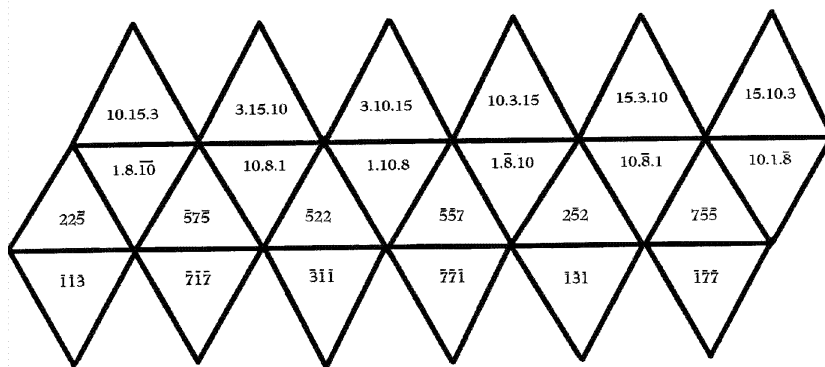


Figure 6. Indexing of a Frank–Kasper polyhedron Z14 in cubic axes. The flat development of the Z14 is shown with Miller indices inscribed on its faces. The $\langle 111 \rangle$ direction of a cubic lattice is parallel to the sixfold symmetry axis of a Z14 polyhedron.

molecule ($C_2B_{10}H_{12}$) having the icosahedral configuration [17]. The scheme of the transformation of the rhombic dodecahedron into the Frank–Kasper polyhedron with 14 vertices was first published by one of the authors for an explanation of certain diffraction anomalies generated in iron and vanadium-based alloys by the ion irradiation [18].

The proposed scheme of the transformation is in intimate proximity to the main concept of the Bain model of the transition from FCC to BCC structure [19]. According to Bain one must find the fragment of the lattice in the initial phase, which will be topologically equivalent to some fragment of the lattice in the resulting phase, and subject this fragment to topological deformations so as to achieve a full coincidence with the structure of the final phase with respect to symmetry and metric relationships.

Such an approach can be called 'a chess-board concept': for a drawing of a chess-board, one need not draw both types of square; it is enough to draw only black (or white) squares. Taking the vertices of the squares as atoms, one can state that these atoms belong to 'a black square phase' and equally well that they belong to 'a white square phase'. Then, the problem of the description of the phase transition is reduced to revealing the intermediate atomic configuration, which will be equivalent to the three-dimensional chess-board formed by atoms. The A15 structure is just this three-dimensional chess-board in which Z12 icosahedra are playing the role of 'white square cells' while Z14 polyhedra are playing the role of 'black square cells', and this three-dimensional chess-board has been found as the substructure of the root lattice E_8 .

Since the local atomic structure of the icosahedral quasicrystal represents some joining of icosahedra, the transition of a such a structure into the B2 phase in the frame of the proposed geometric scheme can be reduced to specified distortions of certain edges of the icosahedra in such a way that the subdivision of space into a set of Frank–Kasper polyhedra with $Z = 14$ will become more distinct. Also, some ordering in the occupation of certain atomic positions by different alloy components must take place if one is furthermore seeking the CsCl stoichiometry and atomic ordering.

Regarding the Al–Cu–Fe system, it was pointed out that the series of intermetallic compounds dealt with in the present paper (namely, icosahedral, B2 cubic and A15-type γ -Al₃₉Cu₆₁) all fall close to a constant electron-to-atom ratio $e/a = 1.8e^-/at$ [20]. This provides further evidence in favour of the transition mechanism that was studied here. In the frame of this approach, the operation for a diagonal throwing over corresponds to changing the selection of the occupation domain in the cut-and-projection algorithm [9]. This circumstance connects a local approach with the global approach in the description of quasicrystal–crystal and crystal–crystal transitions.

3. Conclusion

Our conclusion will be threefold.

- (1) A structural realization of the algebraic geometry approach suggests a structural model for the experimentally observed transformation of an icosahedral phase into a cubic crystalline phase with the BCC disordered B2 (CsCl) structure. This transition between icosahedral and BCC crystalline phase can be described in the framework of the root lattice E_8 in an eight-dimensional space as the hypothetical praphase with the symmetry group playing the role of the supergroup for both participants of the transition. The special subset of vectors of the E_8 coinciding topologically with the unit cell of the A15 structure (Cr₃Si-type) in the three-dimensional Euclidian space was found; this subset can be regarded as an intermediate configuration during transition between FCC, BCC and HCP structures. The properties of the E_8 lattice give foundation to the possibility of mapping a quasicrystalline structure on a crystalline structure (and vice versa).
- (2) For the transformation of the icosahedron of the icosahedral phase into a rhombic dodecahedron of the cubic B2 phase, the cubic A15 structure plays the role of an

intermediate configuration since it can be represented as a three-dimensional packing of linear interlaced chains of Frank–Kasper polyhedra with coordination numbers Z of 12 and 14. The transition between the rhombic dodecahedron of the B2 structure and the Frank–Kasper polyhedron with $Z = 14$ requires insertion of a disclination quadruplet into some rhombic faces of the dodecahedron.

- (3) The symmetry foundation of this model is the only one possible and due to this uniqueness, the proposed model is applicable to the description of any polymorphic transition in metallic tetrahedral structures.

Acknowledgments

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