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To cite this version:
F. Frank. THE ICOSAHEDRAL ORIENTATION MANIFOLD AS A MODEL FOR ICOSAHEDRAL CLOSE-PACKING. Journal de Physique Colloques, 1986, 47 (C3), pp.C3-165-C3-172. <10.1051/jphyscol:1986316>. <jpa-00225727>

HAL Id: jpa-00225727
https://hal.archives-ouvertes.fr/jpa-00225727
Submitted on 1 Jan 1986

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THE ICOSAHEDRAL ORIENTATION MANIFOLD AS A MODEL FOR ICOSAHEDRAL CLOSE-PACKING

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ABSTRACT

Geometrical mappings of the orientation manifold for icosahedral symmetry, both by means of Rodrigues vectors and Quaternion parameter vectors are described. In such mappings the set of 60 points representing the same orientation as the point at the origin provide an array with spherically cyclic closure, in which each point of the array has, topologically, the same icosahedral environment as every other: in which, moreover, the configuration of points in an inner region makes a tolerably good match to the configuration of a low energy packing of 33 or even 45 atoms: so providing a directly visualizable model of an ideal icosahedral close-packing.

Figs.1,2,3 are geometric presentations of the orientation manifold for icosahedral symmetry, according to two different mappings.

An orientation mapping is provided by combining a mapping of rotations with choice of a standard or original orientation to be represented by the point at the origin.

The two different rotation mappings employed here are related to Euler's second method of mathematically specifying the rotations of a three dimensional rigid body. His first method was the use of the so called Euler angles, which are the settings of a three-circle goniometer. His second method, which he recommended for its symmetry, was to specify an axis of rotation, which we may designate as a unit vector \( \mathbf{L} \), and an "amplitude" \( \omega \), of rotation about that axis. These may be combined into a single mathematical entity by multiplying the \( \mathbf{L} \) by \( \omega \) (the crudest combination) or any function \( f(\omega) \) which is odd and monotone increasing within the range \( \omega < \pi \). Two advantageous choices, both employed here, are \( f(\omega) = \tan \left( \frac{1}{2} \omega \right) \) and \( \sin \left( \frac{1}{2} \omega \right) \). These yield:

The Rodrigues vector:

\[
R = \mathbf{L} \cdot \tan \left( \frac{1}{2} \omega \right)
\]

and the Quaternion parameter vector:
The three components of \( Q \), together with \( \cos \left( \frac{1}{2} \omega \right) \), are the quaternion parameters, which may be used to form quaternions, or Cayley-Klein 2x2 complex matrices, convenient for calculating combinations of rotations. When using Rodrigues vectors rotations are combined by use of Rodrigues' formula: Rotations \( R_1 \) followed by \( R_2 \) yield:

\[
R = \frac{R_1 + R_2 - R_1 \times R_2}{1 - R_1 \cdot R_2}
\]

Two particular merits of the Rodrigues mapping are that any continuing rotation about a fixed axis maps as a straight line, and the orientationally equidistant boundary between two given orientations (i.e. the locus of map-points \( R \), such that equal angles of rotation are required to reach a fixed pair of orientations represented by \( R_A \) and \( R_B \) from that represented by \( R_0 \)) is a plane. On transforming to the \( Q \) mapping straight lines in the \( R \)-map become semi-ellipses, terminating on diametrically opposite points of the bounding unit sphere, and planes in the \( R \)-map become hemispheroids bounded by a great circle of the unit sphere.

For our original orientation we choose that of the regular icosahedron with its 12 vertices at: 

\[
(\tau^1, \tau^0, 1), (\tau^0, \tau^1, 1), \text{ and } (\tau^1, 1, \tau^0),
\]

where \( \tau = 2 \cos \frac{\pi}{5} = (\sqrt{5} + 1)/2 = 1.61803... \), the positive root of \( \tau^2 - \tau - 1 = 0 \).

This object has 6 5-fold axes of rotation symmetry, 10 3-fold axes, and 15 2-fold axes. Expressed as unit vectors the 5-fold axes are given (with a two-fold redundancy) by

\[
[0, \tau^1, \tau^1]/(2+\tau)^{1/2}
\]

and its cyclic permutations. The 3-fold axes are given (likewise with 2-fold redundancy) by the unit vectors:

\[
[0, \tau^1, \tau^1]/3^{1/2}
\]

and its cyclic permutations, together with

\[
[1, \tau^1, 1]/3^{1/2}
\]

The two-fold axes are given, again with 2-fold redundancy, by

\[
[\tau^1, \tau^1, 1]/2
\]

and

\[
[1, 0, 0],
\]

both with their cyclic permutations.

Under icosahedral symmetry equivalents of any one orientation are represented by 60 distinct points in the orientation map. In particular, equivalents of the original orientation are represented by: the origin.
plus 4 additional points on each of the 6 5-fold axes,
plus 2 additional points on each of the 10 3-fold axes,
plus 1 additional point on each of the 15 2-fold axes.

The last 15 points appear with a 2-fold redundancy, appearing to be 30, each appearing at points corresponding to \( \omega = \mp \tau \), which are to be regarded as identical. In the Rodrigues mapping these pairs of points are at infinity: in the Quaternion parameter map they are at diametrically opposite points on the boundary sphere of unit radius.

In Rodrigues mapping, the coordinates of these points are:

One at the origin: \((0,0,0)\)

A first shell of 12 at a distance
\[
\tan \frac{\pi}{5} = \left(4 - \frac{1}{2}\right)^{1/2} = 0.72654... \quad \text{from the origin:}
\]
\((0,\mp \tau, \mp \tau) = (0,0.61803, 0.38197)\)
with cyclic permutations.

A second shell of 20 at a distance
\[
\tan \frac{\pi}{3} = 3^{1/2} = 1.73205... \quad \text{from the origin:}
\]
\((0,\mp \tau^2, \mp \tau) = (0,0.61803, 1.61803)\)
with cyclic permutations, and:
\((\mp 1, \mp 1, \mp 1)\).

A third shell of 12 at a distance
\[
\tan 2\pi/5 = (2+\tau)^{1/2}/(2-\tau)^{1/2} = 3.0777... \quad \text{from the origin.}
\]
\((0,\mp \tau/2, \mp \tau/2) = (0,0.61803, 0.80902)\)
with cyclic permutations.

A fourth shell of 30, to be counted as 15, at infinite distance from the origin;
\((\mp 1, \mp 1, \mp 1/2)\),
and \((\mp 1, 0, 0)\),
both with cyclic permutations.

In the Q-map these become:
the origin, \((0,0,0)\);

the first shell of 12 at a distance from the origin of
\[
\sin \pi/5 = (4-\tau)^{1/2}/2 = 0.5878... 
\]
\((0,\mp 1/2, \mp \tau/2) = (0,0.30902, 0.80902)\)
with cyclic permutations:

the second shell of 20 at a distance from the origin of
\[
\sin \pi/3 = 3^{1/2}/2 = 0.8660... 
\]
\((0,\mp 1/2, \mp 1/2) = (0,0.30902, 0.80902)\)
with cyclic permutations, and
\((\mp 1, \mp 1, \mp 1/2) = (\pm 0.5, \pm 0.5, \pm 0.5)\);

the third shell of 12 at a distance from the origin of
\[
\sin 2\pi/5 = (4-\tau^2)^{1/2}/(\tau/2) = 0.95106... 
\]
\((0,\mp \tau/2, \mp 1/2) = (0,0.80902, 0.5)\)
with cyclic permutations:

and the fourth shell of 30 points on the bounding sphere of unit radius of which diametrically opposite points are to be regarded as identical:
\((\mp \tau/2, \pm 1/2, \pm \tau/2) = (\pm 0.30902, \pm 0.5, \pm 0.80902)\) and \((\mp 1, 0, 0)\),
both with cyclic permutations.

If, say, one wishes to display by one of these mappings the experi-
mentally determined orientation of a grain in a polygranular specimen of an icosahedral phase, one will not wish to record all sixty map-points representing the same orientation. One suffices. The most natural convention is to select that one for which \( \omega \) has the smallest value. All points selected by this convention will lie within a fundamental cell near the origin, bounded by planes in the \( R \)-mapping at a distance
\[
\tan \pi/10 = (2-\tau)^{1/2}/(2+\tau)^{1/2} = 0.32492\ldots
\]
from the origin, perpendicular to the lines (along pentad axes) joining the origin to the 12 points at a distance \( \tan \pi/5 = (3-\tau)^{1/2}/\tau = 0.72654\ldots \) from the origin representing the first shell of points representing equivalents of the original orientation. These 12 planes satisfy equations
\[
R \cdot P_i = \tau^{-1}
\]
where the \( P_i \) are vectors of the form
\[
P_i = (\pm \tau, \pm 1, 0)
\]
with cyclic permutations.

They form a regular dodecahedron with vertices at
\[
R = (\pm \tau^{-2}, 0, \pm \tau^{-4}) = (\pm 0.38197, 0, 0.14590)
\]
with cyclic permutations, and at
\[
R = (\pm \tau^{-3}, \pm \tau^{-3}, \pm \tau^{-3}) = (\pm 0.23607, \pm 0.23607, \pm 0.23607),
\]
all at a distance \( 3^{1/2}\tau^{-3} = 0.40888\ldots \) from the origin.

Corresponding proximity cells may be defined around each of the points representing the same orientation as the origin (which, for brevity, we shall call aboriginal points) thus dividing the entire map into 60 cells. They are the equivalent of Dirichlet-Voronoi cells, except that in their definition distance is replaced by angle of rotation. All (in \( R \)-mapping) are pentagonal dodecahedra, but increasingly distorted from the regular dodecahedron with increasing distance from the origin. 15 of them are divided into two parts, in the neighbourhood of plus and minus infinity. In the \( Q \)-mapping, in which these latter 15 cells are halved by the boundary sphere, all cell boundaries which are not radial planes are spheroidally curved.

All 60 cells are equivalent to each other, and a continuous transformation of the map, corresponding to a rotation of the standard object represented by the point at the origin, can bring any one of the aboriginal points (or any other point of the map) to the origin. It is convenient to say that the topological symmetry of the map at any point is that symmetry which it has when brought to the origin. Each aboriginal point has icosahedral topological symmetry. The line joining any neighbouring pair of aboriginal points is a five-fold axis of topological symmetry for the map. Each cell edge (at which 3 cells meet) is a 3-fold axis of topological symmetry. These lines remain 5-fold and 3-fold axes of ordinary symmetry for the map if displaced from the origin along any radius so that by prolongation they still pass through the origin. A similar statement may be made for 2-fold axes.

Each cell vertex, where 4 cells meet, has tetrahedral topological symmetry.

Every face of a cell, if extended, passes through the aboriginal points.
of 5 neighbouring cells (and 10 more at a greater distance). Every
cell edge, if extended, passes through the aboriginal points of 2
neighbouring cells (and another at greater distance).

The ideal ordinary symmetries present at the origin are approximately
realized in an extensive neighbourhood of the origin. Thus, consi-
dering, in R-mapping, the fundamental cell together with the cell-
-boundaries radiating from each of its edges, the internal dihedral
angle at each edge of the cell is 116.6°... and the two external
dihedral angles 121.7°..., while the three dihedral angles at each edge
radiating from its vertices are 120°.

Three of the angles between the four edges meeting at a vertex are 108°
and the other three are 110.9°..., comparing with the ideal tetrahedral
angles of 109.5°...

The 60 aboriginal points (inclusive of the original point) thus make a
closed spherically cyclic array in which each point may be said to have
the same surroundings. It thus provides a visualizable model of an
idealized icosahedral packing of spheres which by introduction of
disclinations could be extended infinitely. About half of its points,
nearest to the origin, match fairly well a packing of spheres, or of
atoms. 12 icosahedrally packed around one in the same configuration as
in the icosahedral orientation manifold are the stabllest configuration
for 13 atoms interacting with Lennard-Jones forces. A further 20,
each contacting 3 in the shell of 12, in positions simulating the
second shell in the orientation map, will also be in stable positions.
A third shell of 12 atoms radially outward from those of the first
shell and each equidistant from 5 atoms of the second shell may or may
not make a stable configuration according to the interatomic force law.
A fourth shell of 30 in positions analogous to the fourth shell of the
icosahedral orientation manifold would probably not: but the analogy
is good at least for a spherical aggregate of 33 or 45 atoms.

It may be of interest to observe also that the array of cell-vertex
points (of which there are 300) also form a spherically cyclic closed
array of points with tetrahedral topological symmetry. However the two
sets of three bonds from either end of one bond are exclusively in the
"eclipsed" position relative to each other: so that this makes an
unduly restrictive idealised model for a fluid with 4-coordinated
atoms.

It is of interest to see how far we can go in constructing a packing of
equal hard spheres, having icosahedral symmetry using the icosahedral
orientation manifold as a model. We do this, taking spheres of unit
diameter, by surrounding one at the origin with a first shell of 12
with centres at radius \(a_1\) situated on the pentad axes, followed by a
second shell of 20 at radius \(a_2\) with centres on the triad axes, then a
3rd shell of 12 at radius \(a_3\), again on the pentad axes, and a 4th shell
of 30 with centres on the diad axes: adjusting the shell radii in turn
so that spheres in each shell touch spheres within it. This procedure
yields

\[
\begin{align*}
  a_1 &= 1 \\
  a_2 &= 2\sqrt[3]{2/5} \cdot \frac{\sqrt[3]{3}}{3} = 1.58931... \\
  a_3 &= 2 \\
  a_4 &= (2\sqrt[5]{2/5} \cdot \frac{\sqrt[5]{3}}{3}) \left[1+\sqrt{1/2-87\sqrt{4}/4}\right] \\
  &= 2.30834...
\end{align*}
\]
Each sphere in the 1st shell touches the central sphere, 5 in the 2nd shell, and 1 in the 3rd shell. Its 5 neighbours in the 1st shell are at a distance (between centres) of:
\[ d_{11} = a_2 (2 - 2/\sqrt{5})^2 = 1.05146 \ldots \]

Each sphere of the 2nd shell touches 3 of the 1st shell, and 4 of the 4th shell. Its 3 neighbours in the 2nd shell are at a distance between centres of:
\[ d_{22} = a_2 (2 - 2/\sqrt{5})^2 = 1.13420 \ldots \]

Considering just the first 33 spheres, it is sufficient that constraints on those of the 2nd shell from its surroundings inhibit their outward displacement to make these 33 a rigid pack. That is not the case for spheres of the 3rd and 4th shells. Those of the 3rd shell make only a single contact each with a sphere of the 2nd shell. Those of the 4th shell, of which each 2nd shell sphere touches 4, each touch only 2 spheres of the 2nd shell. Each is free to break the symmetry by toppling, maintaining these two contacts, in either of two ways towards adjacent pentad axes, impacting a sphere of the 2nd shell, and moving closer to the centre of the pack. These displacements yield a large number of alternative configurations with broken symmetry and closer packing for the 3rd and 4th shells, in which (with some exceptions) each 2nd shell sphere is displaced from its pentad axis and pinned in position by 4 contacts. Packing density cannot be well defined for any finite number of spheres, but by one reasonable test it is, for equal hard spheres, identically the same at the core of this icosahedral pack as in cubic or hexagonal close-packing. The smallest sphere enclosing thirteen has the same radius in all three. By any reasonable test the density diminishes away from the core of the icosahedral pack.

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Fig. 1 Rodrigues vector map of aboriginal points for icosahedral symmetry. A, B, C, D, label points of the first, second, third and fourth shell around the origin. Coordinates are shown in the positive octant only: \( R_1 = 0, R_2 = 0, R_3 = 0 \) are planes of mirror symmetry for the map.
Fig. 2 Quaternion parameter map of aboriginal points for icosahedral symmetry. A, B, C, D, have the same significance as in Fig. 1. Coordinates are shown in the positive octant only. \( Q_1 = 0, Q_2 = 0, Q_3 = 0 \) are planes of mirror symmetry for the map.

Fig. 3 Rodrigues vector map for icosahedral symmetry showing the fundamental cell, the greater part of its 12 adjoining cells, and some part of the next shell. Coordinates of cell vertices are labelled in the positive octant. Aboriginal points shown in this figure are not labelled but can be identified by comparison with Fig. 1 which is at a smaller scale.
R. MOSSERI.- There is an interesting relation between the subject of this talk and the curved space model exposed elsewhere in this book. Pr. FRANK constructs a representation of the icosahedral group in the $SO(3)$ group manifold. Now, $SO(3)$ is not simply connected. Its covering group $SU(2)$ is isomorphic to the hypersphere $S^3$ as a group manifold. It is then possible to construct the lift of the icosahedral group in this covering manifold. One then get a set of 120 points on $S^3$ which are the vertices of polytope $\{3,3,5\}$ described in the curved space approach.