CFU

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29 June 2004
http://homepage.mac.com/whitby/

http://web.me.com/whitby/Octahedron/Welcome.html

Reference

Octahedron1stEd.pdf–bookmark CFU–pages 85-92

Introduction

This material is excerpted from *Octahedron*. It shows how atoms assemble in identical units which join to form a crystal. The unit is a *crystal forming unit* or CFU..

CFU

Introduction

Crystal data is given on the basis that matter is a fluid capable of filling any volume without voids. From the symmetry of the crystal and spectral data a unit cell shape is determined. A chemical analysis is done. A density is determined. The atoms are placed in locations within the cell based on chemical data. Then the number of groups per cell is determined. Then the axial lengths which determine the size of the unit cell are determined. The weight of the number of groups is divided by the density of the crystal which gives the volume of the unit cell, and the axial lengths are calculated based on this volume.

But the shape of the epn determines the shape of the atom, and the shapes of the atoms determines the shape of the group, and the shapes of the groups determine the shape of the *crystal forming unit,* or CFU, whose shape determines the direction of the join and the length of the join, and it is this which determines the shape of the unit volume and its size. The crystal is formed by its particles; the particles are not formed by the crystal[1].

Molecular volume considerations

For a cfu which consists of many groups, there is adequate room in the unit cell to fit the groups, as in the glu-glu cells. For cfus consisting of just one or two atoms, there is almost no room. For one water group there is no space. For ten water groups there seems as much room as for benzyl glutamate.

Defining the Crystal Forming Unit (CFU)

It is essential to the concept of the crystal that the groups of atoms which join to produce it are identical and in identical orientation. It follows that these identical groups exist before they join. If they are to be identical, then they are made of identical groups. It follows that these identical groups exist before they join to form the group. If the groups are to be identical, then they are made of identical atoms. It follows that these atoms exist before they join to form the groups. The pattern is established that identical assemblies require identical parts. The crystal is built from just one kind of assembly whatever its complexity. These assemblies are *crystal forming units* or CFUs.

The volume of the CFU

A CFU in a given position and orientation has places where an identical CFU in identical orientation can attach itself. An attached CFU differs from the reference CFU by a translation, a move of a given length in a given direction with no rotation. If the place of attachment of the reference CFU is called *A* and the place where *A* attaches is called *A*', then, since the CFUS are identical, it must be that the reference CFU has an *A*' place of attachment. That is, if *A* to *A*' then *A*' to *A*. Each of these moves has the same length but opposite direction. This is true for each of the places of attachment. Each move belongs as well to each of the two positions.

The half move in every attachment direction defines the volume of the CFU in the following manner. At the junction of the half moves of adjacent units, a plane is defined which is perpendicular to the move direction. As stated before, the half move in a given direction has an equal and opposite half move. This, too, defines a plane which is parallel to the first. Thus, each move direction provides a pair of parallel join planes. Where a plane meets one other plane, an edge is defined. Where a plane meets more than one plane, a vertex is defined. The edges define the faces. With the faces, edges, and vertexes defined, the CFU is defined.

Locations of CFUs

For identical groupings of epns as crystal forming units, the location of one CFU relative to another in a join direction is expressible with three integers representing the axial direc-

1. C. W. Bunn *Chemical Crystallography* refers to the cfu as the “unit of pattern” (p.224) or “pattern-unit” (p.118).

tions. This distance is the same from any vertex of any epn of one CFU to the equivalent vertex of the equivalent epn of the adjoining CFU. These locations are points on a line. A third epn added to the first in a different join direction is expressible with another set of integers. This location establishes a second line with the first location. The three locations define a plane, and the plane is defined by the vertexes or edges or faces of the epns which constitute the cfus. The points of the plane lie at intervals which are described by the distance between pairs of adjoining cfus. The only plane distances are those which are expressible with integral multiples of the epn vertexial semi-diameters. There are no other points between them. The points have the qualities of the cfu. In a crystal, the cfu has an integral number of join directions. An extension of the crystal in any two join directions produces a pair of planes defined by the diameter of the cfu perpendicular to the planes, no part of which may extend beyond the two planes. The planes are the material limits of the cfu.

There are no decimals on such a plane. No circles. No pi. No infinities. No curves. No fractions of a join distance.

Crystalline lines and planes

A crystalline line is formed by the repeated addition of cfus in a single join direction. A crystalline plane is formed by the addition of a parallel line which establishes a second join direction. A second plane is established by the addition of units to the units of the first line in a third join direction. The first line is common to both planes.

Specifying a crystal plane

The plane of a crystal intersects one or more of the crystal axes. These intersections are termed axial intercepts of the plane. In the Miller system, the planes are expressed as integers which are the reciprocals of fractions which represent the relation between the axial intercepts. In an actual crystal, the planes are defined by cfus. The positions of the cfus which define a plane are related by moves between adjoining cfus. These moves are in the directions of the joins, and each is counted and referred to a set of axes.

Regular polygonal crystal prisms

For the crystal forming unit to produce a regular polygonal prism, the join directions between adjacent units must be symmetrical about the axis of the prism. The projections of the join directions upon a plane normal to the axis of symmetry will have the same symmetry as the polygon they produce. If the polygon has an odd number of sides, then there must be as many moves as there are sides. Polygons with an even number of sides require one half the number of moves as there are sides. The sides of the hexagon and the equilateral triangle have the same directions.

Besides the symmetrical directions, the moves must have the same length, and the joins must be identical. Thus the group itself must be symmetrical. And this symmetry results from symmetrical groups produced by symmetrical atoms produced by symmetrical particles.

Facial diameter changes resulting from cfu moves

If two units are on the same facial plane, the sum of the two lowest absolute values of the differences between their xyz-coordinates will equal the absolute value of the third difference. That is, $|x_1-x_2|,|y_1-y_2|,|z_1-z_2|$ without regard to order is equivalent to m, n, m+n.

Unit Cells defined by CFUs

The idea of building crystals with unit cells leads to crystal surfaces defined by diced portions of the CFUs. It also promotes the idea that the volume determines the content, and leads to the idea of “populating the cell” with atoms. The crystal concept requires that the CFUs be whole and that the CFU joins define its volume. The cubic system unit cells provide an example of the effect that this realization has upon the understanding of the crystalline structure.

Crystal forming units of the cubic system

The cubic system has three main cells in which the CFU are located in different places within the cube which is the unit cell. The types are the *simple*, the *face-centered*, and the *body-centered*. Each will be examined.

Relationships between cube and octahedron

The cube and the octahedron are related—
•the cube has eight vertexes and the octahedron has eight faces
•the cube has twelve edges and the octahedron has twelve edges
•the cube has six faces and the octahedron has six vertexes
•the cubal facial diameter is parallel to the octahedral vertexial diameter
•the cubal edgial diameter is parallel to the octahedral edgial diameter
•the cubal vertexial diameter is parallel to the octahedral facial diameter.

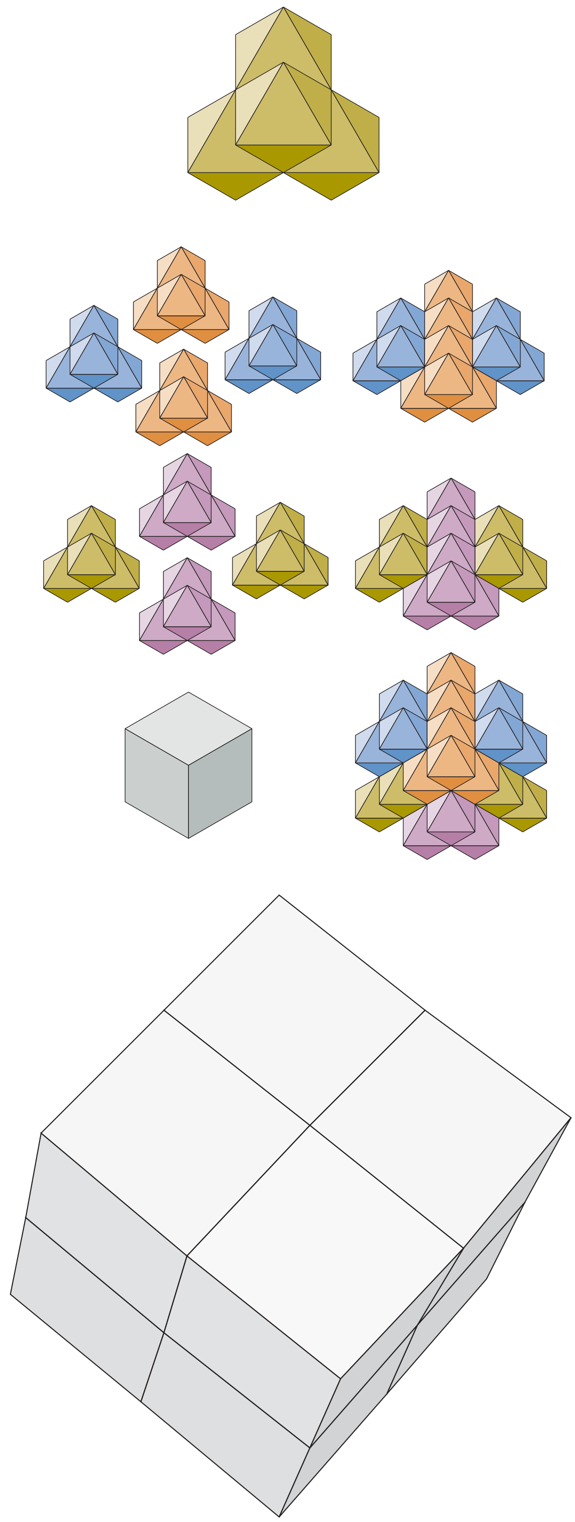
The Cubic Lattices

Simple Cubic

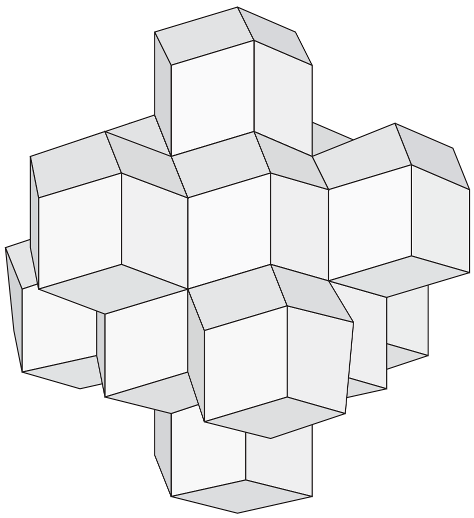
In the simple cubic crystal, CFUs join in directions which are parallel to the cubal facial diameters and the octahedral vertexial diameters. The volume defined by these join directions is a cube. The volume is not fully occupied; but, because of the crystalline order, the volume defined by the join directions belongs wholly and solely to the individual CFU. The length of the join in the octahedral vertexial direction is $n \times HeEdge/\sqrt{2}$. There are three join directions.

At the top of the figure on the right, there is a tetrahedral group consisting of four octahedra. This could be a simple cubic CFU. Below it is shown how eight identical units join cleftly to produce a simple cubic crystal. Each of the CFU centroids is at a vertex of a cube.

The volume defined by the CFU attachment moves is not the unit cell. The simple cubic unit cell is constructed so that a CFU is at each vertex of cube, and the unit cell contains a eighth of each of eight different CFUs. In the figure to the right, a compound cube is shown which is composed of eight smaller cubes.



Each of the smaller cubes is a CFU-volume. The centroid of each of the cubes is located at a vertex of a cube which is the unit cell.

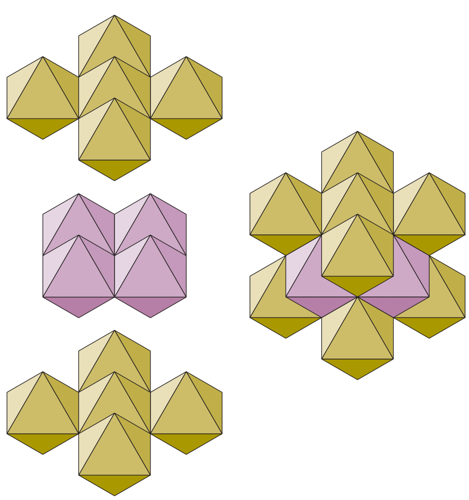


The FCC CFU.

The figure at the top shows a cube composed of fourteen rhombic dodecahedra.

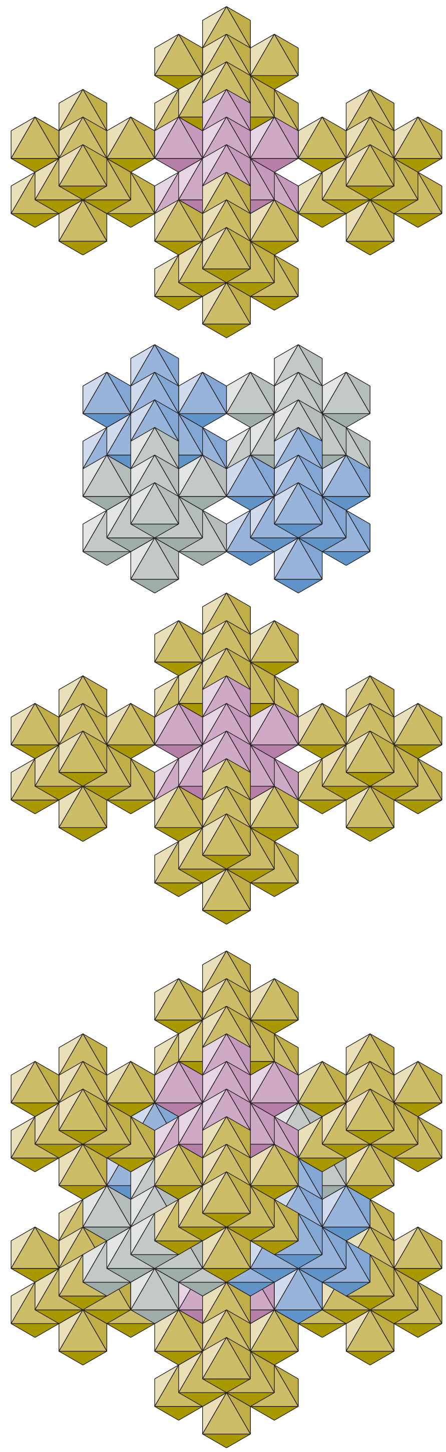
The figure at the bottom shows the assembly of a CFU composed of fourteen octahedra which will be used to construct an FCC crystal. The join between two CFUs will involve an edge of each of two octahedra of each CFU.

An assembly of fourteen CFUs to form a cube is shown on the right.

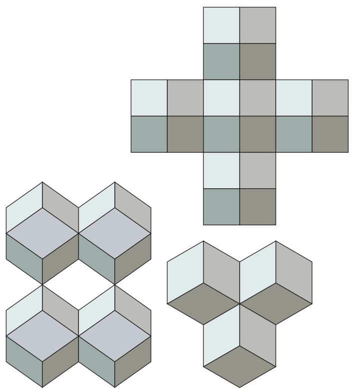


Face-centered Cubic

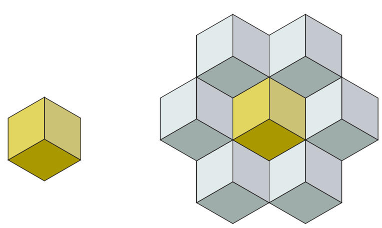
The face centered cubic cell requires attachment moves parallel to the facial diagonals and this produces a rhombic dodecahedral CFU



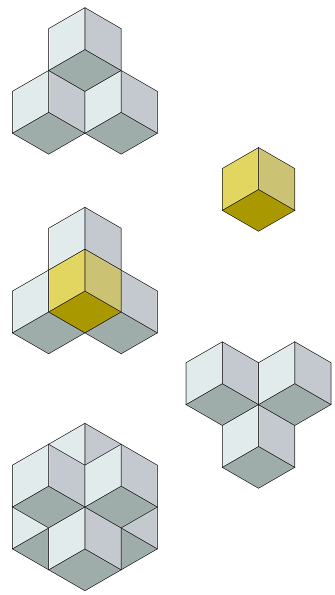
volume which wholly contains a single CFU. The unit cell contains one eighth of each of the eight vertexial CFU volumes and one half of each of the six facial CFU volumes.



Facial, edgial, and vertexial layers of FCC
Three types of planes of the FCC crystal which are defined by features of the CFU-volume are shown here. The 4-vertexes of the top group of five rhombic dodecahedra define a 100-plane. Below it is a rhombic dodecahedral triplet whose 3-vertexes define a 111-plane. To the left of it is a group of four rhombic dodecahedra whose faces define a 110-plane.

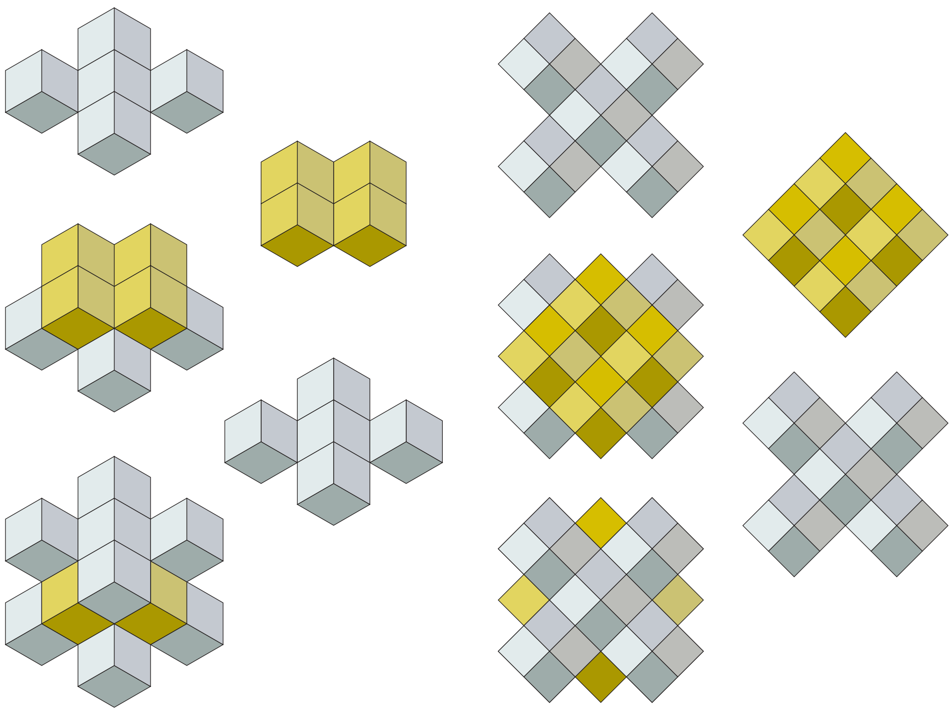


Intralayer (111) joins of FCC cfu
The dodecahedron colored yellow on the left can be joined facially to six identical dodecahedra within a 111-plane of an FCC-crystal.



Interlayer (111) joins of FCC cfu.
The figure shows the relationship between the CFUs of adjoining 111-planes of the FCC-crystal. The assembly depicted is composed of two triplets joined by a single dodecahedron. The assembly progresses from in the left-hand column from top to bottom. The adding units are shown in the righthand column. There are three layers in the final assembly.

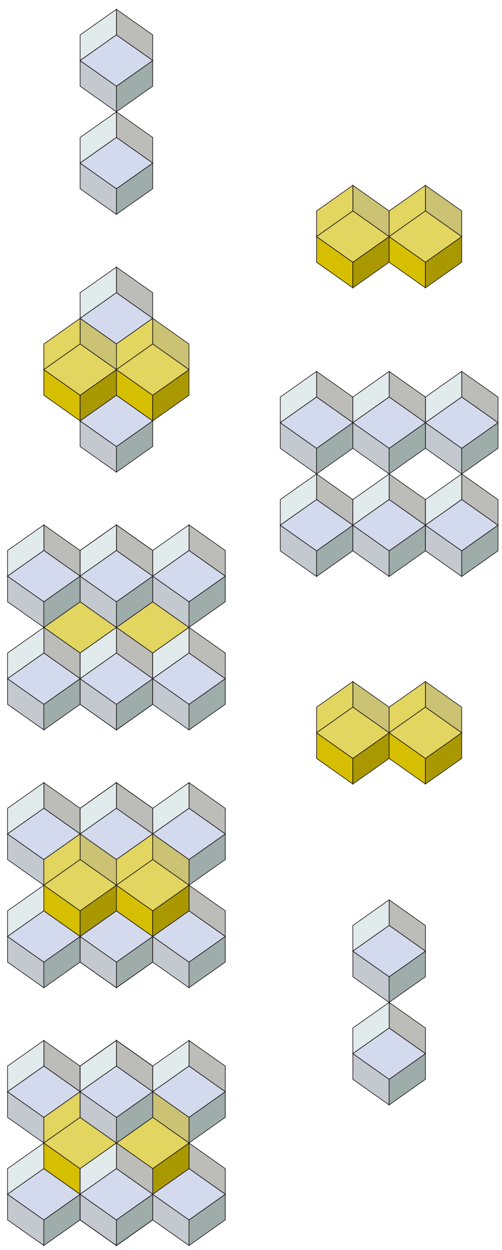
Facial layers (111) of FCC cube



Cubal facial layers of the FCC-crystal.

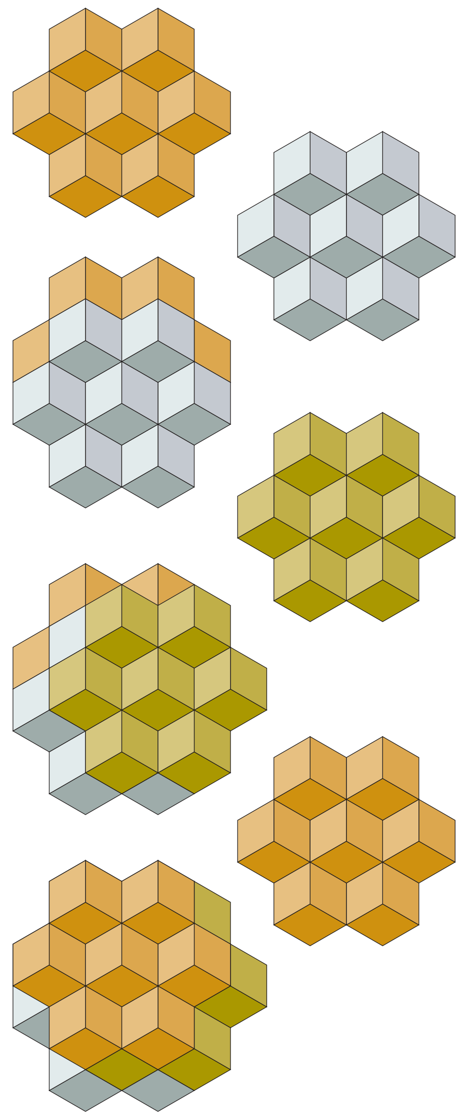
Two views of the assembly of rhombic dodecahedra in three layers are shown above. The assembly on the right is perpendicular to an FCC 100-face. The assembly on the left is perpendicular to an FCC 111-face. The fourteen dodecahedra in each assembly form an FCC cube.

Edgial layers (110) of FCC cube



Edgial layers of the FCC-cube.
The fourteen dodecahedra that form an FCC-cube are shown as an assembly of 110-layers. The assembly progresses from top to bottom in the lefthand column through the addition of the layers shown in the righthand column.

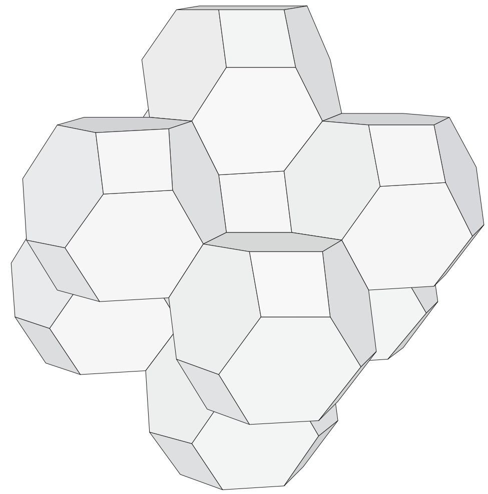
Relationship of (111) planes

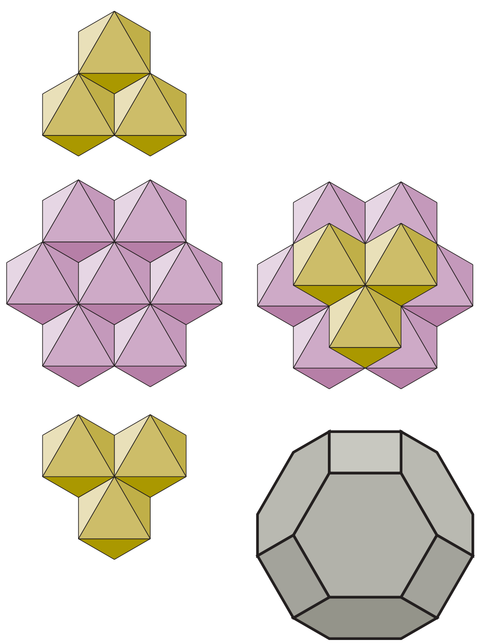


Vertexial layers of the FCC crystal.
The figure shows the addition of 111-layers to form a stack. The assembling stack is on the left, the adding layers are on the right. The stack at the bottom has four layers. The projections of the first and fourth layers are congruent.

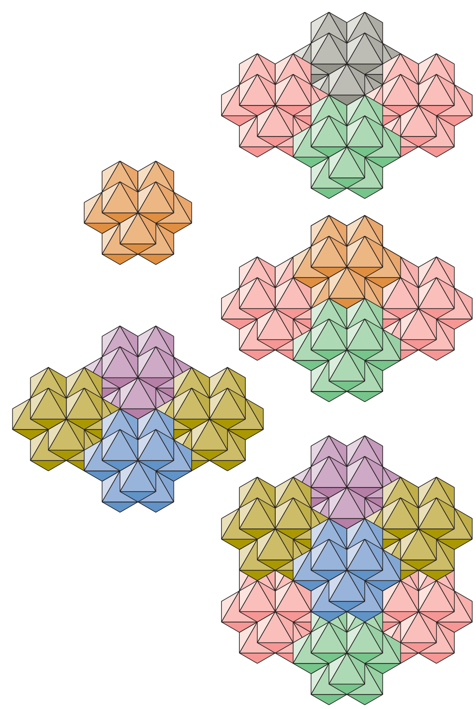
Body-centered Cubic

The body centered cubic cell requires attachment moves from the cube center to the cube vertexes which produces a cuboctahedral CFU volume. The next figure shows a cube composed of nine cuboctahedra. The centroid of one of the cuboctahedra coincides with the centroid of the cube. The centroids of the others are at the vertexes of the cube.





Assembly of a CFU for a BCC.
The three layers of an octahedral assembly which can serve as the CFU for a BCC are shown in the left hand column. The triplet at the top of the column is the bottom layer of the assembly shown in the right hand column..



Cube assembled from BCC CFUs.
The assembly is composed of three layers. The assembly progresses from the top of the right hand column to the bottom. There is a triplet join between adjoining CFUs.