# Chapter 4, Bravais Lattice

A Bravais lattice is the collection of all (and only those) points in space reachable from the origin with position vectors:

$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$

n_1, n_2, n_3 integer (+, -, or 0)

a_1, a_2, and a_3 not all in same plane

The three primitive vectors, a_1, a_2, and a_3, uniquely define a Bravais lattice. However, for one Bravais lattice, there are many choices for the primitive vectors.

A Bravais lattice is infinite. It is identical (in every aspect) when viewed from any of its lattice points.

This is not a Bravais lattice.

Honeycomb: P and Q are equivalent. R is not.
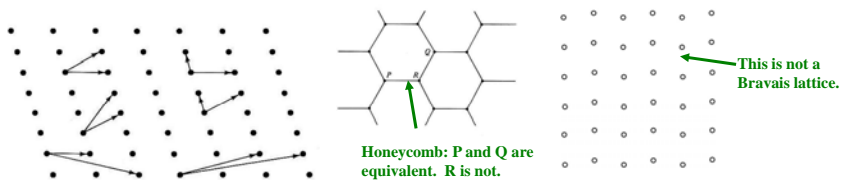
A Bravais lattice can be defined as either the collection of lattice points, or the primitive translation vectors which construct the lattice.

POINT ⇔ OBJECT: Remember that a Bravais lattice has only points. Points, being dimensionless and isotropic, have full spatial symmetry (invariant under any point symmetry operation).

Primitive Vectors

There are many choices for the primitive vectors of a Bravais lattice.

One sure way to find a set of primitive vectors (as described in Problem 4.8) is the following:

(1) a_1 is the vector to a nearest neighbor lattice point.

(2) a_2 is the vector to a lattice points closest to, but not on, the a_1 axis.

(3) a_3 is the vector to a lattice point nearest, but not on, the $a_1 \otimes a_2$ plane.
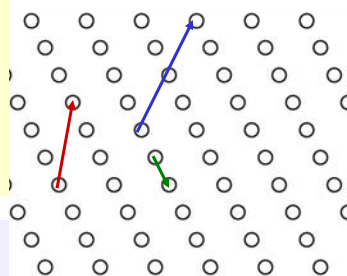
How does one prove that this is a set of primitive vectors?
Hint: there should be no lattice points inside, or on the faces (parallolegrams) of, the polyhedron (parallelepiped) formed by these three vectors.

simul exam01

Actually, a_1 does not need to be a vector between nearest neighbors (e.g. green arrow). It just needs to be a finite vector which is not a multiple of another vector (i.e. we can't pick the blue vector). What happens if we choose the red vector as our a_1?

CONCLUSION: The three primitive vectors can be chosen with considerable degree of freedom.
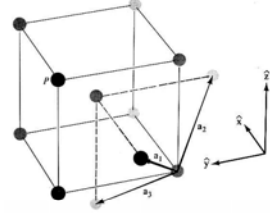
Bravais Lattice Examples

Simple Cubic

$a_1 = [a, 0, 0];$

$a_2 = [0, a, 0];$

$a_3 = [0, 0, a];$
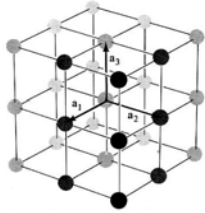
Body-Centered Cubic (bcc)

$a_1 = [-0.5, 0.5, 0.5]a;$

$a_2 = [0.5, -0.5, 0.5]a;$

$a_3 = [0.5, 0.5, -0.5]a;$

Face-Centered Cubic (fcc)

$a_1 = [0, 0.5, 0.5]a;$

$a_2 = [0.5, 0, 0.5]a;$

$a_3 = [0.5, 0.5, 0]a;$
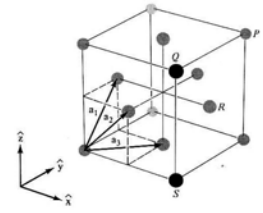
Lattice Points In A Cubic Cell

s.c. (0, 0, 0)   b.c.c. (0, 0, 0), (0.5a, 0.5a, 0.5a)

f.c.c. (0, 0, 0), (0.5a, 0.5a, 0), (0, 0.5a, 0.5a), (0.5a, 0, 0.5a)

Verify for bcc and fcc:
1. Every lattice point is reached.
2. Every lattice point is equivalent.
3. Agree w/ prescribed method.
4. Volume of primitive cell.

Primitive Unit Cell

PRIMITIVE UNIT CELL: A volume of space that, when translated through all the vectors in a Bravais lattice, just fills all of space without overlapping. There is an infinite number of choices for primitive unit cell. Two common choices are the parallelepiped and the Wigner-Seitz cell.

Parallelipiped

$$\vec{r} = x_1\vec{a}_1 + x_2\vec{a}_2 + x_3\vec{a}_3 \qquad 0 \le x_1, x_2, x_3 < 1$$

Wigner-Seitz Cell: primitive cell with full symmetry of the Bravais lattice

Volume of Primitive Cell
$$V_{cell} = |\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)|$$
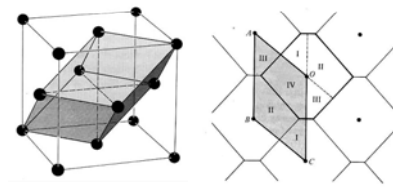
A primitive cell contains precisely one lattice point and has a volume of v=1/n where n is the density of lattice points.

Given any two primitive cells of arbitrary shape, it is possible to cut the first one into pieces, which, when translated through lattice vectors, can be reassembled to give the second cell.

If space is divided up into subspaces belonging to each lattice point. A primitive cell is the space associated with one lattice point.

Portions of the same unit cell don't even need to be connected.

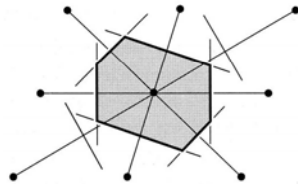examples of valid primitive cell
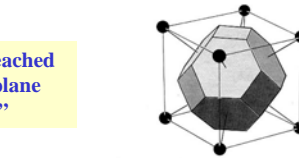

2
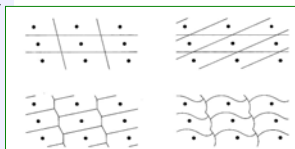
Wigner-Seitz Cell

Wigner-Seitz cell about a lattice point is the region of space that is closer to that point than to any other lattice point.

What if a point in space is equidistance to two lattice points? three lattice points? ….

Construction of Wigner-Seitz Cell: space reached from a lattice point without crossing any "plane bisecting lines drawn to other lattice points"


Generally, the larger the facet on a Wigner-Seitz cell, the closer is the nearest neighbor distance along that direction.

As we will see, all point symmetry operations of the Bravais lattice are also symmetry operations on the Wigner-Seitz cell, and vice versa.

Conventional Unit Cell

A **non-primitive** unit cell is conventionally chosen for convenience. Typically, these unit cells have a few times the volume of the primitive cell. They can fill space without overlaps and gaps through translational vectors which are sums of multiples of lattice constants. Conventionally, lattice points are assumed to occupy corners of the parallelepiped cells.

bcc
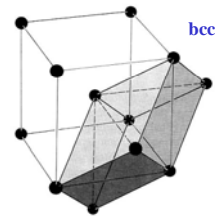
lattice constant ⇔ primitive vector length

bcc ➜ simple cubic with two Bravais lattic points in a unit cell

fcc ➜ simple cubic with four Bravais lattic points in a unit cell

centered tetragonal, centered monoclinic, base-centered orthorhombic, body-centered orthorhombic ➜ two Bravais lattic points in a unit cell

face-centered orthorhombic ➜ four Bravais lattic points in a unit cell

Homework

Homework assignments (and hints) can be found

http://academic.brooklyn.cuny.edu/physics/tung/GC745S12

Ch 4: 2, 5, 6, 8(a)

Ch 5: 1 – 2

Ch 6: 1, 3

Ch 7: 2 – 5

Ch 4-7 Homework Due Date: 3/2

Beginning of Chapter 7

Bravais Lattice Classification

Bravais lattices are classified according to the set of rigid symmetry operations which take the lattice into itself. (.. meaning that the old position of every lattice point will be occupied by a(nother) lattice point after the operation.) Examples of symmetry operations: translation, rotation, inversion, reflection.

The set of symmetry operations is known as a symmetry group or space group.

All translations by lattice vectors obviously belong to the space group.

The order of any space group is infinite. (Why?)

All rules of group theory apply: e.g. the identity operation, the inverse of operation, the product of any two operations all belong to the group.

A sub-group of the space group can be formed by taking those symmetry operations which leave at least one lattice point unchanged. This is known as the point group, which still displays all properties of a group.

The order of a point group is finite.

Point Symmetry Operations

Any symmetry operation of a Bravais lattice can be compounded out of a translation T_R through a lattice vector R and a rigid operation leaving at least one lattice point fixed.
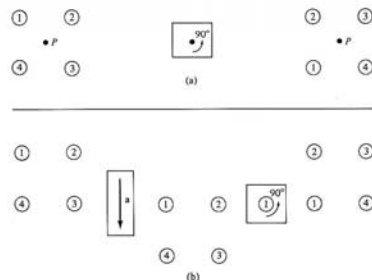
The full symmetry group of a Bravais lattice contains only operations of the following form:

1. Translations through lattice vectors.

2. Operations that leave a particular point of the lattice fixed.

3. Operations that can be constructed by successive applications of (1) and (2).

Point Symmetry Operations

|		
E	The identity transformation.	
i	The inversion operator.	
C_n	Rotation (clockwise) through an angle of $2\pi/n$.	
C_n^k	Rotation (clockwise) through an angle of $2k\pi/n$. Both n and k are integers.	
S_n	An *improper* rotation through an angle of $2\pi/n$ radians. Improper rotations (*rotation-reflections*) are regular rotations followed by a reflection in the plane perpendicular to the axis of rotation. (S_2 the same as i).	
σ	A mirror plane.	
σ_h	*Horizontal* reflection plane - passing through the origin and perpendicular to the axis with the `highest' symmetry.	
σ_v	*Vertical* reflection plane - passing through the origin and the axis with the `highest' symmetry.	
σ_d	*Diagonal* or *dihedral* reflection in a plane through the origin and the axis with the `highest' symmetry, but also bisecting the angle between the twofold axes perpendicular to the symmetry axis.	

Proper and improper operations.

What about mirror planes that do not contain any lattice points?

Point Groups ↔ Crystal Systems

There are seven distinguishable point groups of Bravais lattice. These are the **seven crystal systems.**

Crystal System	# Lattices	Conventional Cell
Cubic	3	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 90^\circ$
Hexagonal	1	$a_1 = a_2 \neq a_3$ $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$
Tetragonal	2	$a_1 = a_2 \neq a_3$ $\alpha = \beta = \gamma = 90^\circ$
Trigonal	1	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma \neq 90^\circ$
Orthorhombic	4	$a_1 \neq a_2 \neq a_3$ $\alpha = \beta = \gamma = 90^\circ$
Monoclinic	2	$a_1 \neq a_2 \neq a_3$ $\alpha = \beta = 90^\circ \neq \gamma$
Triclinic	1	$a_1 \neq a_2 \neq a_3$ $\alpha \neq \beta \neq \gamma$
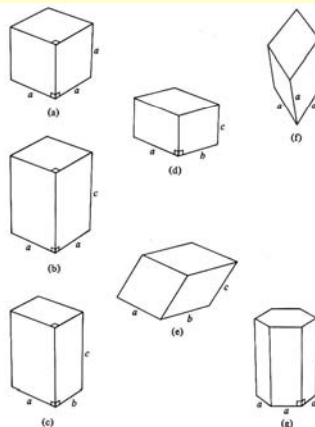
What are the differences and the similarities between "Bravais lattices" belonging to the same "crystal system"?

The 7 Crystal Systems

Crystal System	Operations	Order	Schönflies Symbol
Cubic	E, $8C_3$, $6C_2$, $6C_4$, $3C_2'$, i, $6S_4$, $8S_6$, $3\sigma_h$, $6\sigma_d$	48	O_h
Hexagonal	E, $2C_6$, $2C_3$, C_2, $3C_2'$, $3C_2''$, i, $2S_3$, $2S_6$, σ_h, $3\sigma_d$, $3\sigma_v$	24	D_{6h}
Tetragonal	E, $2C_4$, C_2, $2C_2'$, $2C_2''$, i, $2S_4$, σ_h, $2\sigma_v$, $2\sigma_d$	16	D_{4h}
Trigonal	E, $2C_3$, $3C_2$, i, $2S_6$, $3\sigma_d$	12	D_{3d}
Orthorhombic	E, C_2, C_2', C_2'', i, σ, σ', σ''	8	D_{2h} (V_h)
Monoclinic	E, C_2, i, σ_h	4	C_{2h}
Triclinic	E, i	2	C_i (S_2)

The orders of the point groups can be more easily visualized by counting the number of different ways to orient a lattice.

The 14 Bravais Lattices

From the full symmetries (point operations and translations) of the Bravais lattice, 14 different space groups have been found.

Cubic(3): simple cubic, face-centered cubic, body centered cubic

Tetragonal (2): simple tetragonal, centered tetragonal

Orthorhombic (4): simple orthorhombic, body-centered orthorhombic, face-centered orthorhombic. base-centered orthorhombic

Why can't we have a orthorhombic lattice which is centered on two perpendicular faces?

Monoclinic (2): simple monoclinic, centered monoclinic

Trigonal (1)

Hexagonal (1)

Triclinic (1)

NOTE: All Bravais lattices belonging to the same crystal system have the same set of "point" operations which bring the lattice to itself. For example, any point symmetry operation for a single cubic is also a point symmetry operation for a b.c.c. or an f.c.c. lattice.

not translation operations!!

In other words, a "crystal system" does not uniquely define a Bravais lattice.

Crystal Structure: Lattice With A Basis

A Bravais lattice consists of lattice points. A crystal structure consists of identical units (basis) located at lattice points.

Diamond Structure
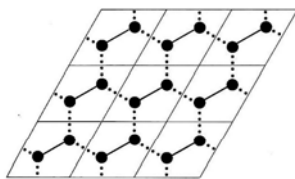
Honeycomb net:

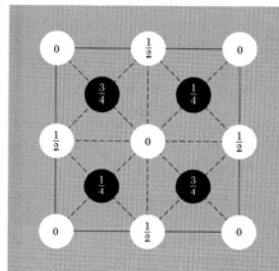Advice: Don't think of a honeycomb when the word "hexagonal" is mentioned.

Figure 22 Atomic positions in the cubic cell of the diamond structure projected on a cube face; fractions denote height above the base in units of a cube edge. The points at 0 and $\frac{1}{2}$ are on the fcc lattice; those at $\frac{1}{4}$ and $\frac{3}{4}$ are on a similar lattice displaced along the body diagonal by one-fourth of its length. With a fcc space lattice, the basis consists of two identical atoms at 000 and $\frac{1}{4}\frac{1}{4}\frac{1}{4}$.
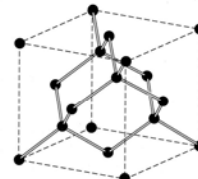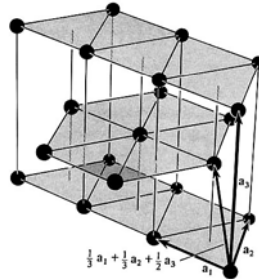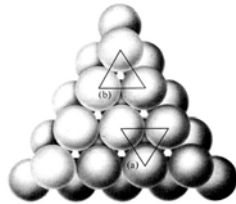
Figure 23 Crystal structure of diamond, showing the tetrahedral bond arrangement.

Close-Packed Structures

Hexagonal Close-Packed Structure

Ideal HCP c/a ratio $c=\sqrt{\dfrac{8}{3}}\,a=1.63299\,a$

two-atom basis
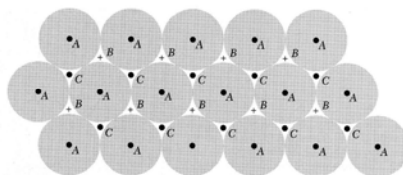
Close-Packed Structures

Figure 19 A close-packed layer of spheres is shown, with centers at points marked A. A second and identical layer of spheres can be placed on top of this, above and parallel to the plane of the drawing, with centers over the points marked B. There are two choices for a third layer. It can go in over A or over C. If it goes in over A, the sequence is ABABAB . . . and the structure is hexagonal close-packed. If the third layer goes in over C, the sequence is ABCABCABC . . . and the structure is face-centered cubic.

hexagonal polytypes
twins
stacking faults
antiphase domains
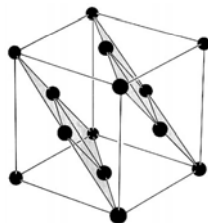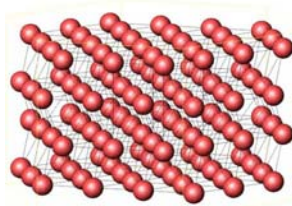
fcc
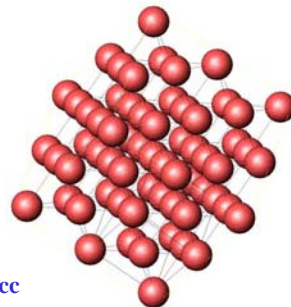
Symmetry Operations For Real Crystal Structures

Bravais lattice constructed from translation of lattice point (point is spherically symmetric).

Real (perfect) crystals are constructed from translation of object (unit cell) in space.

A symmetry operation for the crystal structure is one which takes the crystal to itself (indistinguishable from before).

Crystal symmetry depends not only on the symmetry of the Bravais lattice of the crystal, but also on the symmetry of the unit cell.

Point symmetry operations (those with position of at least one point unchanged) form a sub-group (crystal point group) of any full crystal space symmetry group.

There are 32 different crystallographic point groups.

Cubic Point Groups

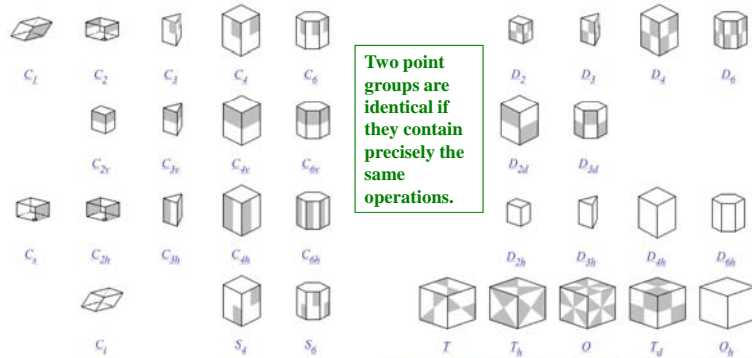The cubic group is identical to the octahedral group.

O: no inversion

T_h: no 4-fold, horiz. planes

T_d: no 4-fold, diag. planes

T: no inv., no 4-fold rot.

Why is T still cubic. When does a structure cease to be cubic?

Operations	Order	Schönflies Symbol
E, $4C_3$, $4C_3^2$, $3C_2$	12	T
E, $8C_3$, $3C_2$, $3\sigma_v$, i, $8S_6$	24	T_h
E, $6C_4$, $8C_3$, $3C_2$, $6C_2'$	24	O
E, $8C_3$, $3C_2$, $6S_4$, $6\sigma_d$	24	T_d
E, $8C_3$, $6C_2$, $6C_4$, $3C_2'$, i, $6S_4$, $8S_6$, $3\sigma_h$, $6\sigma_d$	48	O_h

Example: if we painted the top and the bottom of a cube black, the rest of the faces white, to what point symmetry group does this crystal belong?

32 Crystallographic Point Groups

Two point groups are identical if they contain precisely the same operations.

Schoenflies Notation: Non-cubic Crystallographic Point Groups

C_n	n-fold rotation axis
C_{nv}	n-fold rotation axis + vertical mirror planes
C_{nh}	n-fold rotation axis + horizontal mirror plane
S_n	n-fold rotation-reflection axis
D_n	n-fold rotation axis + 2-fold axis perpendicular to n-fold axis
D_{nd}	D_n + vertical mirror planes (bisecting 2-fold axes)
D_{nh}	D_n + horizontal mirror plane

What crystallographic point group does one get by putting trigonal objects (e.g. NH_3) on tetragonal Bravais lattice sites?

**Moral of story: Translation vectors do not determine crystallographic point group.**

Crystallographic Space Groups

There are 230 crystallographic space groups.

New symmetry operations (not available for Bravais lattices) become possible for crystals.
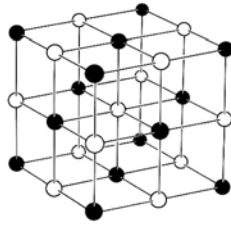
hcp

Example: Screw axis. non-Bravais translation + rotation about same axis

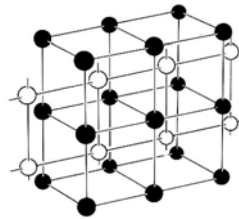**glide plane: non-Bravais translation + reflection in plane containing vector**
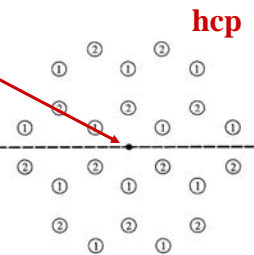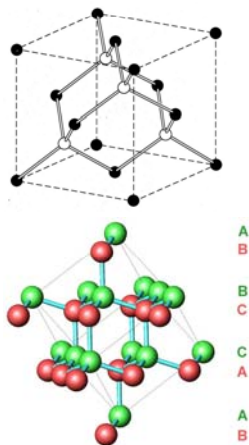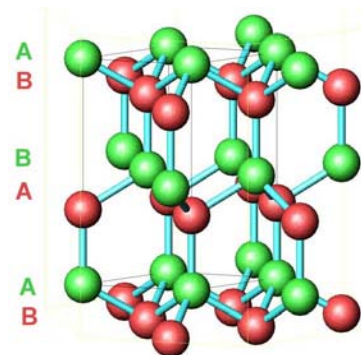
Common Crystal Structures

NaCl

CsCl

You are expected to know the details of these structures by name.

Technologically Important Structures
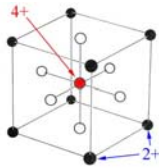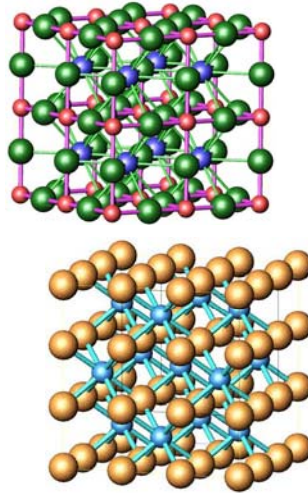
zincblend

Wurzite

These structures follow the stacking of layers with sequences the same as discussed before for fcc and hcp. However, unlike fcc and hcp, these structures are not close-packed.

Other Important Structures

Provskite (SrTiO$_3$)
and high TC superconductors.

Fluorite (CaF$_2$)

Summary Of Crystal Symmetry

1. Bravais lattice consists of points.

2. Unit cell + Bravais lattice = crystal lattice

3. Symmetry operations of Bravais lattice determine its point group and space group.

4. Symmetry operations of real crystal lattice determine its crystallographic point group and space group.

5. 14 different Bravais lattices (space groups) can be found, falling into 7 different crystal systems (point groups).

6. 230 different crystallographic space groups can be found, falling into 32 different point groups.