Lecture #11

Program:

1. The description of systems with discrete translational symmetry periodic systems – The Bravais lattice
2. Examples of cubic lattices (SC, BCC, FCC) and elements that have corresponding Bravais lattices underlying their crystal structure.
3. Primitive lattice vectors, coordination number, primitive unit cell, Wigner-Seitz cell.
4. Crystal structures – lattice with a basis.
5. Examples
6. Reciprocal lattice – reciprocal lattice vectors
7. Brillouin zone
8. Bloch's Theorem

References:

1. Ashcroft and Mermin Solid State Physics

Bravais Lattice

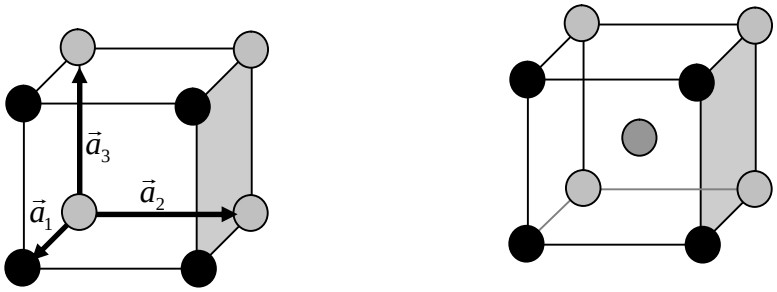
A fundamental concept in the description of any crystal lattice is the Bravais lattice:
Definition:

1. A Bravais lattice is an infinite array of discrete points with an arrangement and orientation that appears exactly the same from whichever of the points the array is viewed.
2. A Bravais lattice consists of all points with position vector $\vec{R}$ of the form:

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

where $\vec{a}_1$, $\vec{a}_2$, $\vec{a}_3$ are called primitive vectors and are any three vectors that do not lie on the same plane and the n's are integers.

Examples: A 2D Bravais lattice and a honeycomb that is not a Bravais lattice



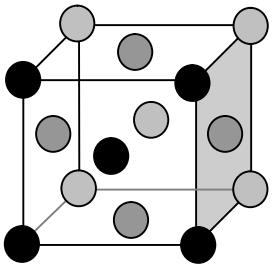
Simple Cubic and Body Centered Cubic Bravais lattices showing primitive lattice vectors

The primitive lattice vectors for the SC structure:

$$\vec{a}_1 = a\hat{x},\ \vec{a}_2 = a\hat{y},\ \vec{a}_3 = a\hat{z}$$

One particular choice of primitive lattice vectors for the BCC lattice can be:

$$\vec{a}_1 = \frac{a}{2}\left(-\hat{x}+\hat{y}+\hat{z}\right),\ \vec{a}_2 = \frac{a}{2}\left(\hat{x}-\hat{y}+\hat{z}\right),\ \vec{a}_3 = \frac{a}{2}\left(\hat{x}+\hat{y}-\hat{z}\right)$$



Face centered cubic (FCC) Bravais lattice

$$\vec{a}_1 = \frac{a}{2}\left(\hat{x}+\hat{y}\right),\ \vec{a}_2 = \frac{a}{2}\left(\hat{x}+\hat{z}\right),\ \vec{a}_3 = \frac{a}{2}\left(\hat{y}+\hat{z}\right)$$

Elements with FCC crystal structure:

Element	a (angstrom)	Element	a (angstrom)
Ar	**5.26**	**Ni**	**3.52**
Ag	**4.09**	**Pb**	**4.95**
Al	**4.05**	**Pd**	**3.89**
Ca	**5.58**	**Pt**	**3.92**

Elements with BCC crystal structure:

Element	a (angstrom)	Element	a (angstrom)
Ba	**5.02**	**Li**	**3.49**
Cr	**2.88**	**Mo**	**3.15**
Fe	**2.87**	**Na**	**4.23**
K	**5.23**	**Rb**	**5.59**

The Coordination Number

The points in a Bravais lattice that are closest to a given point are called its nearest neighbors (n.n.). The number of n.n is called the coordination number and is a property of the lattice since each point in the lattice has the same coordination number (SC=6, BCC=8, FCC=12)

Primitive Unit Cell

A volume of space that, when translated through all Bravais lattice vectors just fills all of space without either overlapping itself or leaving voids is called a primitive cell or primitive unit cell of the lattice. There is no unique way of choosing a primitive cell. The primitive cell must contain precisely one lattice point (mention points on the cell surface). The volume of the primitive cell is thus also a property of the lattice and is inversely related to the density of points.

$$v = \frac{1}{n}$$

The obvious choice for a Primitive Unit Cell is the volume defined by all points satisfying:

$$\vec{r} = x_1\vec{a}_1 + x_2\vec{a}_2 + x_3\vec{a}_3$$

$$0 \le x_i \le 1$$

which defines a parallelepiped.

Wigner Seitz cell

The volume of space that is closest to a lattice point is a Primitive Unit Cell called the Wigner Seitz cell it too is a property of the Bravais lattice. The method for constructing a Wigner-Seitz cell is by drawing lines connecting the lattice point to all the others and bisecting each line with a plane (perpendicular to the line). The W-S cell is the smallest polyhedron containing the point.

Unit Cell (conventional)
A volume of space that, when translated through a subset of Bravais lattice vectors fills all of space without any overlapping is called a unit cell. Numbers specifying the size of a unit cell are called lattice constants.

Crystal Structure – Lattice with a Basis
A physical crystal can be described by giving it's Bravais lattice and specifying the arrangement of atoms within a particular primitive cell. This completely describes the crystal structure.

Important Examples

A. The diamond structure (p76)

This lattice is not a Bravais lattice because the environment at any point differs from that of its n.n. The diamond structure can be described as an FCC lattice with a 2 atom basis

$$0,\ \frac{a}{4}\left(\hat{x}+\hat{y}+\hat{z}\right)$$

elements crystallizing in the diamond structure are:

Element	a (angstrom)
C	**3.57**
Si	**5.43**
Ge	**5.66**
a - Sn	**6.49**

B. The hexagonal closed packed structure

The Bravais lattice underlying this structure is a simple hexagonal lattice with three primitive lattice vectors:

$$\vec{a}_1 = a\hat{x},\ \vec{a}_2 = \frac{a}{2}\hat{x}+\frac{\sqrt{3}a}{2}\hat{y},\ \vec{a}_3 = c\hat{z}$$

The basis associated with this structure is a 2 point basis:

$$0,\ \frac{\vec{a}_1}{3}+\frac{\vec{a}_2}{3}+\frac{\vec{a}_3}{2}$$

Element	a (angstrom)	c (angstrom)	c/a
Mg	**3.21**	**5.21**	**1.62**
Ti	**2.95**	**4.69**	**1.59**
Cd	**2.98**	**5.62**	**1.89**
Er	**3.56**	**5.59**	**1.57**

C. The Sodium Chloride Structure

FCC Bravais lattice with a basis consisting of one type of atom at position 0 and the other type at $\frac{a}{2}(\hat{x}+\hat{y}+\hat{z})$.

Element	a (angstrom)
NaCl	**4.62**
LiF	**4.02**
AgCl	**5.55**
MgO	**4.21**

D. The Cesium Chloride Structure

Bravais lattice is simple cubic, with two atom basis:

Cs at 0, Cl at $\frac{a}{2}(\hat{x}+\hat{y}+\hat{z})$

Element	a (angstrom)
CsCl	**4.12**
CsBr	**4.29**
CsI	**4.57**
TlCl	**3.83**

E. Zincblende Structure

The diamond structure can be described as an FCC Bravais lattice with a 2 atom basis

Zn at 0, Sulfur at $\frac{a}{4}(\hat{x}+\hat{y}+\hat{z})$

Element	a (angstrom)
GaAs	**5.65**
GaP	**5.45**
InP	**5.87**
ZnSe	**5.67**

The Reciprocal Lattice

The set of vectors K which satisfy the relation:

$$e^{i\vec{K}\cdot\vec{R}} = 1$$

where R is the set of Bravais lattice vectors.

The following is a prescription for finding the reciprocal lattice vectors:

$$\vec{b}_1 = 2p\,\frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot \left(\vec{a}_2 \times \vec{a}_3\right)}$$

$$\vec{b}_2 = 2p\,\frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot \left(\vec{a}_2 \times \vec{a}_3\right)}$$

$$\vec{b}_3 = 2p\,\frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot \left(\vec{a}_2 \times \vec{a}_3\right)}$$

The reciprocal lattice is a Bravais lattice with b's being the primitive lattice vectors.

The volume of the reciprocal lattice primitive cell is:

$$\frac{\left(2p\right)^3}{v}$$

First Brillouin Zone

The Wigner Seitz cell of the reciprocal lattice is called the First Brillouin zone.

Bloch's Theorem (draw a periodic potential):

The eigenfunctions of the one-electron Hamiltonian with a periodic potential

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(r)$$

where,

$$V(r+R) = V(r)$$

can be written in the following form:

$$u_{n,k}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} f_{n\vec{k}}(\vec{r})$$

where,

$$f_{n\vec{k}}(\vec{r}+\vec{R}) = f_{n\vec{k}}(\vec{r})$$

another way of stating Bloch's Theorem is:

$$u_{n,k}(\vec{r}+\vec{R}) = e^{i\vec{k}\cdot\vec{R}} u_{n,k}(\vec{r})$$

Proof:

Let us define a discrete translation operator:

$$\hat{T}_d y(x) = y(x+d)$$

one can find eigenfunctions for this operator:

$$\hat{T}_d u(x) = l\,u(x)$$

By inspection the eigenfunctions are:

$$u_k(x) = e^{ikx} f(x)$$

with,

$$f(x+d) = f(x)$$

since,

$$\left[\hat{H}, \hat{T}_d\right] = 0$$

One can find eigenfunctions which are common to the Hamiltonian and the discrete translation operator.

$$u_{n,k}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} f(\vec{r})$$

where,

$$f(\vec{r}+\vec{R}) = f(\vec{r})$$

How do we label our states? What is the conserved quantity in this case?

k is the Bloch wave number (or wave vector, sometimes called the crystal momentum) and represents a conserved quantity associated with the discrete translation symmetry in the crystal. It is related to the eigenvalue of the discrete translation operator in the following way:

$$\hat{T}_d u_{n,k}(x) = e^{ikd} u_{n,k}(x)$$

n is associated with the energy eigenvalue.

$$\hat{H}u_{n,\vec{k}}(x) = E_n u_{n,\vec{k}}(x)$$

Is this conserved quantity identical to the momentum?

$$\frac{\hbar}{i}\frac{\partial}{\partial x}u_{n,\vec{k}}(x) = \frac{\hbar}{i}\frac{\partial}{\partial x}e^{ikx}f(x) = \hbar k e^{ikx}f(x) + e^{ikx}\frac{\hbar}{i}\frac{\partial}{\partial x}f(x) \neq const \times u_{n,\vec{k}}(x)$$