Lecture-1

Introduction & prerequisites are
course structure discussed

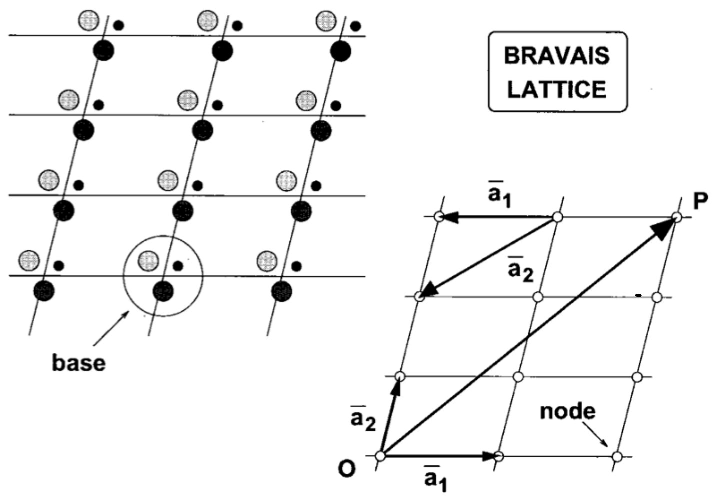
[start - 1:07:00]

Revanth Reddy Pannala
EBIT, Unibo
రేవంత్ రెడ్డి పన్నాల

properties of crystal

Capitolo 20

Proprietà dei cristalli



T. 20.1: Reticolo di Bravais, vettori di traslazione e vettori caratteristici.

→ The first topic we are going to discuss is of CRYSTALS.

The Materials of which semiconductors are made is a crystal.

→ If we look at the figure above we see scheme of a 2 dimentional cross section of a crystal

A crystal by definition is a periodical arrangement of Atoms ~~or~~ group of atoms.

i.e The base in the figure constitutes a group of atoms.

And these group of atoms repeat itself periodically in 3D.

→ The directions in space along which Base is repeated are crystalline directions

∴ The lines in the figure are crystalline directions.

→ First property of the crystals is it's not mandatory that the Crystal line directions in the crystal are mutually orthogonal.

→ It may happen that depending on the structures we may have crystal lines which are angled.

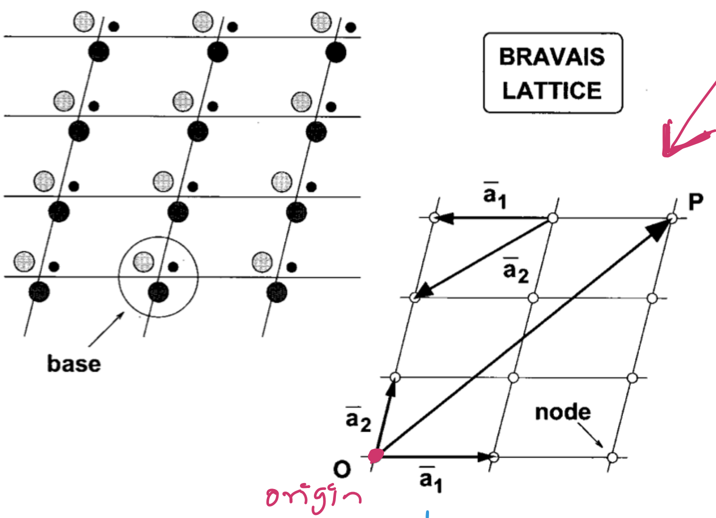
→ The intersection points of Crystalline Directions are called Nodes and then we have offcourse crystalline planes. For instance the plane that is shown in the Figure can be considered as a Crystalline Plane which repeates itself parallelly.

→ It is convenient to associate Geometrical concepts to the physical object that is Crystal.

→ After associating Geometric aspects like crystalline lines, Nodes, planes. we can kind of ignore the atoms and see the

Crystal from a Geometric perspective:

which is clearly illustrated in the figure below on the Rightside.

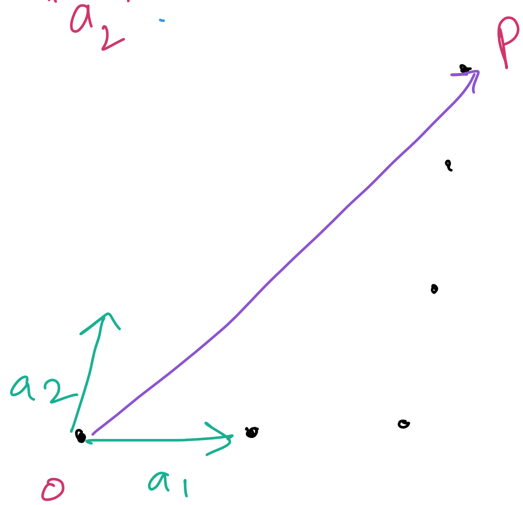


T. 20.1: Reticolo di Bravais, vettori di traslazione e vettori caratteristici.

And from Geometric perspective we assume the Crystal is infinite. and arbitrarily we assume a Node as Origin. "O"

Then we consider another node "P" and the vector that connects "O" & "P" is called $\vec{OP}$ (Translational vector)

→ To reach from "o" to "p" we can go horizontally 2 steps in the direction of "a_1" & 3 steps in the direction of "a_2".



So we have intrinsically defined two vectors that we call a_1, a_2. Such that these two vectors can be combined in the linear combination in which the coefficients are integers.

$$\vec{OP} = 2\vec{a}_1 + 3\vec{a}_2$$

we can see that an linear combination of vectors a_1 & a_2 will allows us to reach any point in the plane.

$\therefore$ a_1, a_2 form a basis in the plane

obviously in 3D we would have an other vector a_3.

$\therefore$ (a_1, a_2, a_3) will be used to describe any translational vector in the crystal

$\therefore$ a_1, a_2, a_3 are called Characteristic vectors of the lattice. In general characteristic vectors are not mutually orthogonal. and the length of the characteristic vectors are not necessarily same.

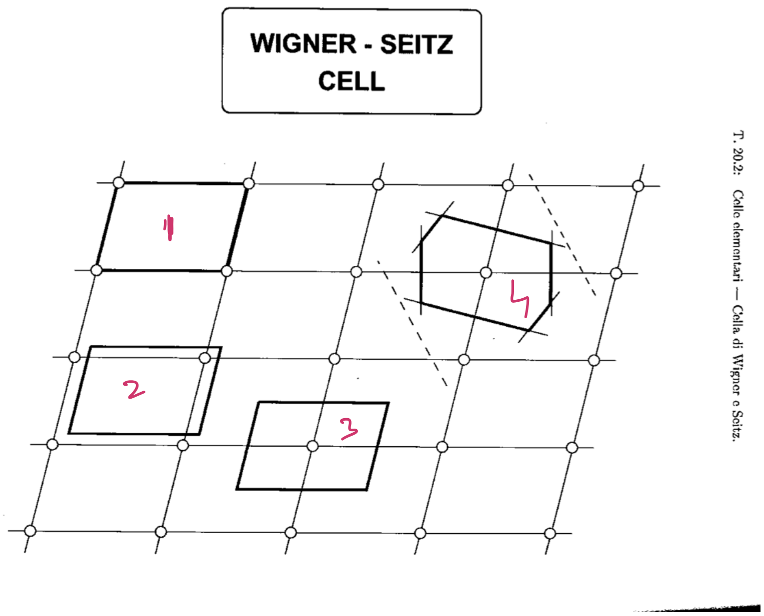
Note:- a_1, a_2, a_3 are Not unit vectors.

& There can be other characteristic vectors which can be defined for the same crystal.

** The Geometrical Representation of crystals is called "Bravis lattice"

The coefficients of the characteristic vectors are Real.

Elementary cell



→ Another concept that is associated to the lattice is the concept of Elementary cell.

→ consider the parallellogram 3 we can say that it is centered along the Node (i.e it is uniquely associated to the Node) & If we replicate it over the whole lattice we will be able to cover the whole lattice.

→ so the parallellogram 3 can be a possible Elementary cell.

→ Elementary cells is also such that it covers the entire lattice.

Similarly 1 & 2 can also be Elementary cells.

→ The strange structure, 4 can also be an Elementary cell. It is also called

"WIGNER-SEITZ CELL".

Q What happens when we have a Finite crystal"?

obviously we will behaving boundaries and it looks like we can nolonger define elementary cell.

In terms of Finite crystal we will consider a Mathematical trick. i.e we assume the crystal is folding at the Boundary. such that Half cell at the top compensates the Halfcell at the Bottom.

(It is a Mathematical Construction)

T. 20.3: Vettori caratteristici del reticolo diretto e di quello reciproco.

Lattice Description

Direct-lattice vectors

$$\boldsymbol{l} = m_1\,\boldsymbol{a}_1 + m_2\,\boldsymbol{a}_2 + m_3\,\boldsymbol{a}_3\,, \qquad \boldsymbol{r} = \mu_1\,\boldsymbol{a}_1 + \mu_2\,\boldsymbol{a}_2 + \mu_3\,\boldsymbol{a}_3$$

Invariant cell-volume (direct lattice)

$$\tau_l = \boldsymbol{a}_1 \bullet \boldsymbol{a}_2 \wedge \boldsymbol{a}_3 = \boldsymbol{a}_2 \bullet \boldsymbol{a}_3 \wedge \boldsymbol{a}_1 = \boldsymbol{a}_3 \bullet \boldsymbol{a}_1 \wedge \boldsymbol{a}_2$$

$$N_c = N_1 N_2 N_3 = \Omega/\tau_l$$

Reciprocal-lattice characteristic vectors

$$\boldsymbol{b}_1 = \boldsymbol{a}_2 \wedge \boldsymbol{a}_3/\tau_l\,, \qquad \boldsymbol{b}_2 = \boldsymbol{a}_3 \wedge \boldsymbol{a}_1/\tau_l\,, \qquad \boldsymbol{b}_3 = \boldsymbol{a}_1 \wedge \boldsymbol{a}_2/\tau_l$$

$$\boldsymbol{a}_i \bullet \boldsymbol{b}_j = \delta_{ij}\,, \qquad \tau_G = \boldsymbol{b}_1 \bullet \boldsymbol{b}_2 \wedge \boldsymbol{b}_3 = \ldots = \boldsymbol{b}_3 \bullet \boldsymbol{b}_1 \wedge \boldsymbol{b}_2 = 1/\tau_l$$

Reciprocal, scaled-lattice vectors

$$\boldsymbol{g} = n_1\,2\pi\boldsymbol{b}_1 + n_2\,2\pi\boldsymbol{b}_2 + n_3\,2\pi\boldsymbol{b}_3\,, \quad \boldsymbol{k} = \nu_1\,2\pi\boldsymbol{b}_1 + \ldots + \nu_3\,2\pi\boldsymbol{b}_3$$

Invariant cell-volume (Brillouin zone)

$$\tau_g = (2\pi)^3\tau_G = (2\pi)^3/\tau_l$$

$$\lambda = m_1 a_1 + m_2 a_2 + m_3 a_3$$

$a_1, a_2, a_3 \Rightarrow$ Characteristic vectors

$\lambda \Rightarrow$ Translational vectors.

→ The volume of the Elementary cell formed by a_1, a_2, a_3 is equal to

$$\boxed{\begin{aligned} \text{volume of cell } T_L &= a_1 \cdot (a_2 \times a_3) = a_2 \cdot (a_3 \times a_1) \\ &= a_3 \cdot (a_1 \times a_2) \end{aligned}}$$

Q: what Happens if we change the form of elementary cell?

Does the volume change?

NO; because all cells are equal to each other ~~ad~~ cells regardless of the form cover completely the volume.

$\therefore$ The volume of the Elementary cell is an invariant property of the lattice.

It does not depend on the form of the cell.

$\therefore$ T_L is same for every cell regardless of form.

In the special case of Finite crystal there's another method to calculated the volume of the Elementary cells.

$$N_C = N_1 N_2 N_3 = \frac{\Omega}{T_L}$$

Ω : Total volume of crystal

N_C = No. of elementary cells

$$\therefore \boxed{T_L = \frac{\Omega}{\text{No. of elementary cells}}}$$

→ to know the value of the No. of cells you just count the No. of cells in all the directions.

$$N_C = N_1 N_2 N_3$$

N_1 = no. of cells in direction 1

N_2 = " " 2

N_3 = " " 3

Reciprocal lattice

→ For every direct lattice, there is a Reciprocal lattice. we must now define it and in order to define it we must define characteristic vectors of new lattice. and we shall call them b_1, b_2, b_3

$$b_1 = a_2 \wedge a_3 / T_L$$

Revanth Reddy Pannala
EBIT, Unibo
రేవంత్ రెడ్డి పన్నాల

$$b_2 = a_3 \wedge a_1 / T_L$$

$\wedge$ = cross product

$$b_3 = a_1 \wedge a_2 / T_L$$

The unit of b_1, b_2, b_3 $\left(1/\text{length}\right)^{\text{cm}}$

$\therefore$ $\boxed{a_i \bullet b_j = \delta_{ij} \text{ (is a pure number)}}$

If $i = j$ The product of $a_i \cdot b_j = 1$

$i \neq j$ The product will be zero

This, defines characteristic vectors b_1, b_2, b_3 of Reciprocal lattice.

& we can also see

$$T_q = b_1 \cdot b_2 \wedge b_3 = b_2 \cdot b_3 \wedge b_1 = b_3 \cdot b_1 \wedge b_2$$

$$= \frac{1}{\tau_L}$$

$$\boxed{T_q = \frac{1}{T_L}}$$

Reciprocal scalled lattice

$$g = n_1 2\pi\, b_1 + n_2 2\pi\, b_2 + n_3 2\pi\, b_3$$

$n_1, n_2, n_3 \longrightarrow$ integer coefficients

$$\boxed{T_g = (2\pi)^3 T_q = (2\pi)^3 / T_L}$$

Invariant cell volume Brillouin zone

→ The weigner-zeit cell of Reciprocal
** scaled lattice is very important and in particular weigner-zeit cell that is centered at origin. and it has got a special name called Brillouin Zone.

Q. Why do we need Reciprocal lattice? & Reciprocal scalled lattice?

The reason is simple, we will be considering periodic structures, the physical properties of these structures will also be periodic. So, when you want to describe periodic functions mathematically it's very convenient to use Fourier series or Fourier transform and Fourier transform will bring one space into another.

→ Fourier Transform

Time $\longrightarrow$ Angular Frequence (ω)

(t)

$$2\pi f = \frac{2\pi}{t}$$

→ But in our case we have periodic structures as functions of SPACE not in Time.

So we shall do F.T in space.

(To be continued)

Revanth Reddy Pannala
EBIT, Unibo
రేవంత్ రెడ్డి పన్నాల