STRUKTUR KRISTAL

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2D Unit Cell example -(NaCl)

We define **lattice points**; these are points with **identical environments**
Choice of origin is arbitrary - lattice points need not be atoms - but **unit cell size should always be the same**.
This is also a unit cell - it doesn’t matter if you start from Na or Cl
- or if you don’t start from an atom
This is **NOT** a unit cell even though they are all the same - empty space is not allowed!
Unit Cell in 3D
Three common Unit Cells in 3D

- Simple cubic
- Body-centered cubic
- Face-centered cubic
Unit Cell in 3D

Crystal Structure
Cara menentukan sel primitif

Diagram:

1. C.P (Cahaya Pada)
2. Bukan C.P

Diagram menunjukkan konsep pembentukan sel primitif dari titik-titik yang diberi tanda C.P dan tidak diberi tanda (Bukan C.P).
Primitive Unit Cell

- **A primitive cell or primitive unit cell** is a volume of space that when translated through all the vectors in a Bravais lattice just fills all of space without either overlapping itself or leaving voids.

- A primitive cell must contain precisely one lattice point.
Solids consist of atoms or molecules executing thermal motion about an equilibrium position fixed at a point in space.

Solids can take the form of crystalline, polycrystalline, or amorphous materials.

Solids (at a given temperature, pressure, and volume) have stronger bonds between molecules and atoms than liquids.

Solids require more energy to break the bonds.
Primitive Unit Cell and vectors

- A primitive unit cell is made of primitive translation vectors $a_1$, $a_2$, and $a_3$ such that there is no cell of smaller volume that can be used as a building block for crystal structures.

- A primitive unit cell will fill space by repetition of suitable crystal translation vectors. This defined by the parallelepiped $a_1$, $a_2$ and $a_3$. The volume of a primitive unit cell can be found by

\[ V = a_1 \cdot (a_2 \times a_3) \quad \text{(vector products)} \]

Cubic cell volume $= a^3$
Primitive Unit Cell

- The **primitive unit cell** must have only one lattice point.
- There can be **different choices** for lattice vectors, but the volumes of these primitive cells are all the same.

P = Primitive Unit Cell
NP = Non-Primitive Unit Cell
Wigner-Seitz Method

A simply way to find the primitive cell which is called Wigner-Seitz cell can be done as follows;

1. Choose a lattice point.
2. Draw lines to connect these lattice point to its neighbours.
3. At the mid-point and normal to these lines draw new lines.

The volume enclosed is called as a Wigner-Seitz cell.
Wigner-Seitz Cell - 3D

- f.c.c Wigner-Seitz cell
- b.c.c Wigner-Seitz cell
Fundamental Types of Lattices

- Crystal lattices can be mapped into themselves by the lattice translations $T$ and by various other symmetry operations.
- A typical symmetry operation is that of rotation about an axis that passes through a lattice point. Allowed rotations of: $2\pi, \frac{2\pi}{2}, \frac{2\pi}{3}, \frac{2\pi}{4}, \frac{2\pi}{6}$
- (Note: lattices do not have rotation axes for $\frac{1}{5}, \frac{1}{7} ...$ times $2\pi$)
Crystal Lattice

Bravais Lattice (BL)
- All atoms are of the same kind
- All lattice points are equivalent

Non-Bravais Lattice (non-BL)
- Atoms can be of different kind
- Some lattice points are not equivalent
- A combination of two or more BL
UNIT CELL

Primitive

- Single lattice point per cell
- Smallest area in 2D, or
- Smallest volume in 3D

Simple cubic (sc)

Conventional & Non-primitive

- More than one lattice point per cell
- Integral multiples of the area of primitive cell

Body centered cubic (bcc)
The Conventional Unit Cell

- A unit cell just fills space when translated through a subset of Bravais lattice vectors.
- The **conventional unit cell** is chosen to be larger than the primitive cell, but with the **full symmetry** of the Bravais lattice.
- The size of the conventional cell is given by the lattice constant $a$. 

*FCC Bravais lattice*
sel konvensional (sel tak primitif) adalah sel yang mempunyai luas atau volume bukan terkecil artinya mempunyai luas atau volume yang besarnya merupakan kelipatan sel primitif.

Gambar sel konvensional
Primitive and conventional cells of FCC

A primitive unit cell  a conventional unit cell

primitive vectors

\[ \vec{a}_1 = \frac{a}{2}(\hat{x} + \hat{y}), \]
\[ \vec{a}_2 = \frac{a}{2}(\hat{y} + \hat{z}), \]
\[ \vec{a}_3 = \frac{a}{2}(\hat{z} + \hat{x}). \]
What is a crystal lattice?

In crystallography, only the geometrical properties of the crystal are of interest, therefore one replaces each atom by a geometrical point located at the equilibrium position of that atom.
Primitive and conventional cells of BCC

Primitive Translation Vectors:

\[ \vec{a}_1 = \frac{1}{2}(\hat{x} + \hat{y} - \hat{z}) \]

\[ \vec{a}_2 = \frac{1}{2}(-\hat{x} + \hat{y} + \hat{z}) \]

\[ \vec{a}_3 = \frac{1}{2}(\hat{x} - \hat{y} + \hat{z}) \]
Primitive and conventional cells

Body centered cubic (bcc):
conventional ≠ primitive cell

Fractional coordinates of lattice points in conventional cell:
000, 100, 010, 001, 110, 101, 011, 111, ½ ½ ½

Simple cubic (sc):
primitive cell = conventional cell

Fractional coordinates of lattice points:
000, 100, 010, 001, 110, 101, 011, 111
Primitive and conventional cells

Body centered cubic (bcc):
primitive (rombohedron) ≠ conventional cell

Fractional coordinates:
000, 100, 101, 110, 110, 101, 011, 211, 200

Face centered cubic (fcc):
conventional ≠ primitive cell

Fractional coordinates:
000, 100, 010, 001, 110, 101, 011, 111, ½ ½ 0, ½ 0 ½, 0 ½ ½, ½ ½ ½, 1 ½ ½, ½ ½ 1
Primitive and conventional cells-hcp

Hexagonal close packed cell (hcp): *conventional* = primitive cell

**Fractional coordinates:**
100, 010, 110, 101,011, 111,000, 001
Unit Cell

- The unit cell and, consequently, the entire lattice, is uniquely determined by the six lattice constants: a, b, c, α, β and γ.
- Only 1/8 of each lattice point in a unit cell can actually be assigned to that cell.
- Each unit cell in the figure can be associated with $8 \times \frac{1}{8} = 1$ lattice point.
**Coordination Number**

- **Coordination Number (CN):** The Bravais lattice points closest to a given point are the nearest neighbours.

- Because the Bravais lattice is periodic, all points have the same number of nearest neighbours or coordination number. It is a property of the lattice.

- A simple cubic has coordination number 6; a body-centered cubic lattice, 8; and a face-centered cubic lattice, 12.
Didalam kristal terdapat kisi-kisi yang ekivalen yang sesuai dengan lingkungannya dan diklasifikasikan menurut simetri translasi. Operasi translasi kisi didefinisikan sebagai perpindahan dari sebuah kristal oleh sebuah vektor translasi kristal, maka persamaannya

\[ \vec{T} = u_1 \vec{a}_1 + u_2 \vec{a}_2 + u_3 \vec{a}_3 \]

Dimana \( u_1, u_2, u_3 \) = bilangan bulat.
- \( a_1, a_2, a_3 \) = vektor translasi primitive
- \( \approx \) sumbu-sumbu kristal
Operasi Translasi Kisi:
Perpindahan dari sebuah kristal oleh sebuah vektor translasi kristal

\[ \vec{T} = u_1 \vec{a}_1 + u_2 \vec{a}_2 + u_3 \vec{a}_3 \]

Keterangan:
\[ \vec{T} \] = vektor translasi kristal
\[ u \] = Bilangan bulat
\[ \vec{a} \] = vektor translasi primitif/sumbu-sumbu kristal
Contoh Operasi Translasi Kisi
Untuk $\overrightarrow{T_1}$

$\overrightarrow{T_1} = u_1 \hat{a_1} + u_2 \hat{a_2} + u_3 \hat{a_3}$

$\overrightarrow{T_1} = -3 \hat{a_1} + 2 \hat{a_2} + 0 \hat{a_3}$

$\overrightarrow{T_1} = -3 \hat{a_1} + 2 \hat{a_2}$

Jadi:

$u_1 = -3$ dan $u_2 = 2$

Untuk $\overrightarrow{T_2}$

$\overrightarrow{T_2} = u_1 \hat{a_1} + u_2 \hat{a_2} + u_3 \hat{a_3}$

$\overrightarrow{T_1} = -1,5 \hat{a_1} + 1,5 \hat{a_2} + 0 \hat{a_3}$

$\overrightarrow{T_1} = -1,5 \hat{a_1} + 1,5 \hat{a_2}$

Jadi:

$u_1 = -1,5$ dan $u_2 = 1,5$

$\overrightarrow{T_1}$: vektor translasi (bilangan bulat)

$\overrightarrow{T_2}$: bukan vektor translasi (bukan bilangan bulat)
Posisi dari sebuah pusat atom \( j \) dari sebuah basis relatif terhadap titik lattice dimana basis diletakkan adalah:

\[
\vec{r}_j = x_j \vec{a}_1 + y_j \vec{a}_2 + z_j \vec{a}_3
\]

Dimana: \( 0 \leq x_j, y_j, z_j \leq 1 \)
The smallest component of the crystal (group of atoms, ions or molecules), which when stacked together with pure translational repetition reproduces the whole crystal.