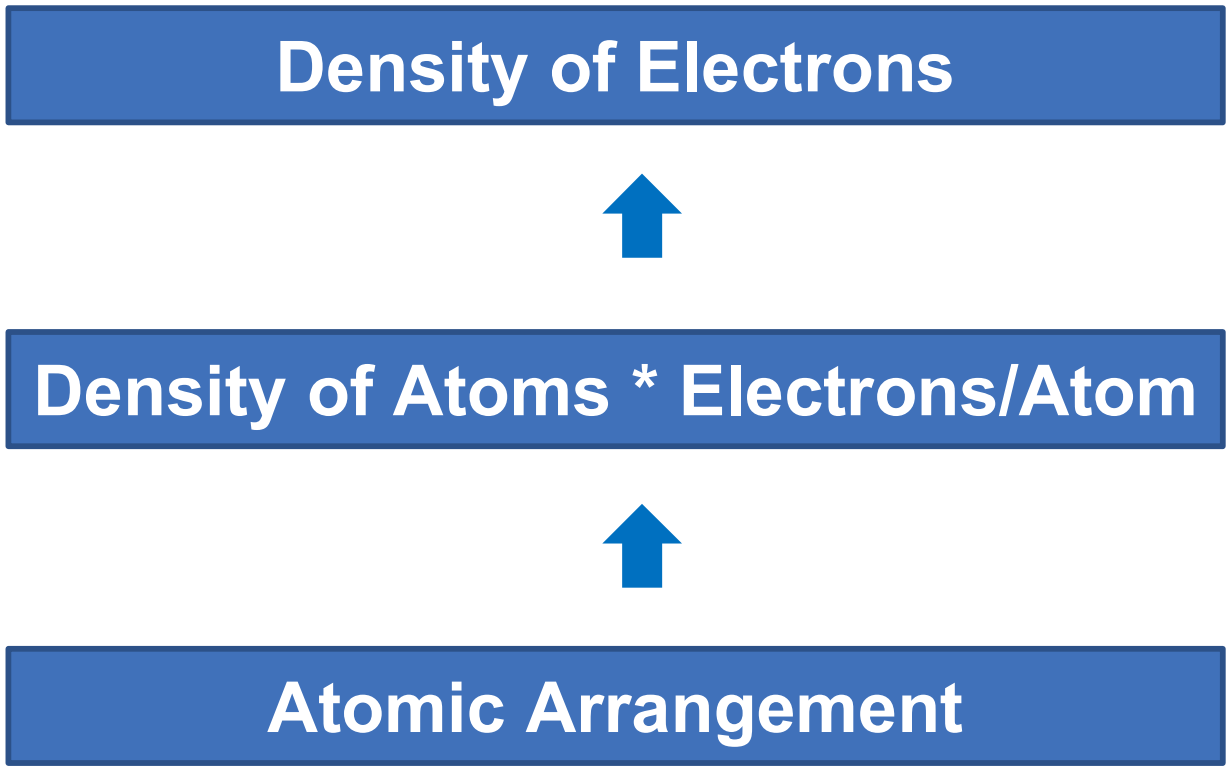
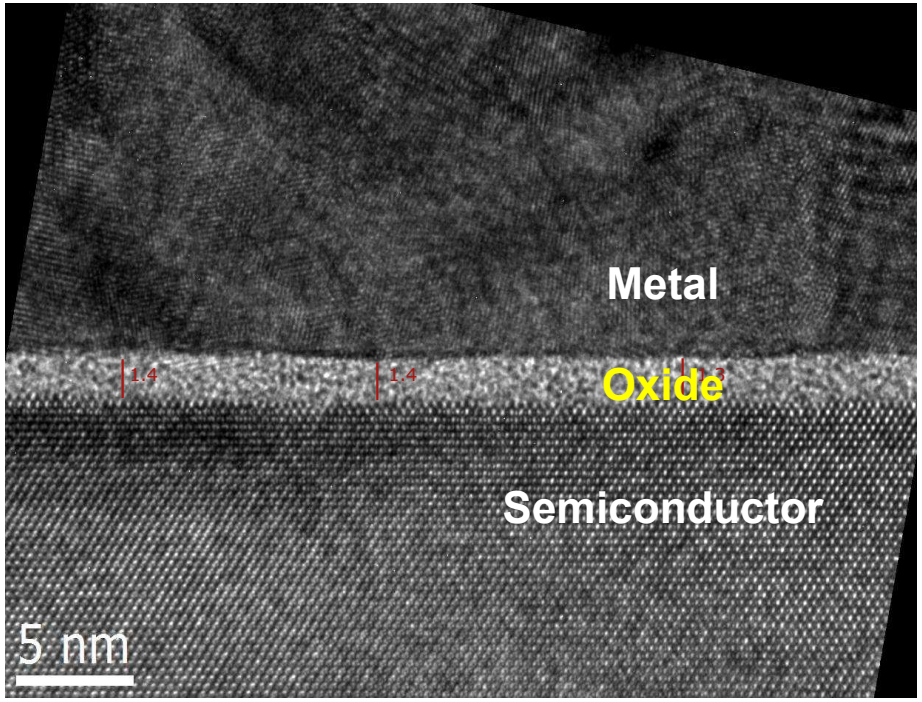
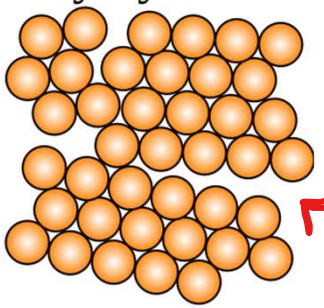
Crystal Structure – why?



Atomic Arrangements



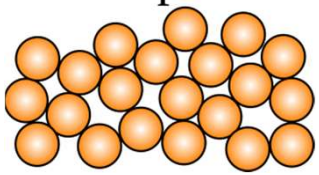
Polycrystalline



grain boundaries

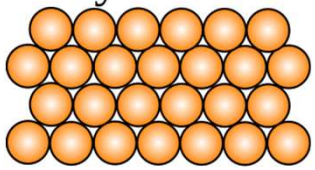
Steel, Aluminum, Brass, SiC, AlO, Polycrystalline silicon (used in

Amorphous



Glass, Polyethylene, Amorphous Silicon

Crystalline



Cu. GaAs. SiO. NaCl

www.nanohub.org

Cu. GaAs. SiO.

Crystal Lattice

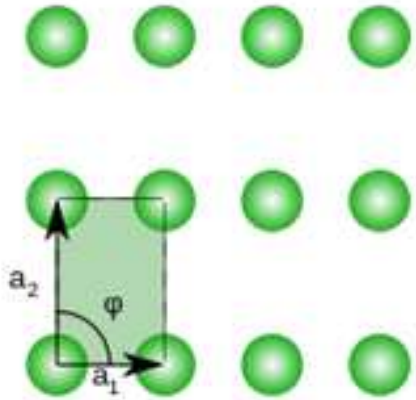
Lattice: Regular, repeated arrangement of points

French physicist Auguste Bravais, who identified that there are 14 unique lattice types in three-dimensional space

***Bravais Lattice*: looks the same from every lattice point**

Including distance and angle.

Infinite, Periodic



Primitive vectors

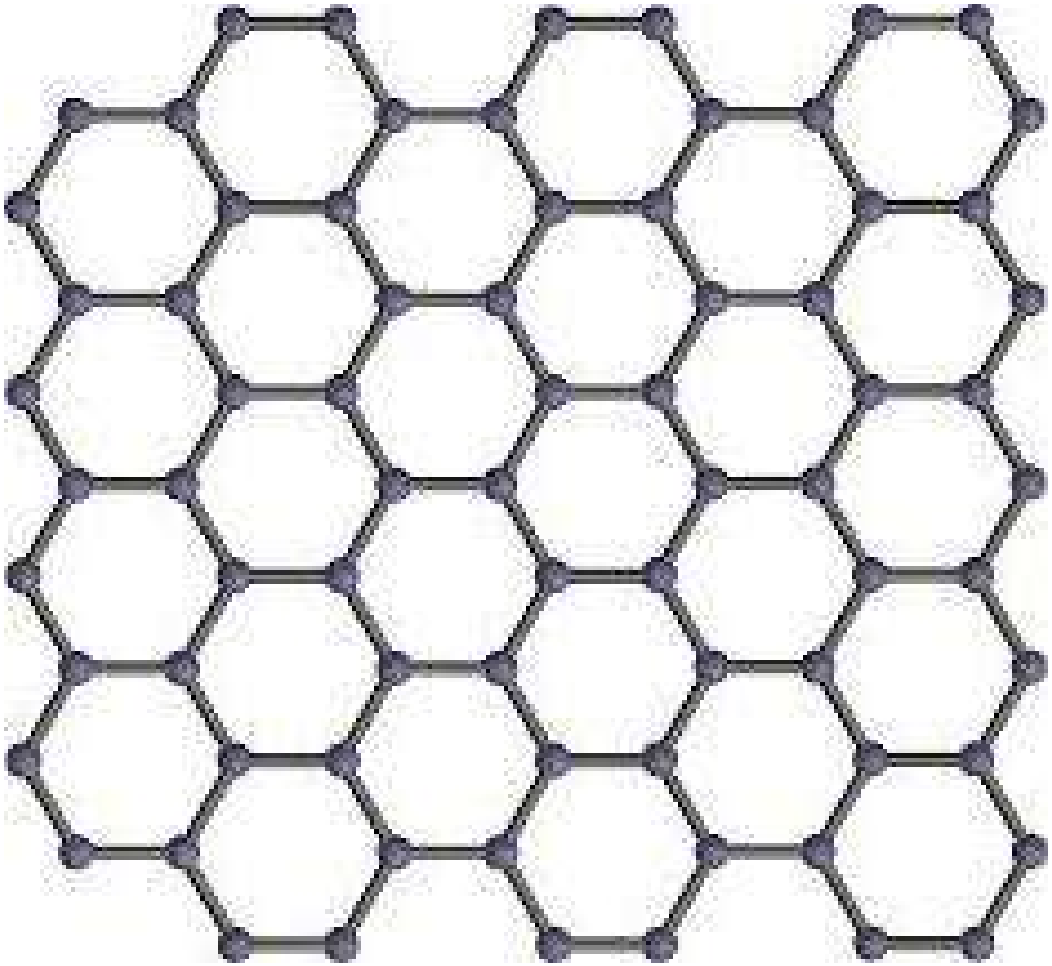
Lattice vector

***Bravais Lattice*: can be generated by**

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

en.wikipedia.org (Prolineserver)

Bravais?

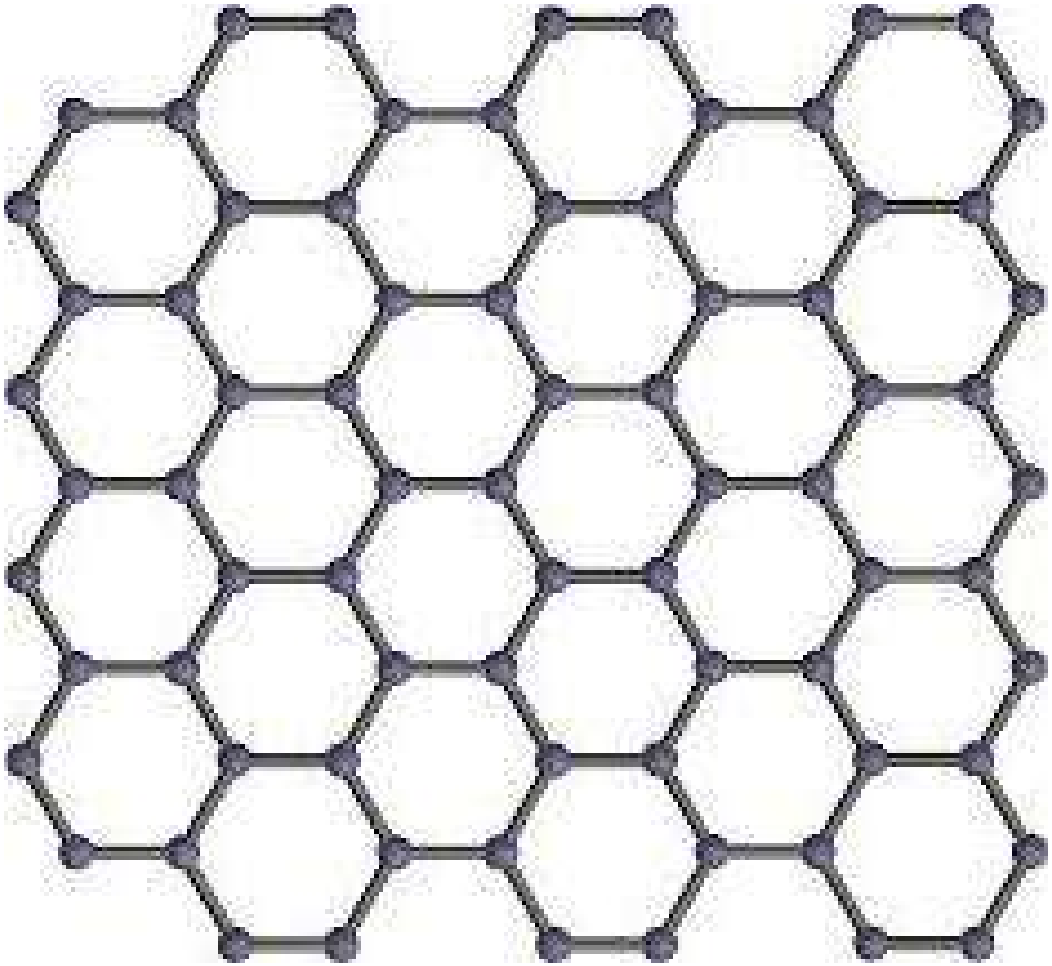


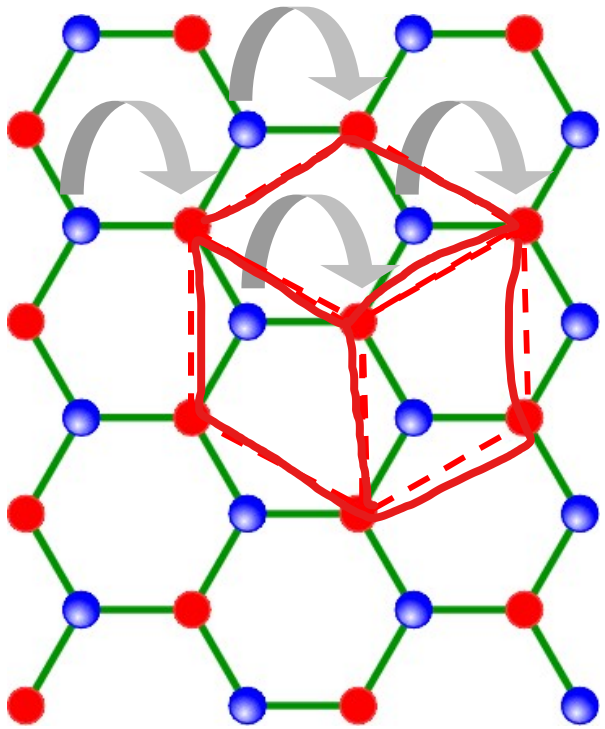
Not a Bravais Lattice because each lattice point doesn't follow the same ordering and orientation

Not Bravais

Basis

We can convert a non-Bravais Lattice into a Bravais Lattice by changing the type of lattice points i.e. making similar configurations associated with a single type of entity and other similar lattice points associated with another type of entity. Example - done below.





Body Centered Hexagonal Lattice

Not Bravais

Bravais (hexagonal) with a basis of two

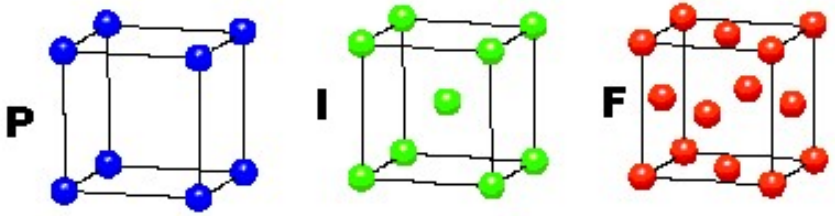
Bravais Lattice Classification – 3D

Learn the Mnemonic to remember them.

CUBIC

$a = b = c$

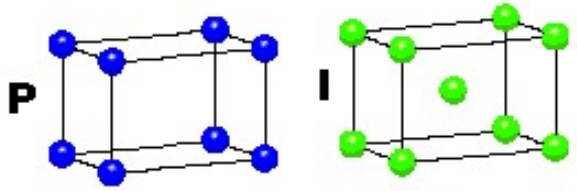
$\alpha = \beta = \gamma = 90°$



TETRAGONAL

$a = b \neq c$

$\alpha = \beta = \gamma = 90°$

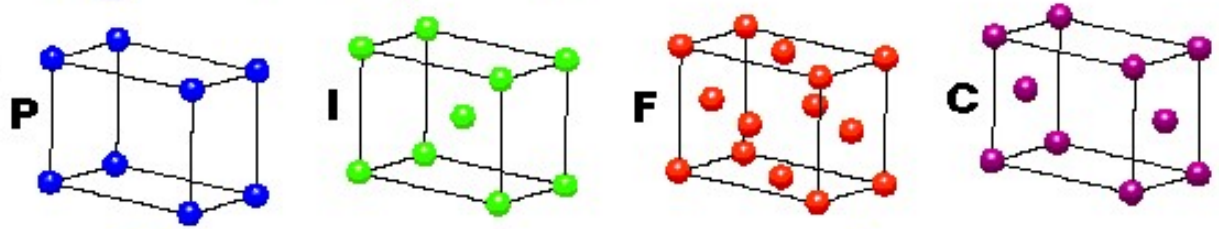


?

ORTHORHOMBIC

$a \neq b \neq c$

$\alpha = \beta = \gamma = 90°$

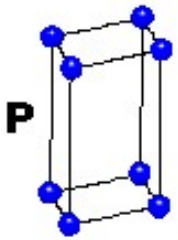


HEXAGONAL

$a = b \neq c$

$\alpha = \beta = 90°$

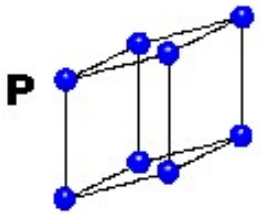
$\gamma = 120°$



TRIGONAL

$a = b = c$

$\alpha = \beta = \gamma \neq 90°$

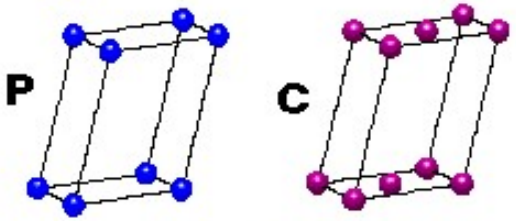


MONOCLINIC

$a \neq b \neq c$

$\alpha = \gamma = 90°$

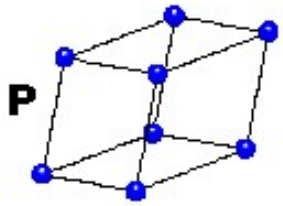
$\beta \neq 120°$



TRICLINIC

$a \neq b \neq c$

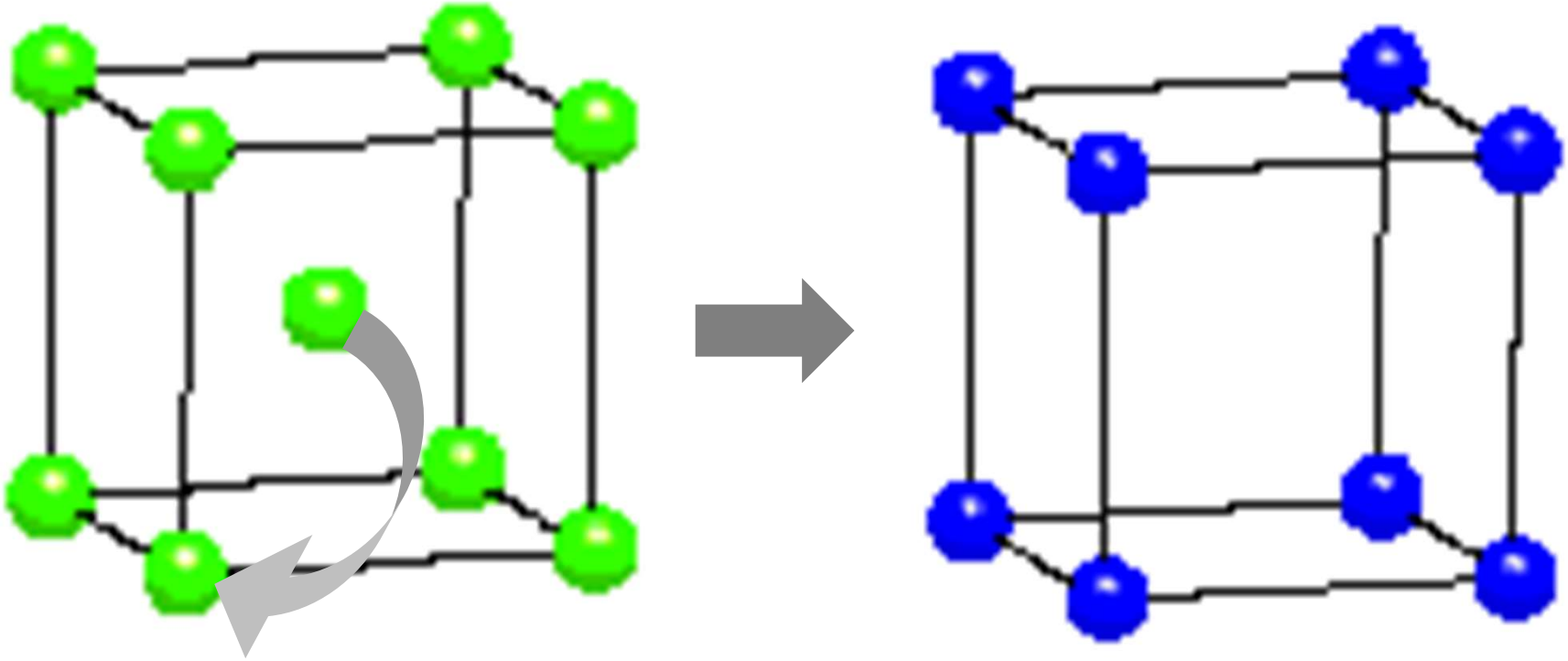
$\alpha \neq \beta \neq \gamma \neq 90°$



4 Types of Unit Cell
P = Primitive
I = Body-Centred
F = Face-Centred
C = Side-Centred
+
7 Crystal Classes
→ 14 Bravais Lattices

Basis (3D)

Changing the position of the Body Centered lattice point to one of the corners will again in turn form another Bravais lattice. This occurs for the whole crystal with the same effects.

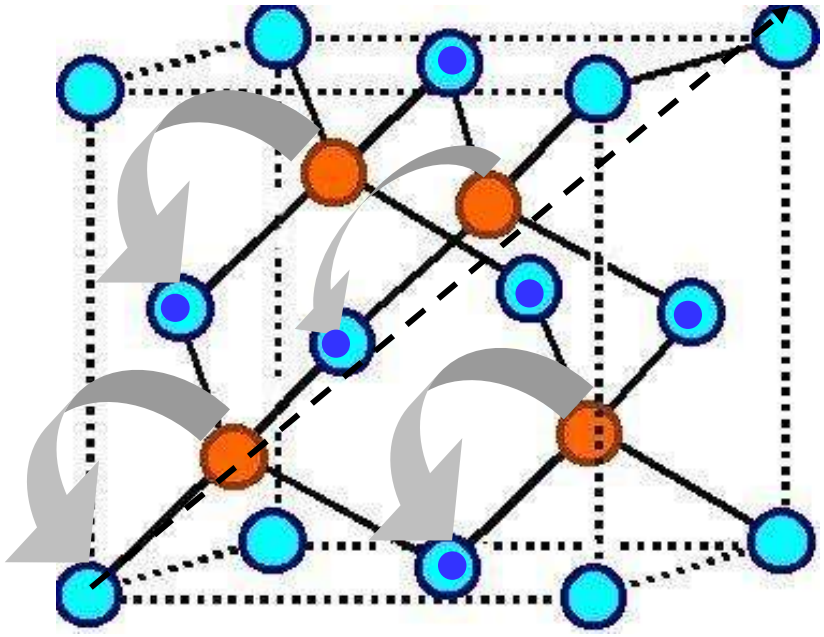


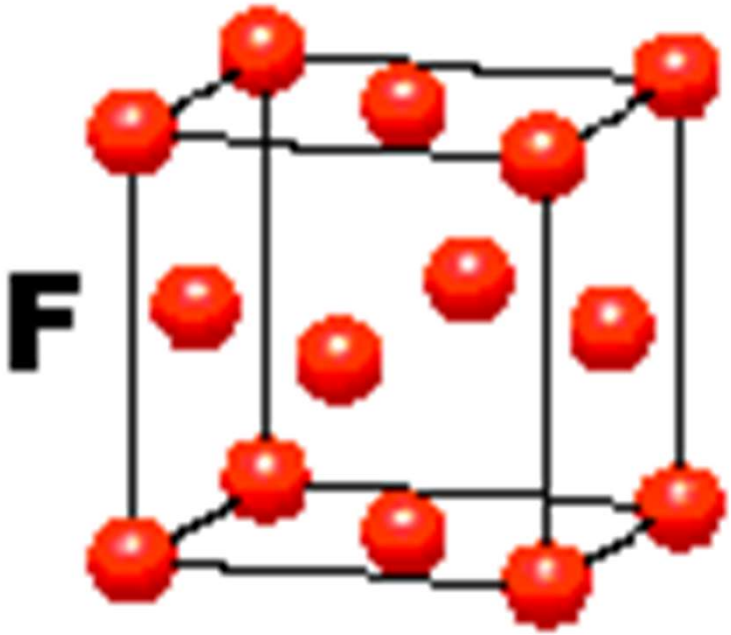
Bravais (BCC)

Bravais (cubic) with a basis of two

Basis (3D)

1 amu = 1.66054e-27 kgs





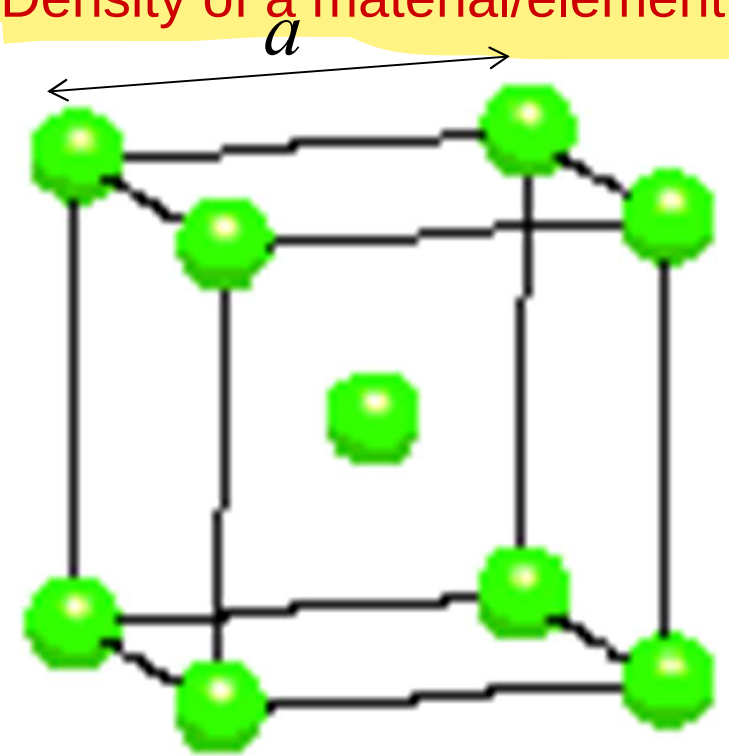
Non-Bravais: Zinc-blende (GaAs), Diamond (Si, Ge)

Bravais (FCC) with a basis of two

Atomic density (volume)

$$\text{Atomic density} = \frac{\text{Effective number of atoms in unit cell}}{\text{Volume of unit cell}}$$

Density of a material/element = mass of one atom (gms) * atomic density (/m3)



Atoms in unit cell: $8 \times 1/8 + 1 = 2$

Vol. of unit cell: a^3

Atomic density: $2/a^3$

(8.6 x 10^22) * 55.845 * (1.6605 x 10^-27) * 10^6 = 7974.8335 kg/m3

For BCC Fe
Lattice constant a = 2.856Å

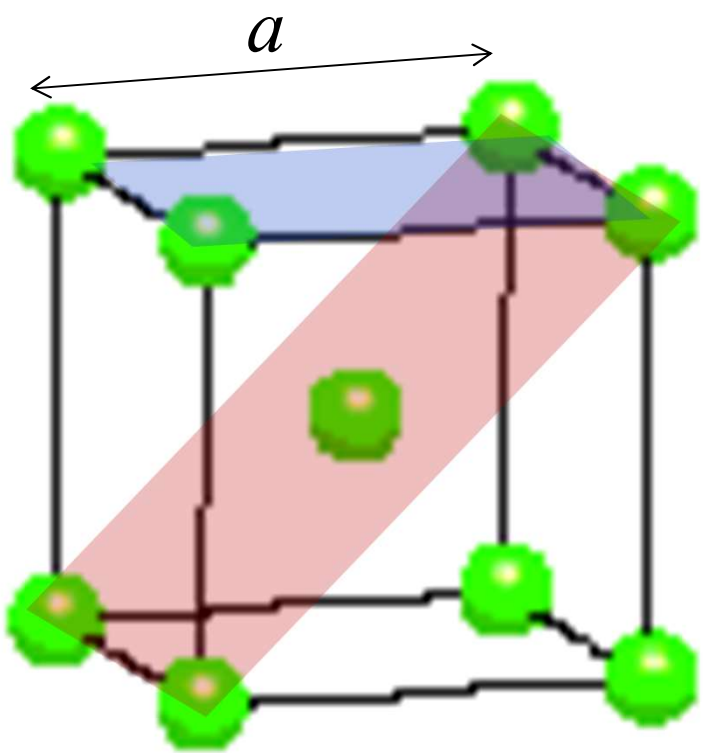
Relative atomic mass = 55.845

Atomic density = 8.6 x 10^{22} cm^{-3}

Calculate the density of Fe; look up its value on the web.

Atomic density (surface)

$$\text{Atomic density} = \frac{\text{Effective number of atoms on 'unit surface'}}{\text{Area of 'unit surface'}}$$



Atoms on 'pink surface' element: $4 \times 1/4 + 1 = 2$

Area of 'pink surface' element: $\sqrt{2}a^2$

Atomic density on 'pink surface': $\sqrt{2}/a^2$

BCC Fe: a = 2.856Å

Atomic density = 1.7×10^{15} cm^{-2}

(i) What is the atomic density for BCC Fe on the 'blue surface'?

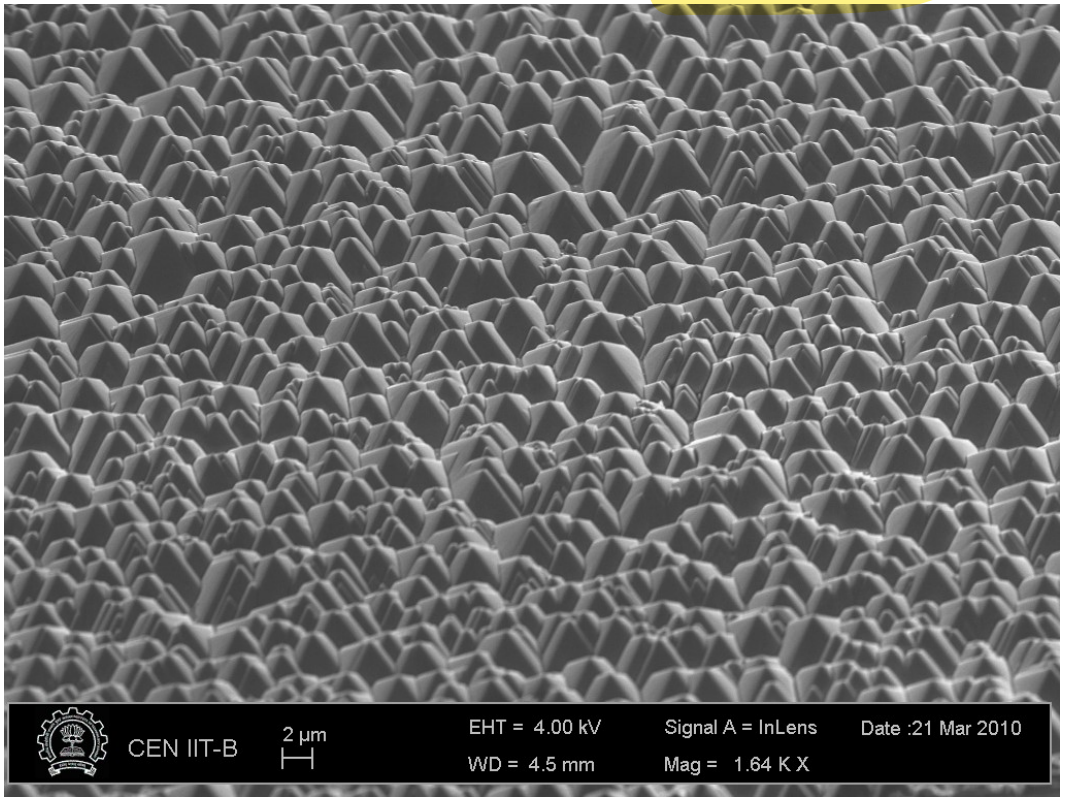
(ii) Will these calculations hold for the *actual* surface of the solid?

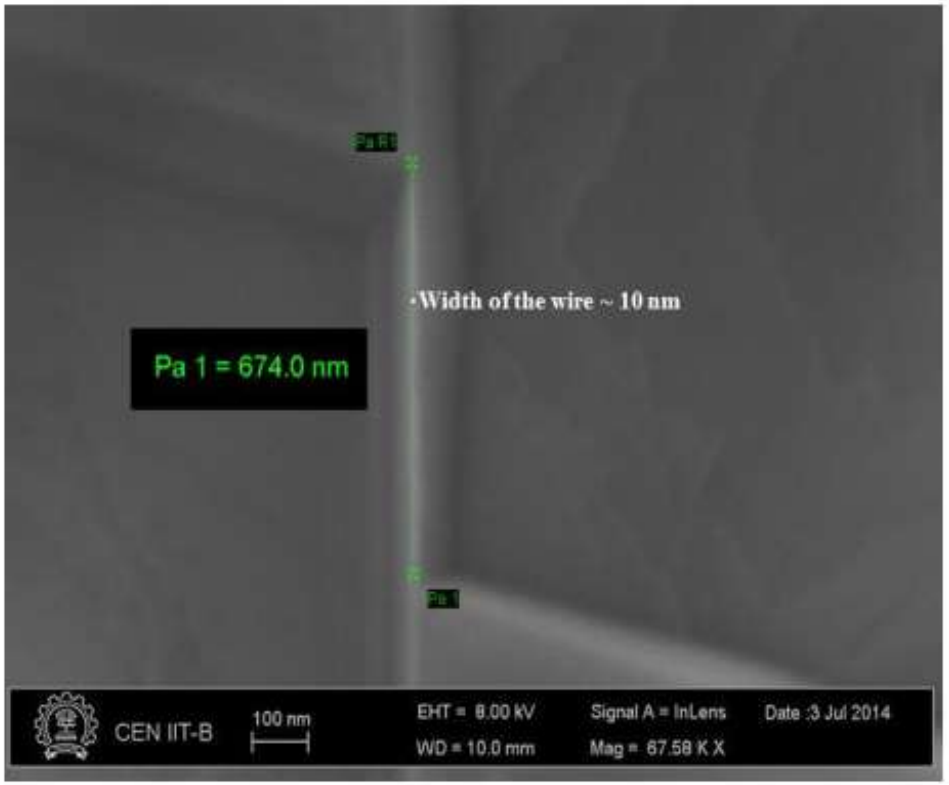
Anisotropic etching is a process used in microfabrication and nanofabrication to selectively remove material from a substrate, where the etch rate depends on the crystallographic orientation of the material. This leads to a highly directional etch, creating well-defined structures with sharp, precise geometries.

Atomic density (surface)

Anisotropic Etching

Anisotropic = Unidirectional and Isotropic = Uniform in all directions





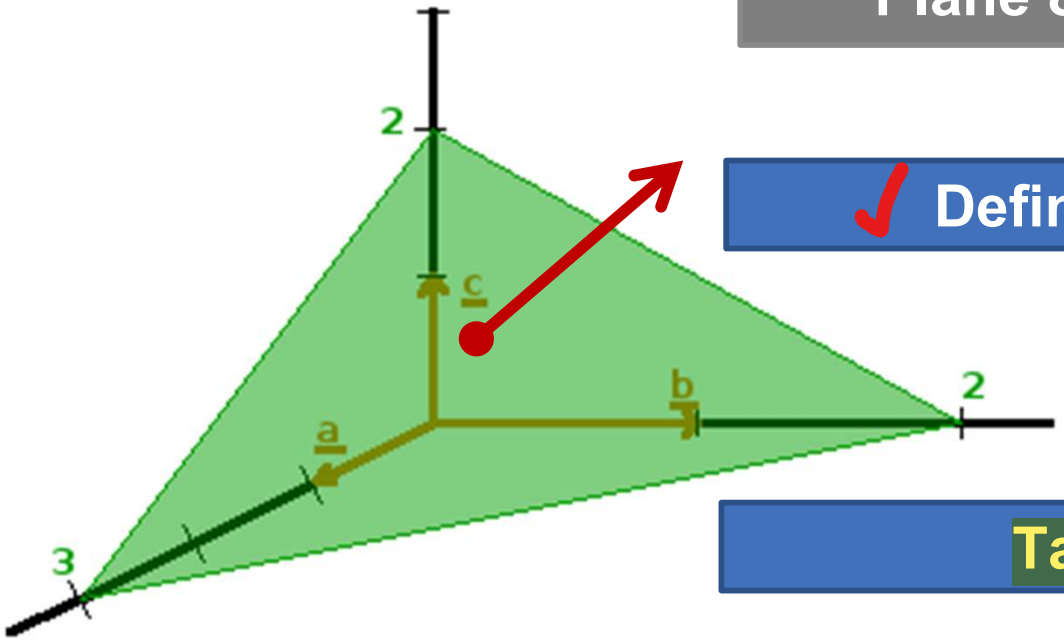
Solar cell surface texturing

III-nitride quantum wire

Benefits: Reduces Reflection of Light, Increases Light Absorption, Enhances Photon Collection, Facilitates Anti-Reflective Coatings

Why does the surface of a solar cell *need to be* rough?

Naming planes & directions: Miller Indices



Plane & Direction (perpendicular to it)

✓ Define axes along unit cell edges

Take *normalized* intercepts ✓

Form ordered triplet: (3,2,2) ✓

Negative numbers:
(-a b c) → (ā b c)

Invert and rationalize (1/3,1/2,1/2) → (2 3 3) ✓ ✓

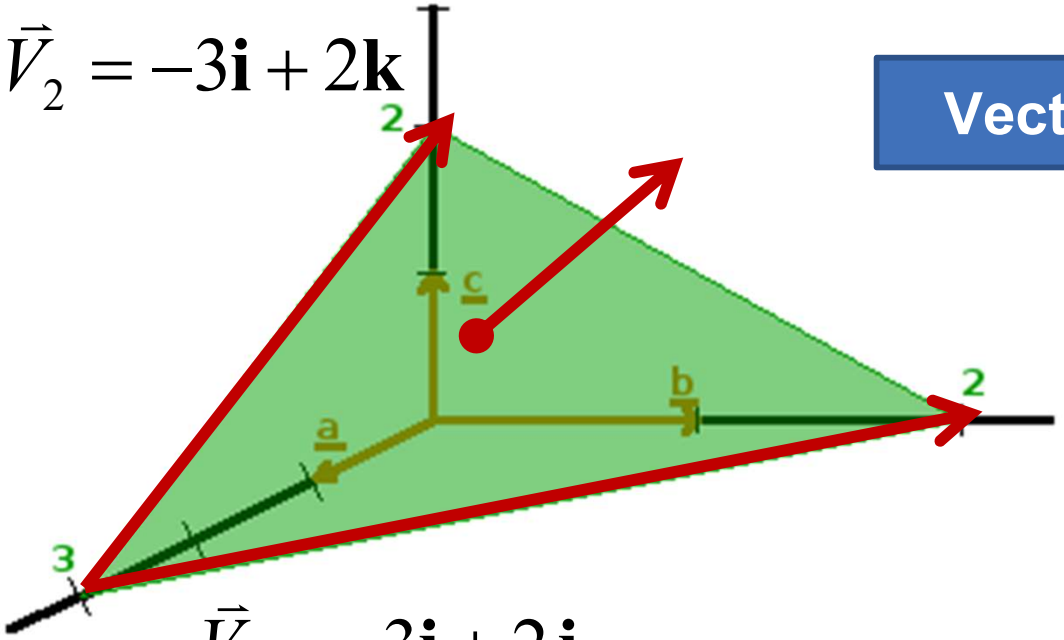
Rationalize --> Denominator = 1

Plane || to Z: (a b 0)

MI for plane: (2 3 3)

MI for direction: [2 3 3]

Naming planes & directions: Miller Indices



$\vec{V}_2 = -3\mathbf{i} + 2\mathbf{k}$

$\vec{V}_1 = -3\mathbf{i} + 2\mathbf{j}$

Vector normal to V_1, V_2 plane: V_1 x V_2

$$\vec{V}_1 \times \vec{V}_2 = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ -3 & 2 & 0 \\ -3 & 0 & 2 \end{vmatrix} = 4\mathbf{i} + 6\mathbf{j} + 6\mathbf{k} \rightarrow [233]$$

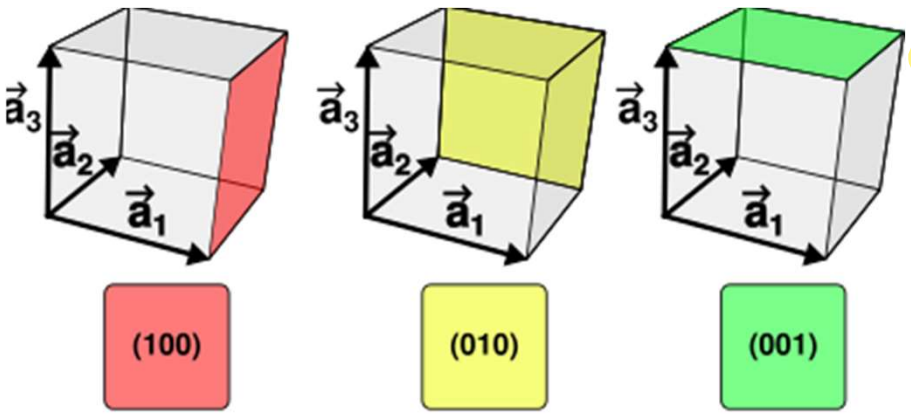
MI for direction: [2 3 3]

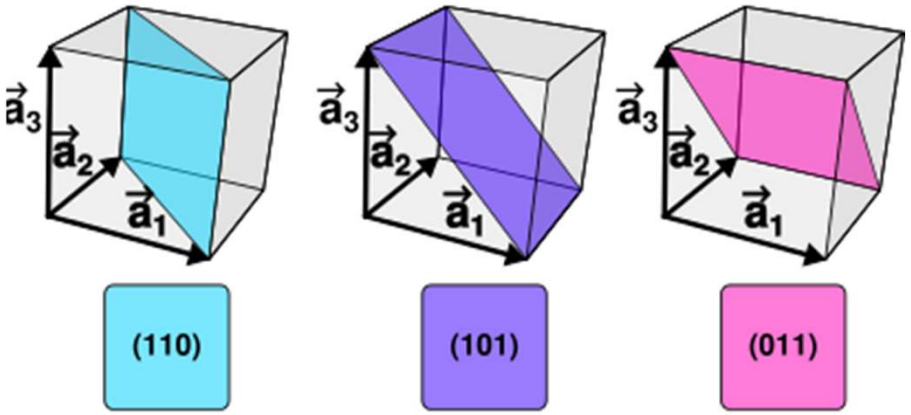
Miller Indices for cubic crystal

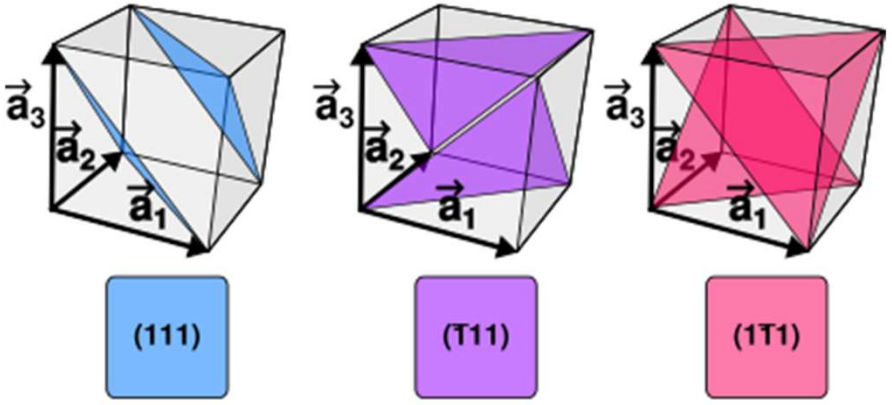
Miller Indices consisting of only 1s and 0s will be the same as the direction triplet (normalized intercepts) because they are already Inverted and Rationalized.

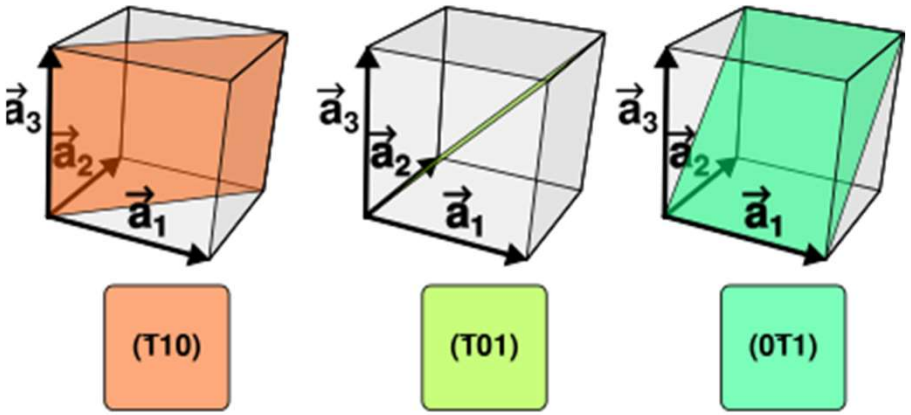
Can you construct MI for hexagonal crystal?

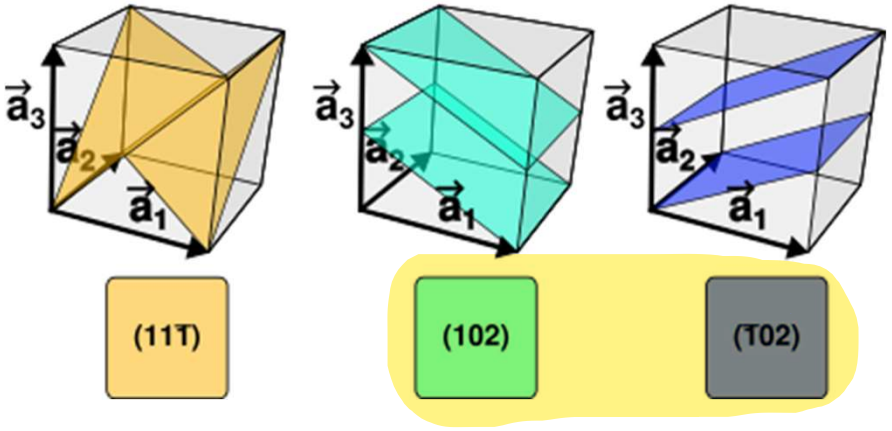
Other than 0s and 1s will have to be Inverted and Rationalized.











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Artwork Sources:

1. www.myscienceacademy.org
2. home.iitk.ac.in
3. www2.latech.edu
4. www.tf.uni-kiel-de
5. users.aber.ac.uk
6. www.flickriver.com
7. commons.wikimedia.org