Section 3 – Crystals

3.4 Surfaces, Miller Index

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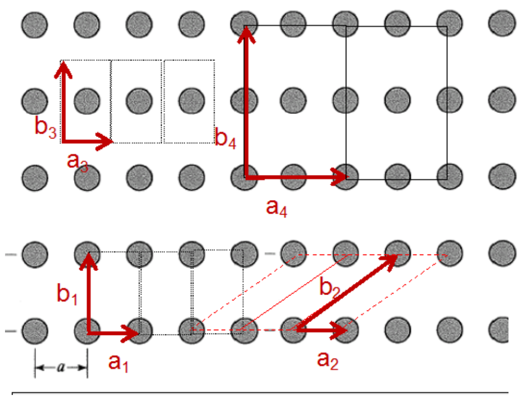
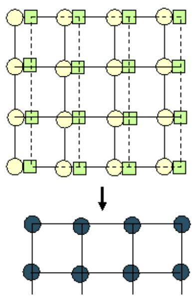
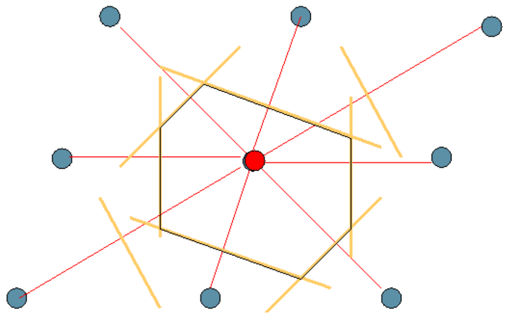
Section 3
Crystals

One Video Segment

- 3.1 Crystal definitions
  - » One-dimensional Crystals – simple primitive cell
  - » Unit cells of a Periodic 2D Lattice
  - » Bravais lattice
  - » Bravais lattice with a basis
  - » Non-periodic repeated cells
  - » Definition of ONE Primitive Cell – Wigner-Seitz Cell







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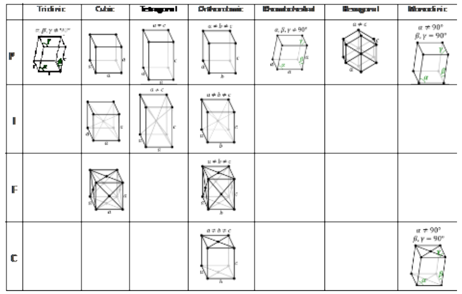
- 3.2 Tables of Bravais Lattices
  - » Bravais Lattices in 2D (5 types)
  - » Bravais Lattices in 3D (14 types)
  - » 3 Dominant Bravais Lattices in Nature



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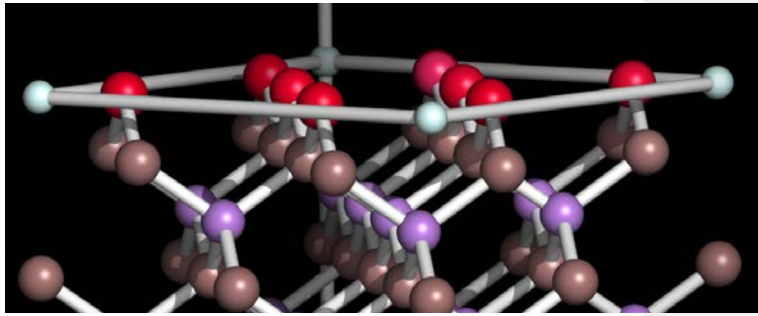
- 3.3 Density Definitions and Applications to Common Materials
  - » Number, Packing, and Areal Density
  - » Common Crystals – Non-Primitive Unit Cells (NaCl, GaAs, CdS)



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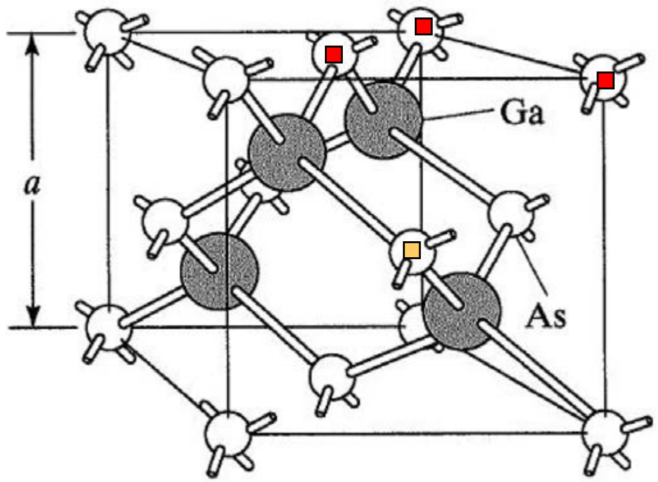
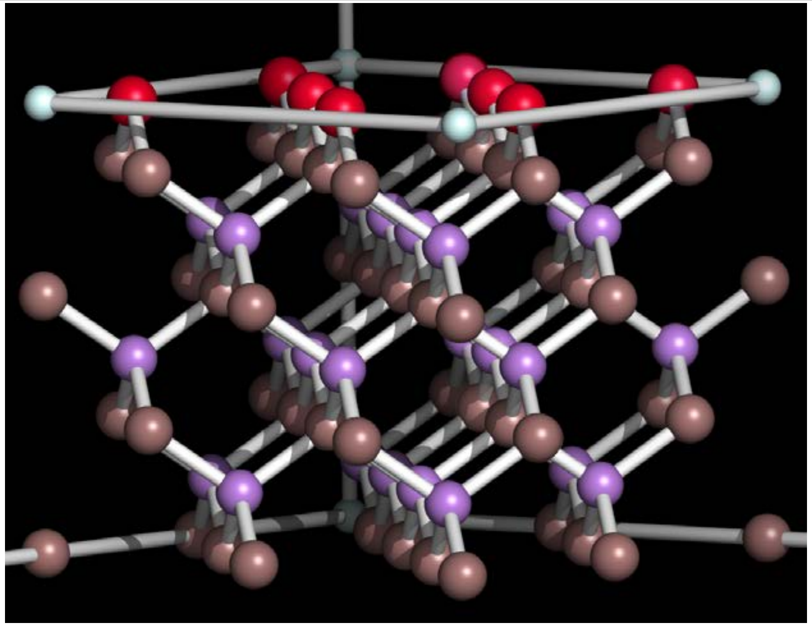
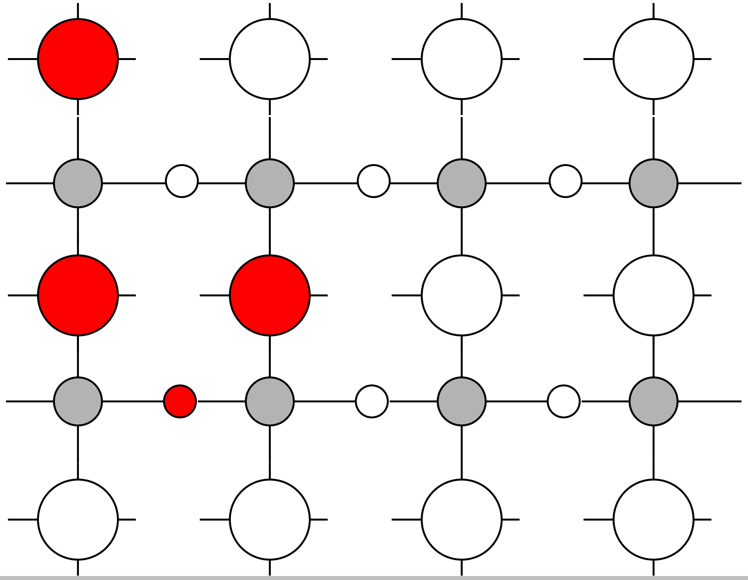
- 3.4 Surfaces, Miller Index

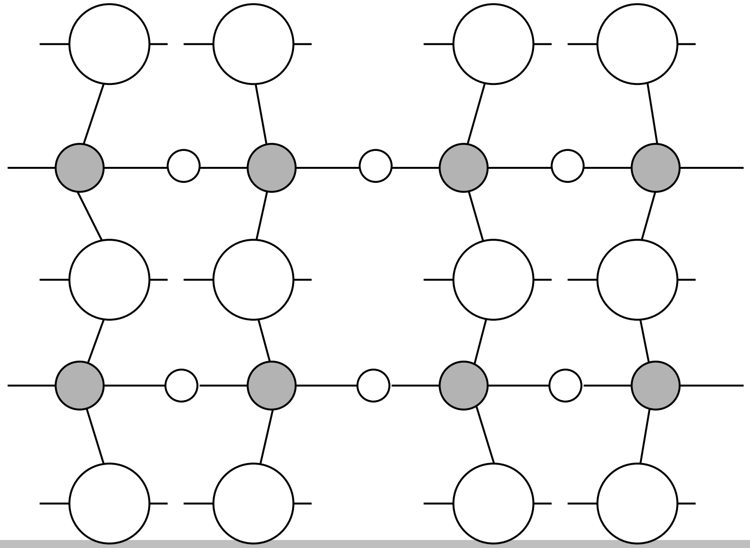
Reference: Vol. 6, Ch. 1, ABACUS tool at nanohub.org/tools/abacus and "Crystal Viewer Lab, https://nanohub.org/resources/crystalviewer

Surface Reconstruction

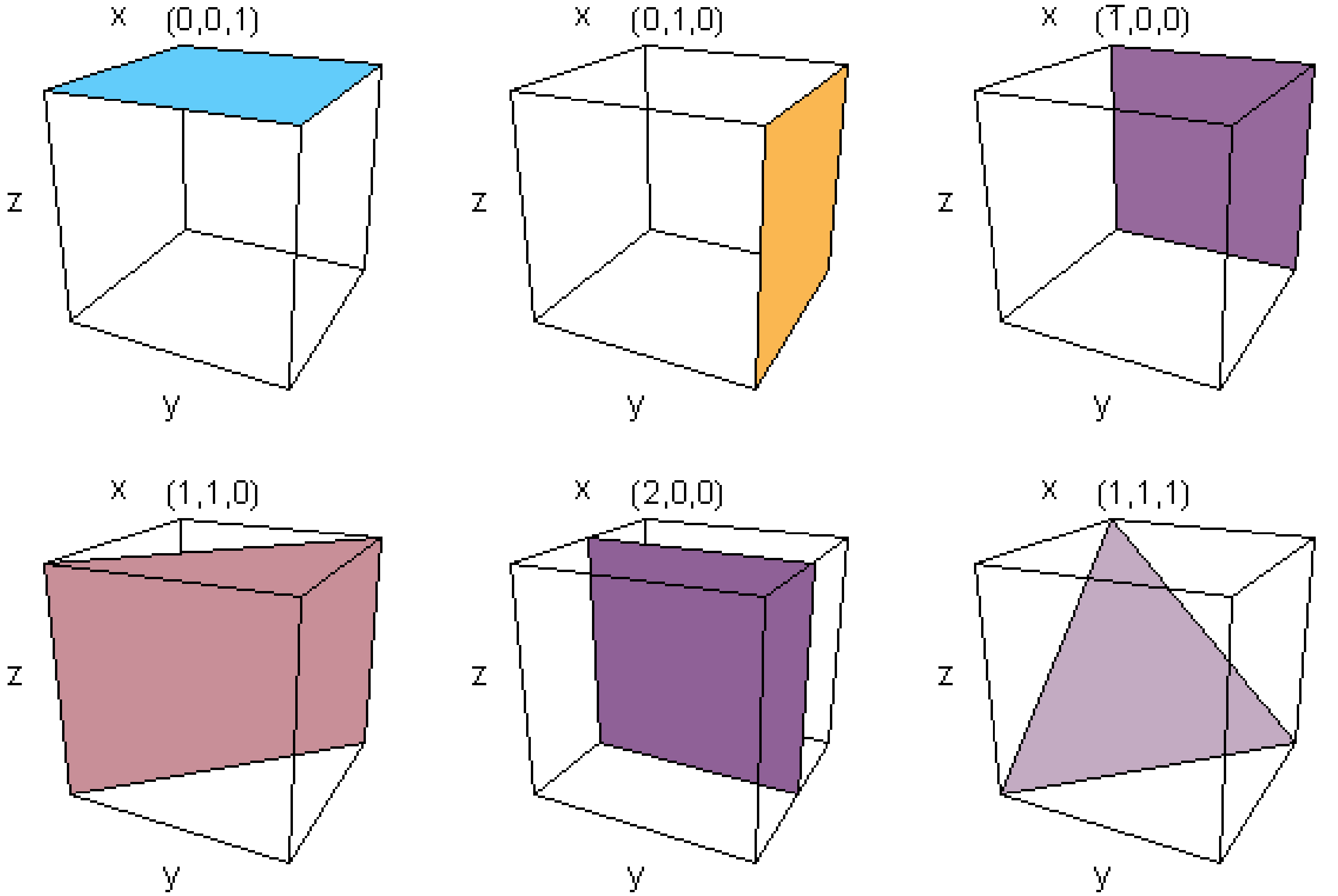




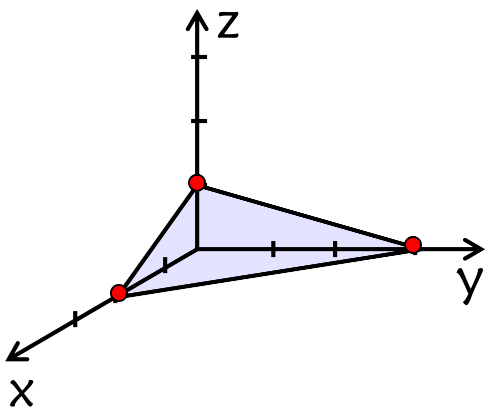




Miller-Indices and Definition of Planes



Miller Indices: Simple Construction Process



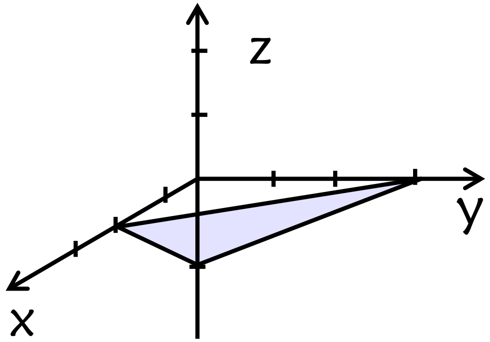
1. Set up axes along the edges of unit cell
2. Normalize intercepts …. 2, 3, 1
3. Invert/rationalize intercepts … 1/2, 1/3, 1

   3/6, 2/6, 6/6
4. Enclose the numbers in curvilinear brackets

   (326)

Miller Indices: Additional Cases

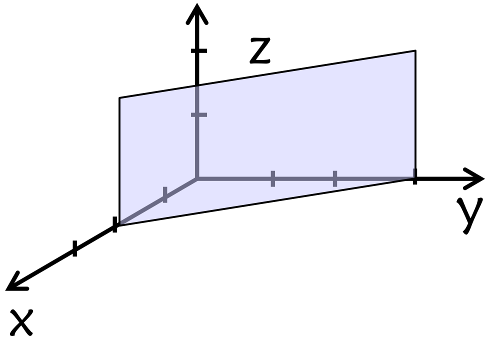
Negative Intercept



2,	3,	-2
1/2,	1/3,	-1/2
3,	2,	-3

$(3\ 2\ \bar{3})$

Intercept at infinity

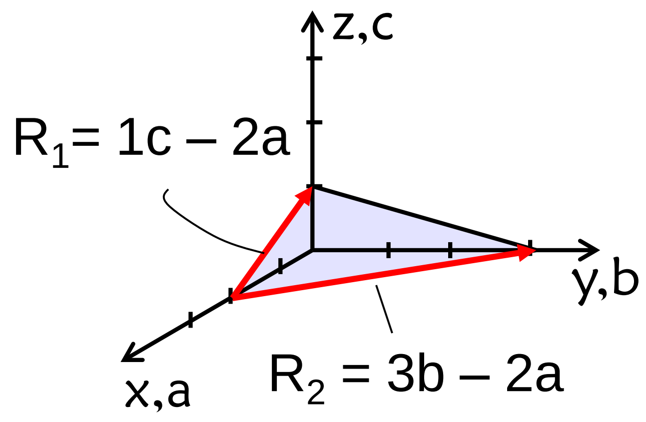


2,	3,	∝
1/2,	1/3,	0
3,	2,	0

(3 2 0)

Miller Indices and Vector Algebra

Miller indices: (326)



$$\vec{R}_1 = \begin{pmatrix} -2 \\ 0 \\ 1 \end{pmatrix} \quad \vec{R}_2 = \begin{pmatrix} -2 \\ 3 \\ 0 \end{pmatrix}$$

Normal to the surface and R_1,R_2

$$R_2 x R_1 = \begin{vmatrix} a & b & c \\ -2 & 3 & 0 \\ -2 & 0 & 1 \end{vmatrix} = 3a + 2b + 6c$$

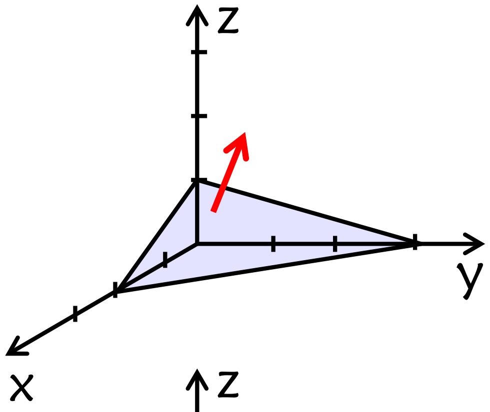
Vector indices same as Miller indices !

(326) vs. [326]

Specification of vectors normal to a particular plane!

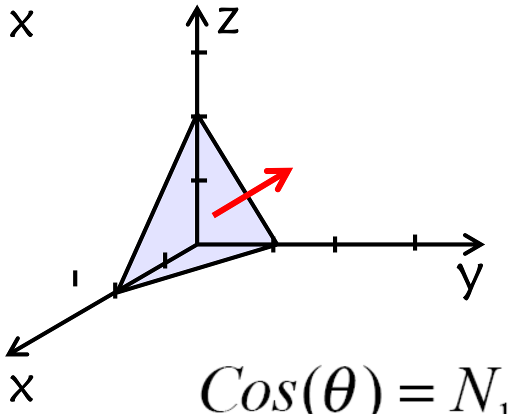
⇒Angle between two vectors

⇒Dot product / inner product between two vectors



Unit vector normal to plane 1:

$$N_1 = (h_1\vec{a} + k_1\vec{b} + l_1\vec{c})/(h_1^2 + k_1^2 + l_1^2)^{1/2}$$



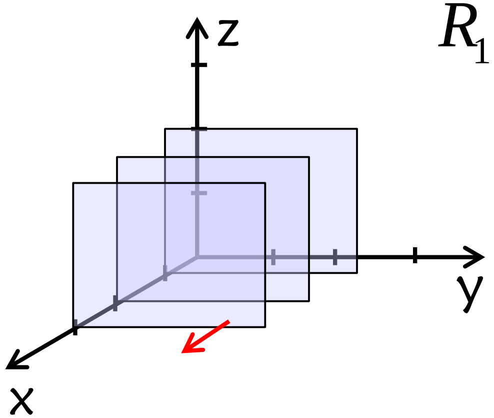
Unit vector normal to plane 2:

$$N_2 = (h_2\vec{a} + k_2\vec{b} + l_2\vec{c})/(h_2^2 + k_2^2 + l_2^2)^{1/2}$$

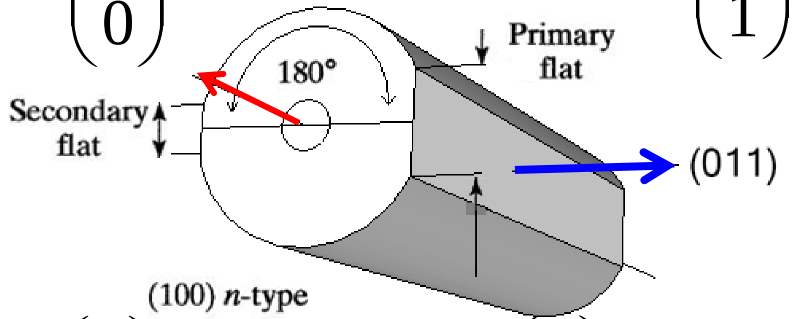
$$Cos(\theta) = N_1 \bullet N_2$$

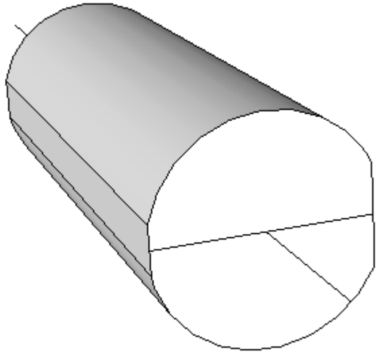
$$= (h_2h_1 + k_2k_1 + l_2l_1)/(h_2^2 + k_2^2 + l_2^2)^{1/2}(h_2^2 + k_2^2 + l_2^2)^{1/2}$$

Examples ...



$$\vec{R}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad \vec{R}_2 = \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}$$





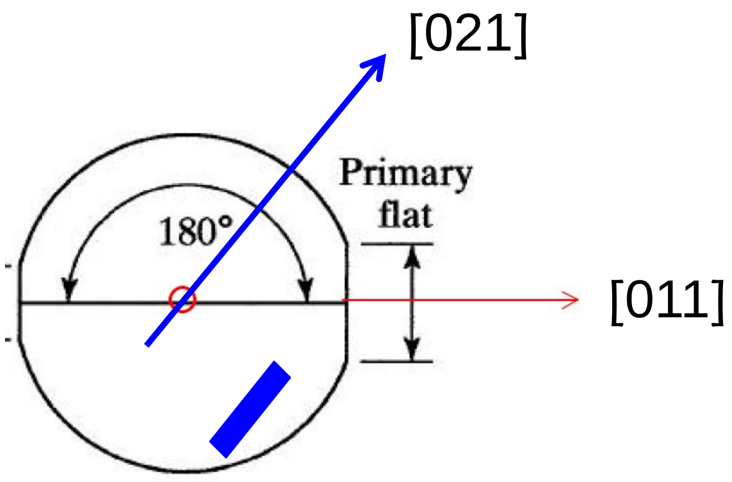
$$\vec{N}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} / \sqrt{1} \qquad \vec{N}_2 = \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} / \sqrt{2}$$

$\cos(\theta)=(1 \times 0+0 \times 1+0 \times 1)/(\sqrt{1} \times \sqrt{2}) = 0$

so θ=90 degrees

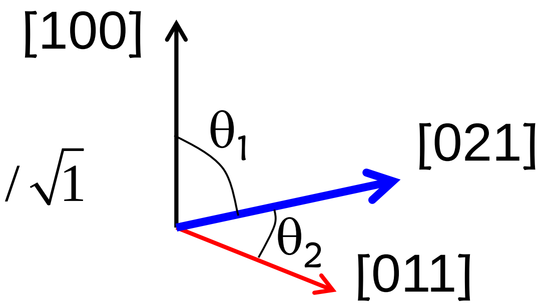
(011) surface is normal to (100) surface

Example: Find the [021] direction



(100) *n*-type

$$\vec{N}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} / \sqrt{1}$$



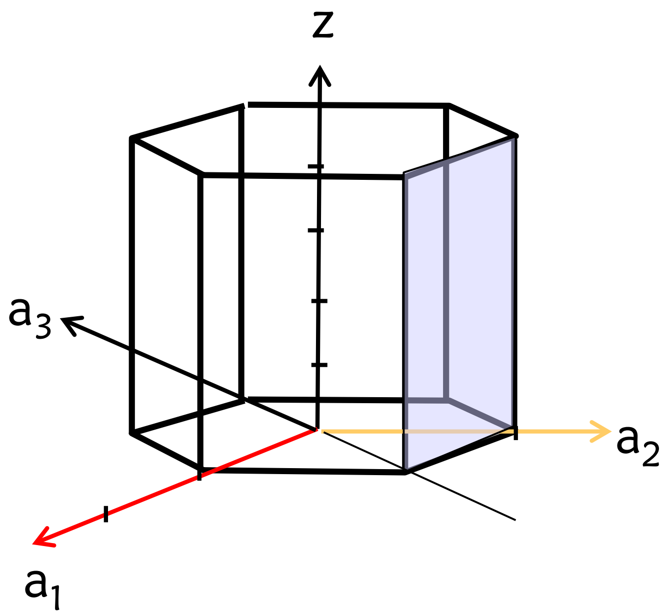
$$\vec{T} = \begin{pmatrix} 0 \\ 2 \\ 1 \end{pmatrix} / \sqrt{1}$$

$$\vec{N}_2 = \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} / \sqrt{2}$$

$N_1 \bullet T = \cos(\theta_1) = (1x0+0x2+0x1)/(1x□5)$ = 0, so θ=90 degrees
[021] vector lies on (100) plane.

$N_2 \bullet T = \cos(\theta_2) = (0x0+2x1+1x1)/(□5 □2)$ = 3/ □10, so θ=18.43 degrees
with respect to [011] direction.

Bravais-Miller Indices



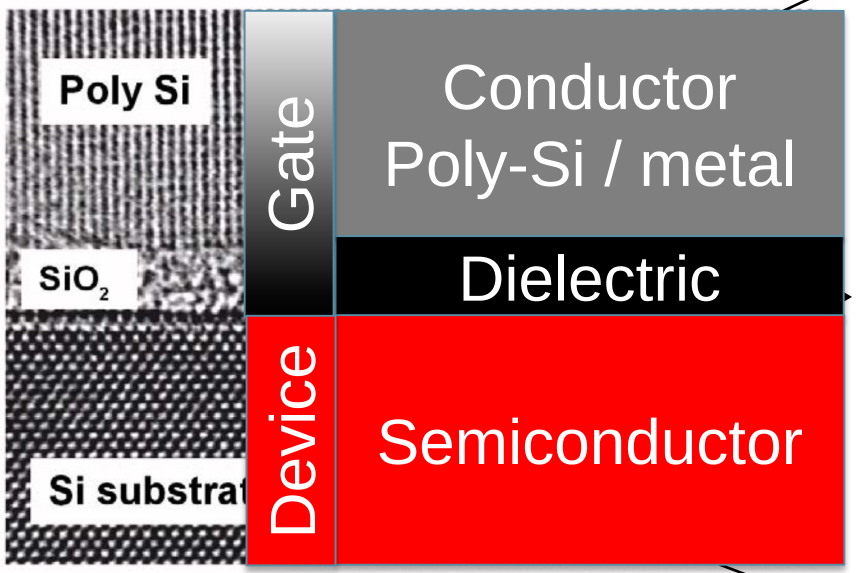
∝,	1,	-1,	∝
0,	1,	-1,	0
0,	1,	-1,	0

$(0\ 1\ \bar{1}\ 0)$

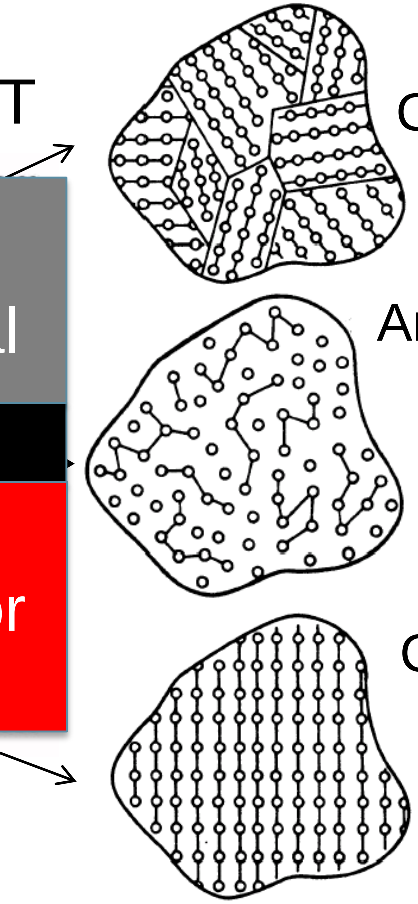
First three indices sum to zero.

Crystals form the Core Device Material

Cross section of a MOSFET



Device is a perfectly arranged crystal



Poly-Crystalline

Conductive
Electron transport
Hold charge

Amorphous Oxides

Non-Conductive
“NO” transport

Crystalline

Highly conductive
Electron transport

- Modern solid state devices use all forms these forms of materials
- Focus on Crystals first – start with 1D => 2D => 3D
- Transfer concepts of electronic behavior in crystals to other materials

Summary

- Crystalline material can be built by repeating the basic building blocks. This simplifies the quantum solution of the material, which will allow us to compute n and v for these systems easily.
- Silicon, GaAs, PbS do not have simple Bravais lattice; but they have Bravais lattice with a basis.
- Often we need to calculate the direction of crystal planes because material properties differ along different planes. Miller indices are one useful way of characterizing crystal planes. It is useful to review some identities of vector calculus to such calculations involving crystal planes.

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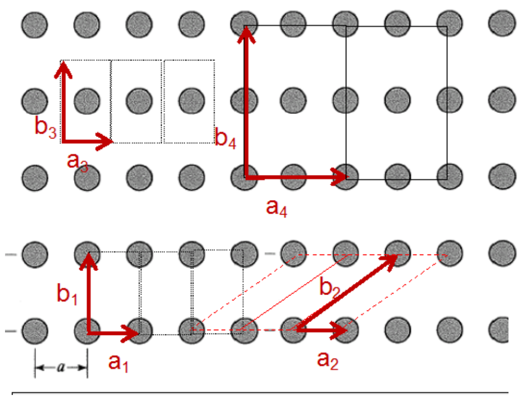

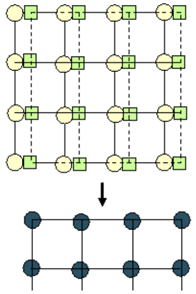

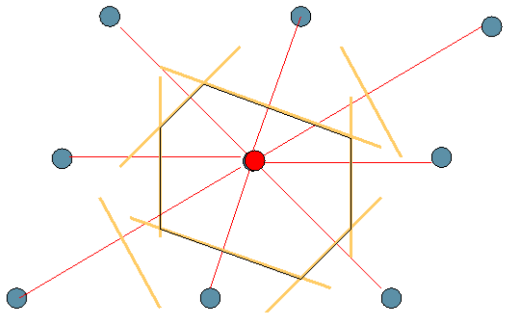

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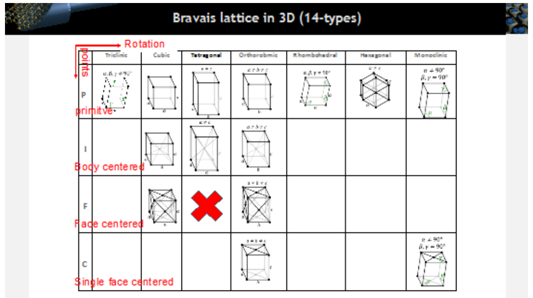

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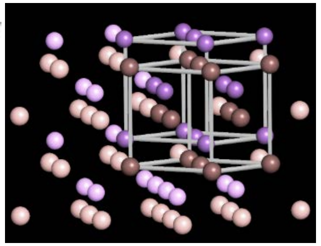

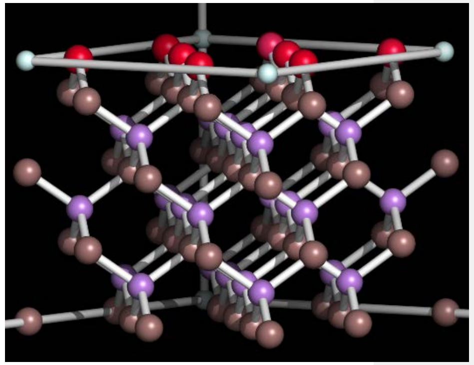

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