ECE606: Solid State Devices
Lecture 1

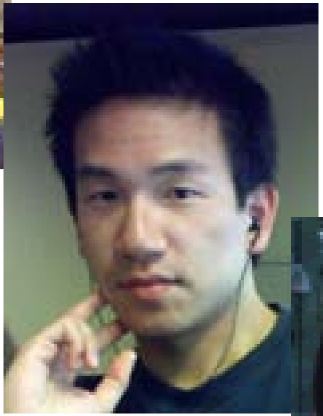
Gerhard Klimeck
gekco@purdue.edu

PURDUE UNIVERSITY

Your Instructor and Teaching Assistants

- Gerhard Klimeck
  - » Prof. at Purdue for 8 years
  - » Principal at NASA/JPL, 6 years
  - » Texas Instruments, 4 years
  - » Over 340 papers on devices/physics
- Parijat Sengupta
  - » 5th year graduate student
- Yaohua Tan
  - » 5th year graduate student
- Matthias Yui-Hong Tan
  - » 3rd year graduate student
- Yuling Hsueh
  - » 2nd year graduate student

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Books

- Advanced Semiconductor Fundamentals (QM, SM, Transport) first 5 weeks
- Semiconductor Device Fundamentals (Diode, Bipolar, MOSFET) Weeks 6-15

HW/Exams

- HW (9 HW, all will be graded; solutions will be provided; distributed every Tuesday, due at the beginning of the lecture
- 3 exams (~5 weeks apart)

Website

- http://cobweb.ecn.purdue.edu/~ee606/
- https://blackboard.purdue.edu (grades and optional notes)
- https://nanohub.org/resources/5749 (full course on-line from Spring 2009)

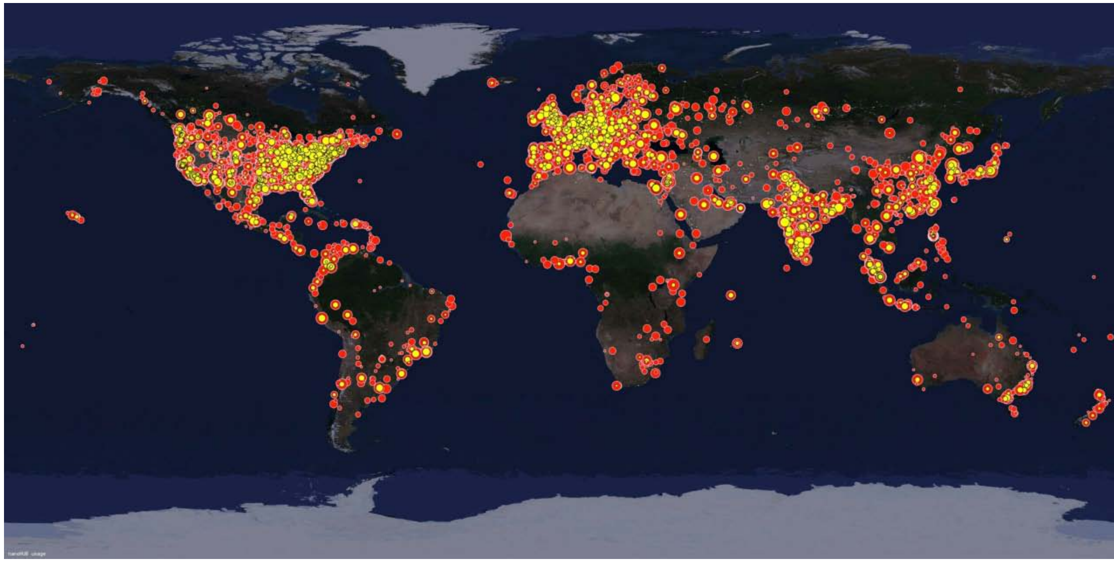
Office hours

- Klimeck: 1:30-2:30 Tue@EE 323, Thu 4:30pm-5:30pm@EE323

Your Purdue Resources

Klimeck

- Leads the Network for Computational Nanotechnology (NCN)
- NCN hosts nanoHUB.org
- >230,000 users
- 172 countries
- ~15 professional staff
- 5 other universities



>3,000 resources on line

Also THIS WHOLE course

nanohub.org/resources/5749

Or search for "nanohub 606"

Outline

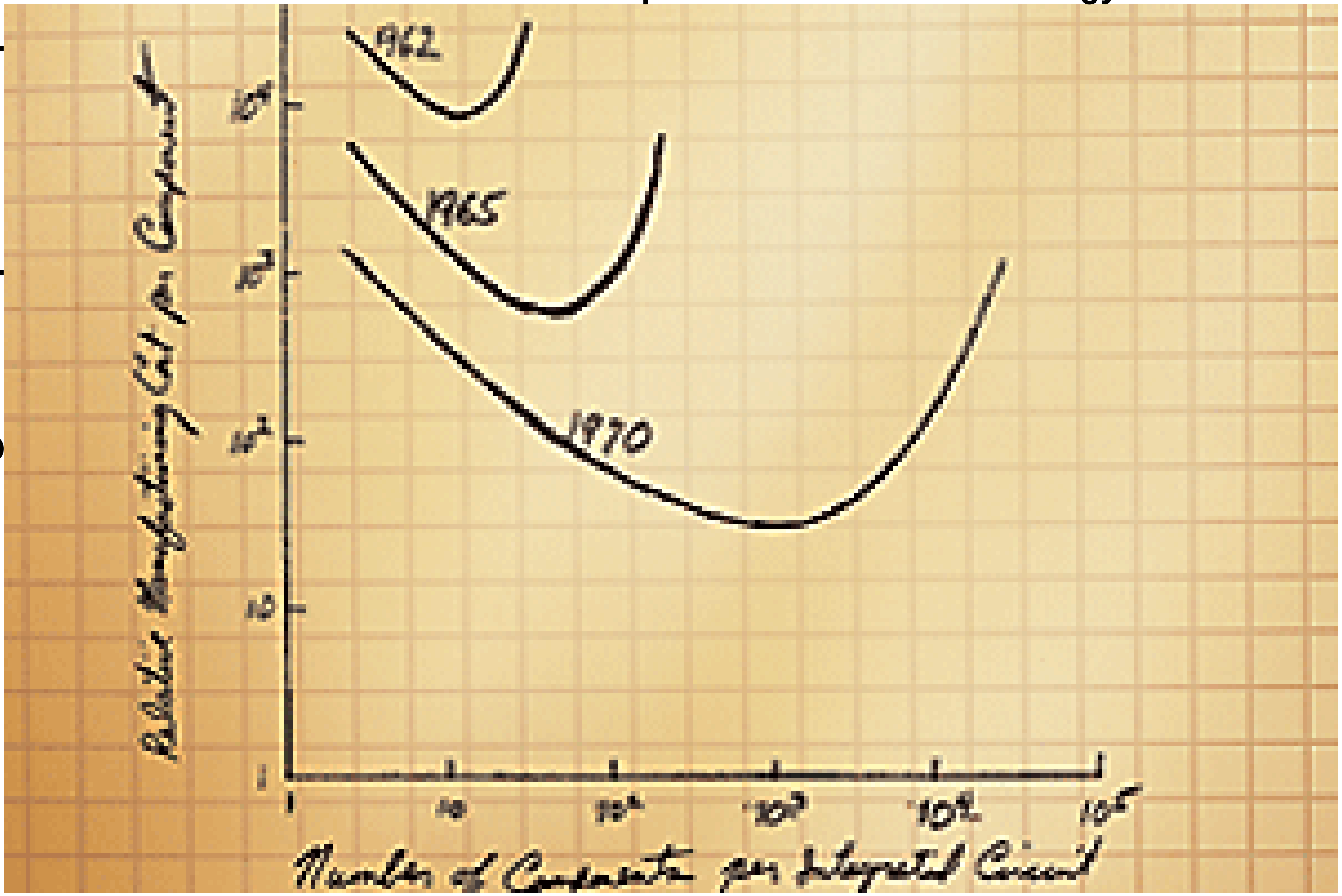
- Course information
- Motivation for the course
- Current flow in semiconductors
- Types of material systems
- Classification of crystals
  - » Bravais Lattices
  - » Packing Densities
  - » Common crystals - Non-primitive cells
    - ✓NaCl, GaAs, CdS
  - » Surfaces

- Reference: Vol. 6, Ch. 1
- Helpful software: Crystal Viewer in ABACUS tool at nanohub.org

1965 Gordon Moore => Moore's Law

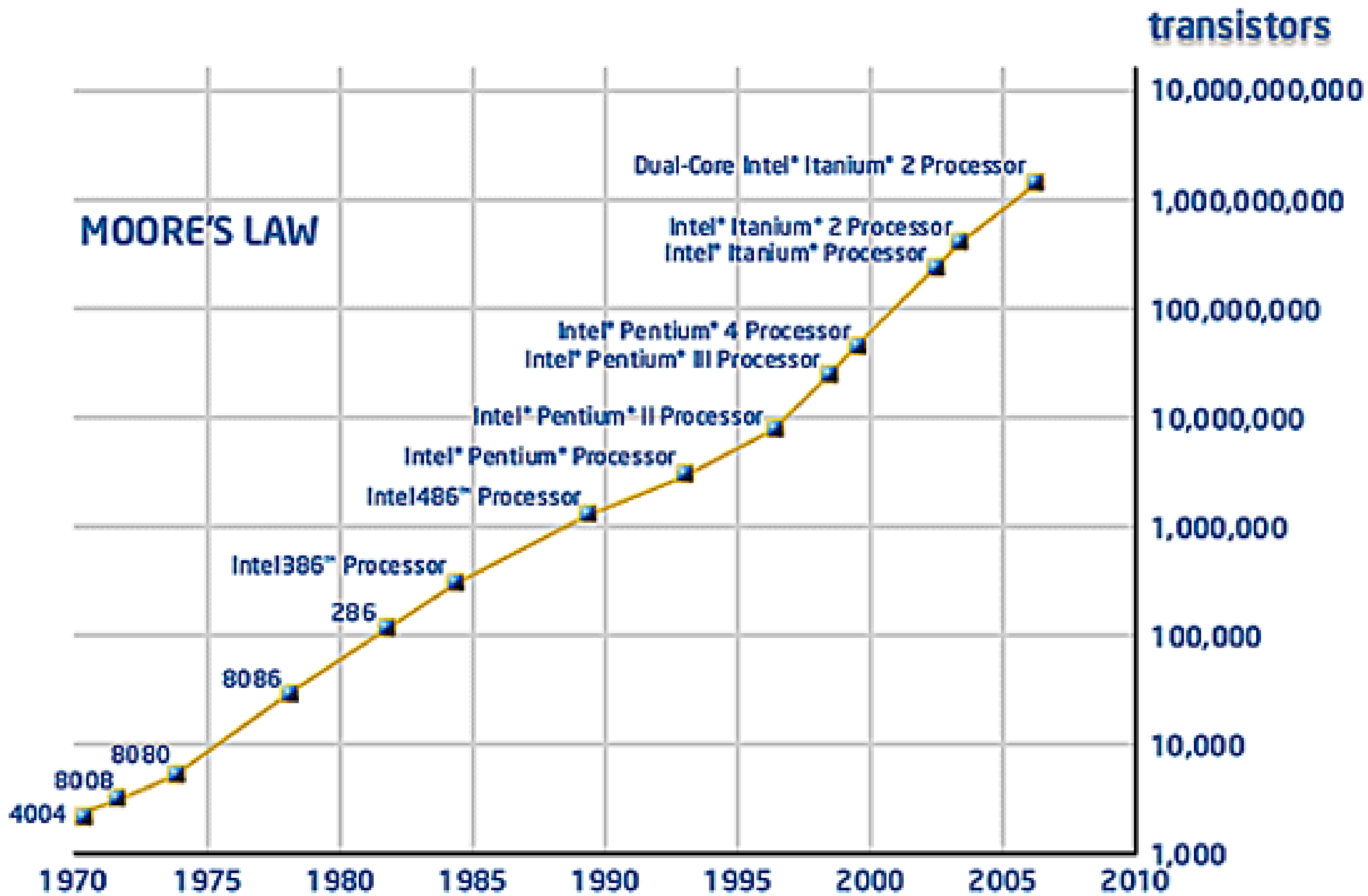
http://www.intel.com/technology/mooreslaw

Relative Manufacturing Cost per Component



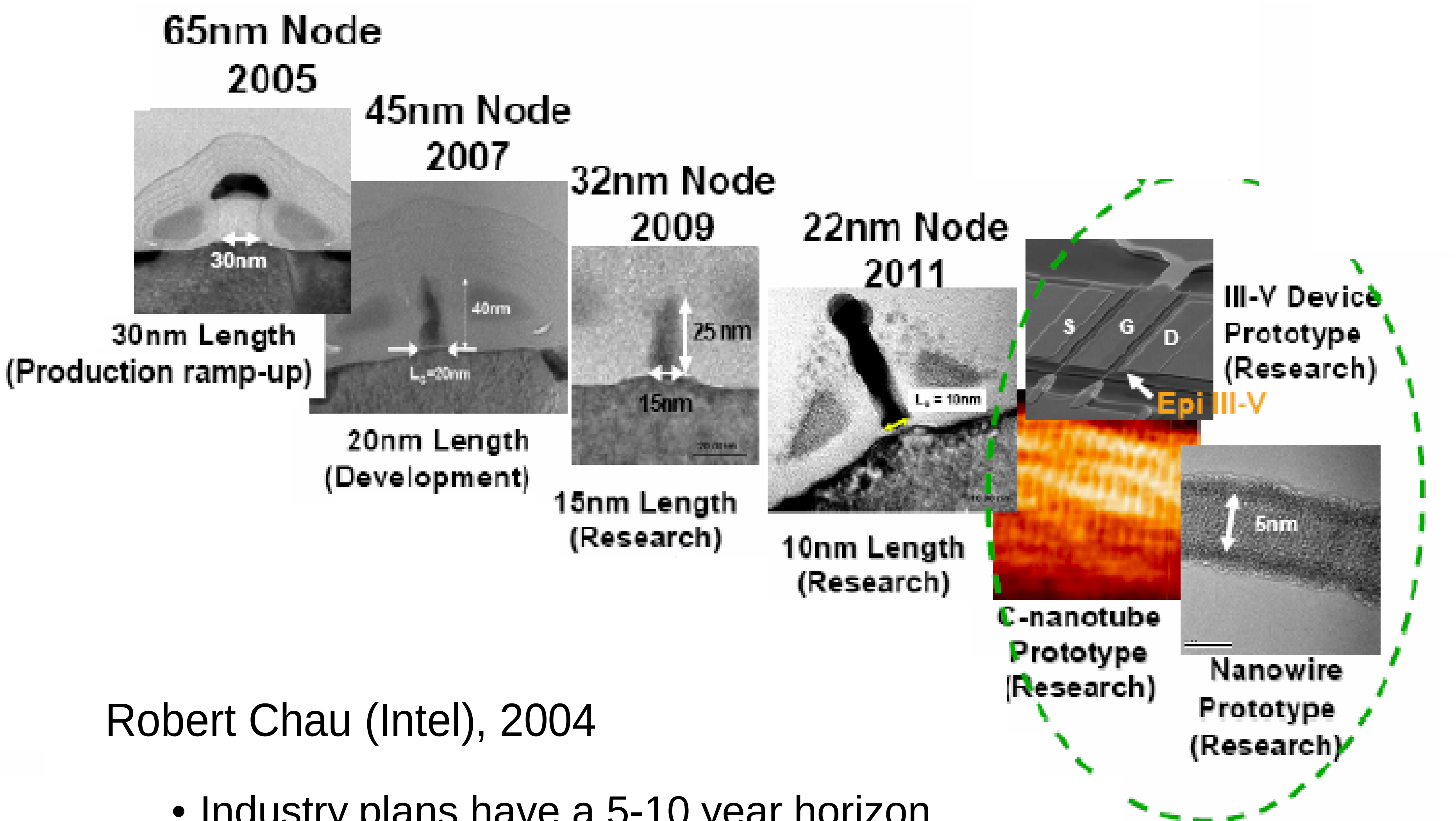
Number of Components per Integrated Circuit

Moore's Law
a Self-Fulfilling Prophesy



- From http://www.intel.com/technology/mooreslaw/index.htm

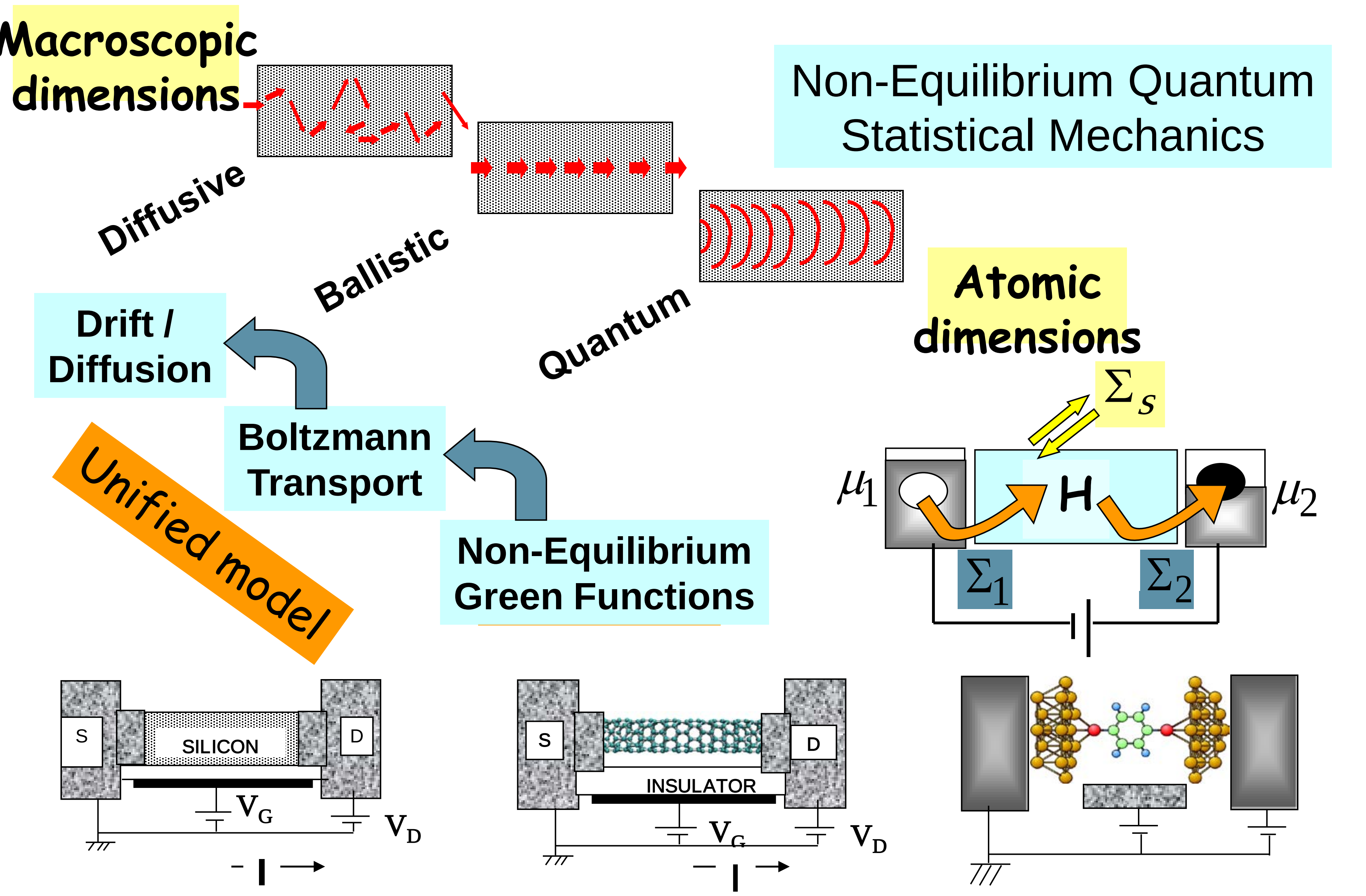
Technical Developments to enable Moore's Law



Robert Chau (Intel), 2004

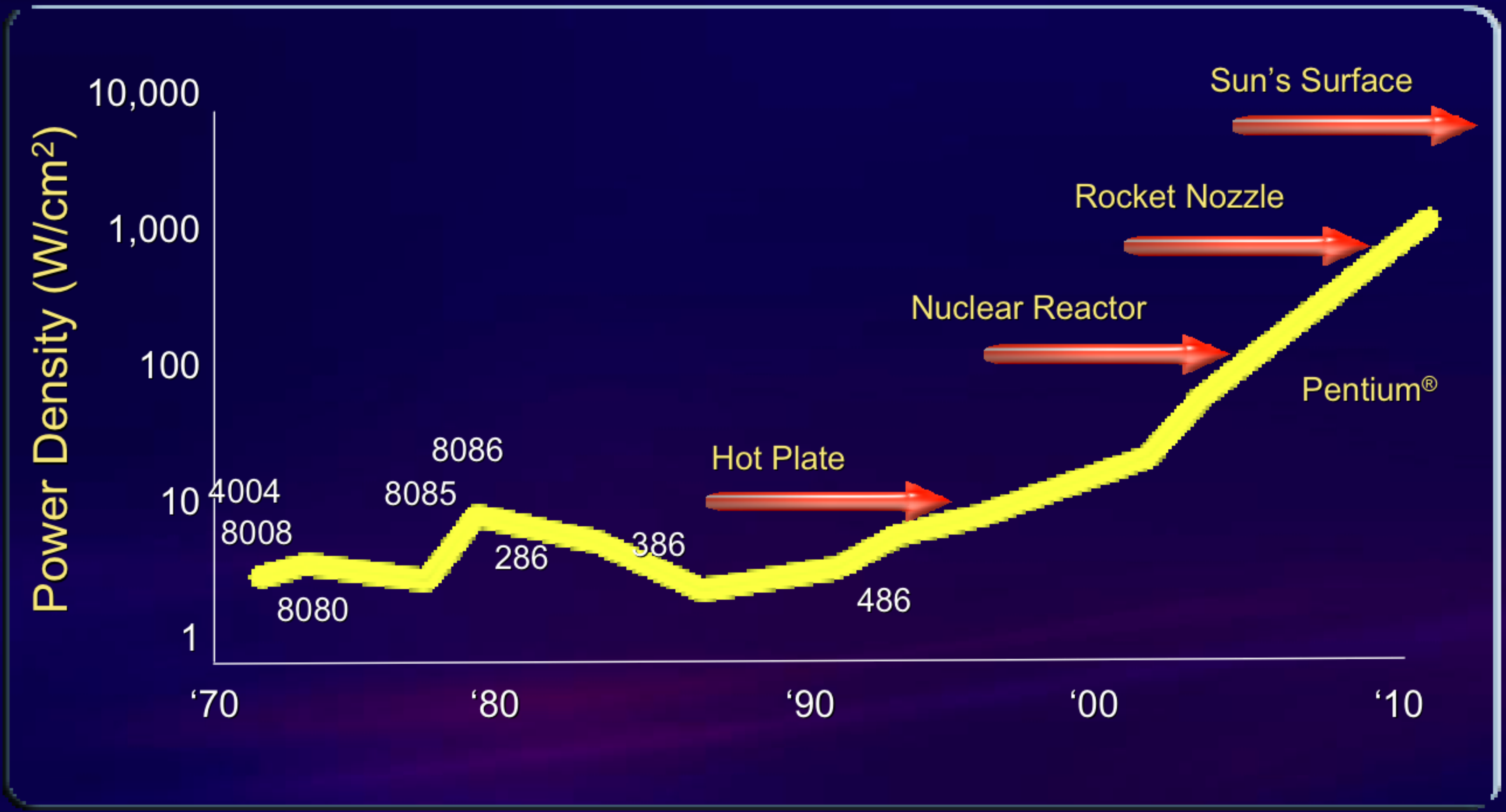
- Industry plans have a 5-10 year horizon
- Industry has been on time:
- 32nm node predicted in 2004 and announced 2009
- **There are NO technically viable solutions beyond 2015**

Device Sizes and Transport Concepts

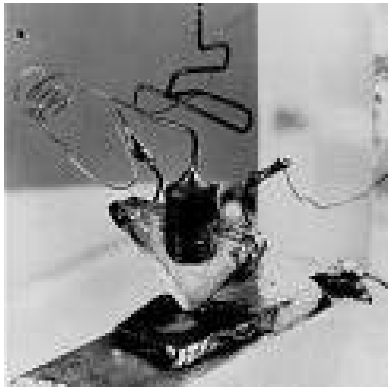
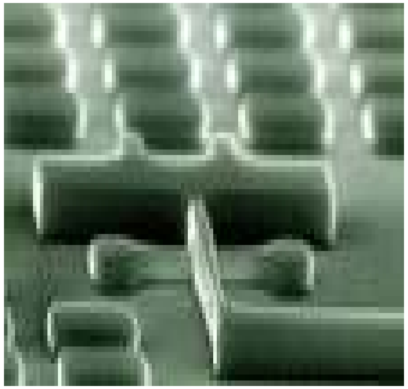


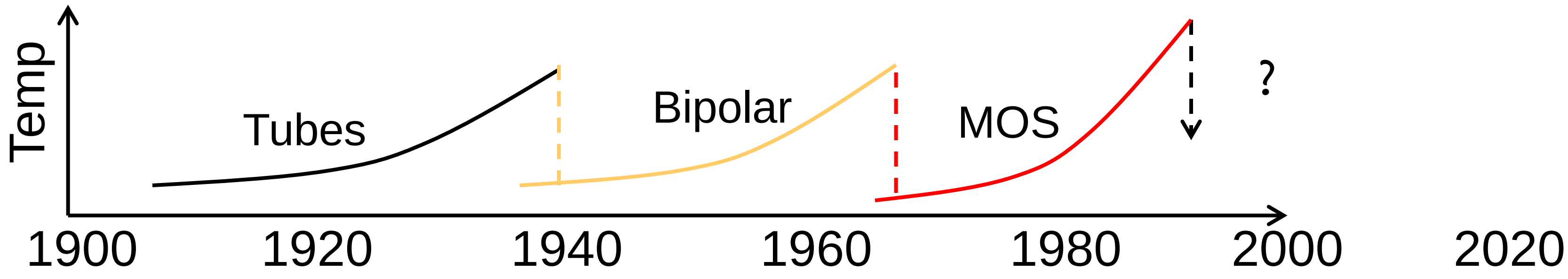
Today's CPU Architecture

Heat becoming an unmanageable problem



Intel Developer Forum, Spring 2004 - Pat Gelsinger

Vacuum Tubes	Bipolar	MOSFET	Now ??
			Spintronics Bio Sensors Displays ….
1906-1950s	1947-1980s	1960-until now	



Outline of the Course

Device-specific system design ← **Application specific device operation** ← **Physical Principle of device operation** ← **Foundation in Physics**

- TFT for Displays
- CMOS-based Circuits for μP
- LASERS for Disk Drives
- MEMS for Read heads

EE606

- Resistors (5 wk)
- Diodes (3 wk)
- Bipolar (3 wk)
- MOSFETs (3 wks)

Quantum Mechanics
+
Statistical Mechanics
↓
Transport Equations

Relation to Other MN-Area Courses

Device-specific system design	EE 695F: RF Design	EE 695E: Opto-system	BME 695A: Bio-system Design
Application specific device operation	EE 654: Advanced Semi Dev.	EE 612: VLSI Devices	EE 520: Bio-Systems
Physical Principle of device Operation	EE 606: Basic Semi Dev.	EE 604 EM, Magnetics	
Foundation	EE 656: Semi-Transport	EE 659: Quantum Transport	PHYS 570B : Bio-physics
	Finite Element, Molecular Dynamics, Monte Carlo	Characterization	ECE 557: Fabrication

Motivation and Importance of 606

- Define "the language"
  - » Specialty area in ECE: MN - Micro – Nano – Electronics
  - » Bridge different communities, Electrical Engineering, Physics

- Fundamentals of Semiconductor Devices
  - » How to "think" about electrons in a semiconductor
  - » Foundation of typical job interviews –
    - ✓ technical interviews will typically not go into more detail
    - ✓ Probe the fundamental understanding of electronic behavior in Semiconductor

  => Your entry into a technical job in Semiconductor Industry

  - » Required knowledge in the MN area Qualifying Exam

  => Your entry into the PhD program in the MN area

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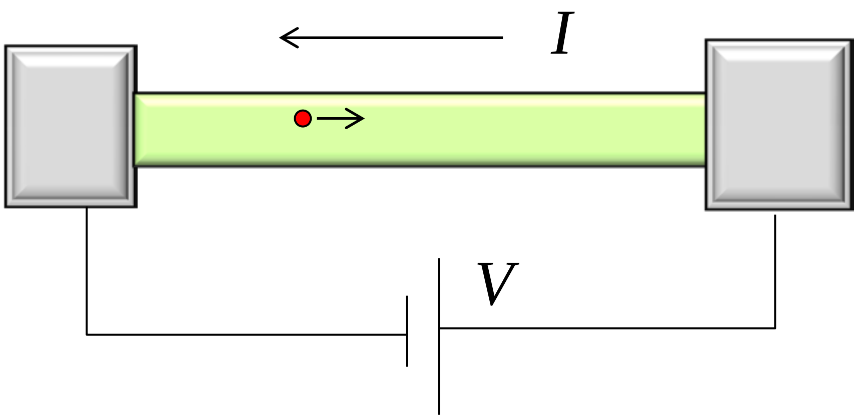
  - » Packing Densities
  - » Common crystals - Non-primitive cells
    - ✓NaCl, GaAs, CdS
  - » Surfaces

- Reference: Vol. 6, Ch. 1
- Helpful software: Crystal Viewer in ABACUS tool at nanohub.org

Current Flow Through Semiconductors (5 weeks)



$$I = G \times V$$

$$= q \times \color{red}{n} \times \color{blue}{v} \times A$$

Carrier Density

velocity

Depends on chemical composition, crystal structure, temperature, doping, etc.
Could be tabulated for "known" materials
Need a theory for engineering of new devices/materials

Quantum Mechanics + Equilibrium Statistical Mechanics

- Encapsulated into concepts of effective masses and occupation factors (Ch. 1-4)

Transport with scattering, non-equilibrium Statistical Mechanics

- Encapsulated into drift-diffusion equation with recombination-generation (Ch. 5 & 6)

Atomic composition

- *number of electrons per atom*

Arrangement of atoms

- *not all electrons are available for conduction*

For Periodic Arrays

- *simplification for computation*
  - Concept of Unit Cells
  - Simple 3-D Unit Cells

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Elemental and Compound Semiconductors

II	III	IV	V	VI
4 Be	5 B	6 C	7 N	8 O
12 Mg	13 **Al**	14 **Si**	15 **P**	16 S
30 **Zn**	31 **Ga**	32 Ge	33 **As**	34 **Se**
48 Cd	49 In	50 Sn	51 Sb	52 Te
80 Hg	81 Tl	82 Pb	83 Bi	84 Po

Si: $260billion industry

Elemental (e.g., Si, Ge, C)

Compound

IV-IV: Si-Ge, Si-C

SiGe: stressors
SiC: radiation

III-V: InP, GaAs, $(In_xGa_{1-x})(As_yP_{1-y})$

Lasers/detectors
expensive

II-VI: CdTe

Far IR detectors
Soft and difficult

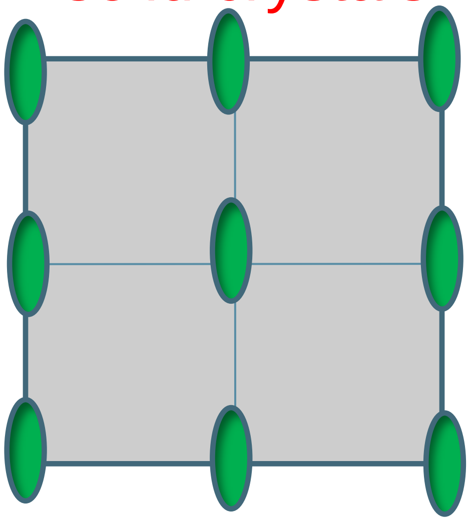
IV-VI: PbS

First semiconductor diodes
Very soft and difficult

Not all combinations possible:
lattice mismatch, room temp. instability, etc. are concerns

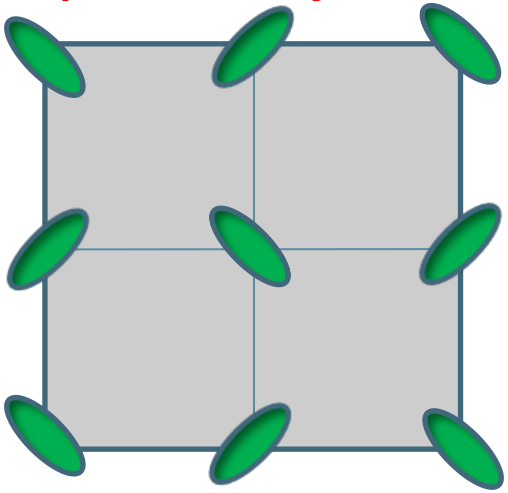
Arrangement of Atoms: orientation vs. position

solid crystals



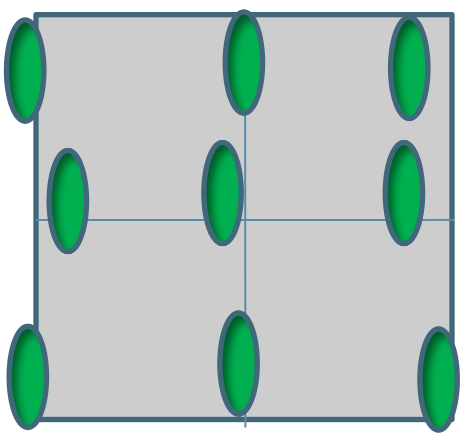
specific position
specific orientation

plastic crystals



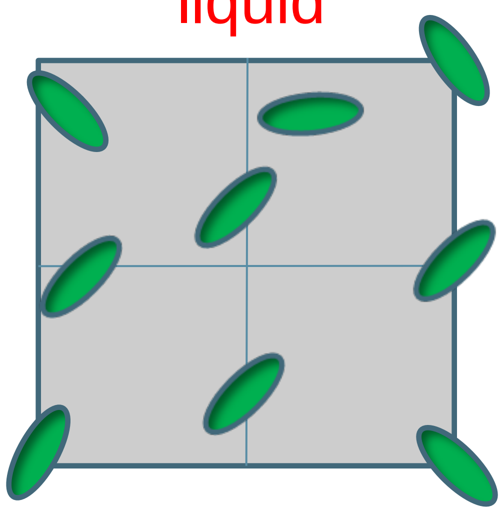
specific position
random orientation

liquid crystals



random position
specific orientation

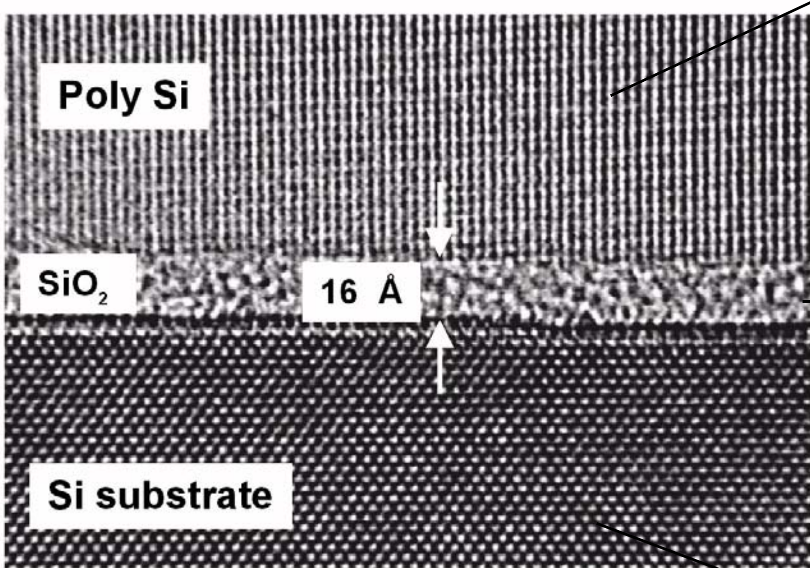
liquid



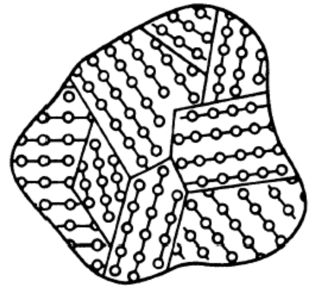
random position
random orientation

Arrangement of Atoms

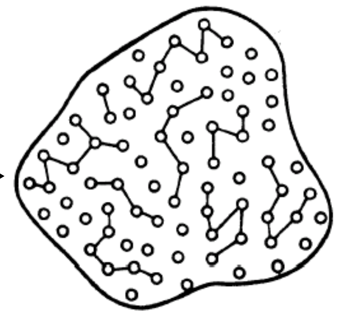
Cross section of a MOSFET



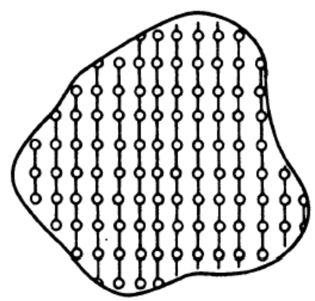
Perfectly arranged Si Crystal



Poly-crystalline
Thin Film
Transistors



Amorphous
Oxides
Why ?



Crystalline
Definition ?

- Quantitative definition: Correlation spectrum and diffraction pattern
- Modern solid state devices use all forms these forms of materials
- Focus on Crystals first – relatively simple
- Transfer knowledge of electronic behavior in crystals to other materials

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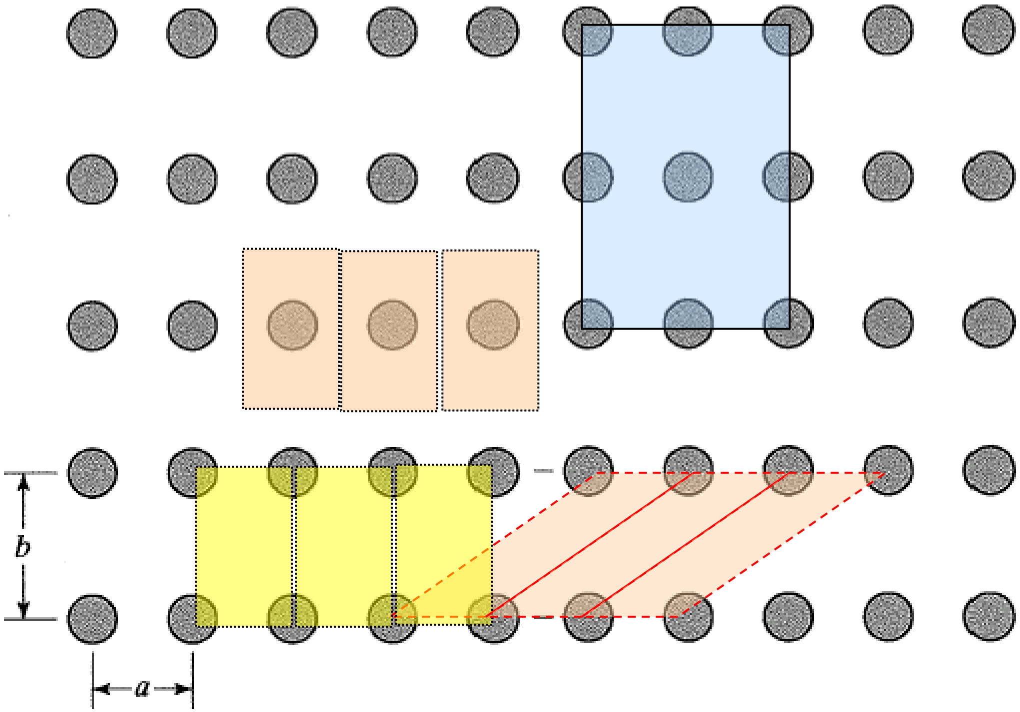
Unit cell of a Periodic Lattice

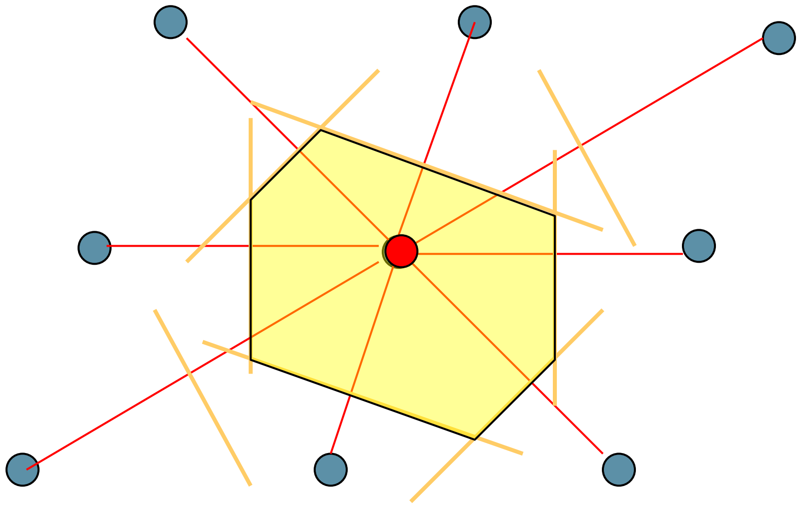


"Infinitely" extended
2D shown
3D same concepts

⇒ N_A=6 x 10^{23}/mol
⇒ Can NEVER solve this, even on the largest computer
⇒ Simplify to a repeated (small) cell

- Unit cells are *not* unique
- Unit cells can be Primitive or Non-primitive
- Property of ONE CELL defines the property of the solid

- Choose a reference atom
- Connect to all its neighbors by straight lines
- Draw lines (in 2D) or planes (in 3D) normal to and at the midpoints of lines drawn in step 2
- Smallest volume enclosed is the Wigner-Seitz primitive cell

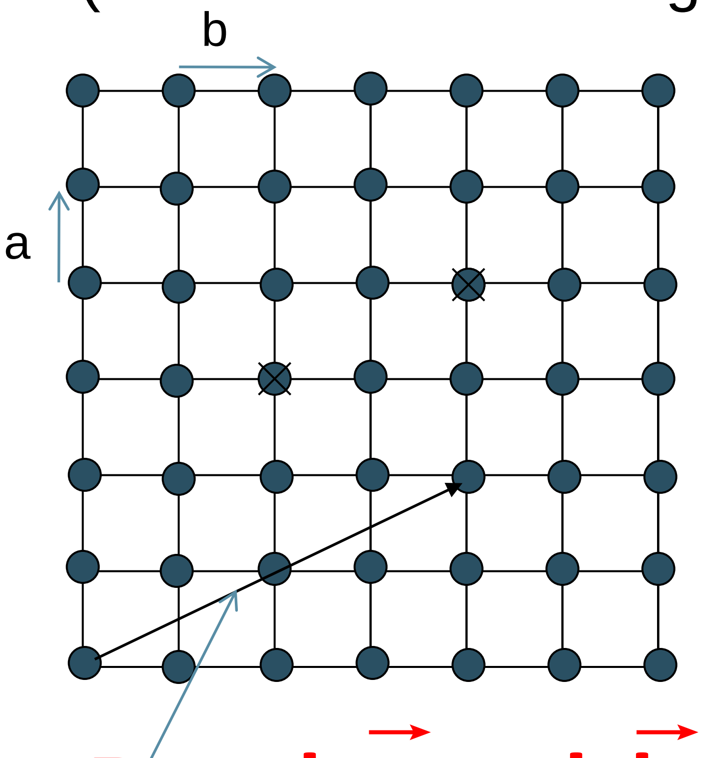


Wigner-Seitz cell is ONE definition of a Unit Cell that always works
There are other ways of construction!

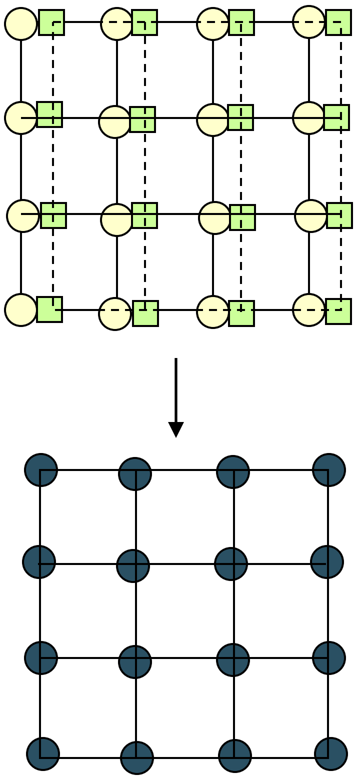
Geometry of Lattice Points

In a Bravais lattice,

- every point in the lattice can be "reached" by *integer* translation of unit vectors
- every point has the same environment as every other point (same number of neighbors, next neighbors, …)

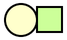


$$R = h\vec{a} + k\vec{b}$$

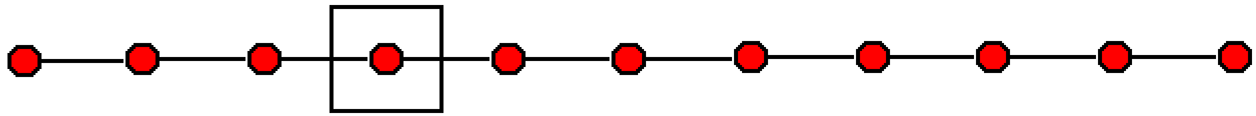


Non-Bravais lattice

Bravais lattice with a basis



Unit Cells in One-dimensional Crystals

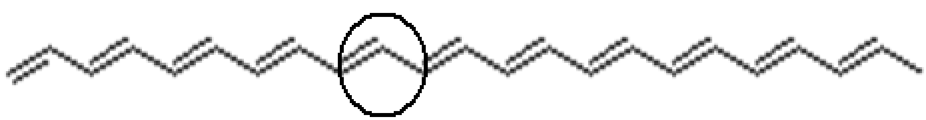


There is exactly ONE primitive unit cell in a 1D system

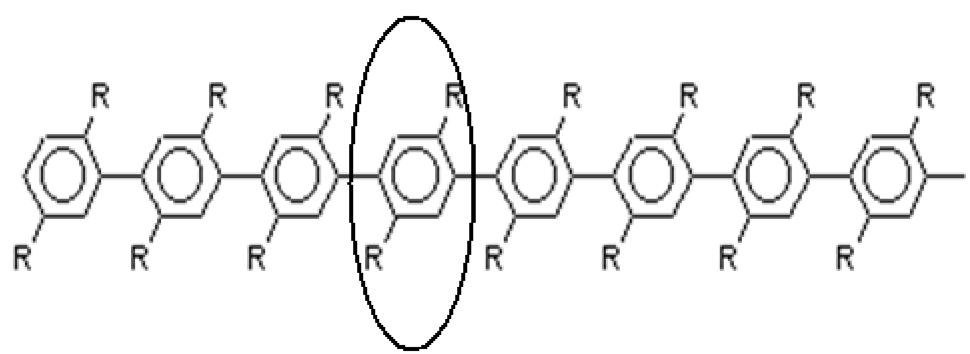
No system truly 1-D, but ….

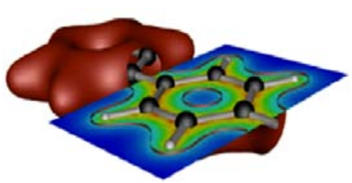
- 1D properties dominate behavior in some material
    - e.g.: polymers, DNA, 1D heterostructures (lasers, RTDs)
- Can often be solved analytically, many properties have 2D/3D analogs

Polyacetylene

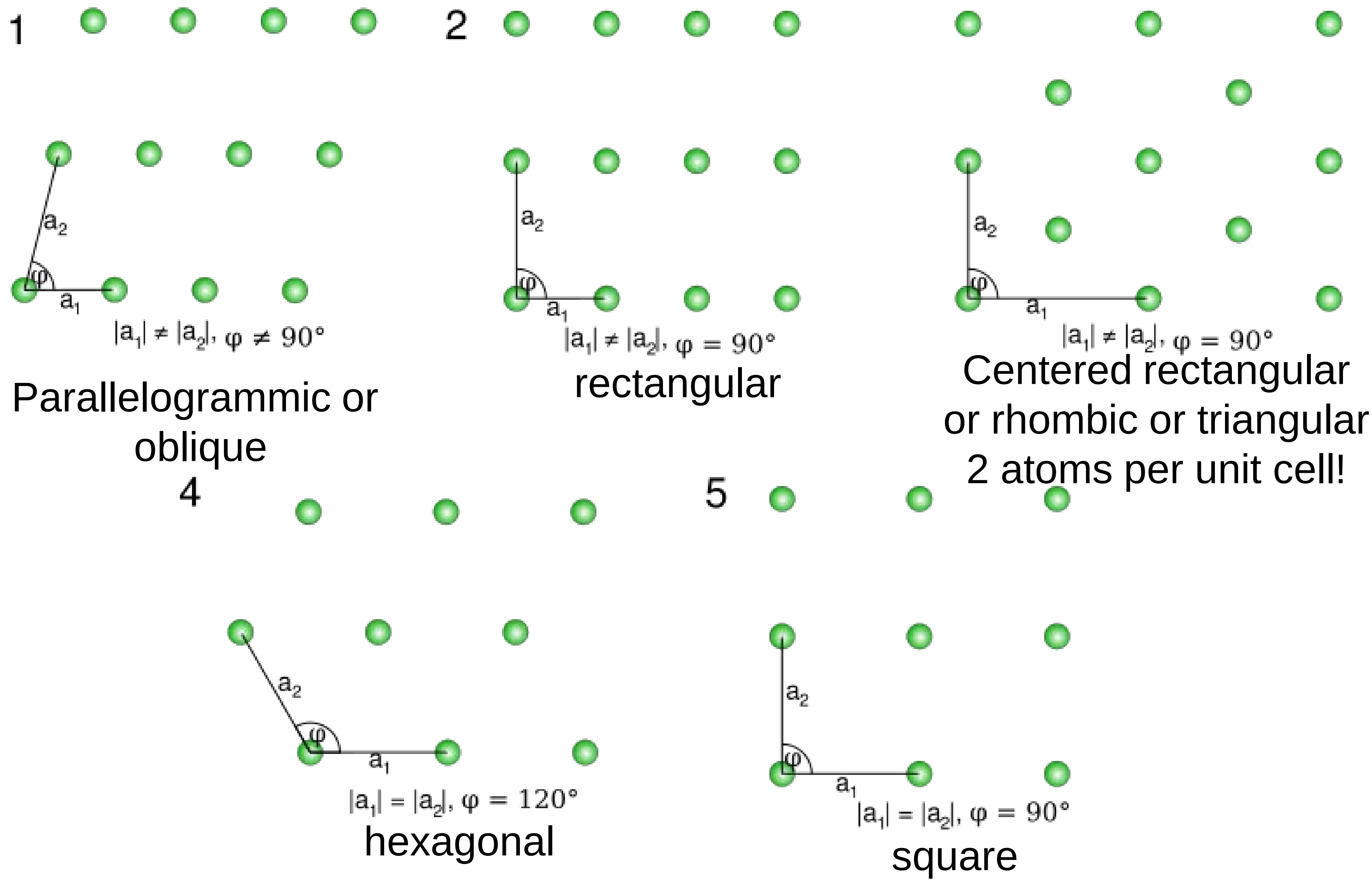


PPP



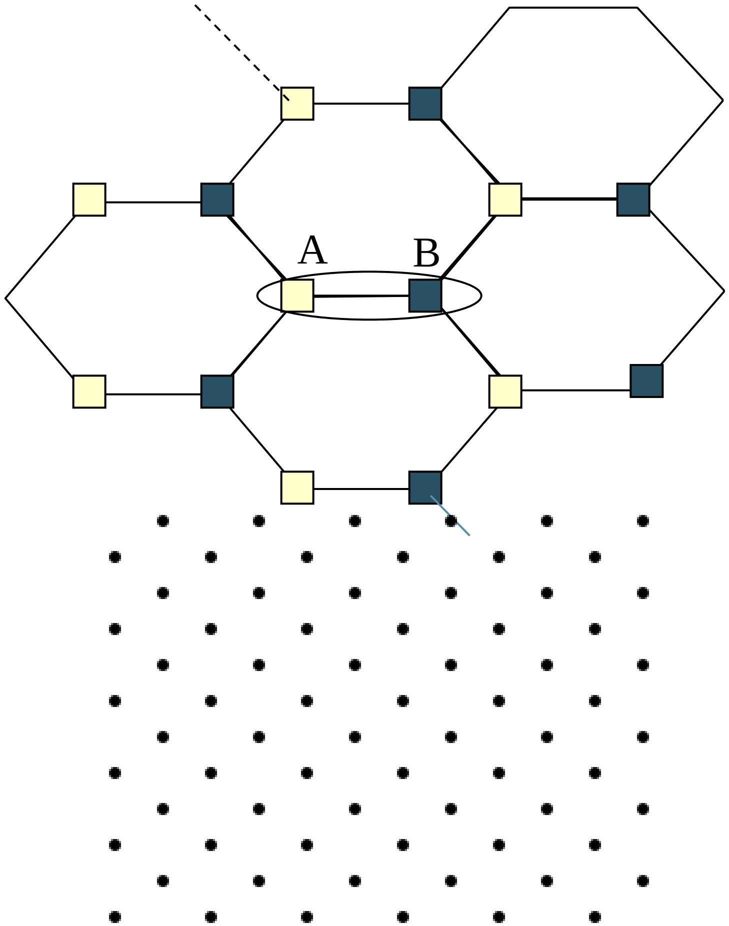


Periodic Lattice in 2D (5-types)



Original image from: http://upload.wikimedia.org/wikipedia/commons/e/ee/2d-bravais.svg

A and B do not have identical environments



This is a Graphene sheet which has recently been isolated from Graphite by adhesive tape stamping.

Ref. Novoselov, Geim, et al. Nature, 438, 197, 2005.

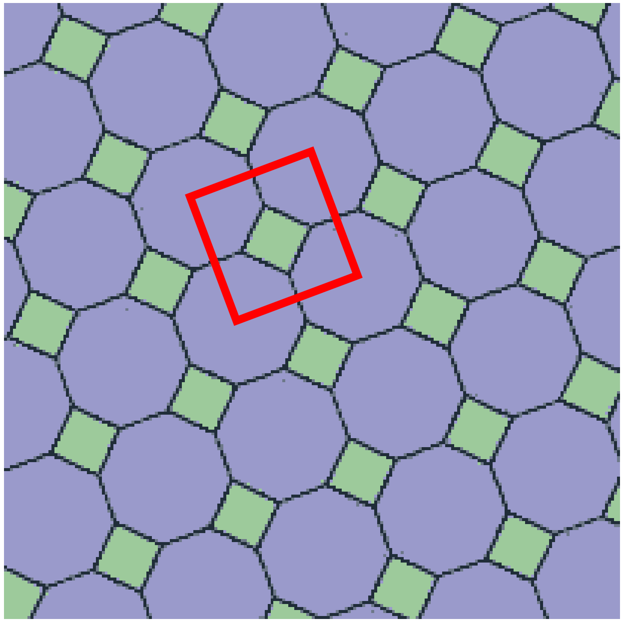
Conversion into a Bravais lattice:
-Combine A and B int a single basis
-Obtain a rhombic Bravais lattice

Original image from: http://en.wikipedia.org/wiki/File:Rhombic_Lattice.svg

Not a Bravais Lattice, but ...

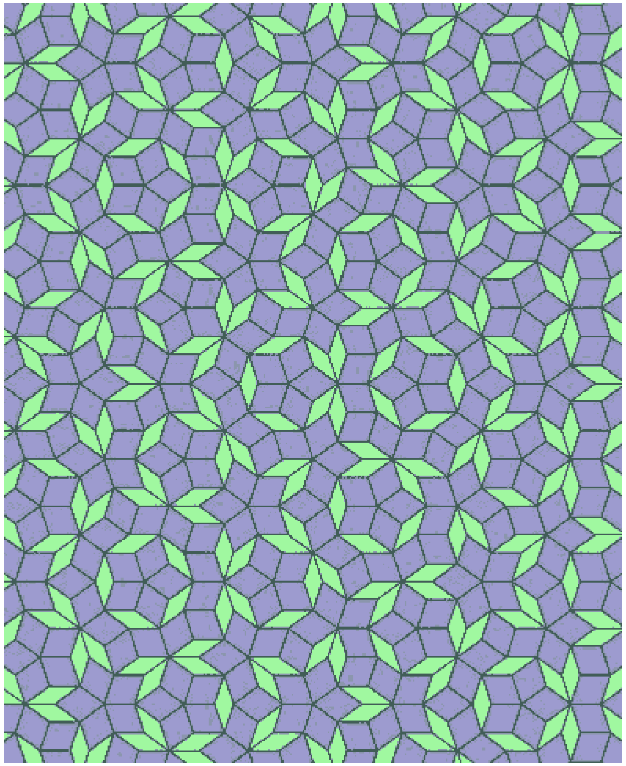
Escher Tiling

Kepler Tiling



....but these can be converted into Bravais lattice

Penrose Tiles



Ancient Tiles

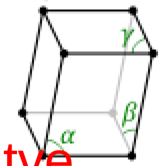
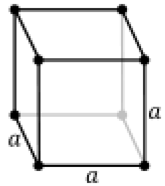
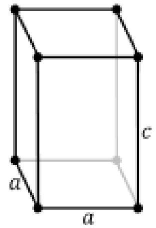
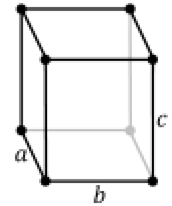
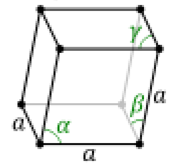
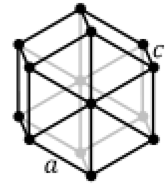
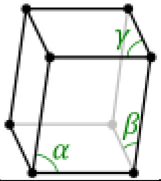
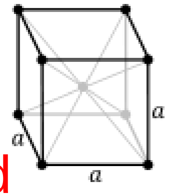
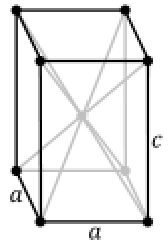
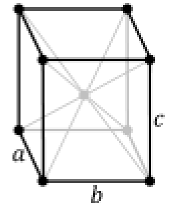
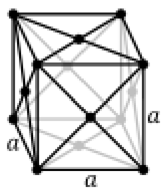
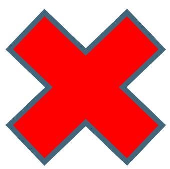
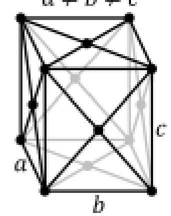
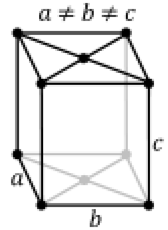
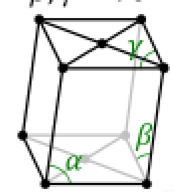
Two different unit cells in **random order**

… these CANNOT be transformed to Bravais lattice
ex. Aluminum-Manganese compounds, non-sticky coats

Bravais lattice in 3D (14-types)

Rotation →

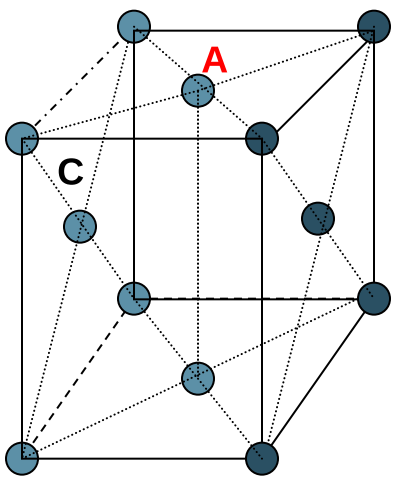
points ↓

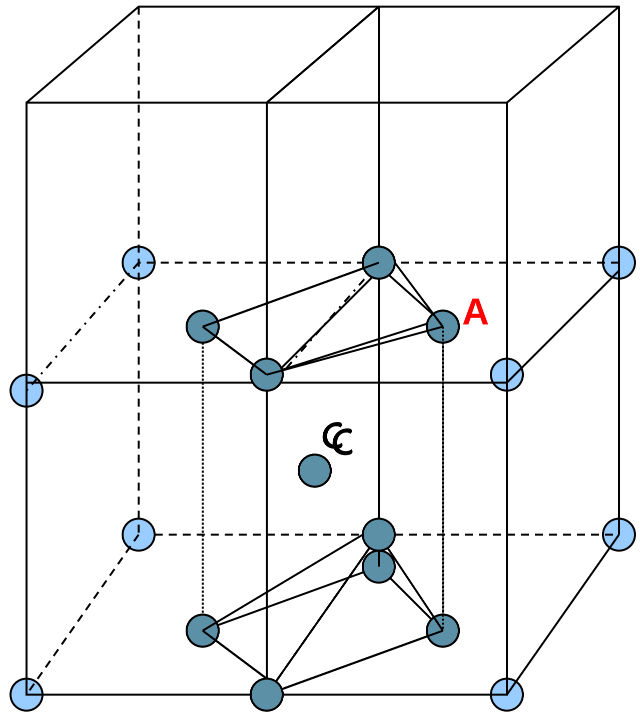
	Triclinic	Cubic	Tetragonal	Orthorobmic	Rhombohedral	Hexagonal	Monoclinic
P (primitve)	$\alpha, \beta, \gamma \neq 90°$ 		$a \neq c$ 	$a \neq b \neq c$ 	$\alpha, \beta, \gamma \neq 90°$ 	$a \neq c$ 	$\alpha \neq 90°$ $\beta, \gamma = 90°$ 
I (Body centered)			$a \neq c$ 	$a \neq b \neq c$ 			
F (Face centered)				$a \neq b \neq c$ 			
C (Single face centered)				$a \neq b \neq c$ 			$\alpha \neq 90°$ $\beta, \gamma = 90°$ 

Duplicated Bravais Lattice

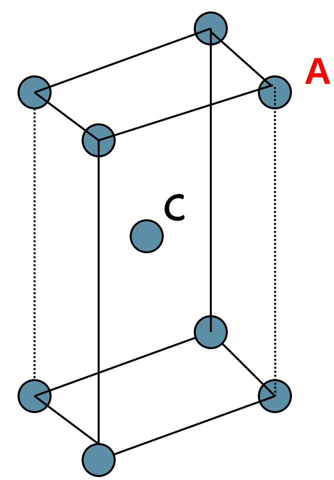
Unlucky Frankenheim (1842) counted 15 unit cells! Bravais pointed out that 2 cells were duplicated

Tetragonal face centered



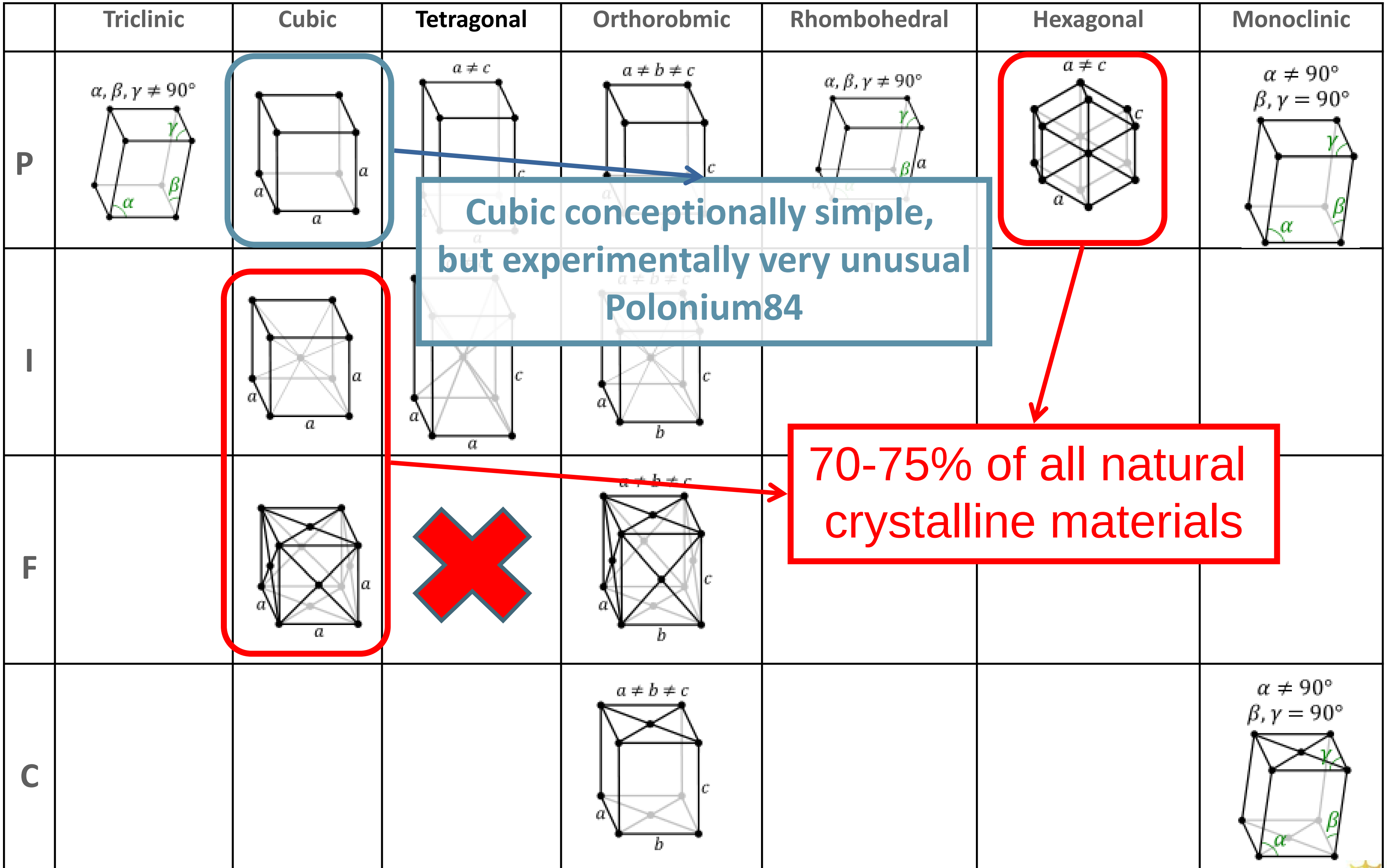


Tetragonal body centered



Tetragonal FC = Tetragonal BC

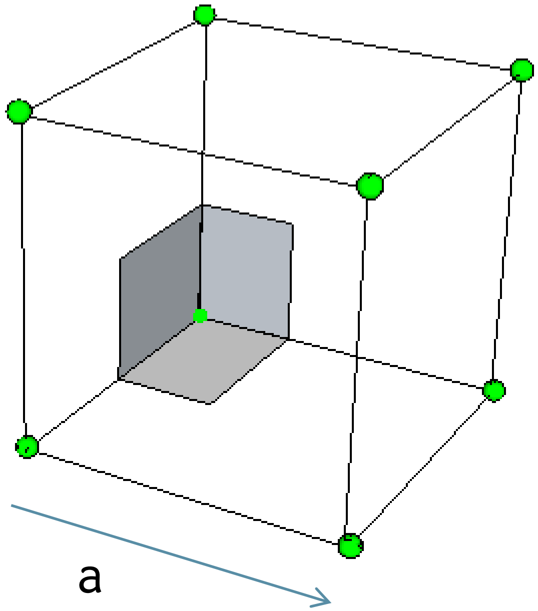
3 Dominant Bravais Lattices



- Course information
- Motivation for the course
- Current flow in semiconductors
- Types of material systems
- Classification of crystals
  - » Bravais Lattices
  - » Packing Densities
  - » Common crystals - Non-primitive cells
    - ✓NaCl, GaAs, CdS
  - » Surfaces

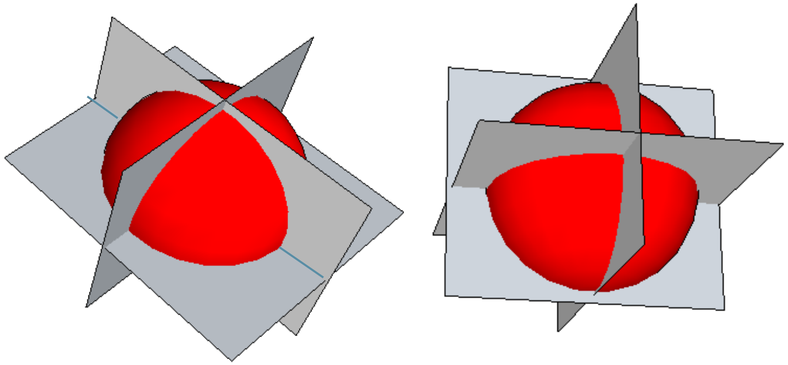
- Reference: Vol. 6, Ch. 1
- Helpful software: Crystal Viewer in ABACUS tool at nanohub.org

Simple Cubic Cubic Lattice: Number of atoms



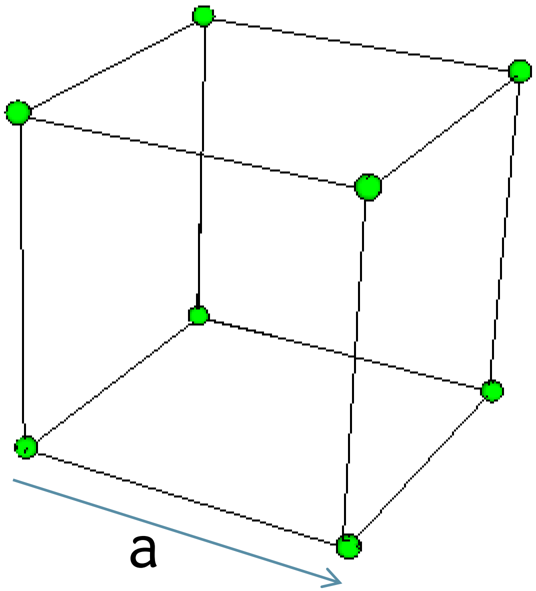
Points per cell
=1/8 points/corner x 8 corners
=1 Point/cell

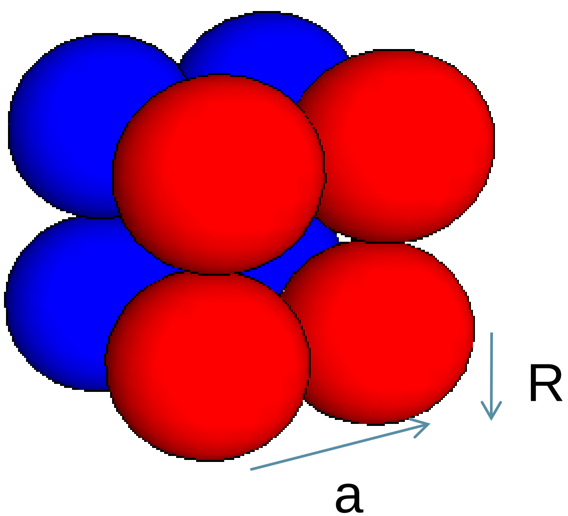
(depends on definition of cell)



Number density
= $(1/a^3)$ points/cm^3

(does not depend on cell definition)





Packing density
=volume filled/total volume

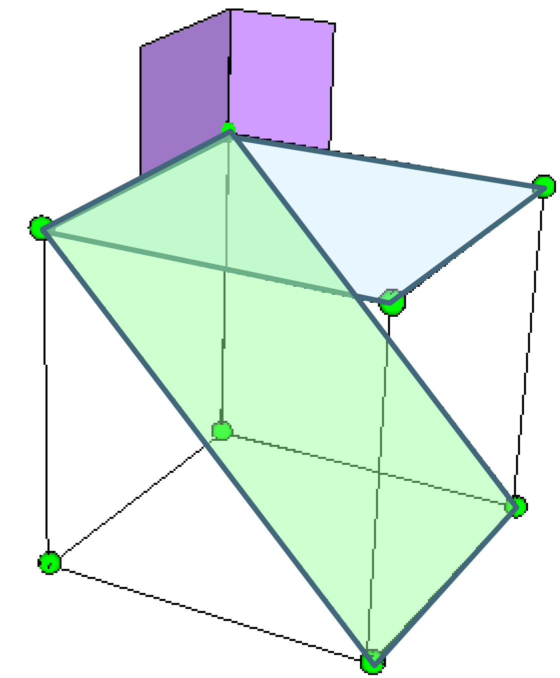
$R=a/2$ maximum radius
$V=(4/3)\pi R^3$ Volume of a sphere

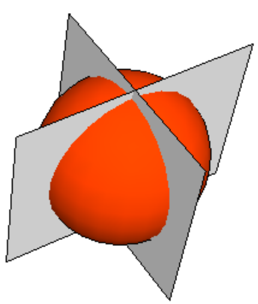
$P= (1/8)x(4/3)\pi R^3$ x (8 corners) $/a^3$

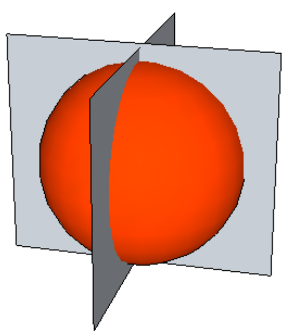
$=\pi/6$
~52%
(about HALF of the volume is EMPTY)
Typical for crystals and amorphous materials

(does not depend on cell definition)

Simple Cubic Cubic Lattice: Areal Density





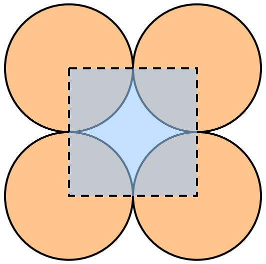


Surfaces are critical in semiconductors:
-Vertical stacking of materials
=> misalignment => dangling bonds => loose electrons
=> Different surface chemistry

Areal Density

=(1/4 per corner) x (4 corners)/a^2

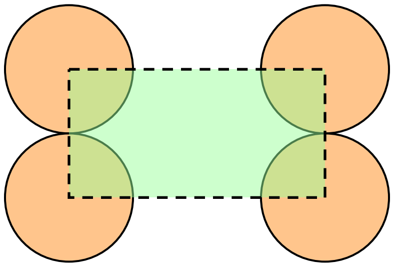
=$1/a^2$ cm^{-2}



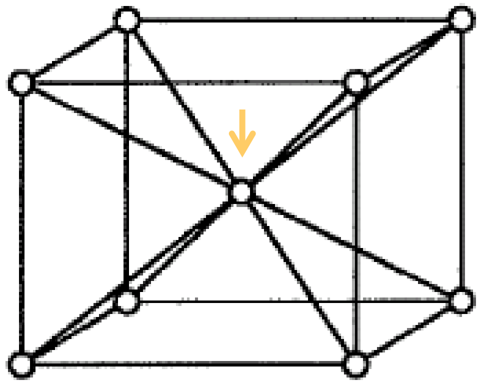
Areal density (face diagonal)

= (1/4 points/corner) x (4 corners)/$\sqrt{2}a^2$ cm^{-2}

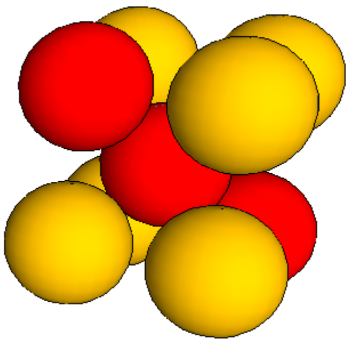
~$0.7/a^2$ cm^{-2}

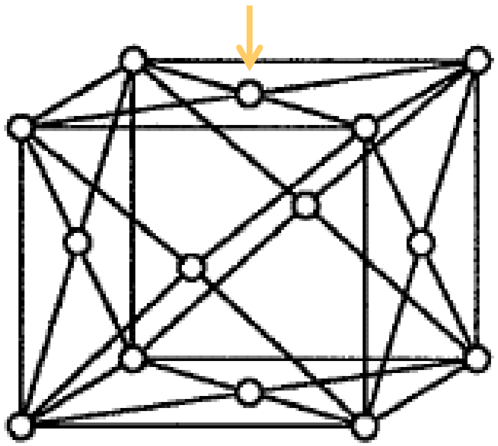


BCC and FCC lattices

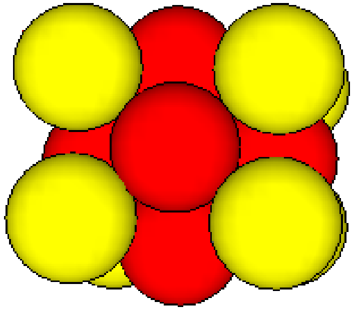


Points per cell
= 1/8 x 8 @corners
+ 1 @inside
=2

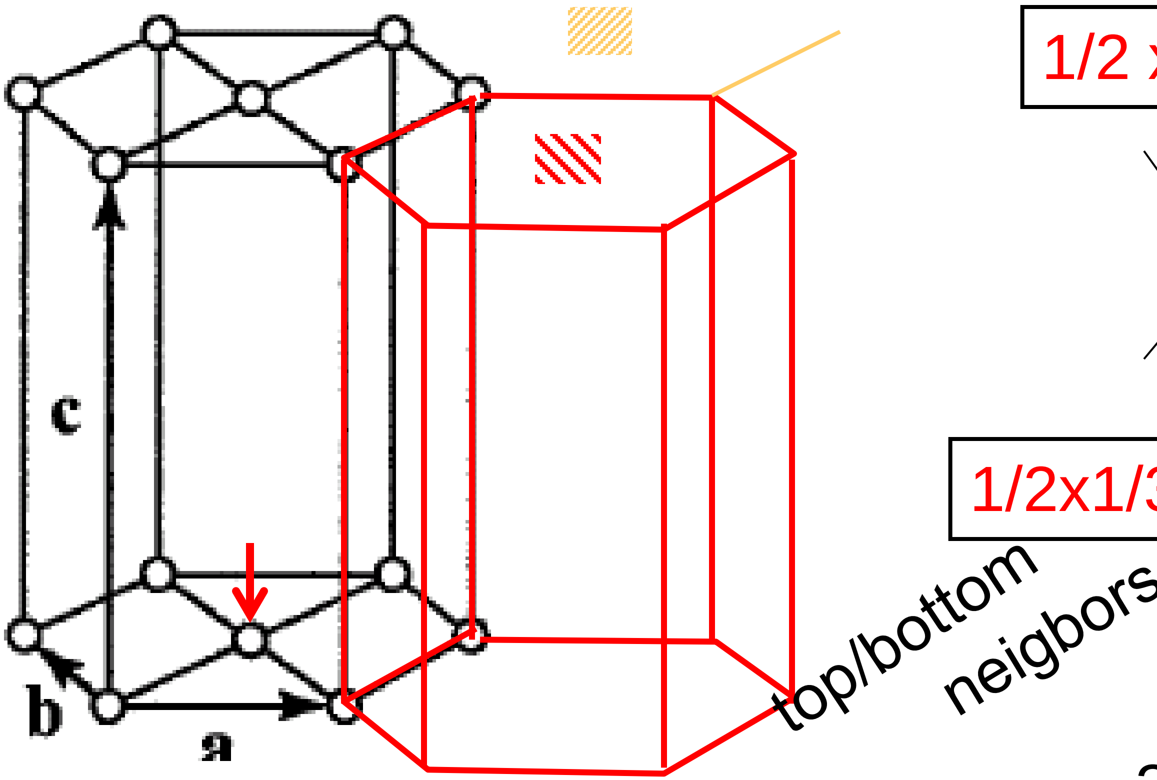




Points per cell
= 1/8 x 8 @corners
+ 1/2 x 6 @faces
=4

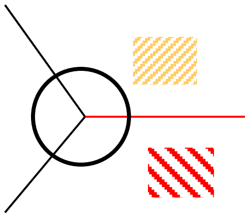


Hexagonal Closed-Packed



Points per cell

1/2 x 2 @faces =1



1/2x1/3 x 12 @corners =2

3 points/cell

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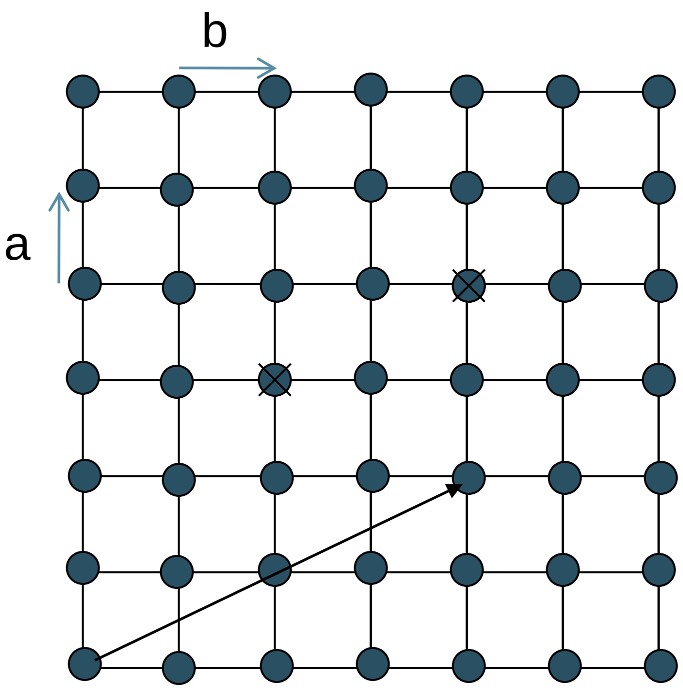
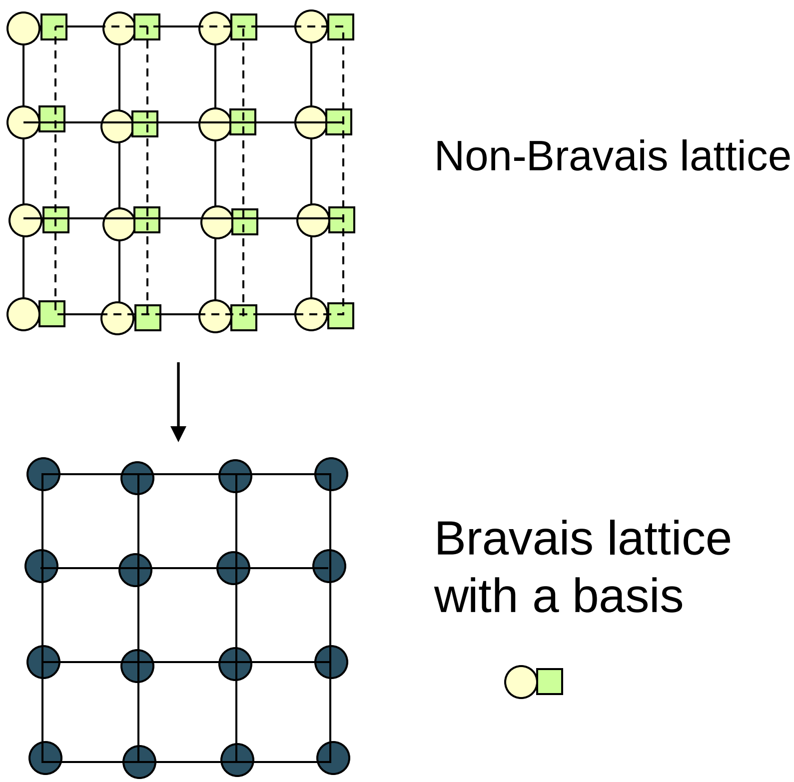
In a Bravais lattice, every point has the same environment as every other point (same number of neighbors, next neighbors, …)

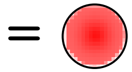


$$R = h\vec{a} + k\vec{b}$$



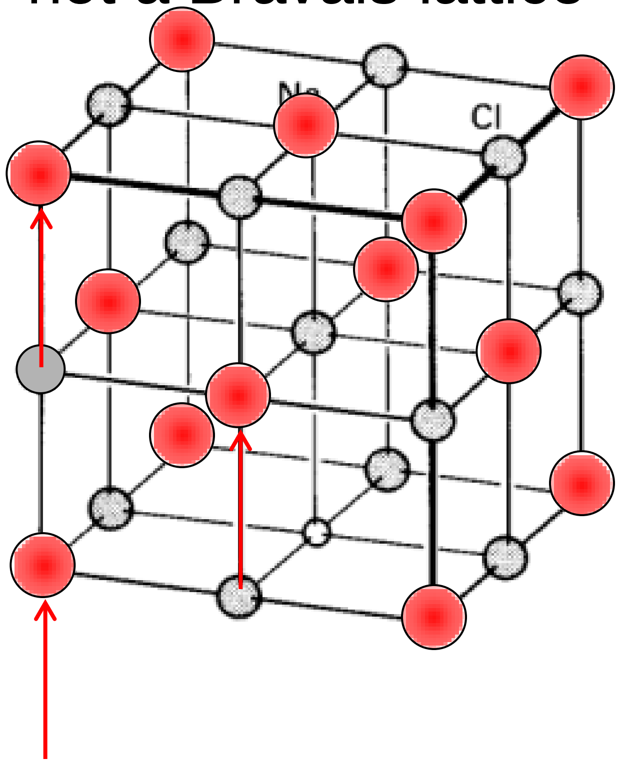
Rock-Salt as FCC lattice

NaCl is normal household cooking salt
We see the crystals every day – what is the crystal structure?
At first glance it looks like a simple cubic cell
⇒one atom on each corner
⇒But they are different => not a Bravais lattice

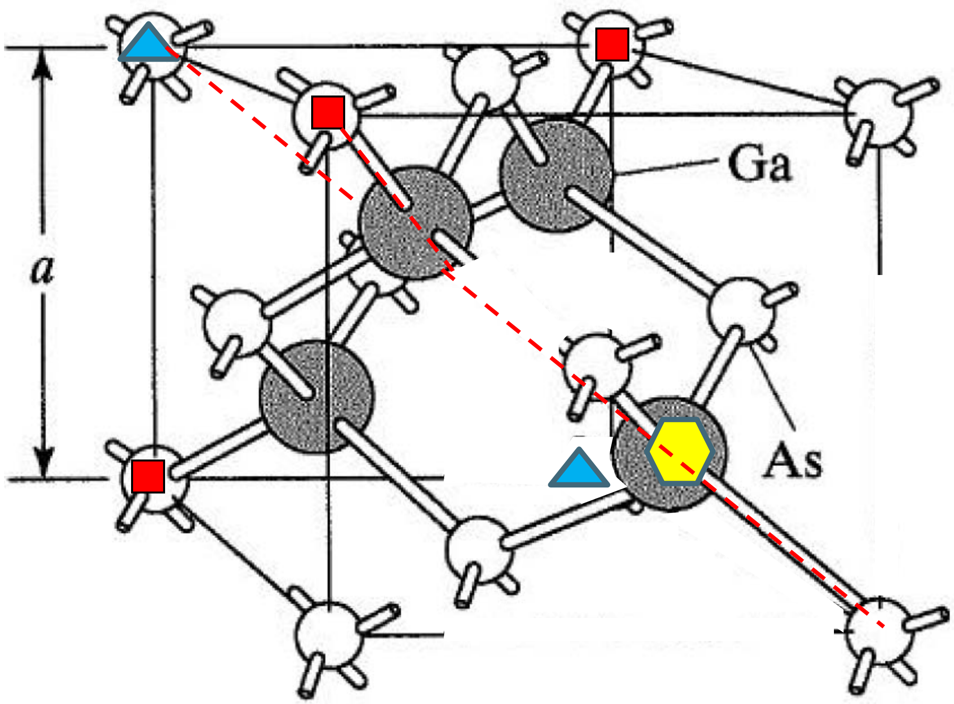


a basis
of 2 atoms

arranged in
FCC

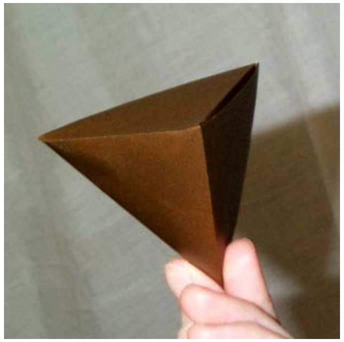


For more discussion, see Kittel and Ashcroft/Mermin

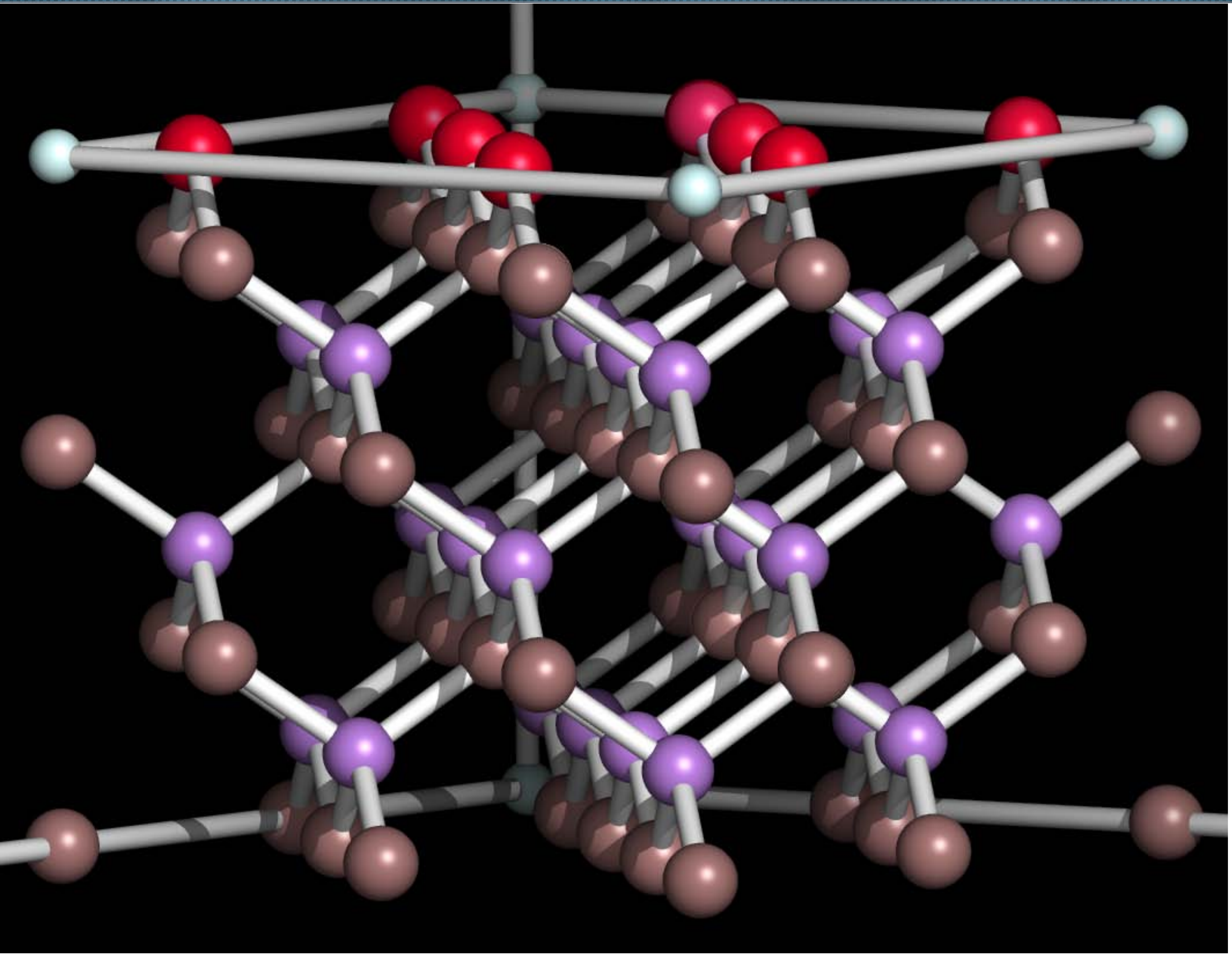


Atoms/cell=(1/8)x8 + (1/2)x6 + 4=8

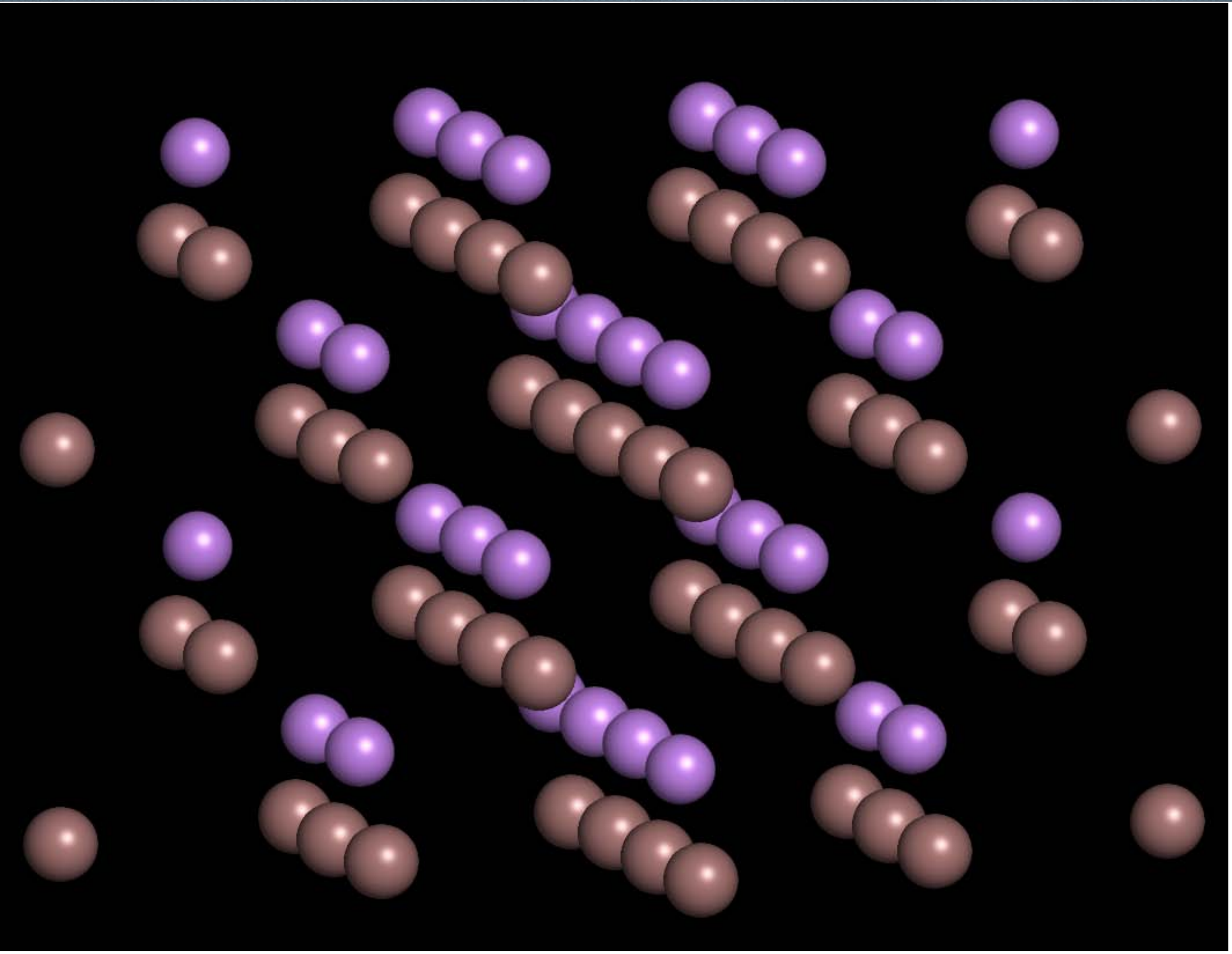
Tetrahedral structure



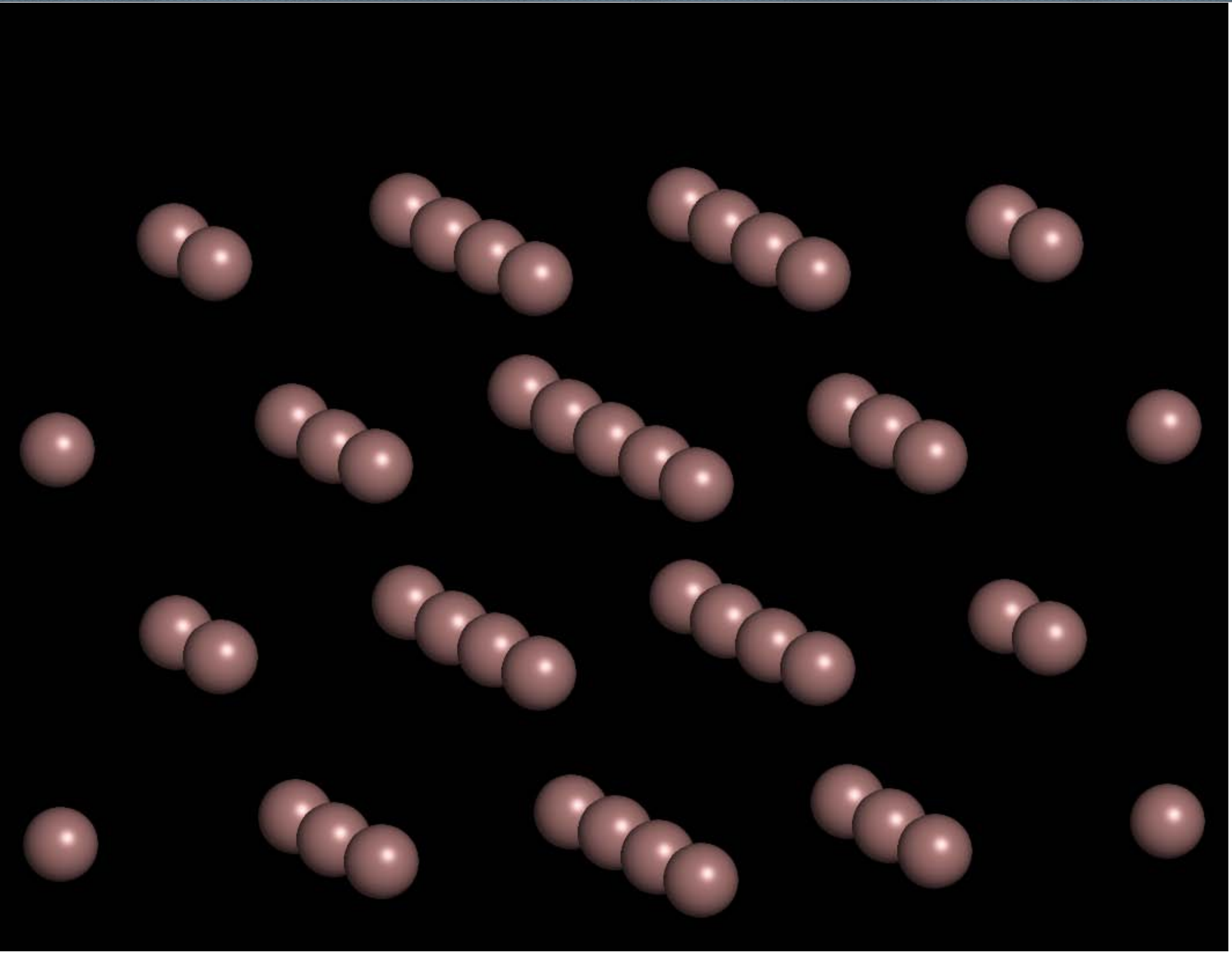
GaAs Crystal Plotted in Crystal Viewer

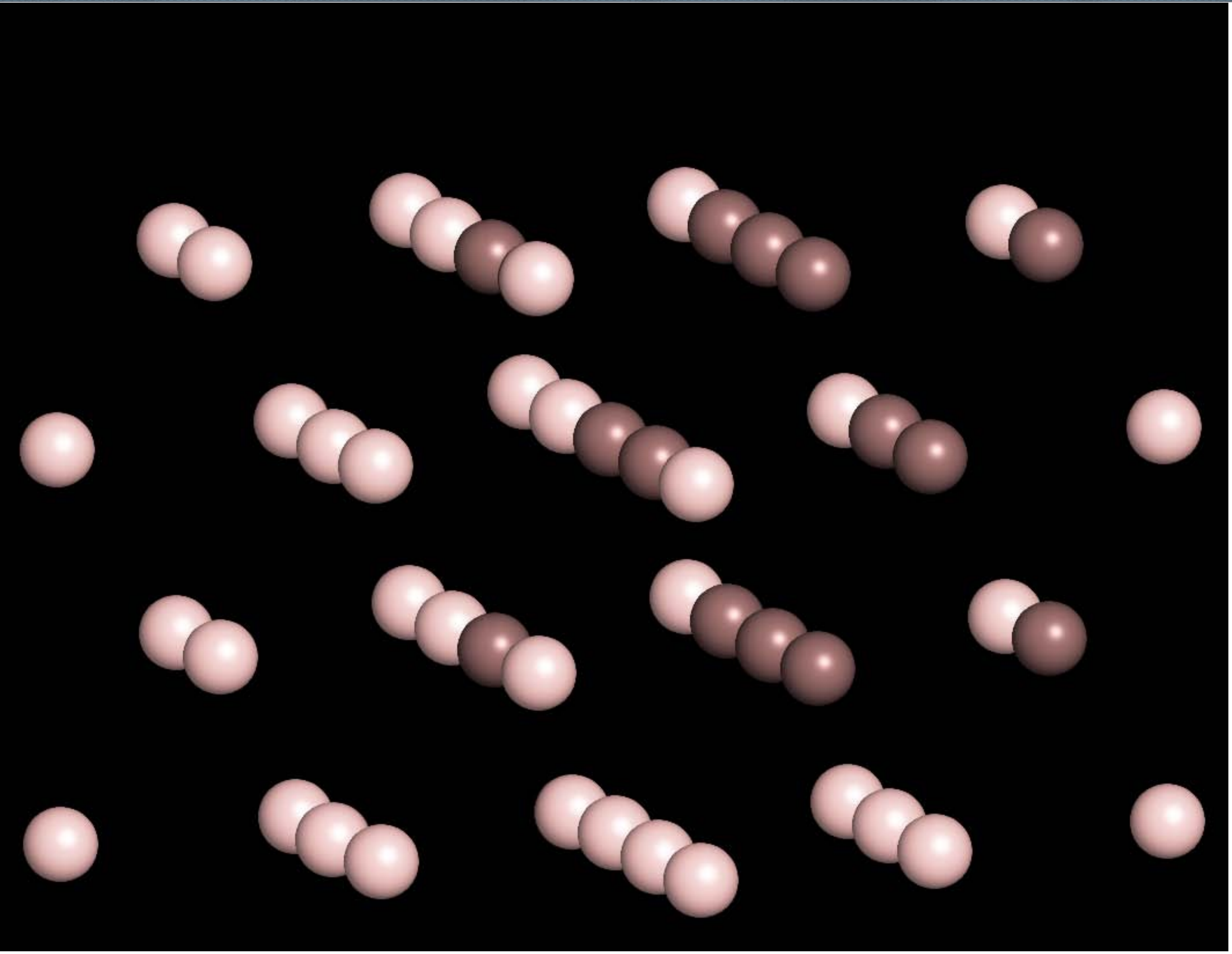


GaAs Crystal Without Bonds

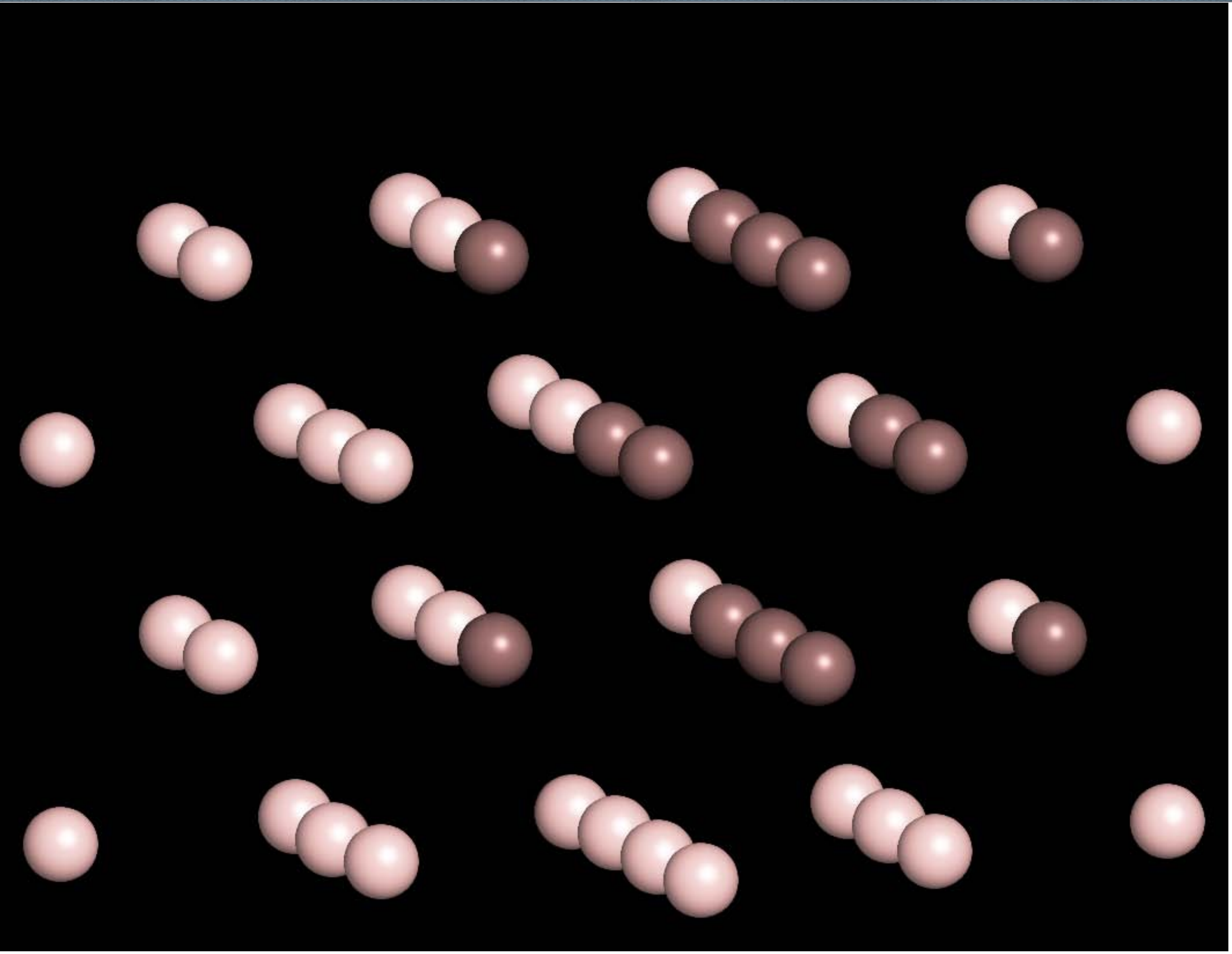


GaAs Crystal Just One Species

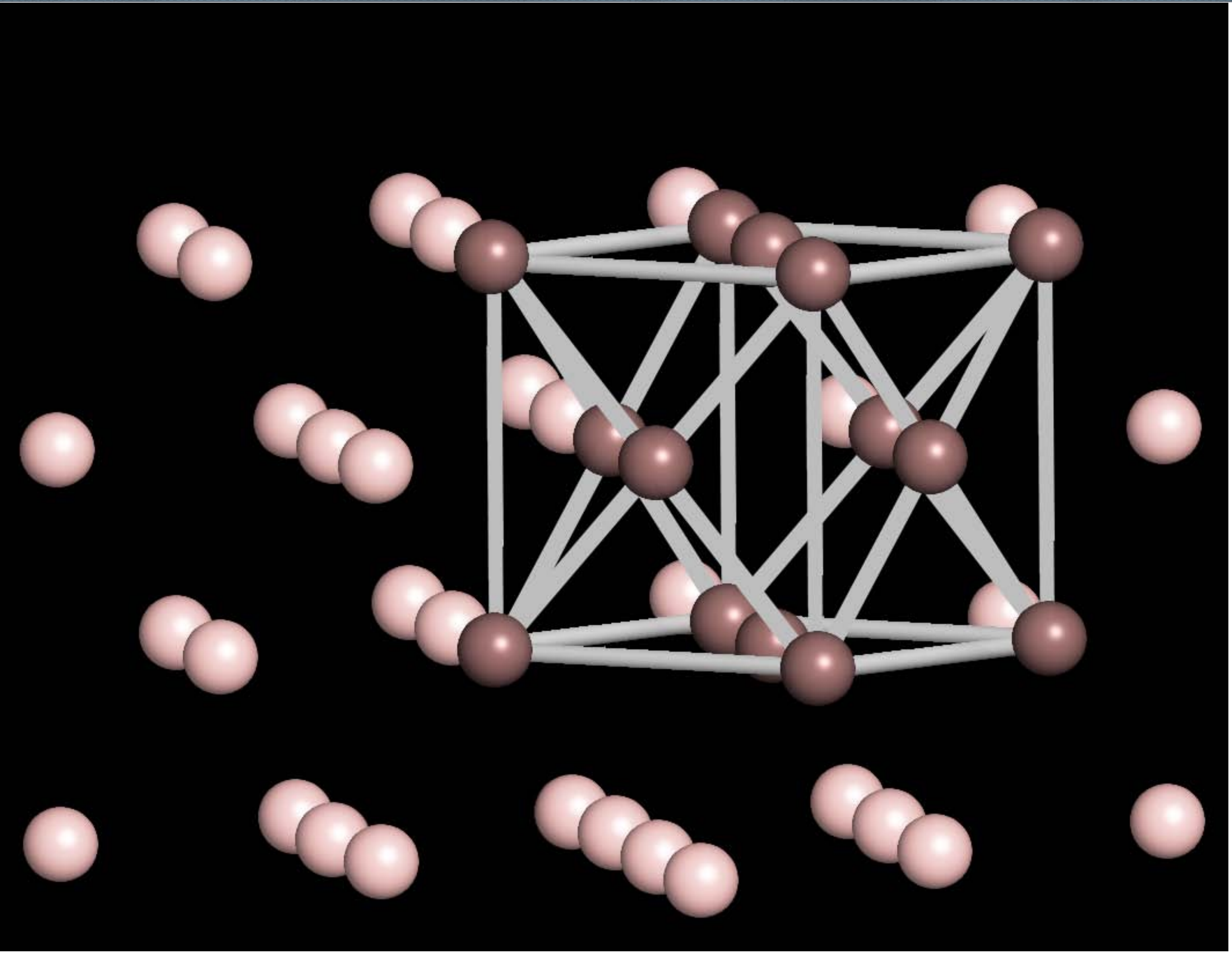




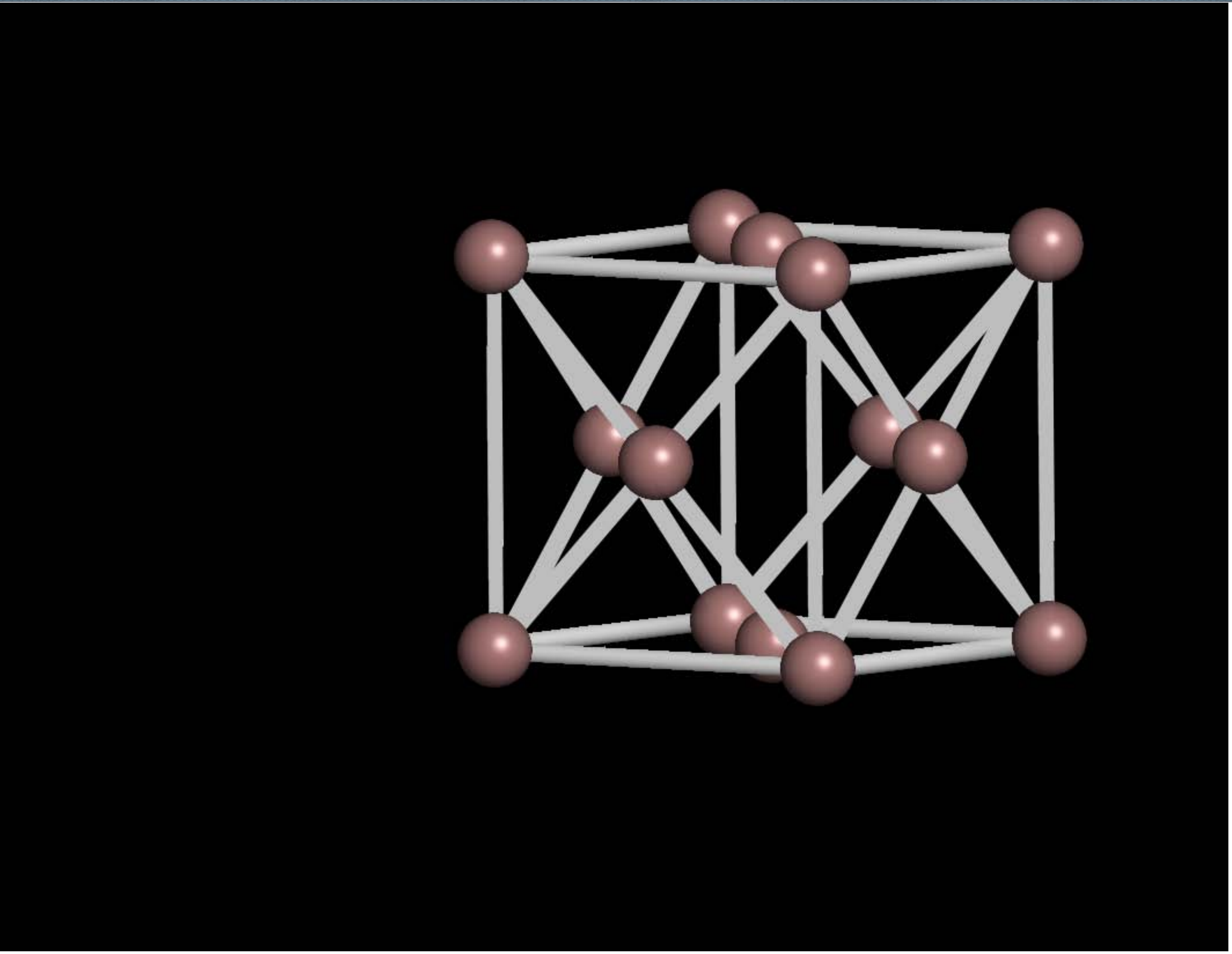
GaAs Crystal Just One Species
Focus on Few - Take out a Few



GaAs Crystal Just One Species A FCC Cell!

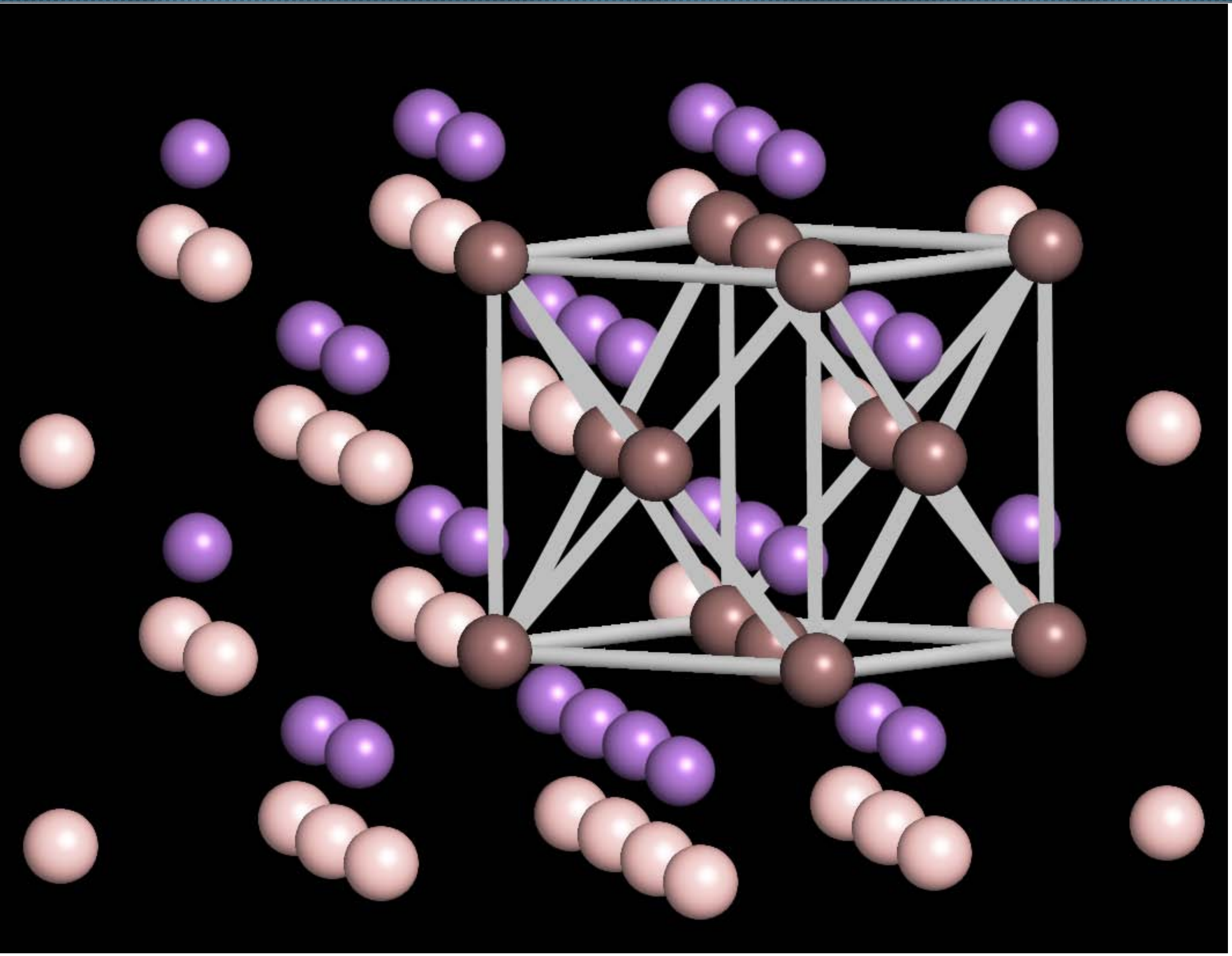


- FCC cell – 4 atoms per unit cell



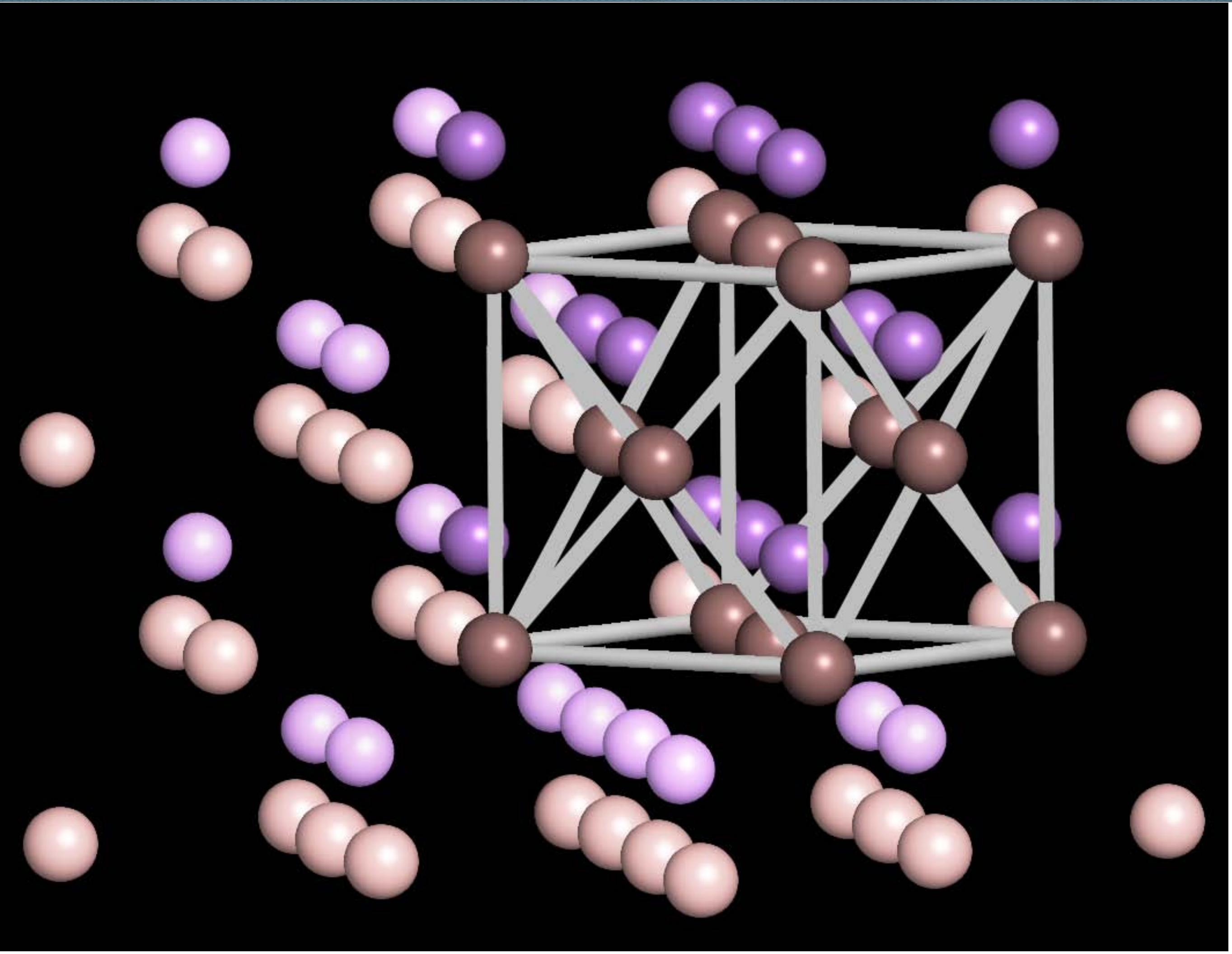
• FCC cell – 4 atoms per unit cell

GaAs Crystal Both Species



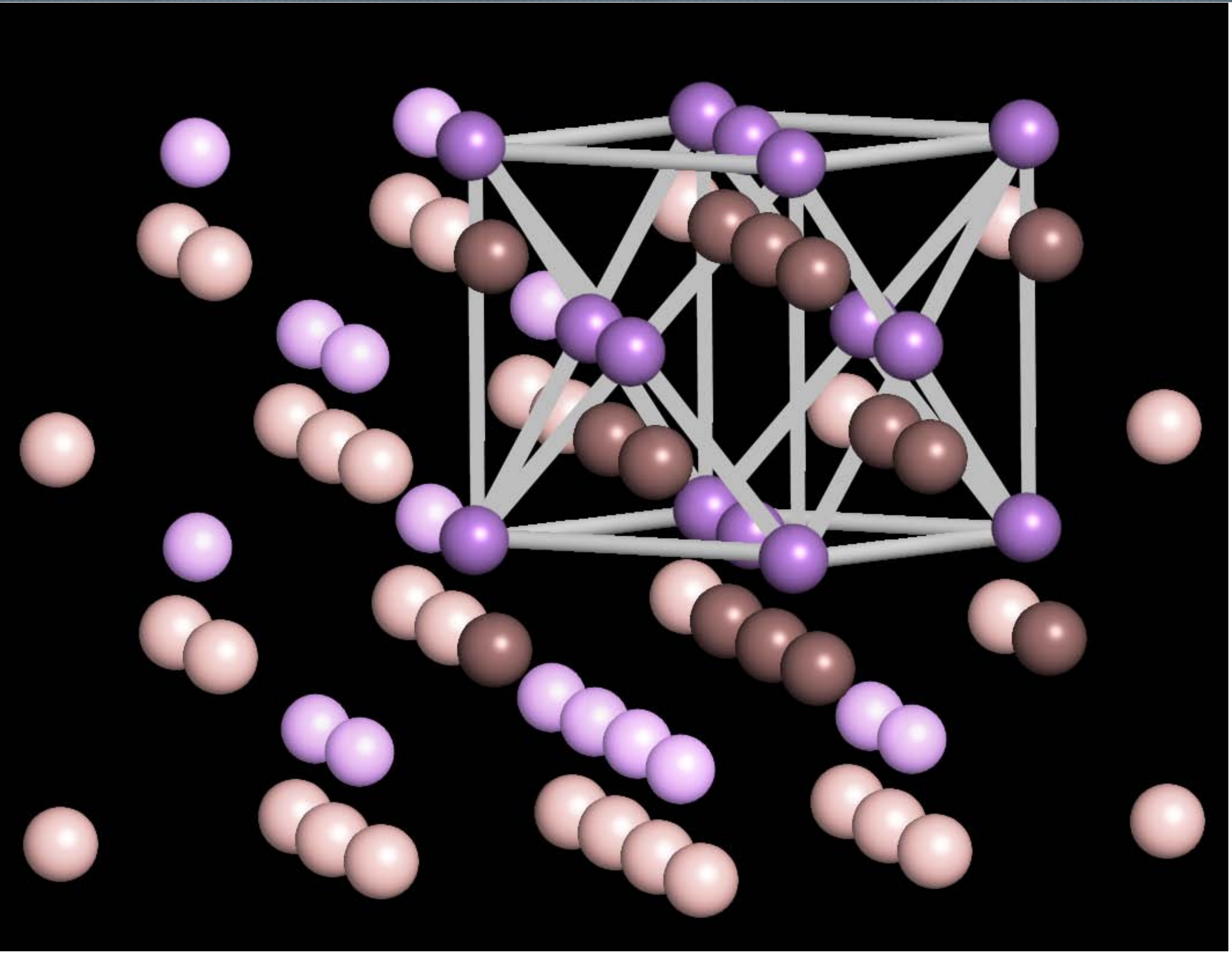
• FCC cell – 4 atoms per unit cell – brown species

GaAs Crystal Both Species



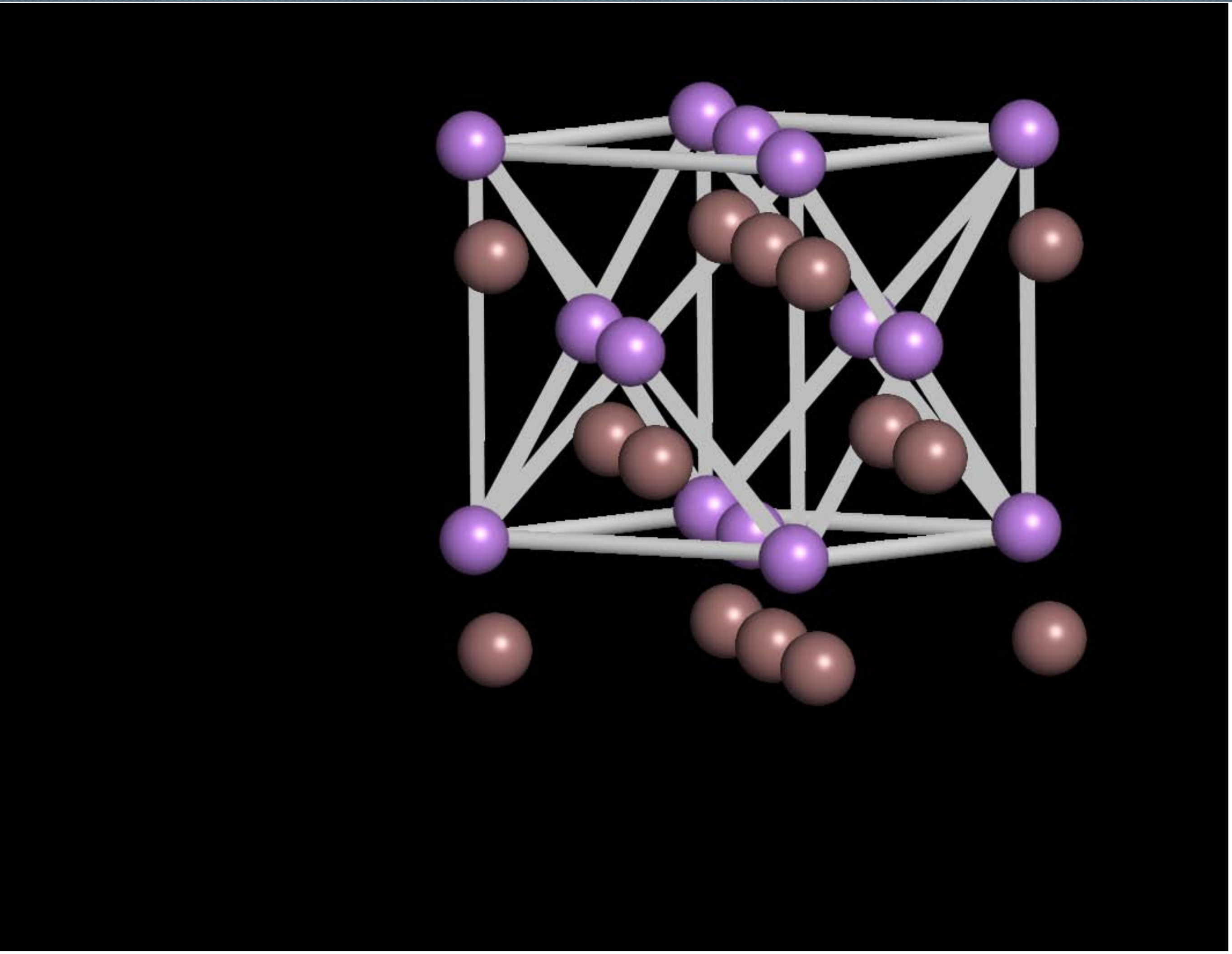
- FCC cell – 4 atoms per unit cell – brown species
- Focus on a few of the “blue species”

GaAs Crystal Both Species



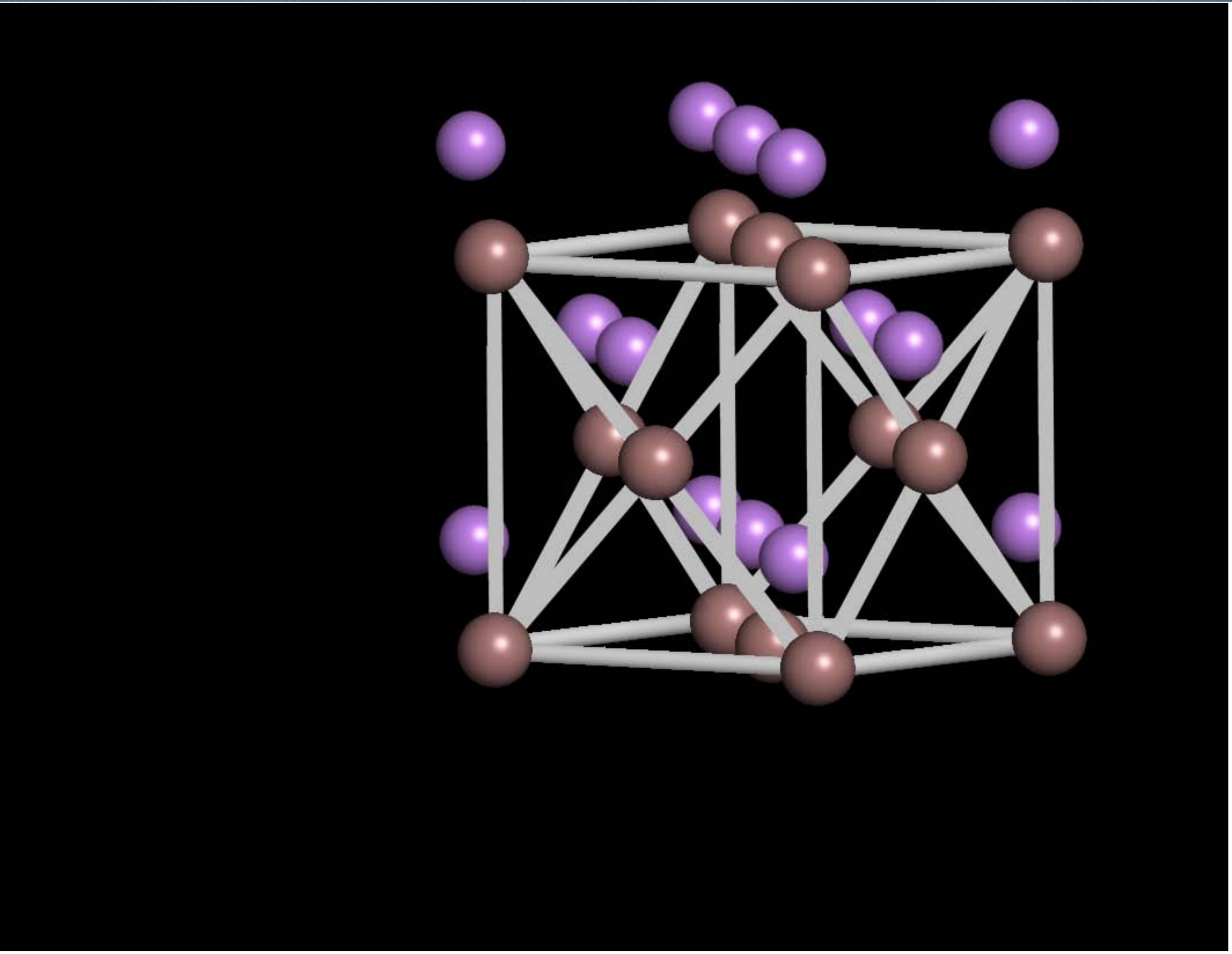
- FCC cell – 4 atoms per unit cell – brown species
- FCC cell – 4 atoms per unit cell – purple species

GaAs Crystal Both Species



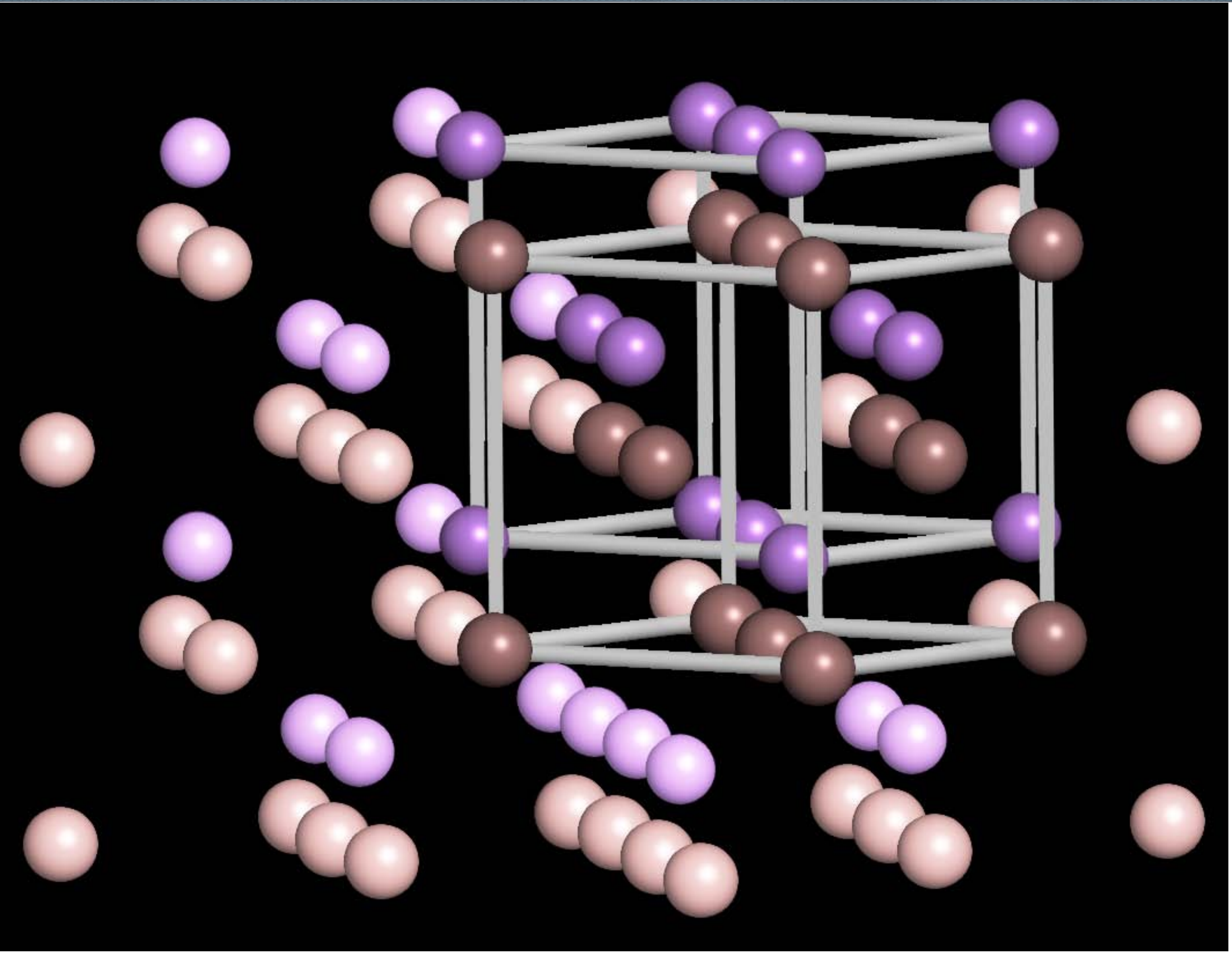
- FCC cell – 4 atoms per unit cell – brown species
- FCC cell – 4 atoms per unit cell – purple species

GaAs Crystal Both Species



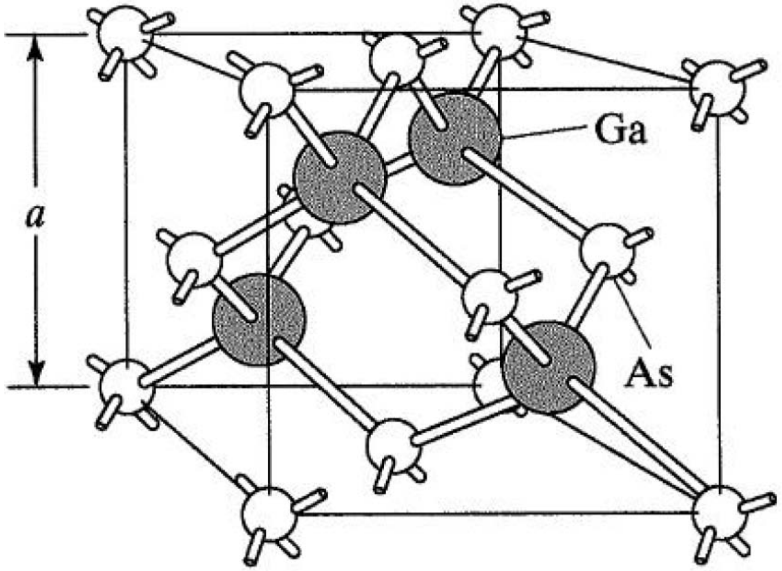
- FCC cell – 4 atoms per unit cell – brown species
- FCC cell – 4 atoms per unit cell – purple species

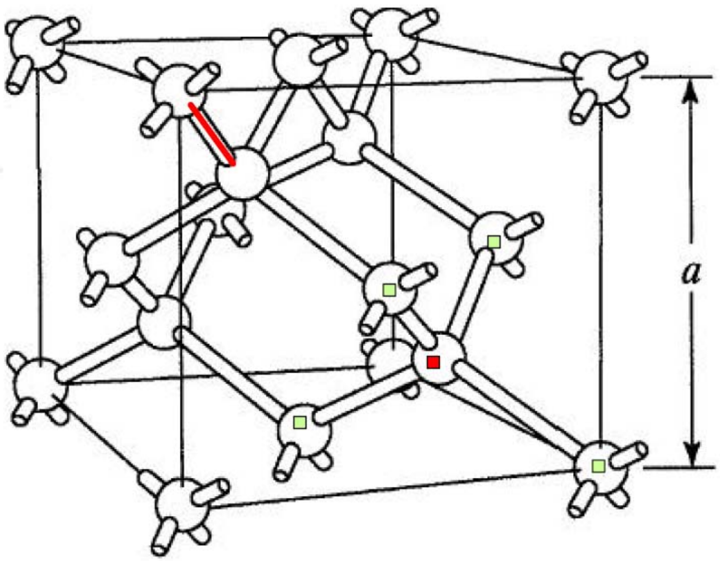
GaAs Crystal - 2 FCC



• Zincblende – 2 FCC bases – separated by [¼ ¼ ¼]

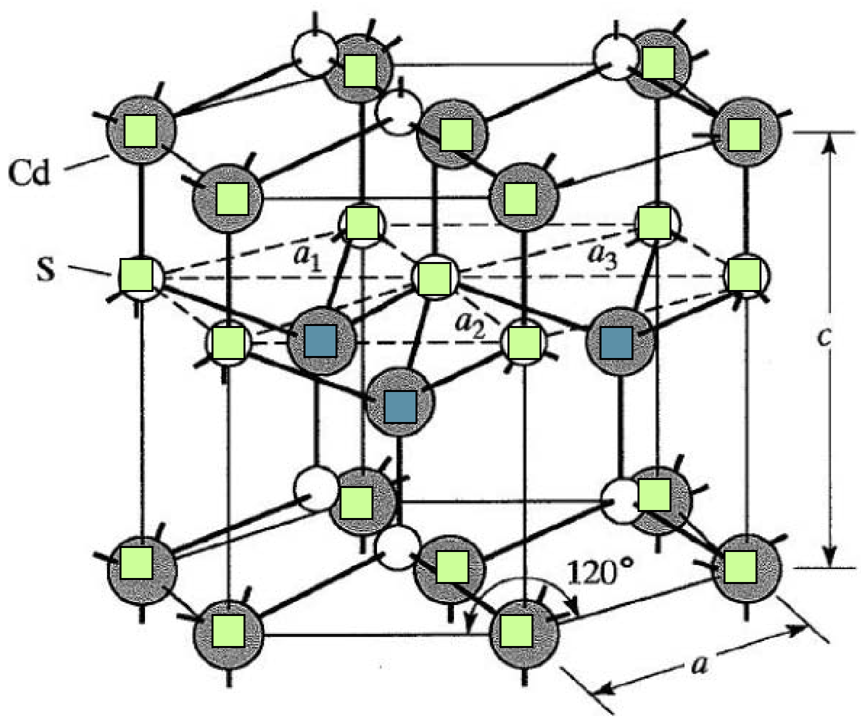
Diamond FCC Lattice for Silicon



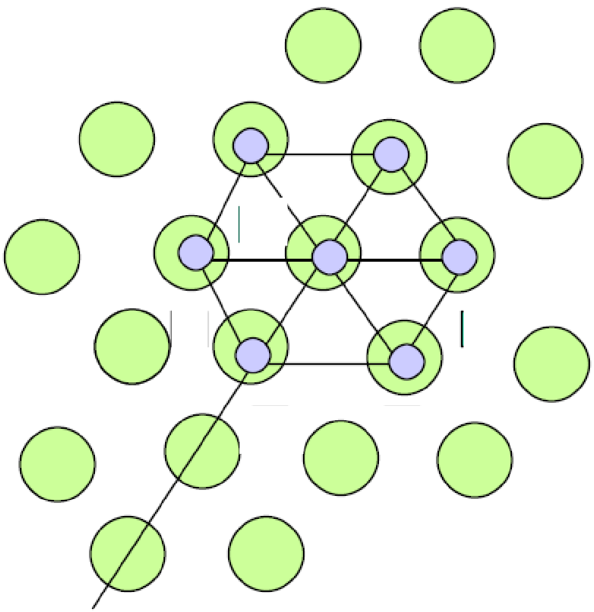


- Zincblende – GaAs - 2 FCC bases – separated by [¼ ¼ ¼]
- Diamond – Si - 2 FCC bases – separated by [¼ ¼ ¼]

Hexagonal Closed-Packed for CdS



Focus on (Cd) …



(Cd) atoms/cell=
(1/6)x12 + (1/2)x2 + 3=6

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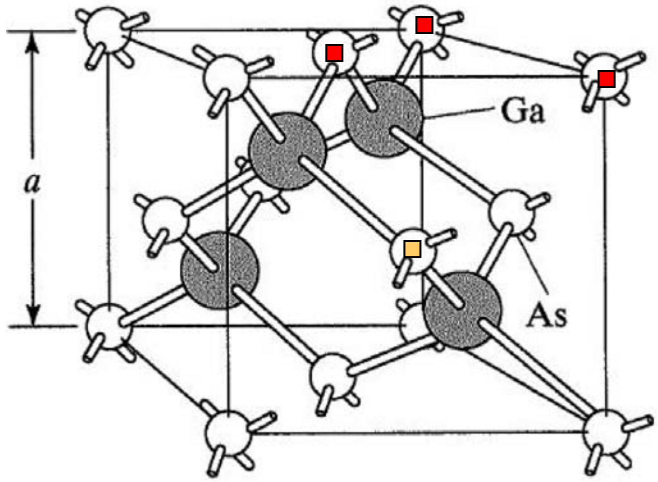
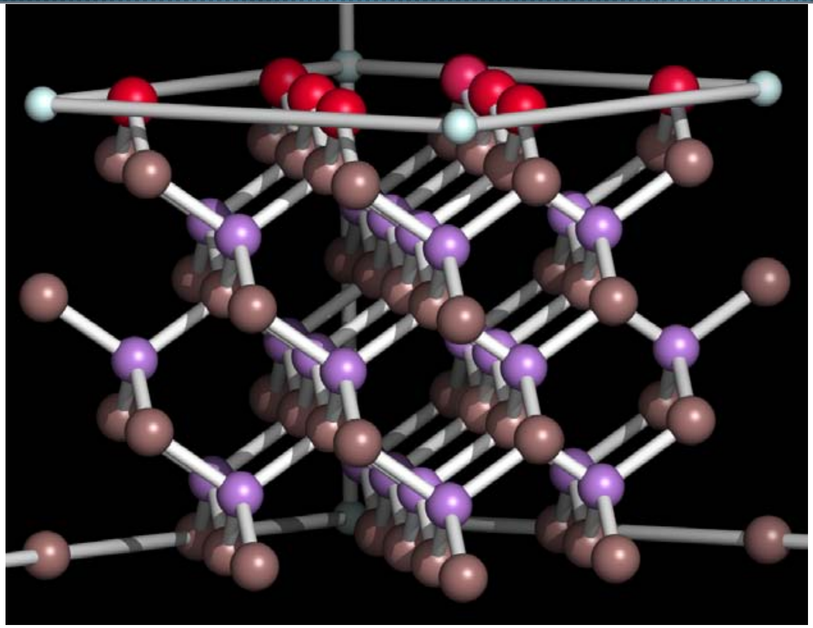
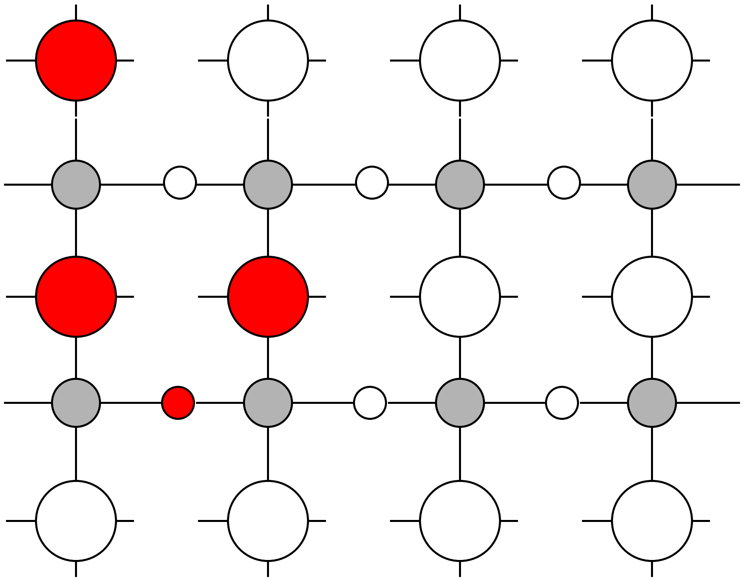
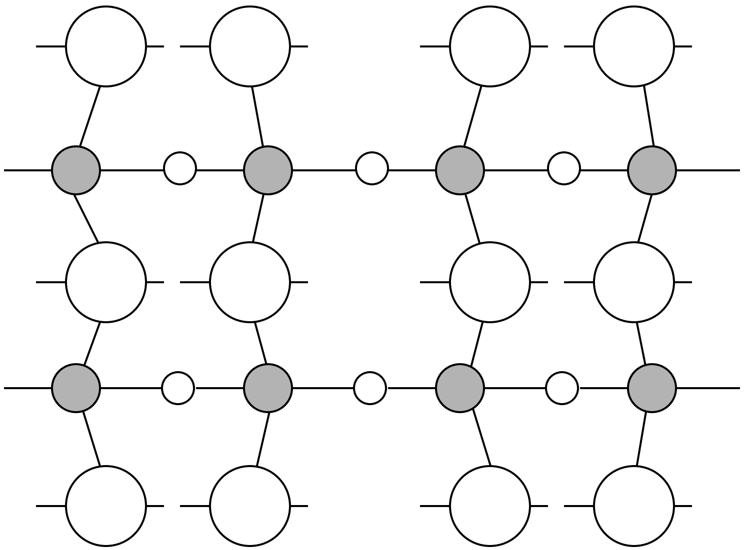
Surface Reconstruction

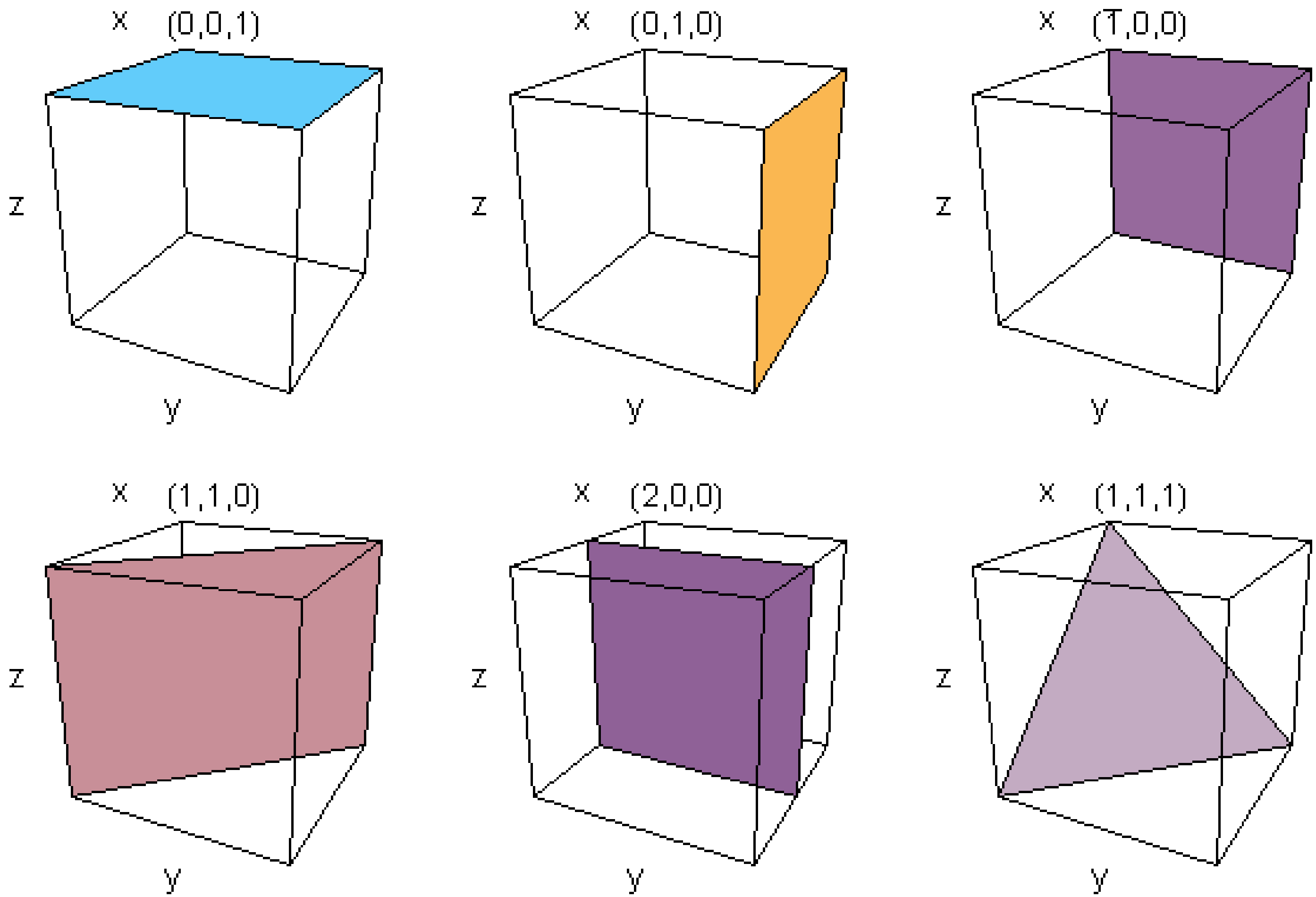




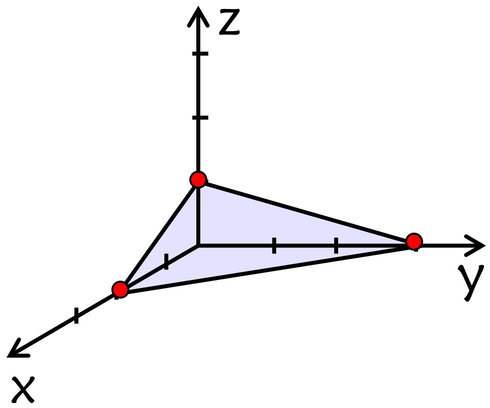




Miller-Indices and Definition of Planes



Miller Indices: Rules



1. Set up axes along the edges of unit cell

2. Normalize intercepts …. 2, 3, 1

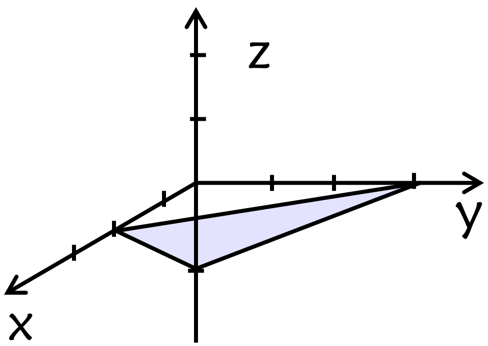
3. Invert/rationalize intercepts … 1/2, 1/3, 1

   3/6, 2/6, 6/6

4. Enclose the numbers in curvilinear brackets
   (326)

Few more rules ...

Negative Intercept



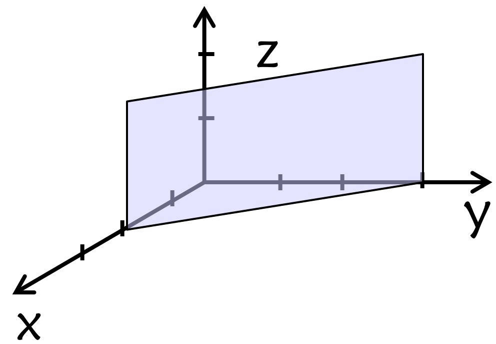
2, 3, -2

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

3, 2, -3

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

Intercept at infinity



2, 3, ∝

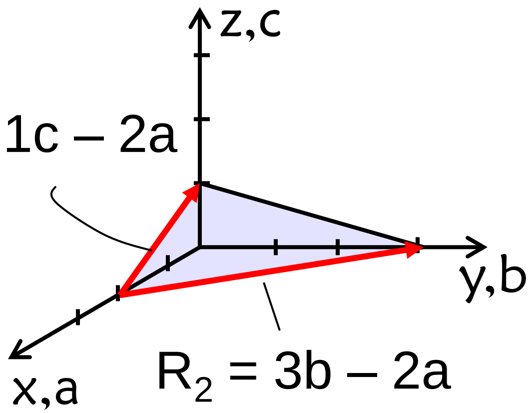
1/2, 1/3, 0

3, 2, 0

(3 2 0)

Where does Miller Indices come from ?

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

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

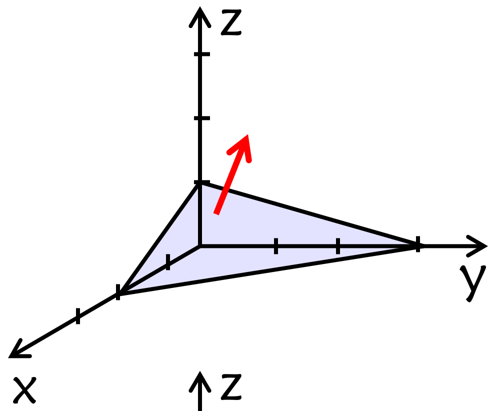
Vector indices same as Miller indices !

(326) vs. [326]

Specification of vectors normal to a particular plane!

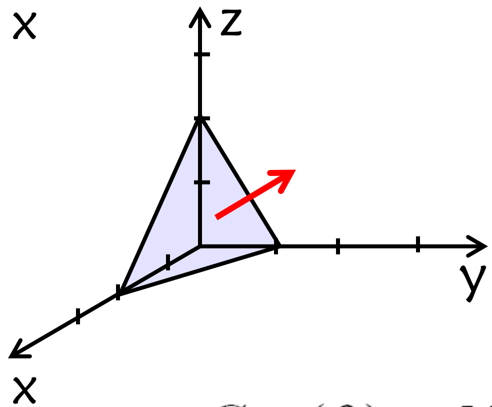
⇒Angle between two vectors

⇒Dot product / inner product between two vectors



Unit vector normal to plane 1:

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



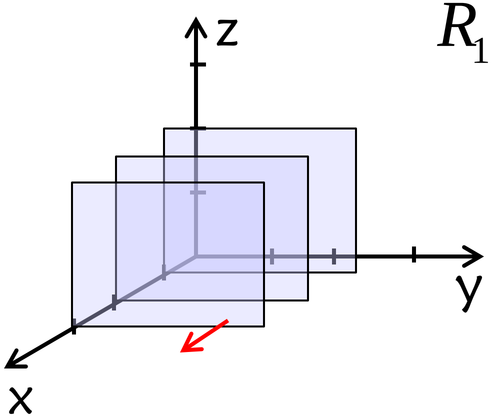
Unit vector normal to plane 2:

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

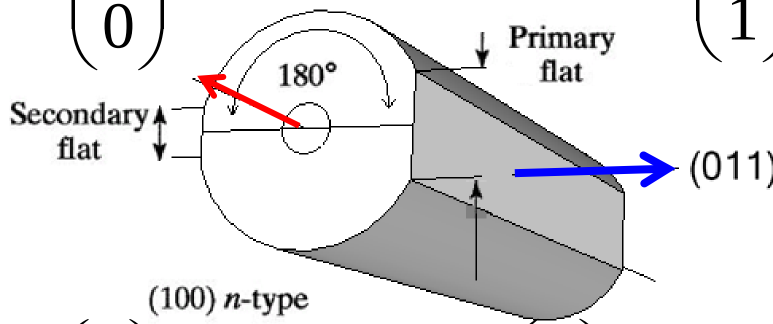
$$Cos(\theta) = N_1 \bullet N_2$$

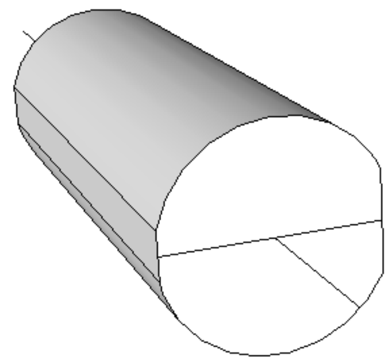
$$= (h_2 h_1 + k_2 k_1 + l_2 l_1)/(h_2^2 + k_2^2 + l_2^2)^{1/2}(h_2^2 + k_2^2 + l_2^2)^{1/2}$$

Examples ...



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





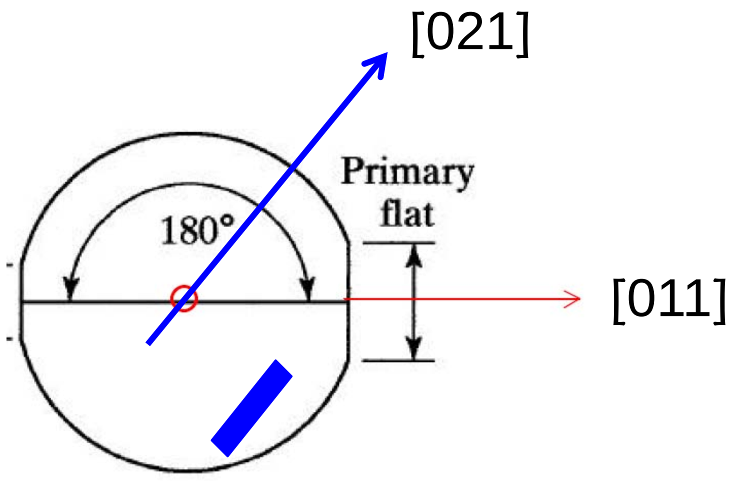
$$\vec{N}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} / \sqrt{1} \qquad \vec{N}_2 = \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} / \sqrt{2}$$

cos(θ)=(1x0+0x1+0x1)/(√1x√2) = 0

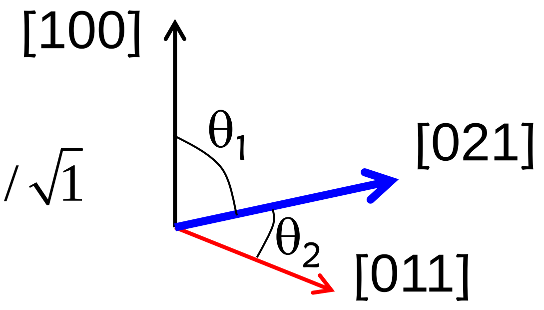
so θ=90 degrees

(011) surface is normal to (100) surface

Example: Find the [021] direction



(100) *n*-type



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

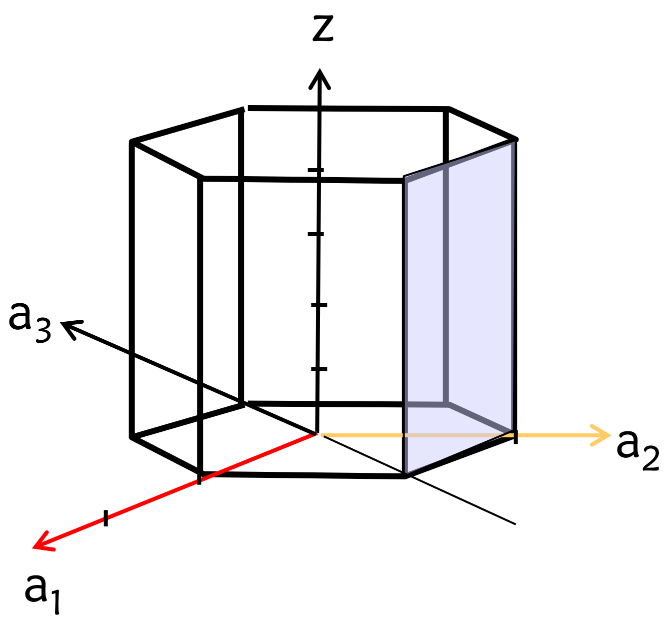
$$\vec{N}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} / \sqrt{1}$$

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

$N_1 \bullet T = \cos(\theta_1) = (1\text{x}0+0\text{x}2+0\text{x}1)/(1\text{x}\sqrt{5}) = 0$, so θ=90 degrees
[021] vector lies on (100) plane.

$N_2 \bullet T = \cos(\theta_2) = (0\text{x}0+2\text{x}1+1\text{x}1)/(\sqrt{5}\ \sqrt{2}) = 3/\sqrt{10}$, 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.

Outline

- Course information
- Motivation for the course
- Current flow in semiconductors
- Types of material systems
- Classification of crystals
  - » Bravais Lattices
  - » Packing Densities
  - » Common crystals - Non-primitive cells
    - ✓NaCl, GaAs, CdS
  - » Surfaces

- Reference: Vol. 6, Ch. 1
- Helpful software: Crystal Viewer in ABACUS tool at nanohub.org

Summary

1. To understand transport in semiconductors, we need to know carrier density (n) and carrier velocity (v). In order to find these quantities, we need to understand the chemical composition and atomic arrangements.

2. 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.

3. Silicon, GaAs, PbS do not have simple Bravais lattice; but they have Bravais lattice with basis.

4. 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. In is useful to to review some identities of vector calculus to such calculations involving crystal planes.