Section 3 – Crystals

3.3 Density Definitions and Applications to Common Materials

Gerhard Klimeck

gekco@purdue.edu

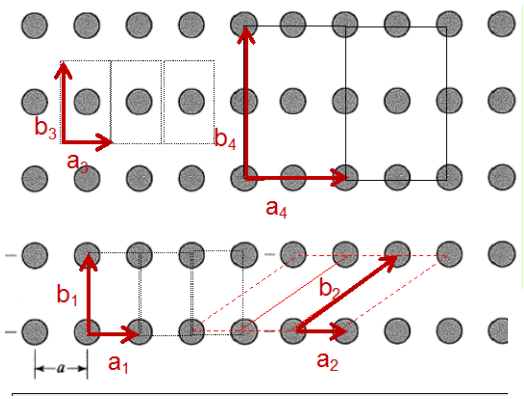
PURDUE UNIVERSITY

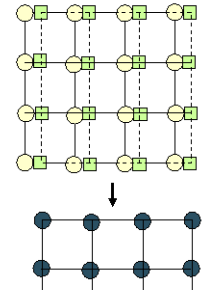
School of Electrical and Computer Engineering

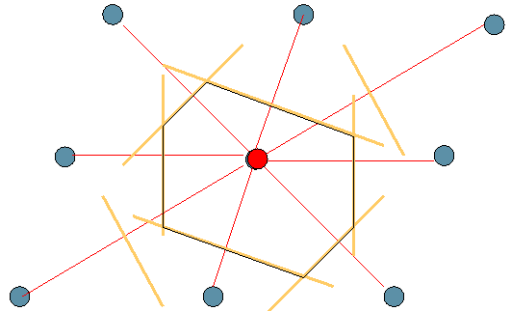
Section 3
Crystals

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

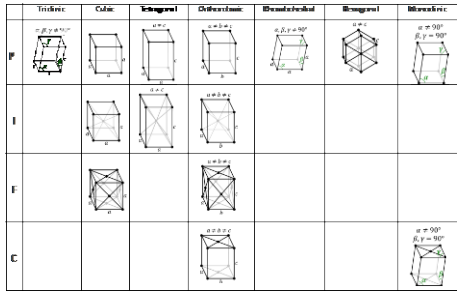






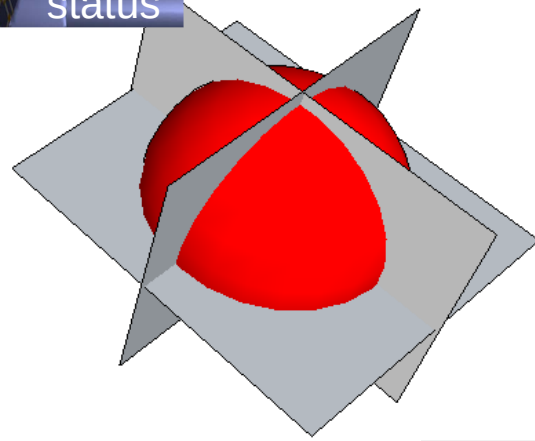
One Video Segment

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



One Video Segment

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

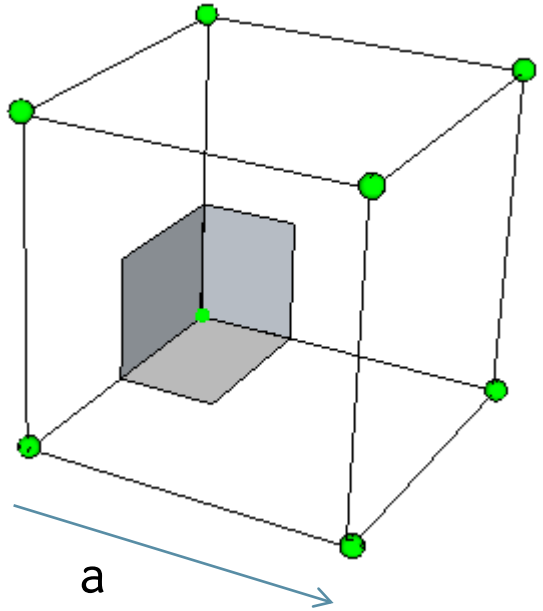


One Video Segment

- 3.4 Surfaces, Miller Index

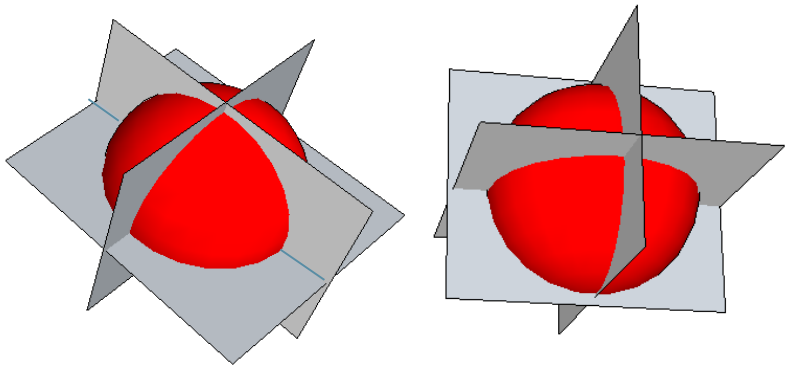
Reference: Vol. 6, Ch. 1, ABACUS tool at nanohub.org/tools/abacus and "Crystal Viewer Lab, https://nanohub.org/resources/crystalviewer

Simple Cubic Cubic Lattice: Number of atoms



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

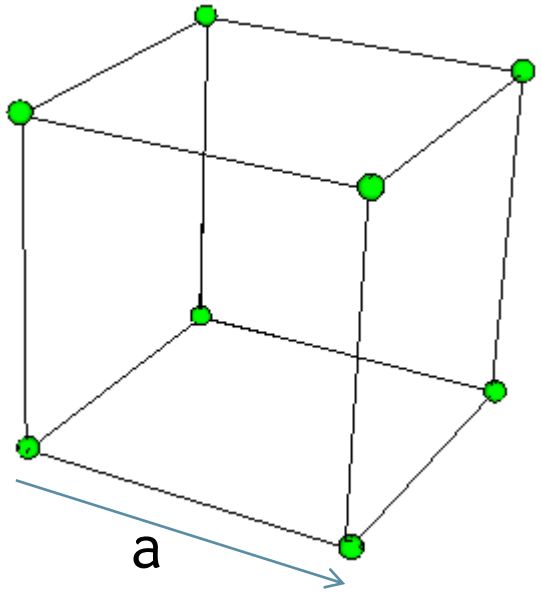
(depends on definition of cell)

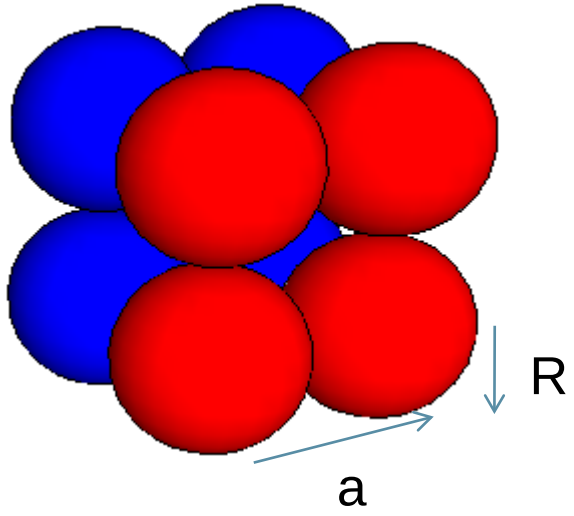


Number density
= $(1/a^3)$ points/cm^3

(does not depend on cell definition)

Simple Cubic Cubic Lattice: Packing Density





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) $/a^3$

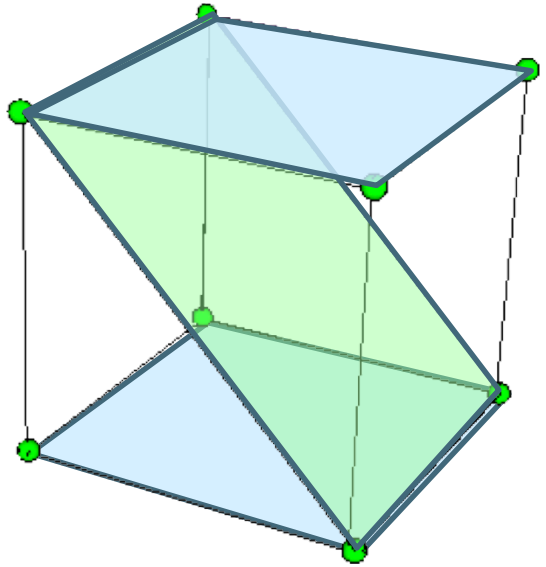
$=\pi/6$

~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

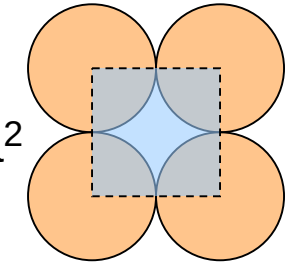


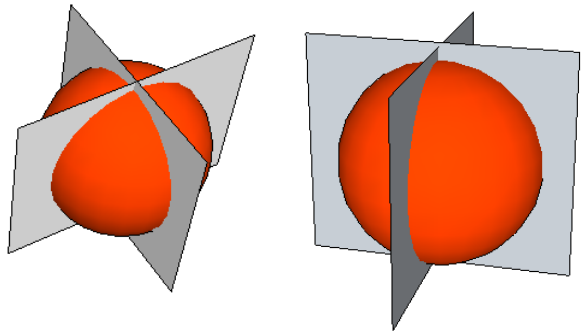
Surfaces are critical in semiconductors:
-Vertical stacking of materials
=> misalignment => dangling bonds => loose electrons
=> Different surface chemistry

Areal Density

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

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

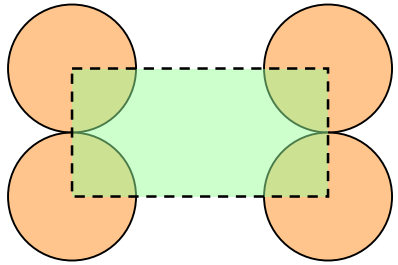




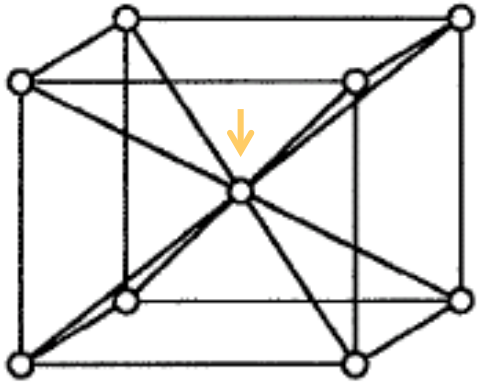
Areal density (face diagonal)

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

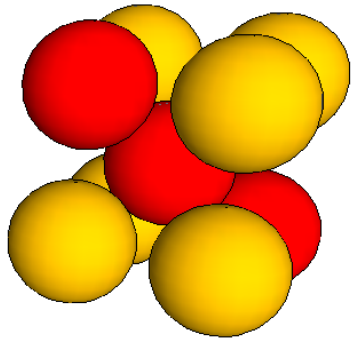
~$0.7/a^2$ cm^{-2}

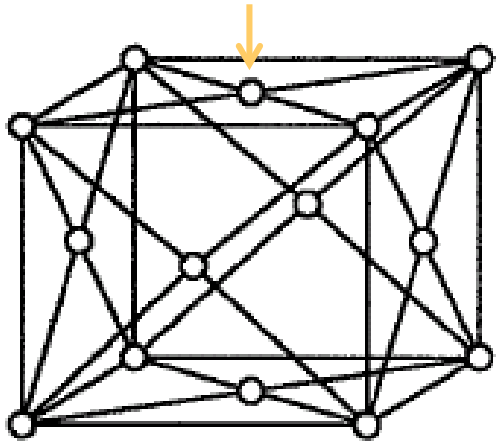


Points per Cell Examples

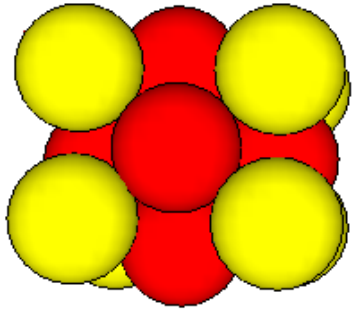


BCC
Points per cell
= 1/8 x 8 @corners
+ 1 @inside
=2

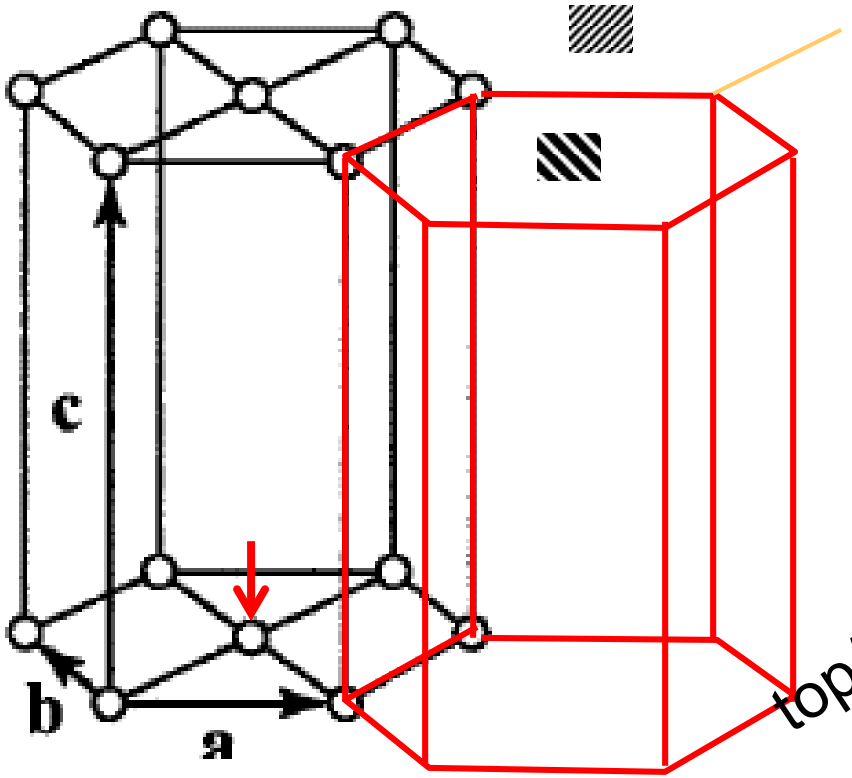




FCC
Points per cell
= 1/8 x 8 @corners
+ 1/2 x 6 @faces
=4

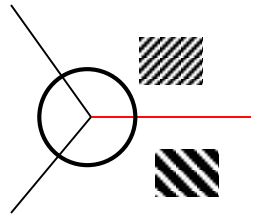


Hexagonal Closed-Packed



Points per cell

1/2 x 2 @faces =1



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

top/bottom neigbors

3 points/cell

Section 3
Crystals

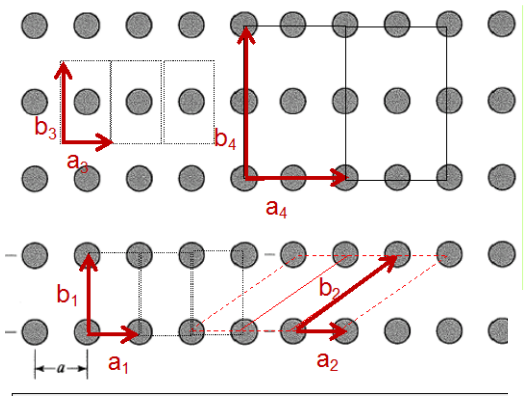
One Video Segment

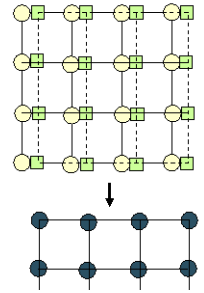
One Video Segment

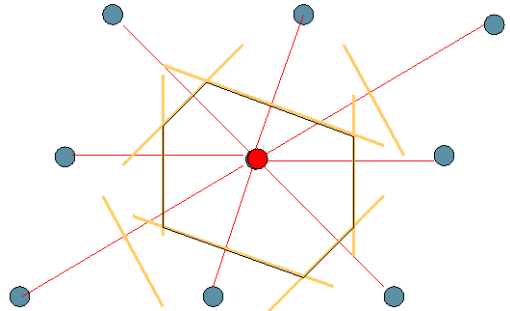
One Video Segment

One Video Segment

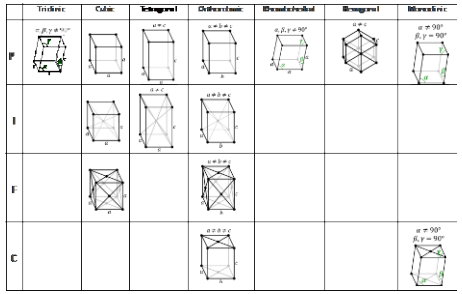
- 3.1 Crystal definitions
  - » One-dimensional Crystals – simple primitive cell
  - » Unit cells of a Periodic 2D Lattice
  - » Bravais lattice
  - » Bravais lattice with a basis
  - » Non-periodic repeated cells
  - » Definition of ONE Primitive Cell – Wigner-Seitz Cell

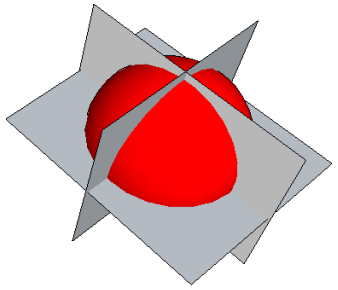






- 3.2 Tables of Bravais Lattices
  - » Bravais Lattices in 2D (5 types)
  - » Bravais Lattices in 3D (14 types)
  - » 3 Dominant Bravais Lattices in Nature





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

- 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

Section 3
Crystals

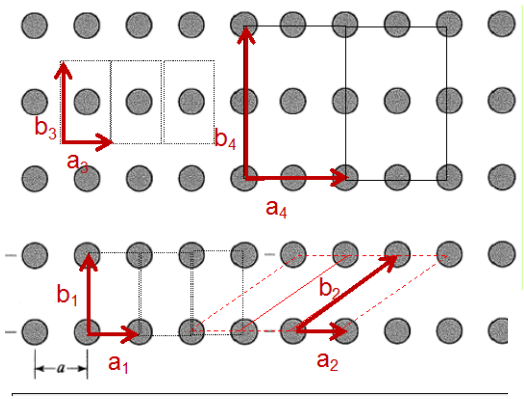
One Video Segment

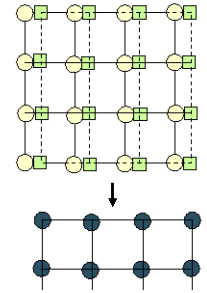
One Video Segment

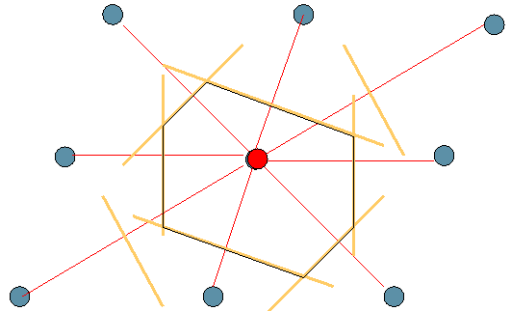
One Video Segment

One Video Segment

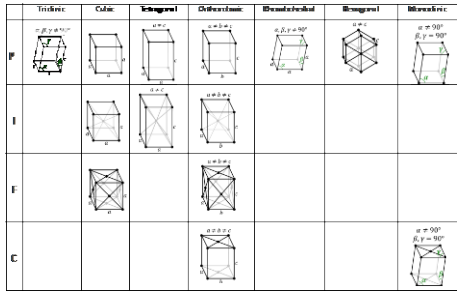
- 3.1 Crystal definitions
  - » One-dimensional Crystals – simple primitive cell
  - » Unit cells of a Periodic 2D Lattice
  - » Bravais lattice
  - » Bravais lattice with a basis
  - » Non-periodic repeated cells
  - » Definition of ONE Primitive Cell – Wigner-Seitz Cell

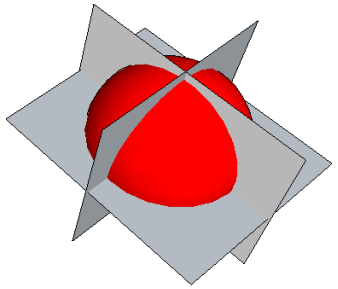




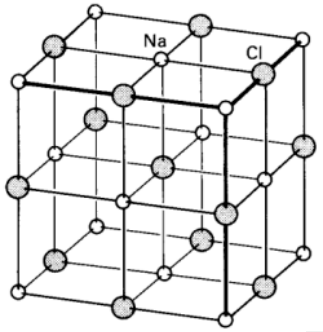


- 3.2 Tables of Bravais Lattices
  - » Bravais Lattices in 2D (5 types)
  - » Bravais Lattices in 3D (14 types)
  - » 3 Dominant Bravais Lattices in Nature





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

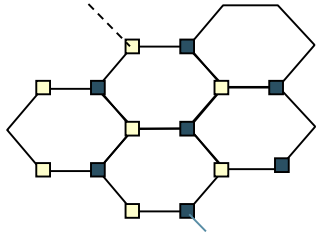


- 3.4 Surfaces, Miller Index

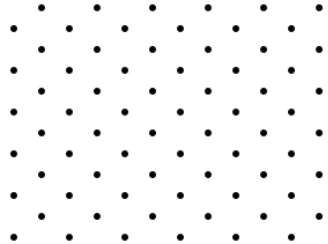
Reference: Vol. 6, Ch. 1, ABACUS tool at nanohub.org/tools/abacus and "Crystal Viewer Lab, https://nanohub.org/resources/crystalviewer

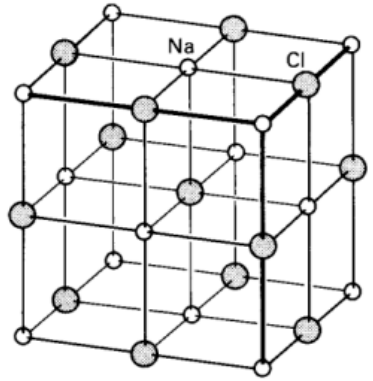
Bravais Lattice with a Basis

Graphene

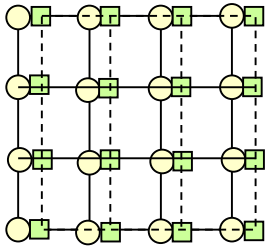


Bravais lattice with a basis

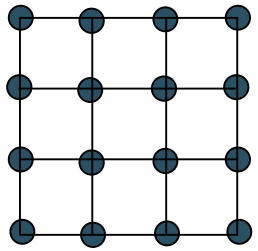




NaCl
Rocksalt



Non-Bravais lattice



Bravais lattice with a basis

Conversion into a Bravais lattice:

- Combine complex components into a single repeated basis
- Establish basis vectors

- Property of ONE CELL defines the property of the solid
- Address every point in the lattice by integer translation of unit vectors
- every point has the same environment as every other point (same number of neighbors, next neighbors, …)

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

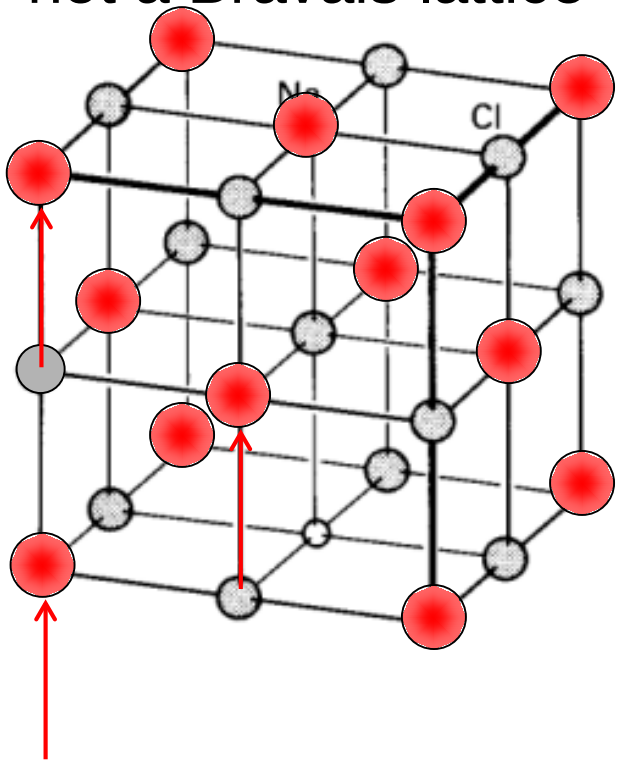
Rock-Salt as FCC lattice

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

= 

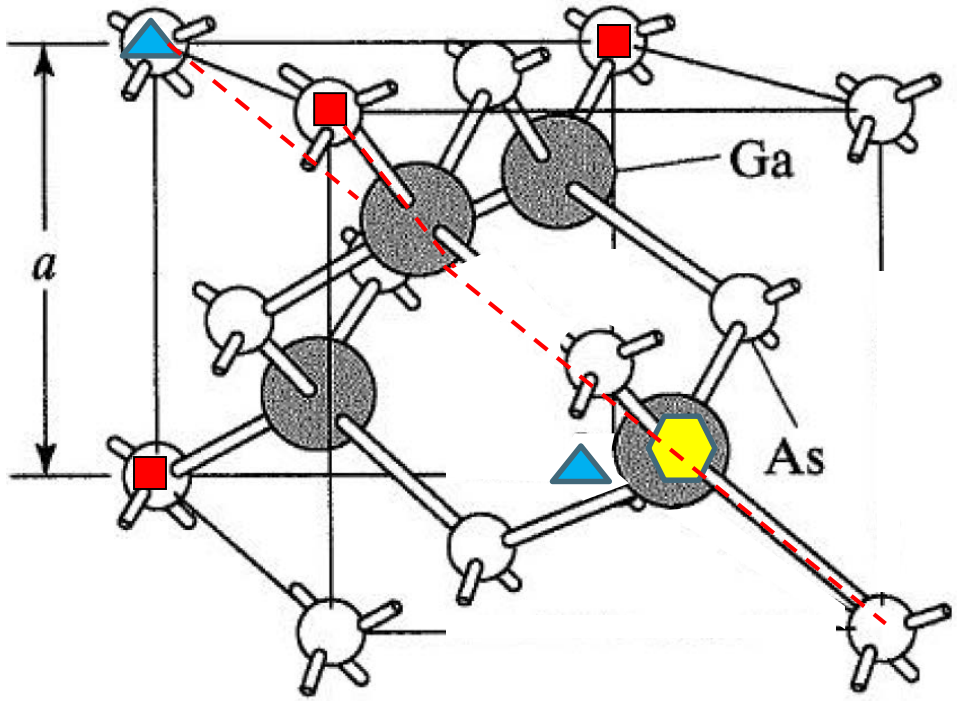
a basis
of 2 atoms

arranged in
FCC



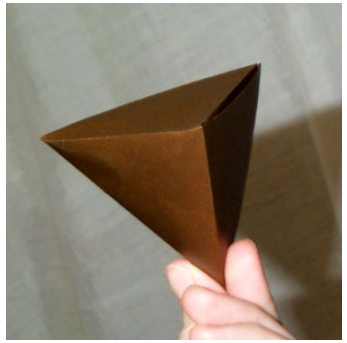
For more discussion, see Kittel and Ashcroft/Mermin

Zinc-Blende Lattice for GaAs

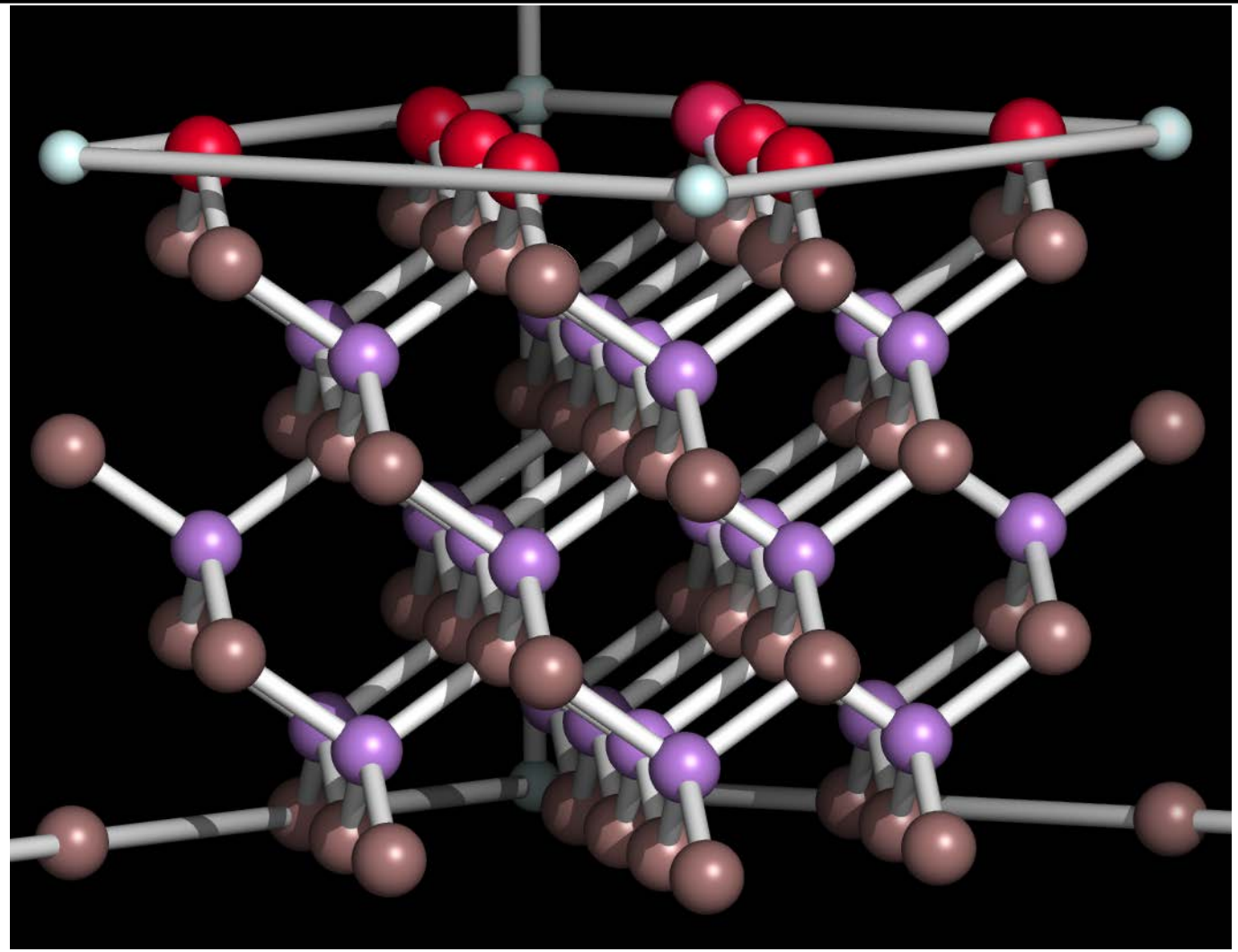


Atoms/cell=(1/8)x8 + (1/2)x6 + 4=8

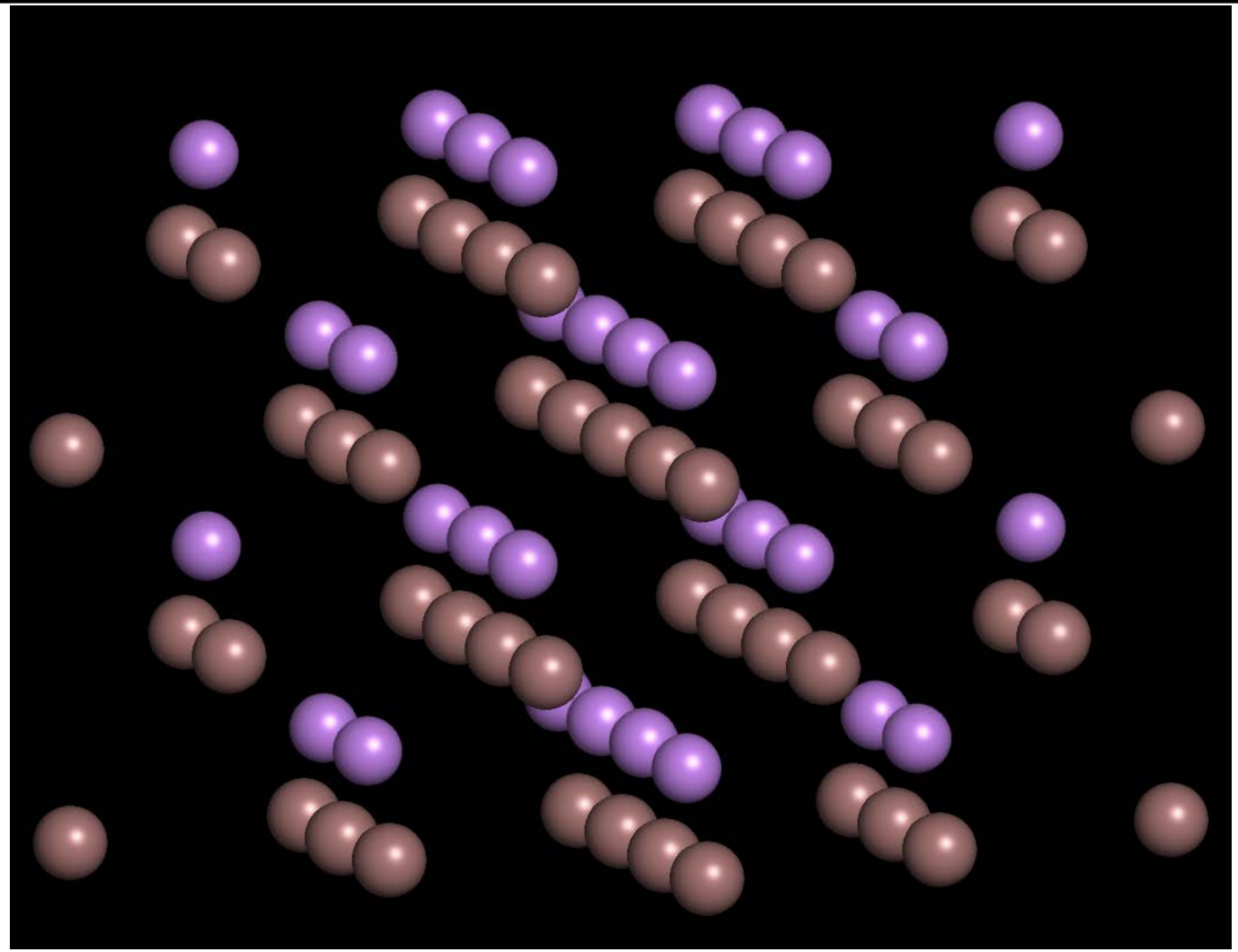
Tetrahedral structure



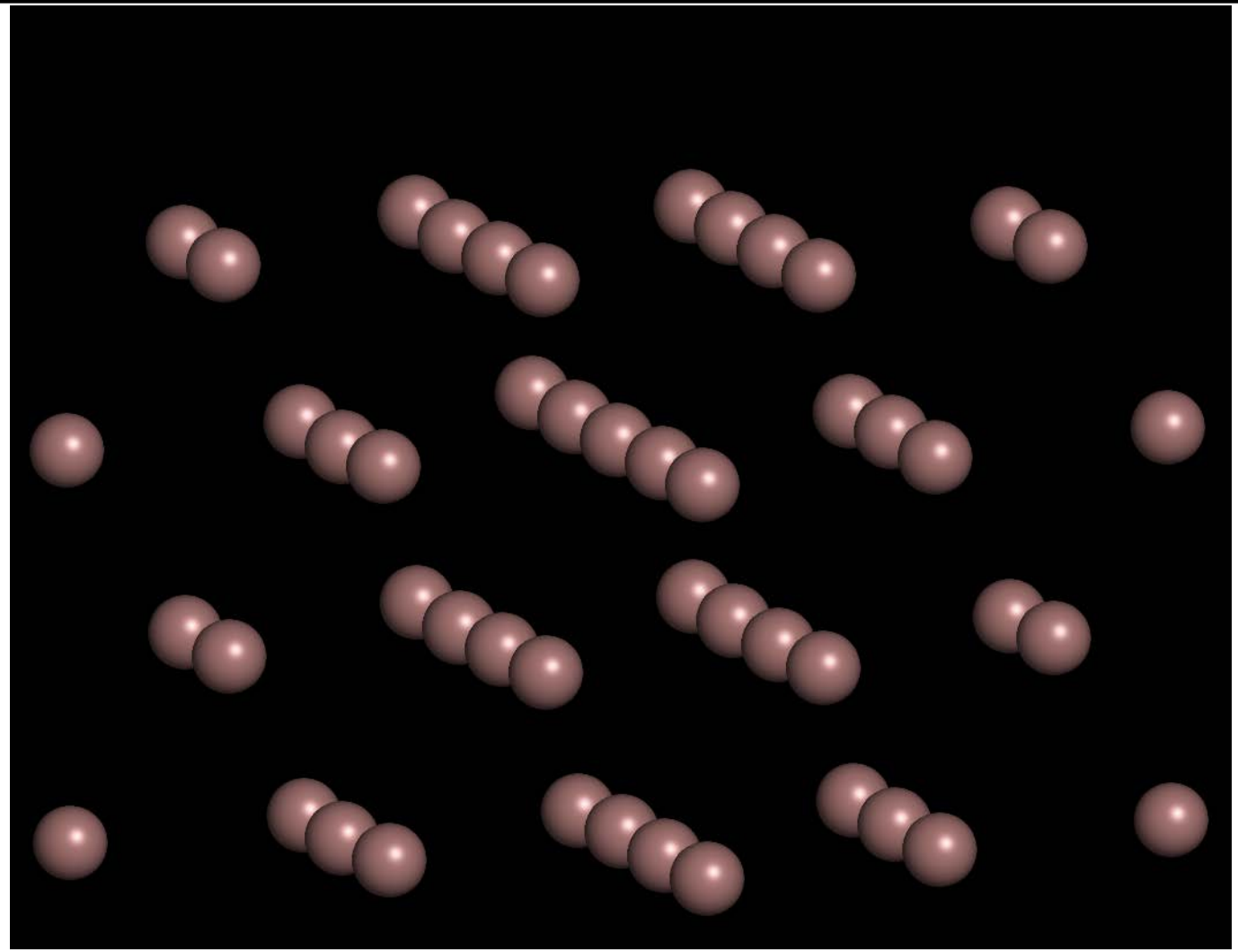
GaAs Crystal Plotted in Crystal Viewer



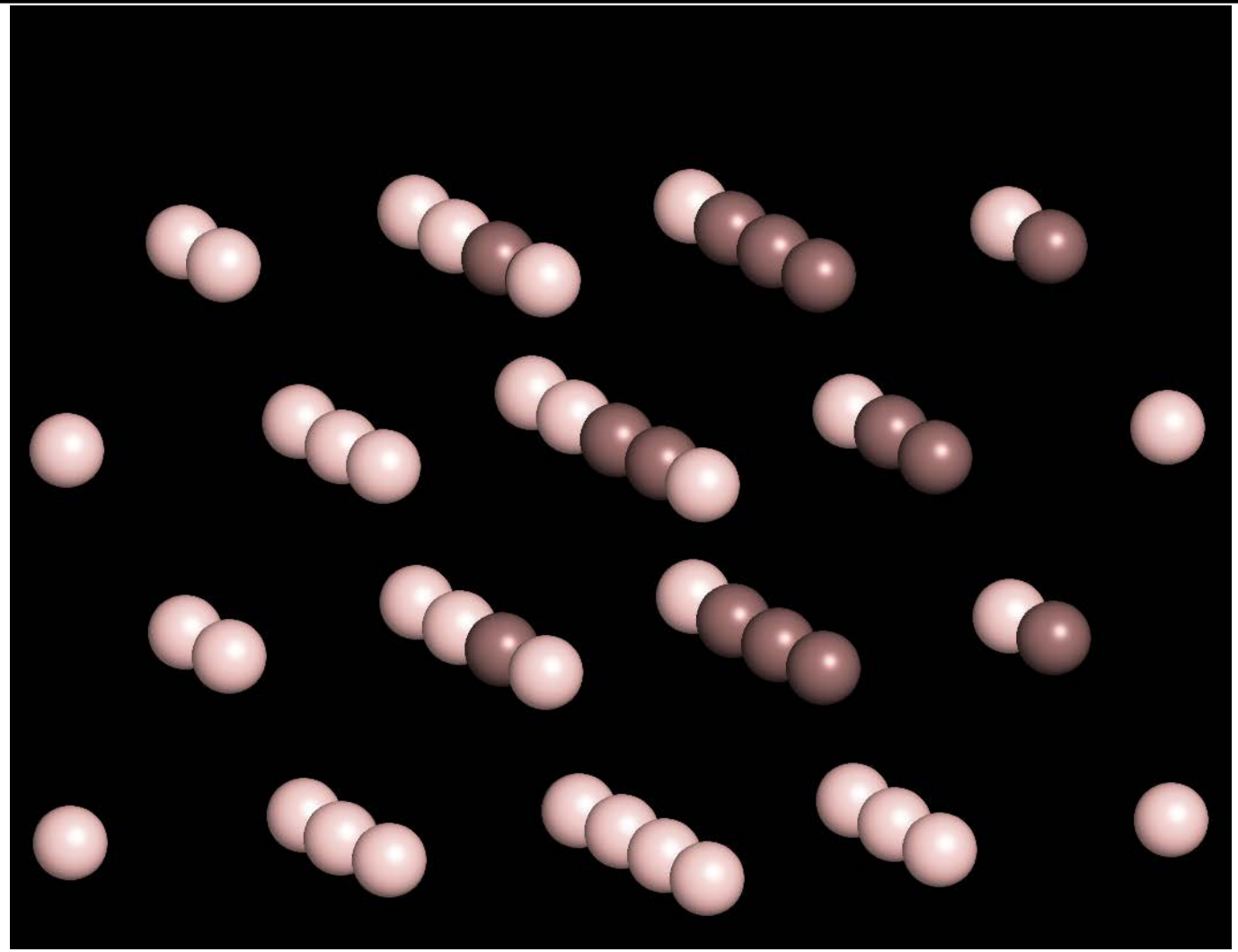
GaAs Crystal Without Bonds



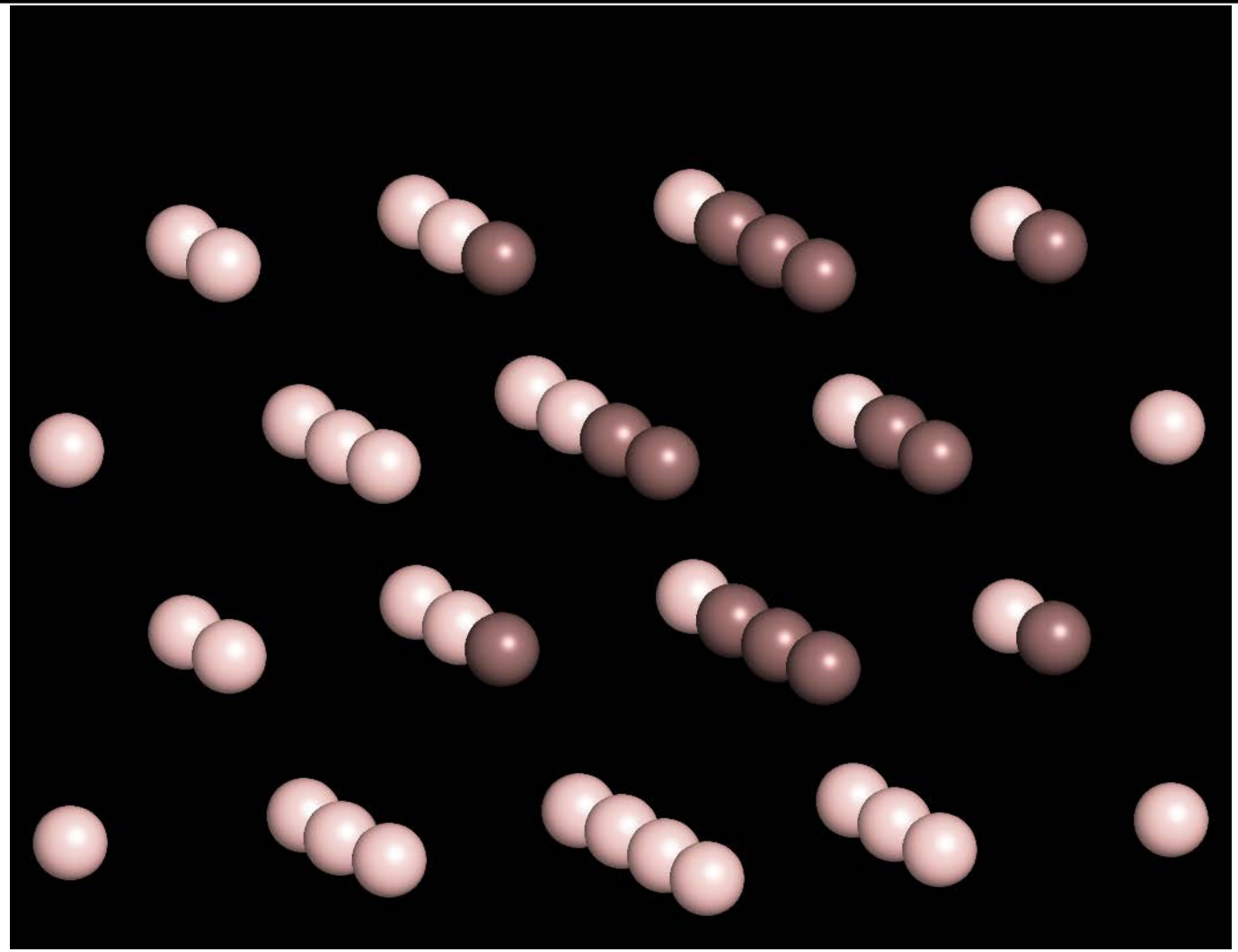
GaAs Crystal Just One Species



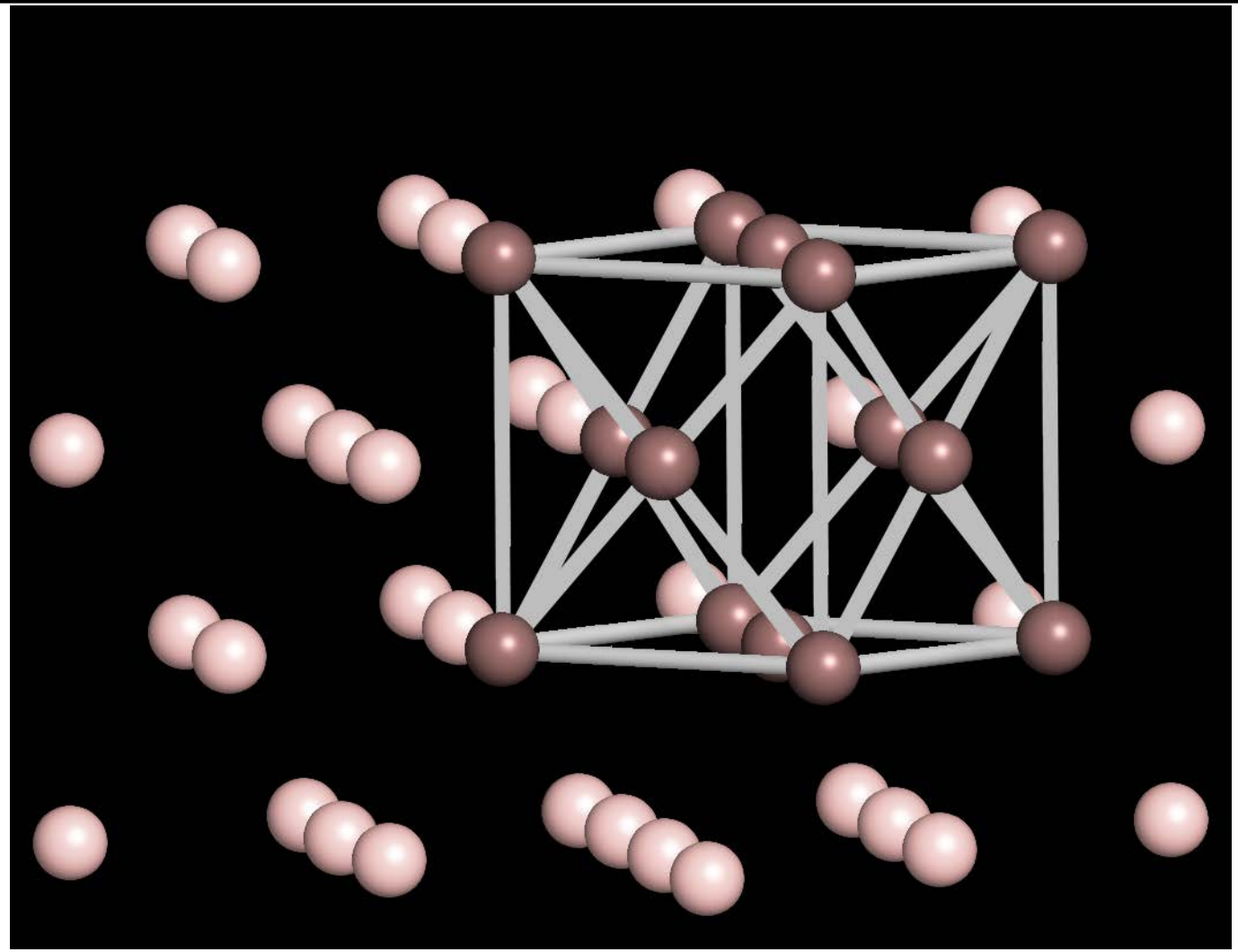
GaAs Crystal Just One Species
Focus on Few



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

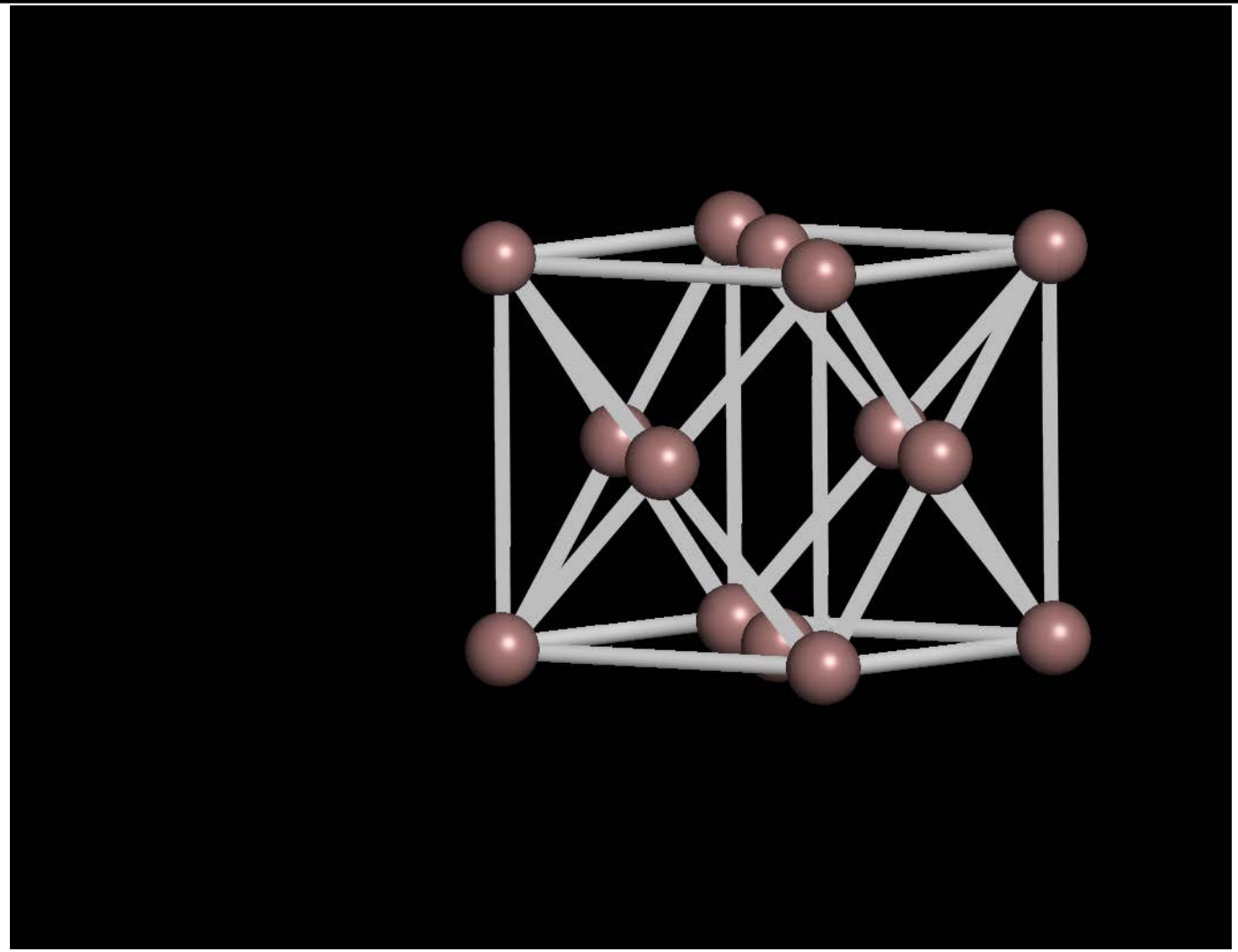


GaAs Crystal Just One Species
A FCC Cell!



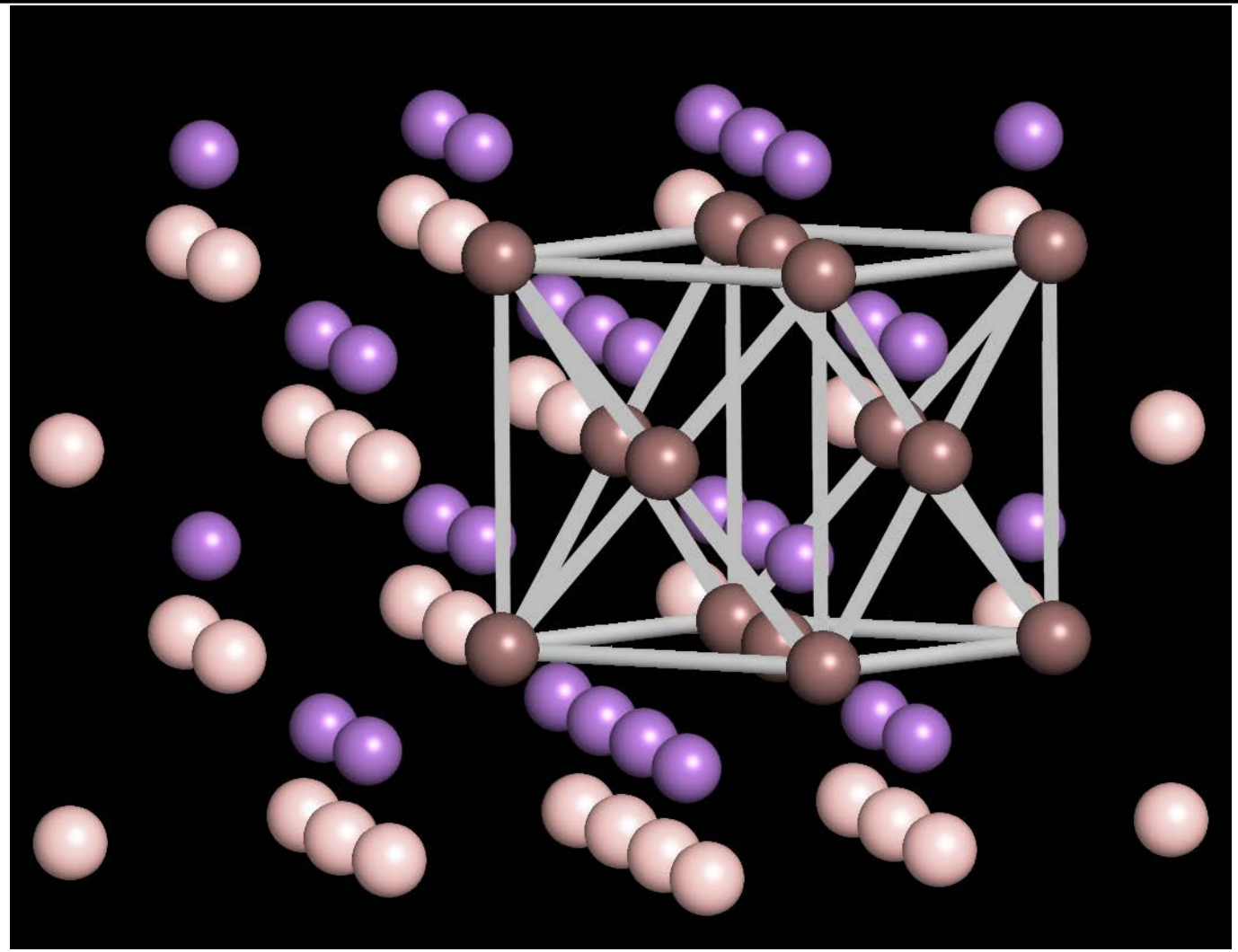
- FCC cell – Atoms/cell = (1/8)x8 + (1/2)x6 = 4

GaAs Crystal Just One Species
A FCC Cell!



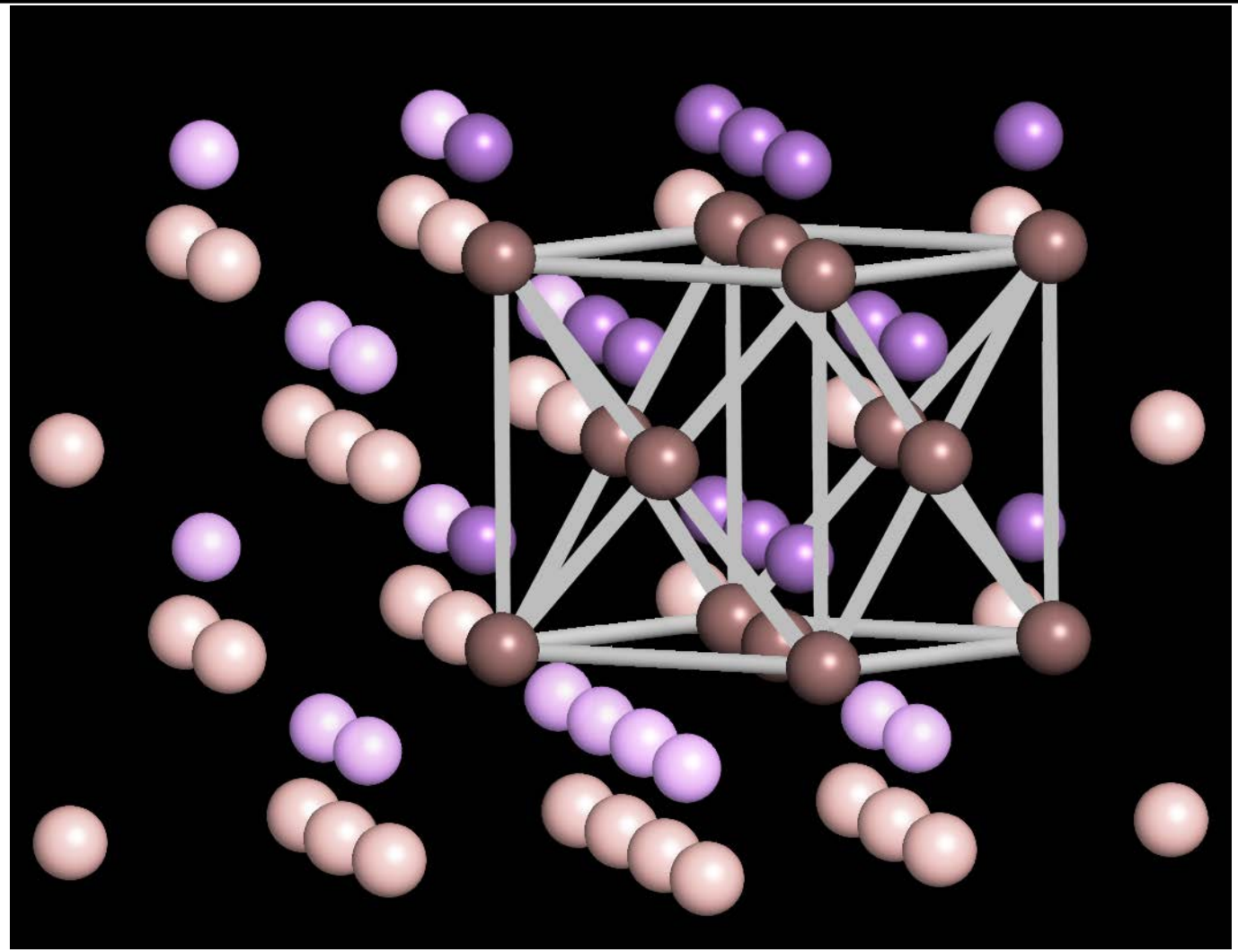
- FCC cell – 4 atoms per unit cell

GaAs Crystal Both Species



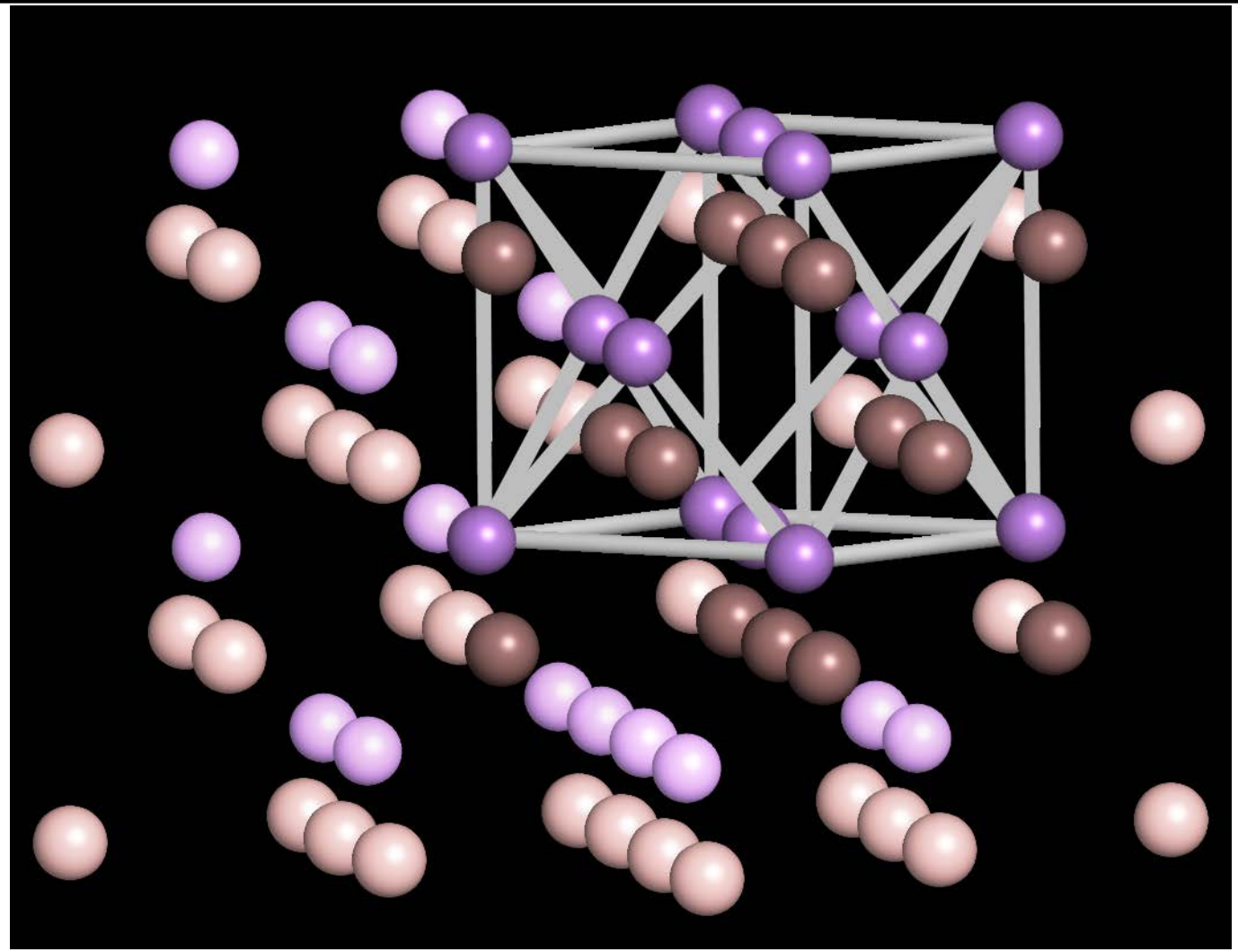
- FCC cell – 4 atoms per unit cell – brown species

GaAs Crystal Both Species



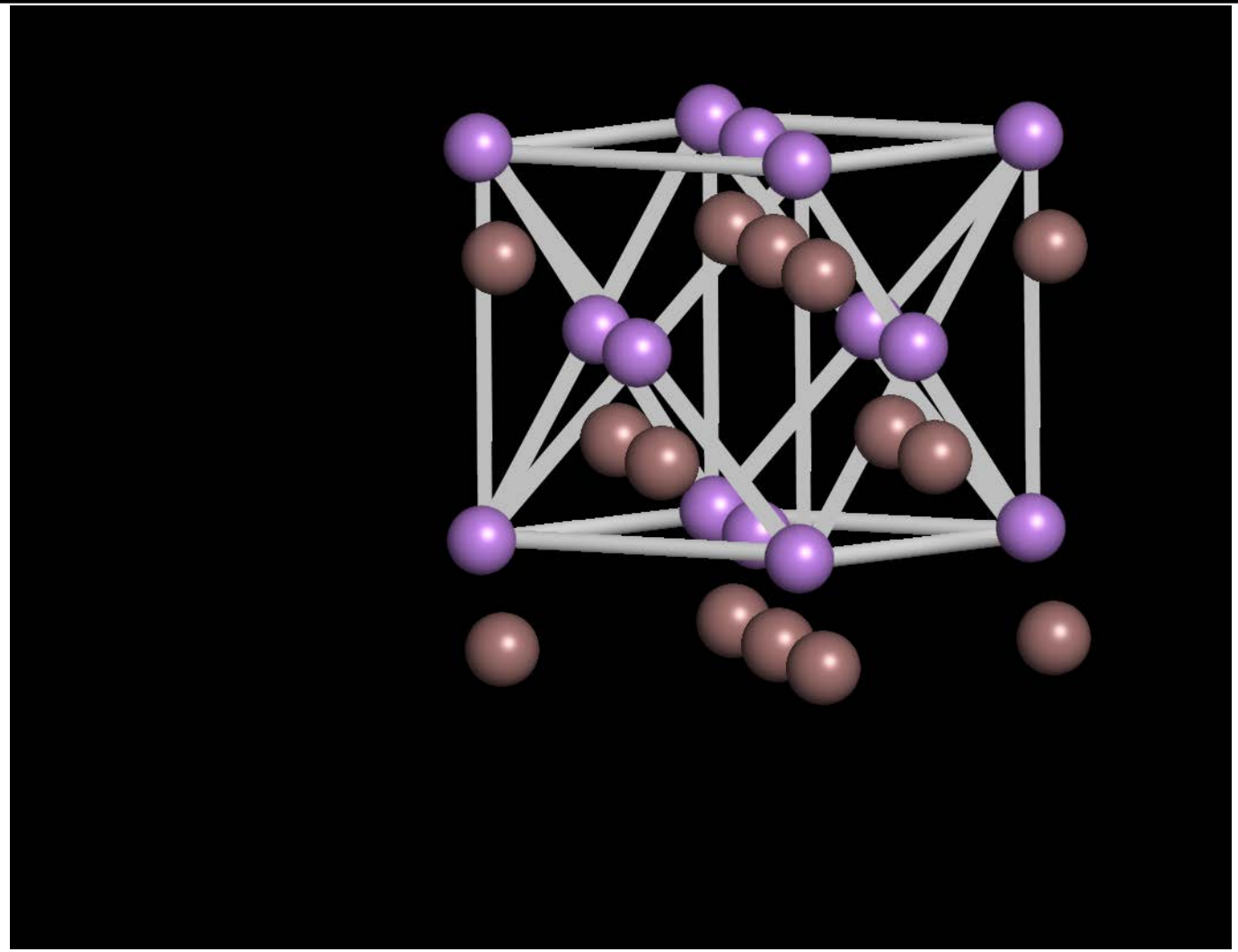
- FCC cell – 4 atoms per unit cell – brown species
- Focus on a few of the “blue species”

GaAs Crystal Both Species



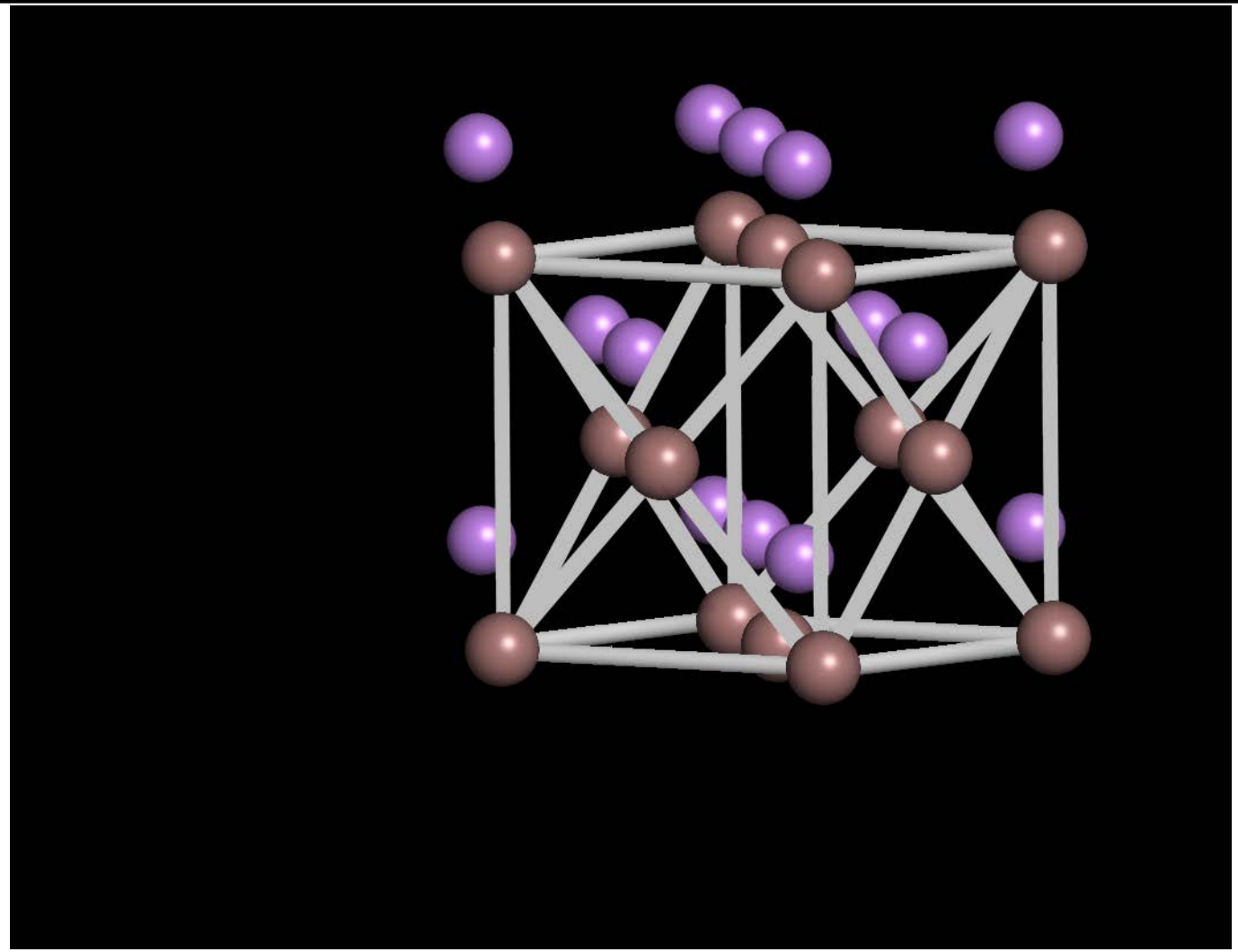
- FCC cell – 4 atoms per unit cell – brown species
- FCC cell – 4 atoms per unit cell – purple species

GaAs Crystal Both Species



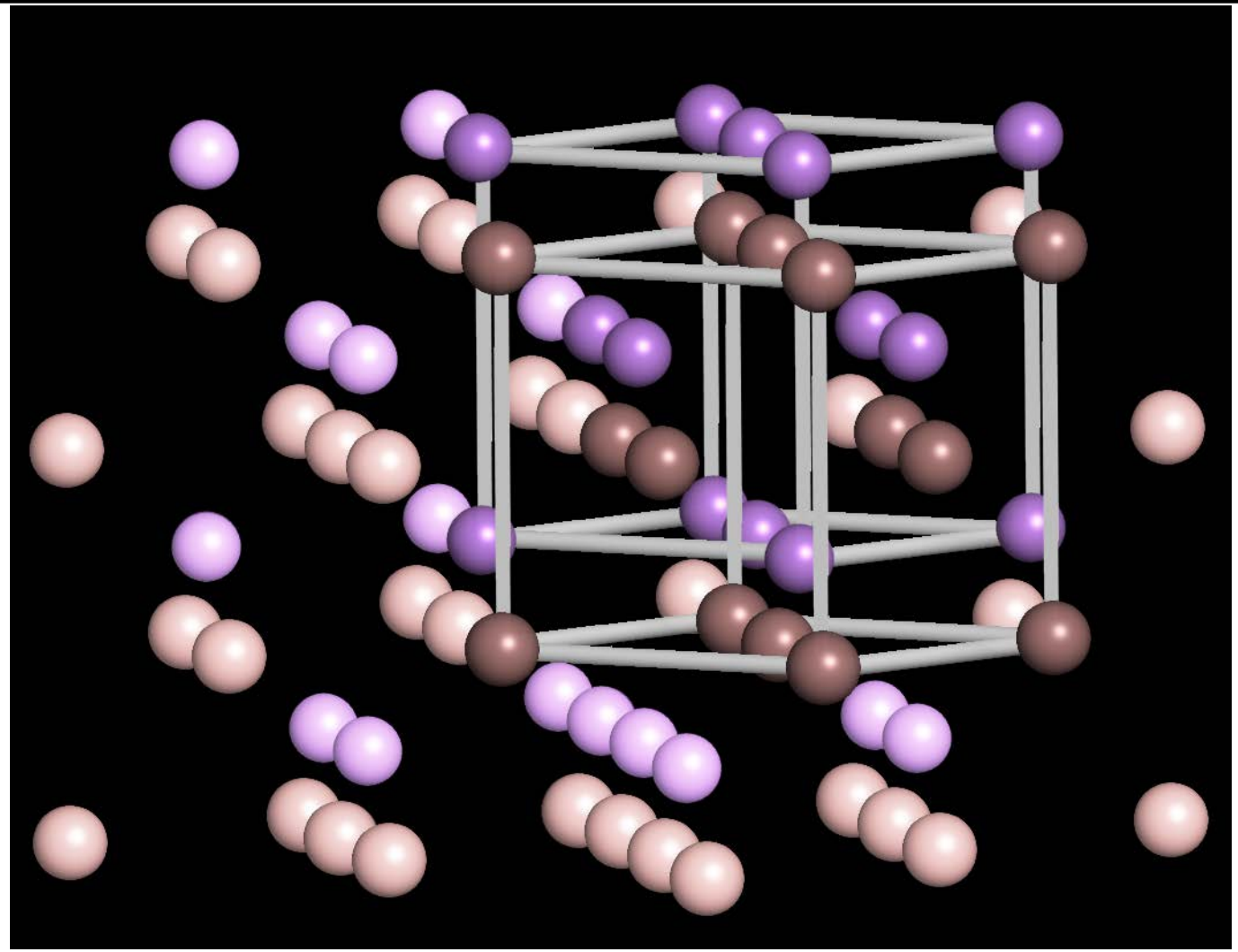
- FCC cell – 4 atoms per unit cell – brown species
- FCC cell – 4 atoms per unit cell – purple species

GaAs Crystal Both Species



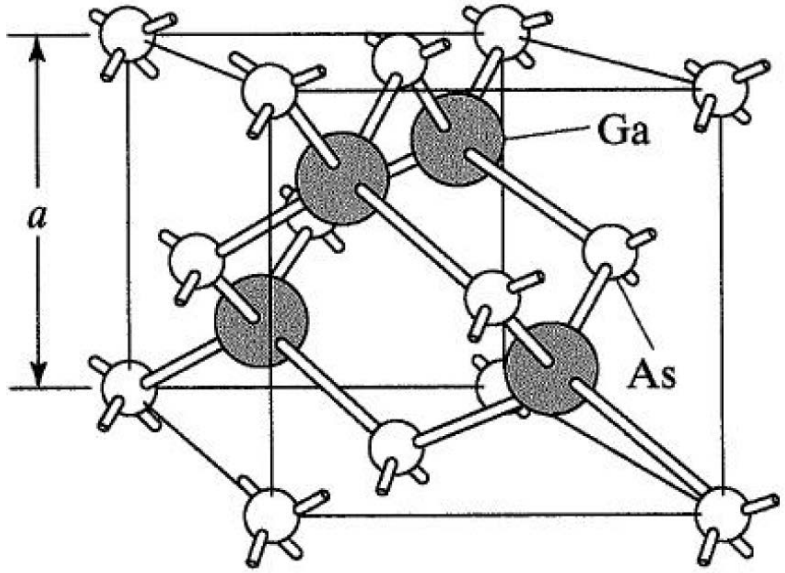
- FCC cell – 4 atoms per unit cell – brown species
- FCC cell – 4 atoms per unit cell – purple species

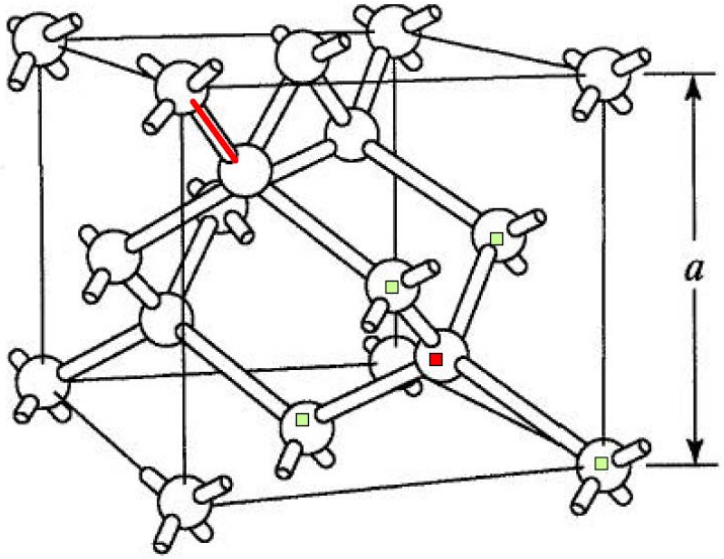
GaAs Crystal – 2 FCC



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

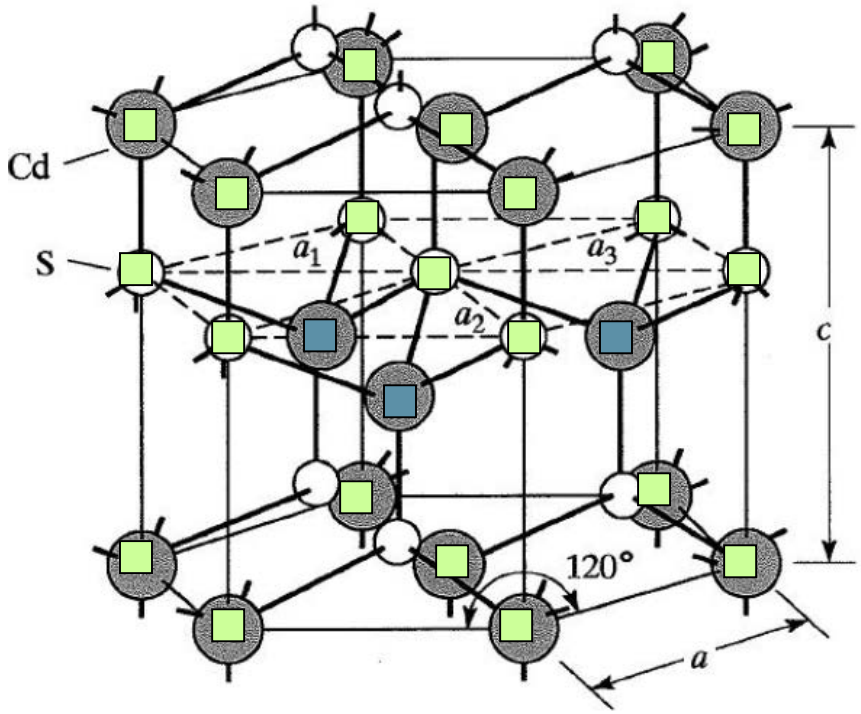
Diamond FCC Lattice for GaAs and Silicon



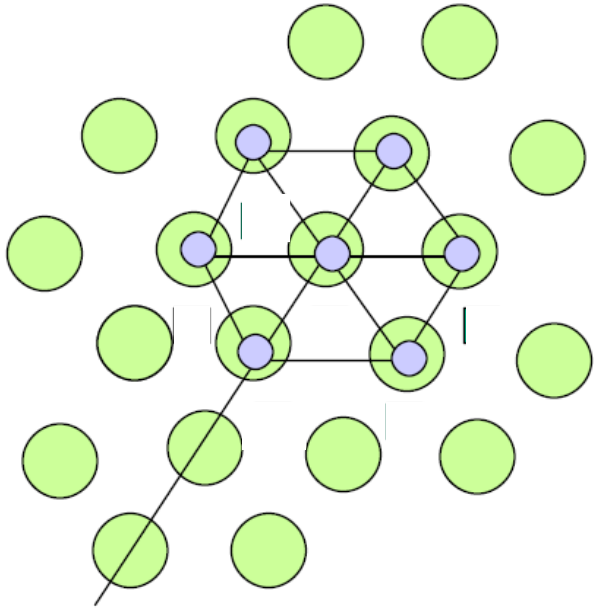


- Zincblende – GaAs - 2 FCC bases – separated by [¼ ¼ ¼]
- Diamond – Si - 2 FCC bases – separated by [¼ ¼ ¼]

Hexagonal Closed-Packed for CdS



Focus on (Cd) …



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

Section 3
Crystals

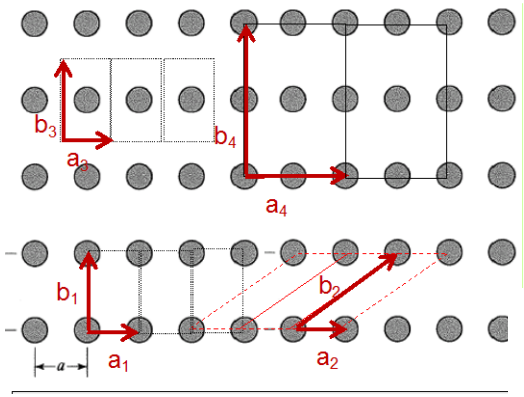
One Video Segment

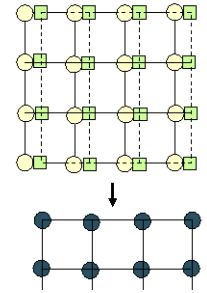
One Video Segment

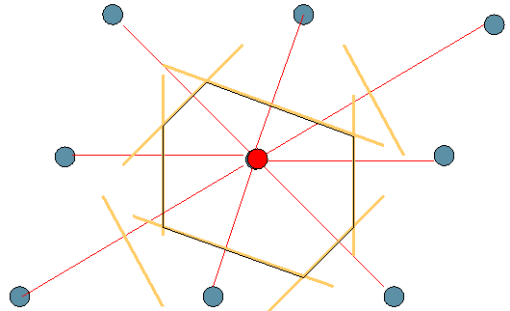
One Video Segment

One Video Segment

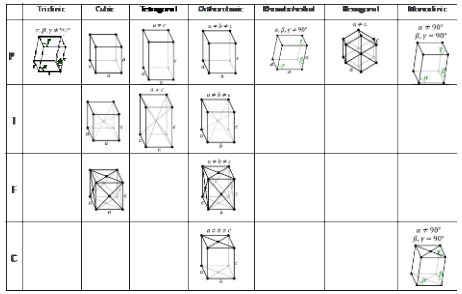
- 3.1 Crystal definitions
  - » One-dimensional Crystals – simple primitive cell
  - » Unit cells of a Periodic 2D Lattice
  - » Bravais lattice
  - » Bravais lattice with a basis
  - » Non-periodic repeated cells
  - » Definition of ONE Primitive Cell – Wigner-Seitz Cell



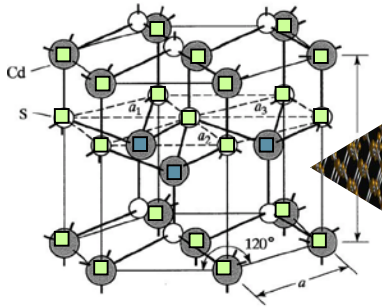




- 3.2 Tables of Bravais Lattices
  - » Bravais Lattices in 2D (5 types)
  - » Bravais Lattices in 3D (14 types)
  - » 3 Dominant Bravais Lattices in Nature



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



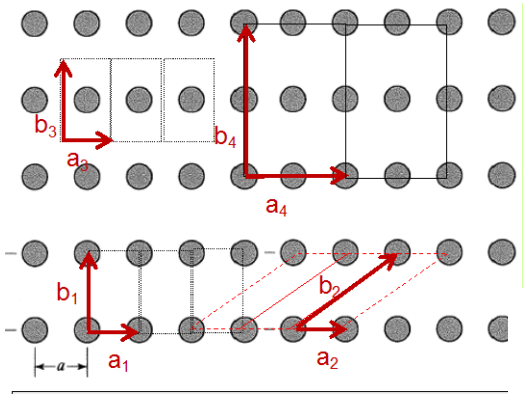
- 3.4 Surfaces, Miller Index

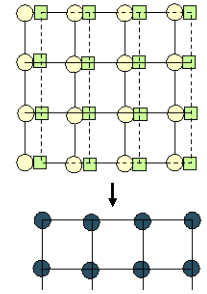
Reference: Vol. 6, Ch. 1, ABACUS tool at nanohub.org/tools/abacus and "Crystal Viewer Lab, https://nanohub.org/resources/crystalviewer

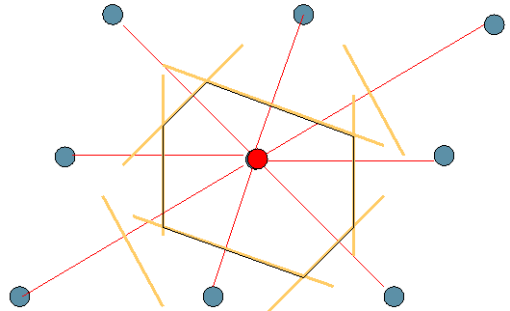
Section 3
Crystals

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

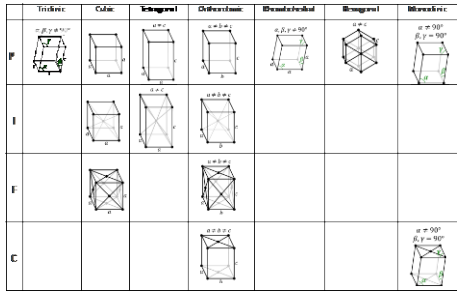






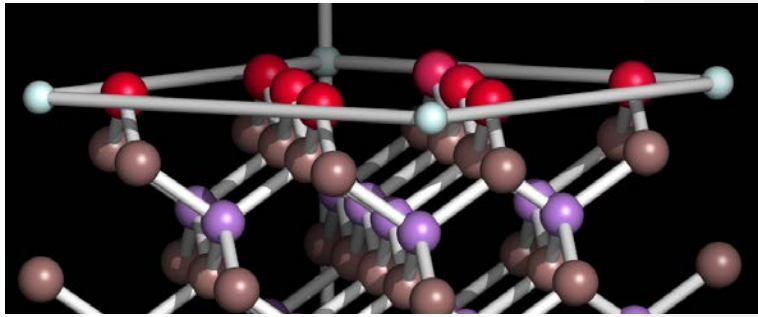
One Video Segment

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



One Video Segment

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



One Video Segment

- 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