ECE 340 Lecture 2
Semiconductor Electronics

Spring 2022
10:00-10:50am
Professor Umberto Ravaioli
Department of Electrical and Computer Engineering
2062 ECE Building

Today's Discussion

- Semiconductor Materials
- Lattices and Crystal Structures

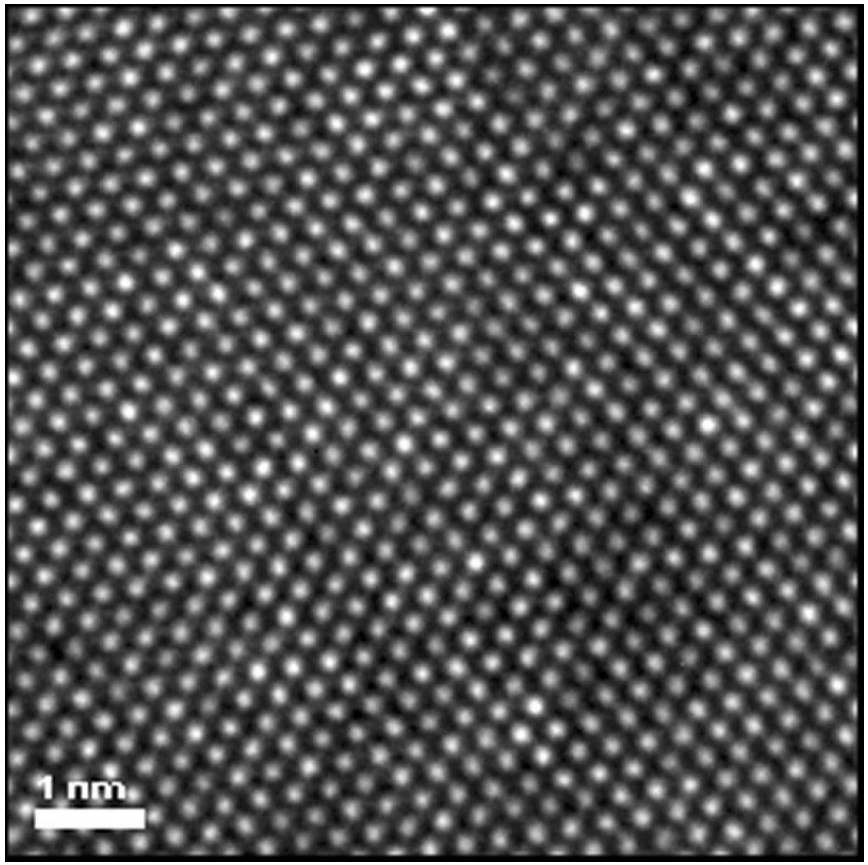
- **Homework #1** will be assigned today and posted on Canvas (due on January 28)
- **Reading Assignment:**

  Chapter 1 of Streetman & Banerjee

Lattices and Crystal Structures

Types of Solids (1) Crystalline

Ki-Bum Kim, Seoul National University (2008)

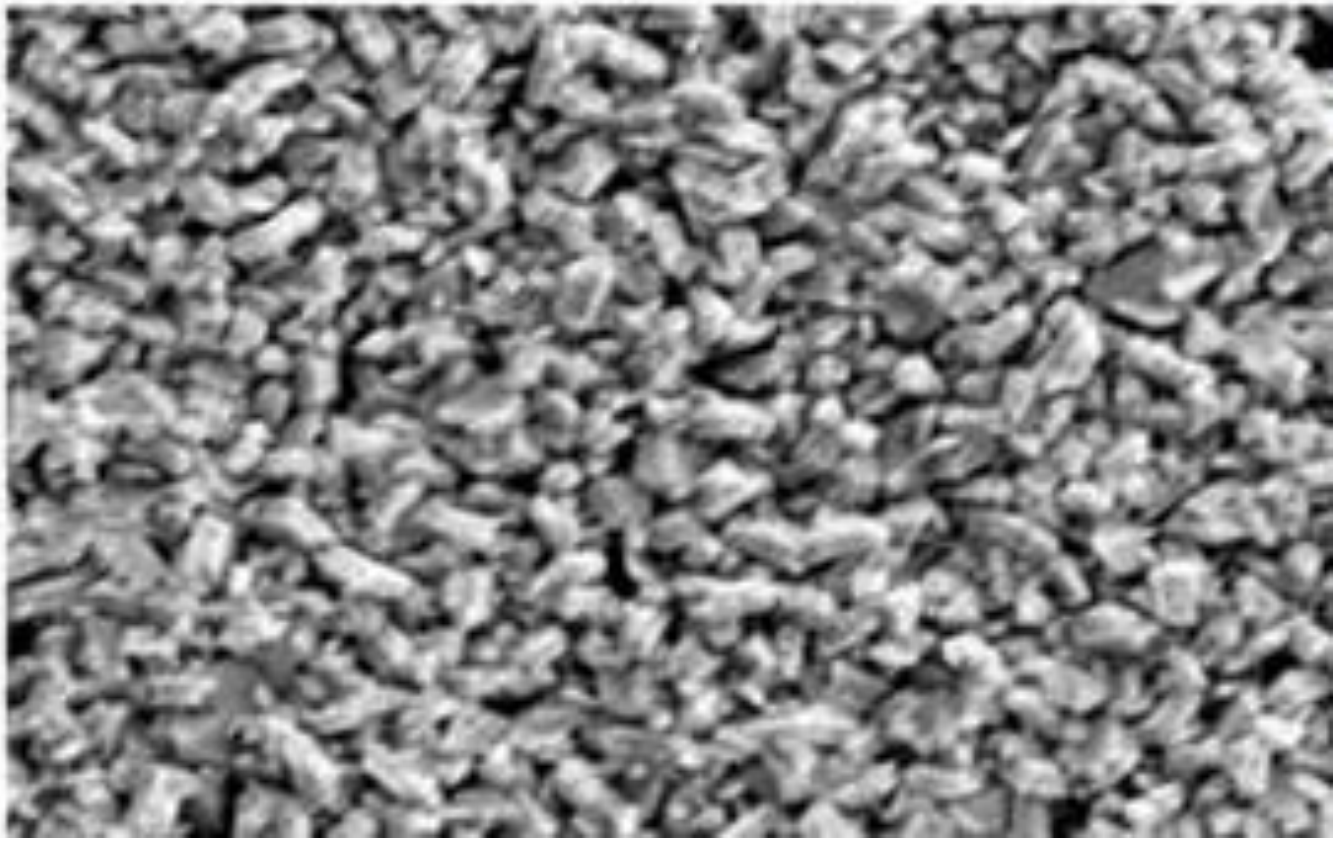


HRTEM image of a silicon (Si) [110] crystallographic zone axis.

In the CRYSTALLINE state the atoms are ordered into a well-defined lattice that extends over very long distances

Types of Solids (2) Amorphous

Rajathi and Berchmans, www.nature.com/scientificreports (2019)

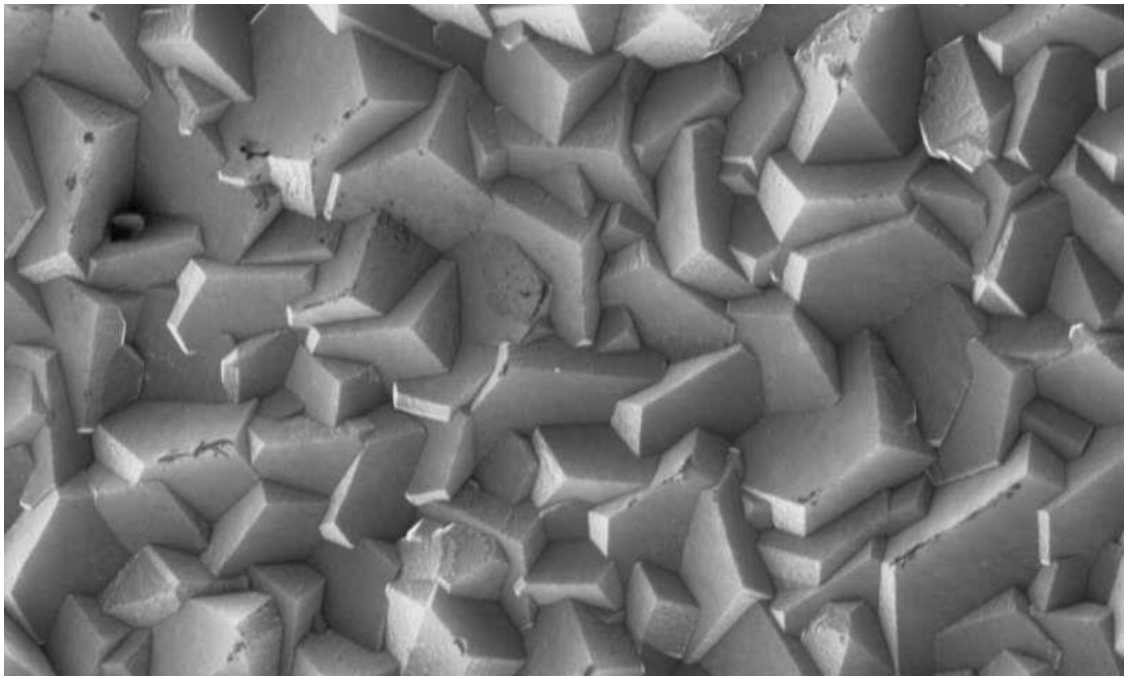


Glassy Palladium

In the AMORPHOUS state there is little or no evidence for long-range crystalline order

Types of Solids (3) Polycrystalline

Tomsk Polytechnic University (2017)



Polycrystalline diamond film

POLYCRYSTALLINE materials consist of small crystallites that are embedded in AMORPHOUS regions of material

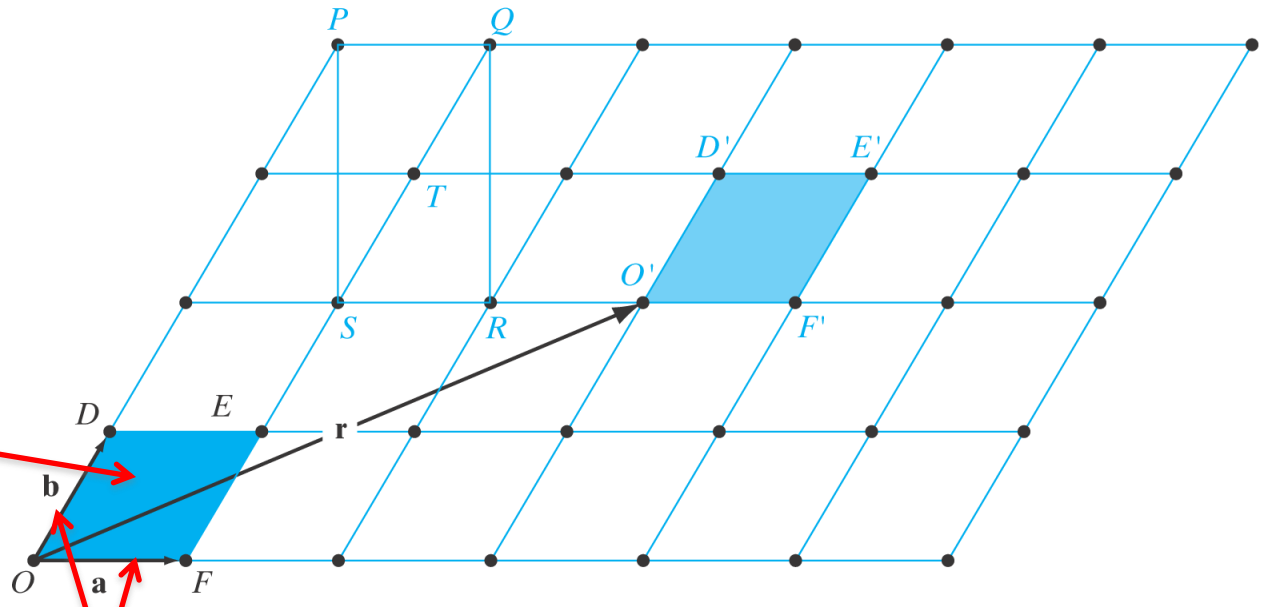
Crystal Lattice – Definitions

- **Lattice:** Periodic arrangement of a substance or "**basis**"
  - Atom, atomic pair, group of atoms, molecule, etc.
- **Unit Cell:** Contains a region which is representative of the lattice which can be regularly repeated to recreate the entire lattice
- **Primitive Cell:** The smallest unit cell that can be repeated in integral steps to produce the lattice
  - Contains a single lattice point
  - The Primitive Cell is a special form of the Unit Cell
- **Primitive Vectors: a, b, c** **(define the cell)**
  - (1 dimension) $r = p\,\mathbf{a}$
  - (2 dimension) $r = p\,\mathbf{a} + q\,\mathbf{b}$
  - (3 dimension) $r = p\,\mathbf{a} + q\,\mathbf{b} + r\,\mathbf{c}$

translation vectors

- **Basis Vectors**: Similar to primitive vectors, but used to replicate the lattice through the translation of a unit cell

Simple Lattices and Unit Cells



Primitive Cell

Primitive Vectors

Figure 1.2

A two-dimensional lattice showing translation of a unit cell by $\mathbf{r} = 3\mathbf{a} + 2\mathbf{b}$.

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Simple Lattices and Unit Cells

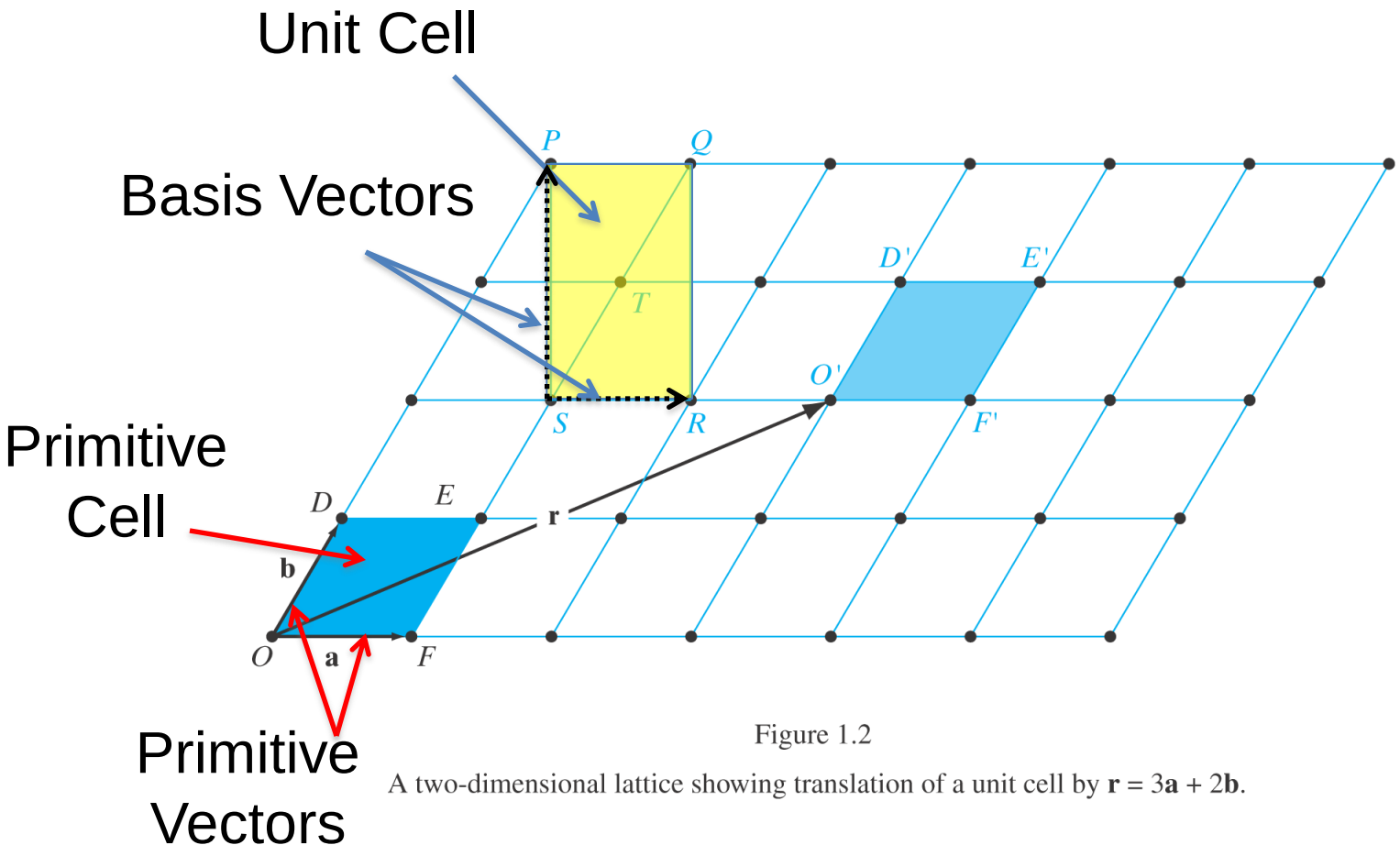

Figure 1.2

A two-dimensional lattice showing translation of a unit cell by $\mathbf{r} = 3\mathbf{a} + 2\mathbf{b}$.

Simple Lattices and Unit Cells

Primitive and Unit Cells are not unique. We can find equivalent geometries.

Possible primitive cells should have the same area (in 2D) or the same volume (in 3D).

Possible units cells can be of different size.

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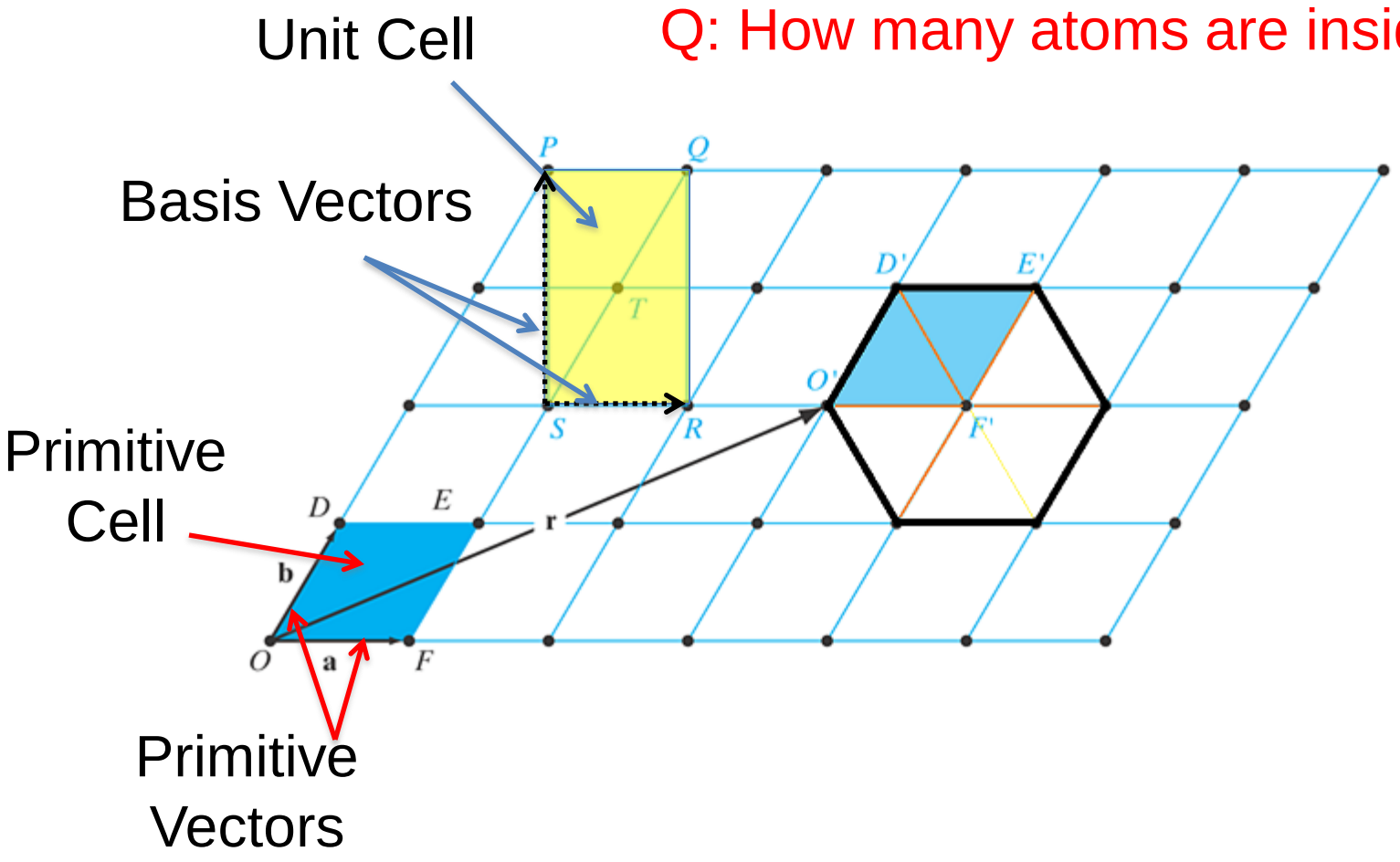
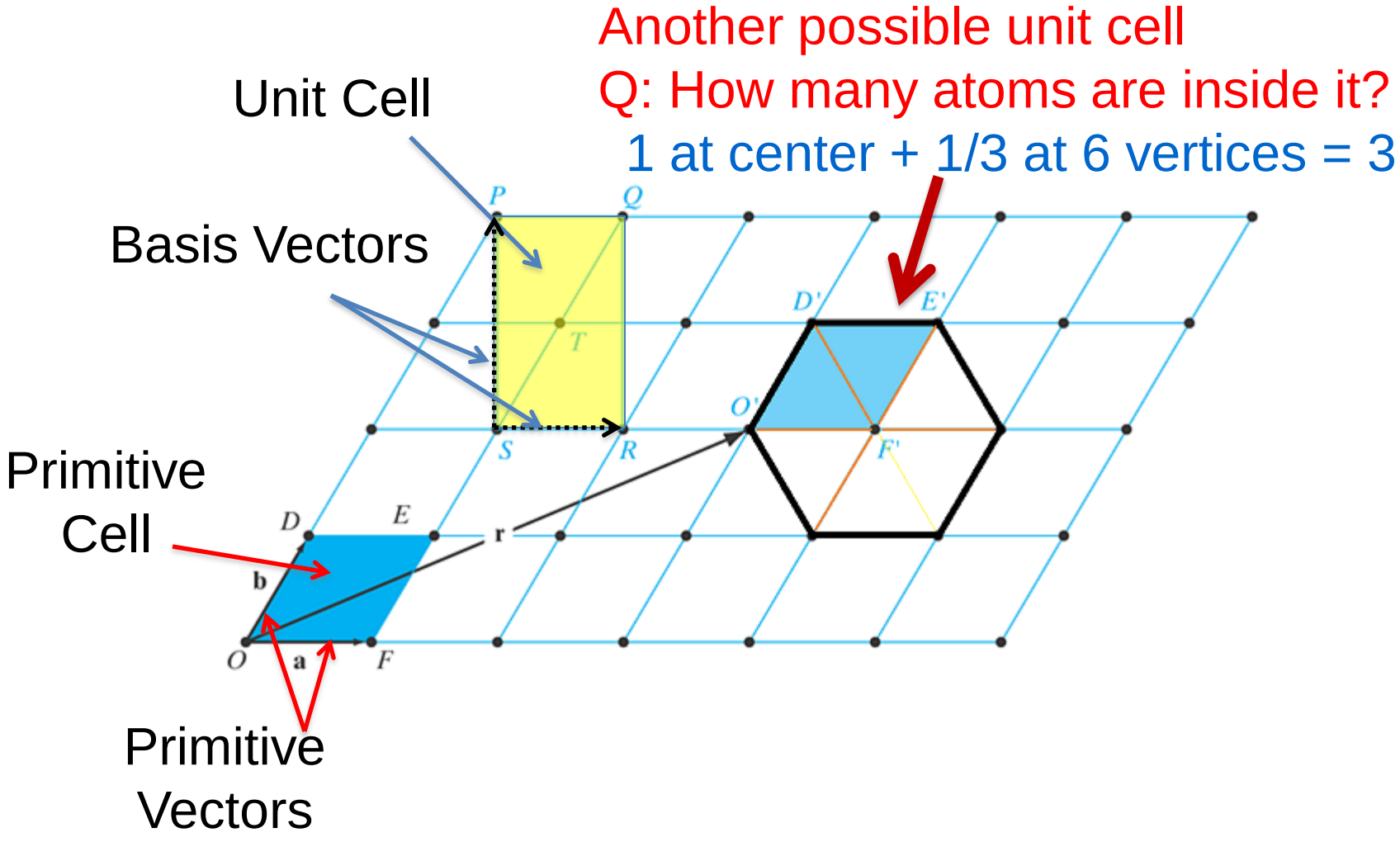
Simple Lattices and Unit Cells

Another possible unit cell

Q: How many atoms are inside it?

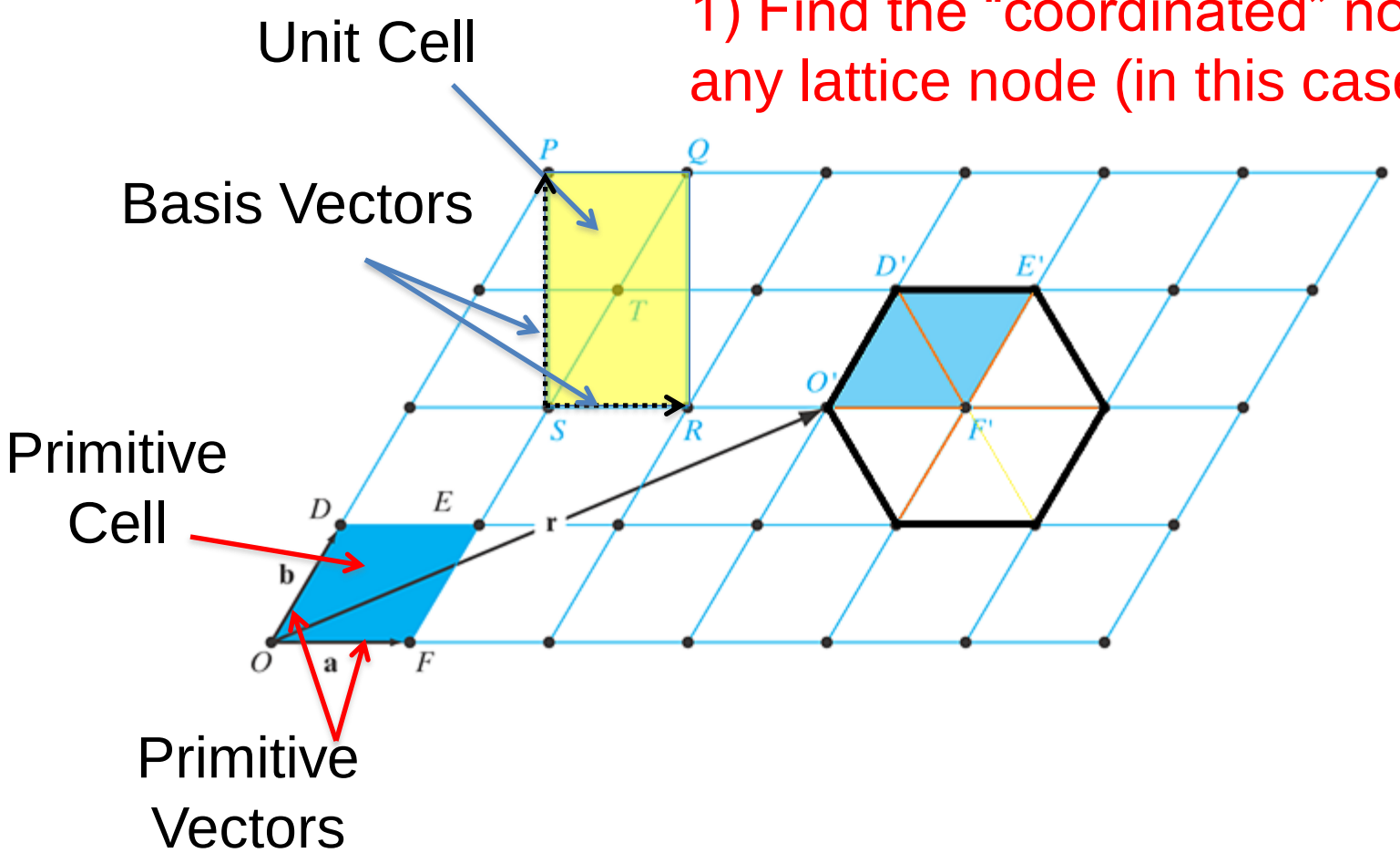


Simple Lattices and Unit Cells



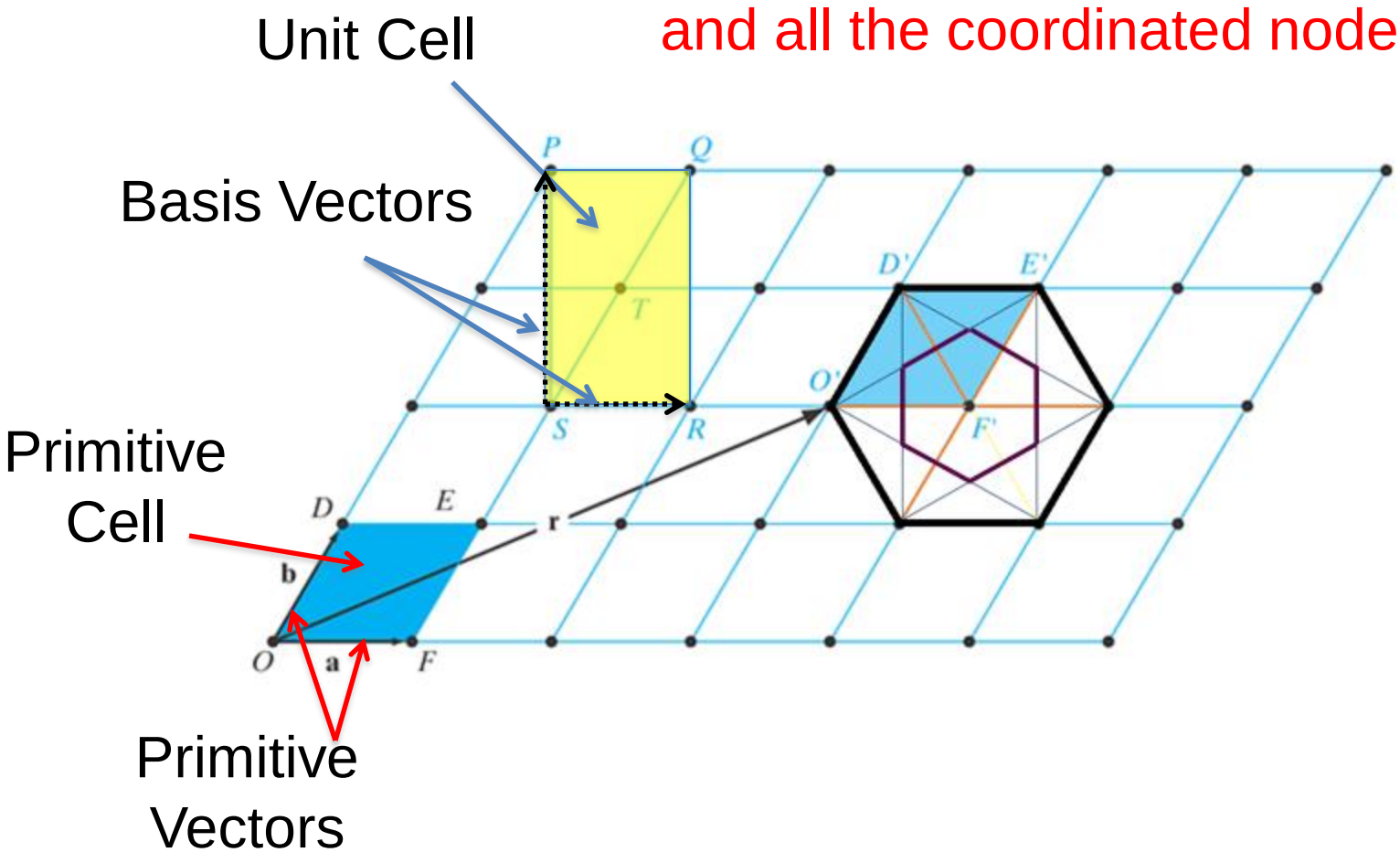
Simple Lattices and Unit Cells

A formal way to find a primitive cell
1) Find the "coordinated" nodes for any lattice node (in this case *F'*)



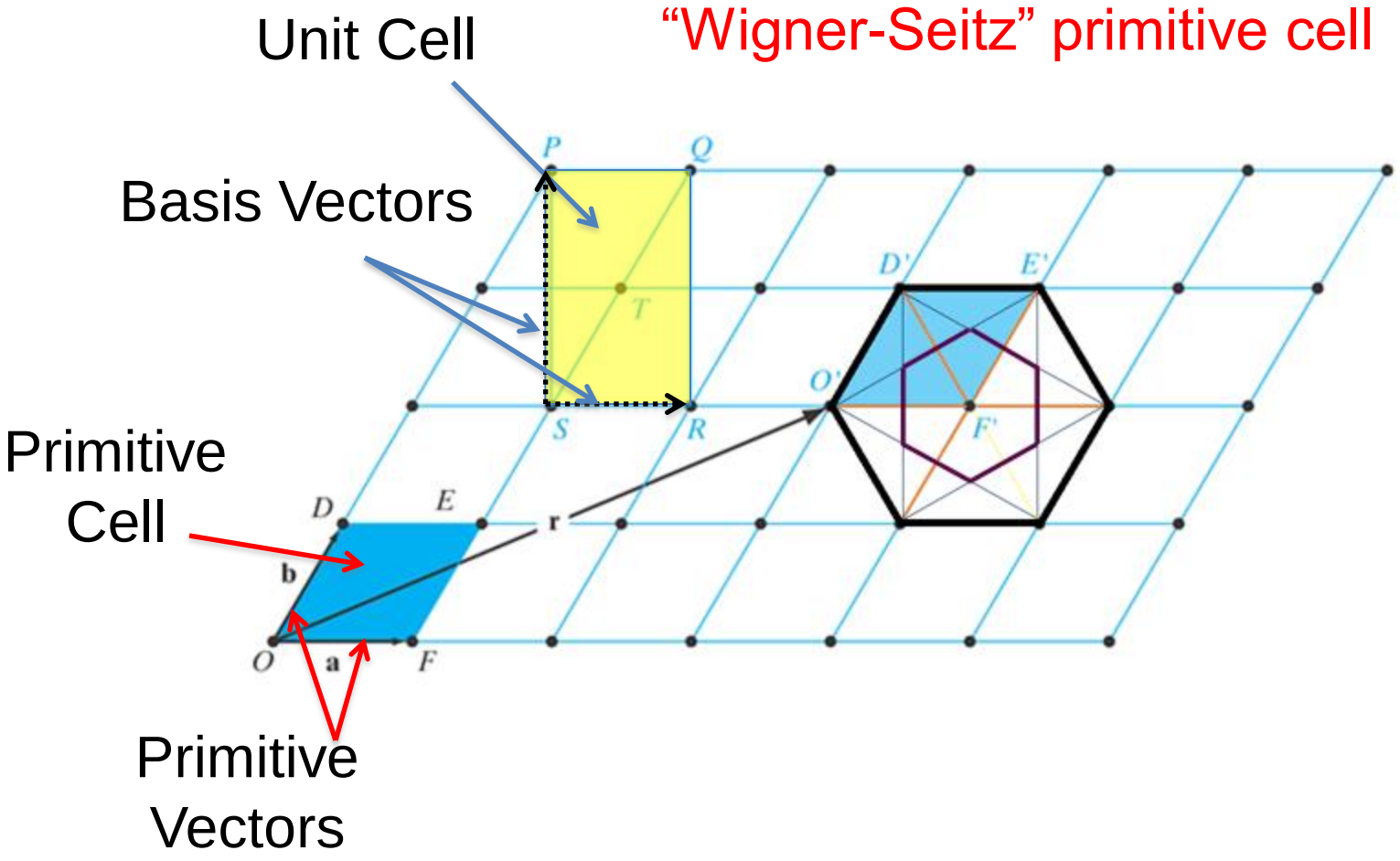
Simple Lattices and Unit Cells

2) Bisect the segments between *F'* and all the coordinated nodes



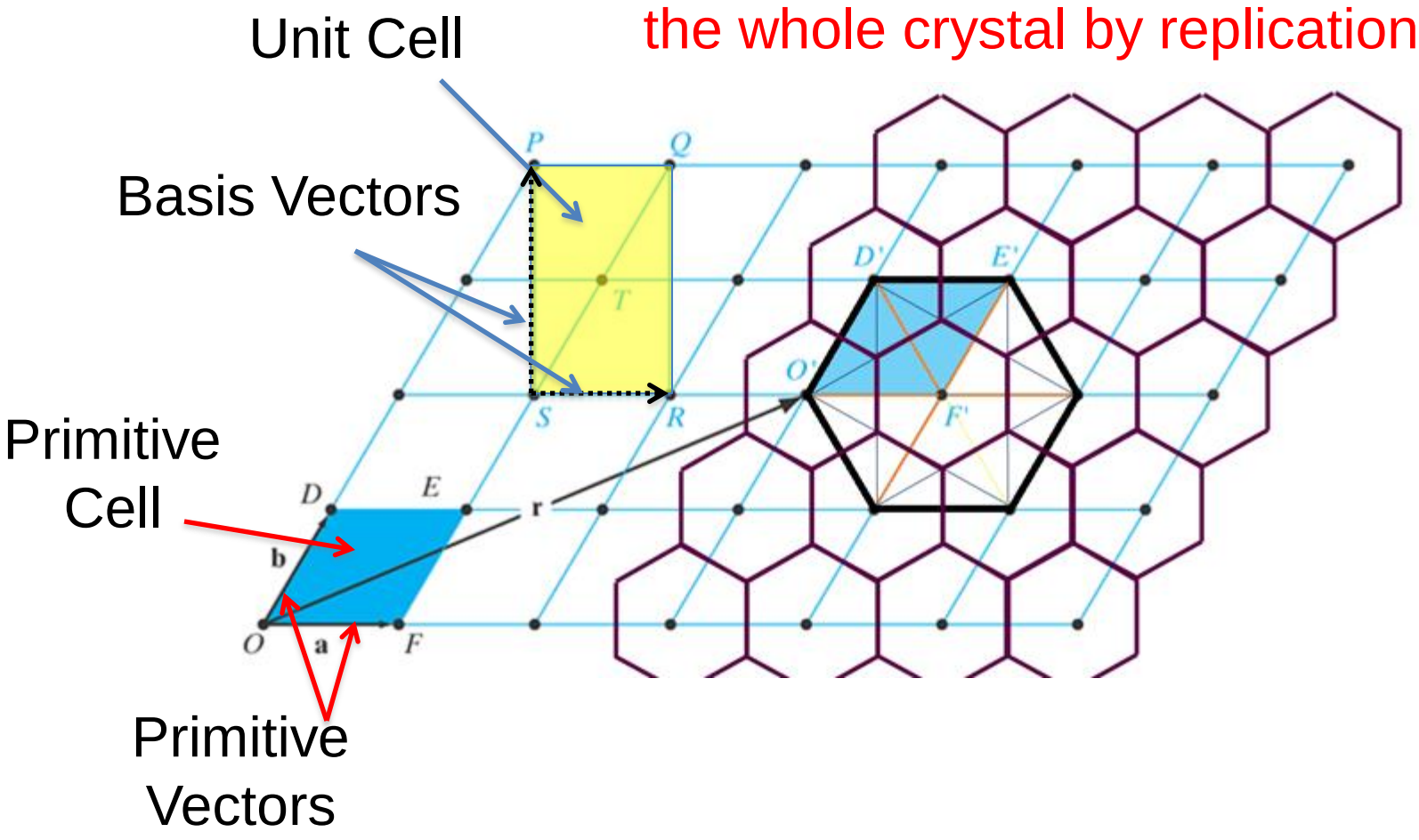
Simple Lattices and Unit Cells

3) The inner hexagon is the "Wigner-Seitz" primitive cell



Simple Lattices and Unit Cells

3) The new primitive cell will cover the whole crystal by replication

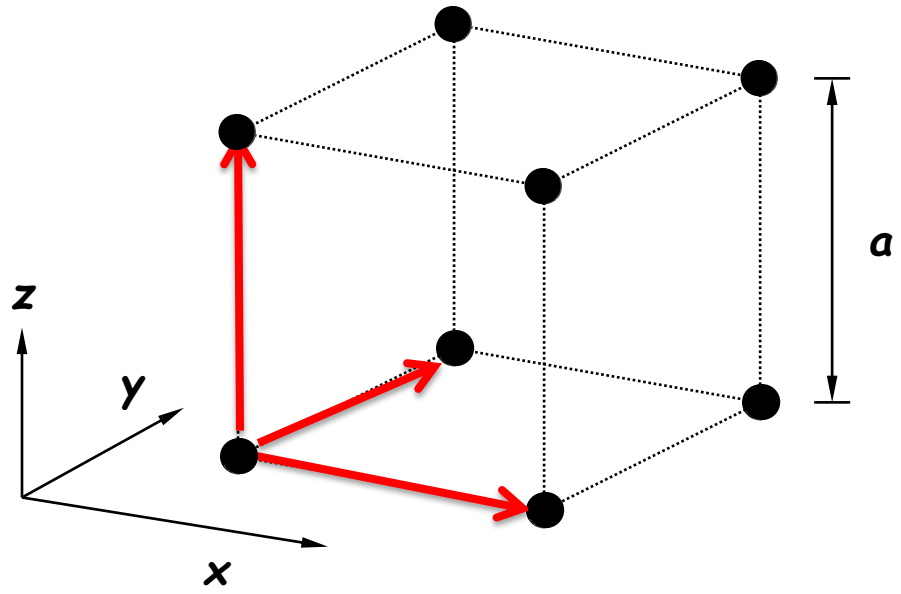


Other Important Definitions

- **<u>Lattice Constant:</u>** distance along the edge of a cubic unit cell ("a" in examples that follow)

NOTE: The lattice constant is **NOT** necessarily the distance between nearest neighbor atoms (bond length).

Cubic Crystal Structures



- **primitive vectors** are equal in all three dimensions.
- The balls represent the **lattice** points.

a = lattice constant

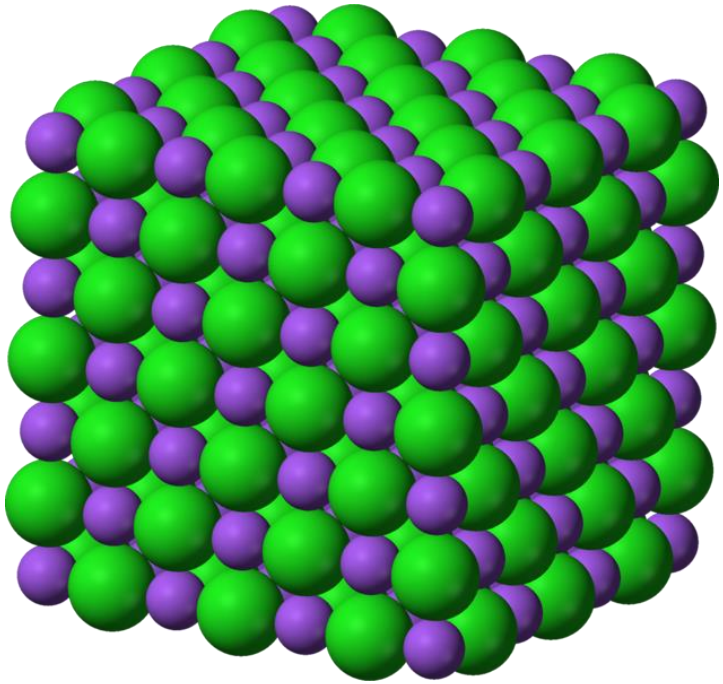
$$\mathbf{a}_1 = a\hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a\hat{\mathbf{y}}$$

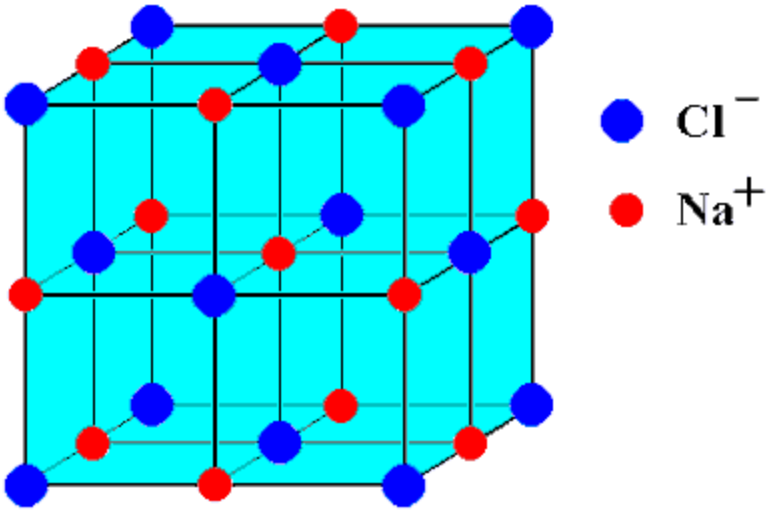
$$\mathbf{a}_3 = a\hat{\mathbf{z}}$$

The only element with simple cubic crystal is α-polonium

Cubic Crystal Structures

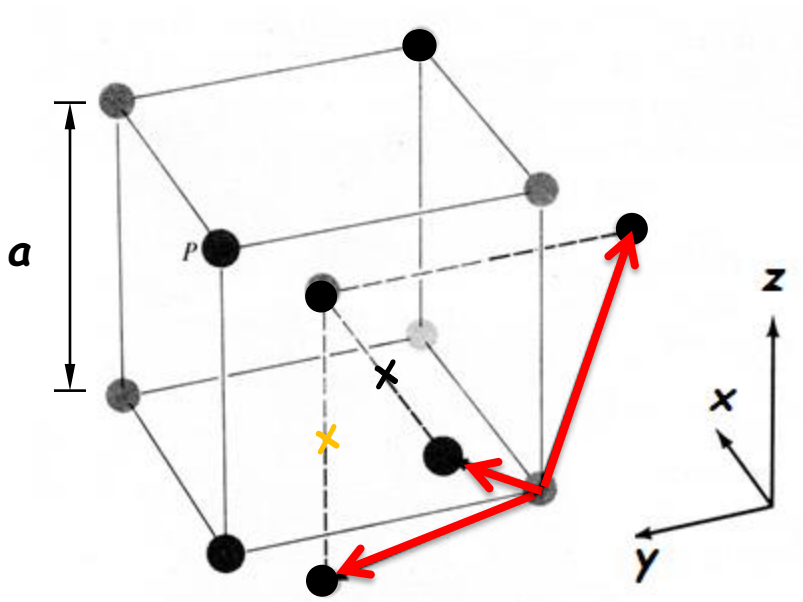


unit cell



NaCl has a cubic structure but it has two elements (more complicated)

Body-Centered Cubic Crystal Structure



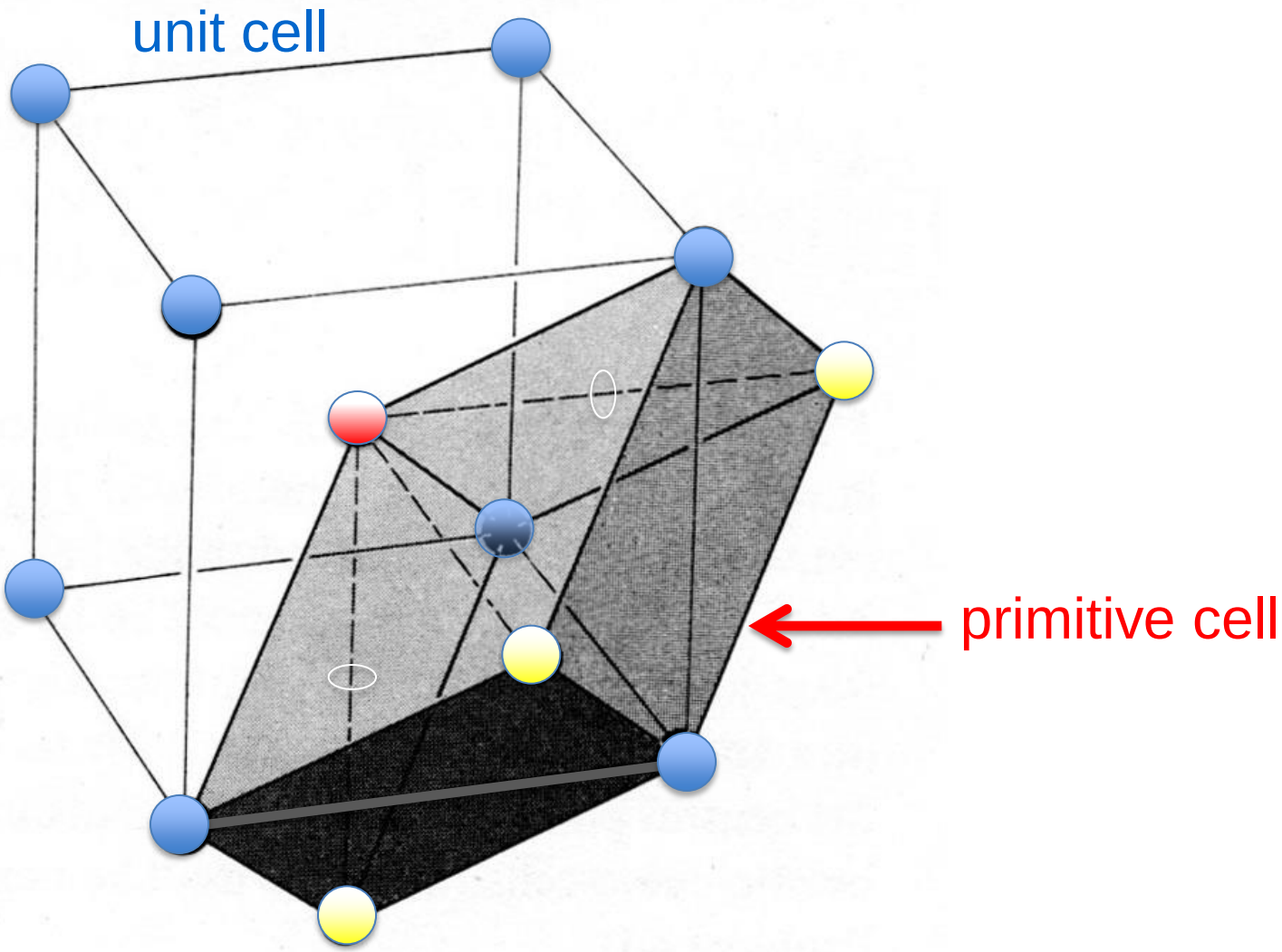
- Same as simple cubic but with an additional atom at the center of the cell.
- One set of possible primitive lattice vectors

$$\mathbf{a}_1 = \frac{a}{2}\left[\hat{\mathbf{x}} + \hat{\mathbf{y}} - \hat{\mathbf{z}}\right]$$

$$\mathbf{a}_2 = \frac{a}{2}\left[-\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}}\right]$$

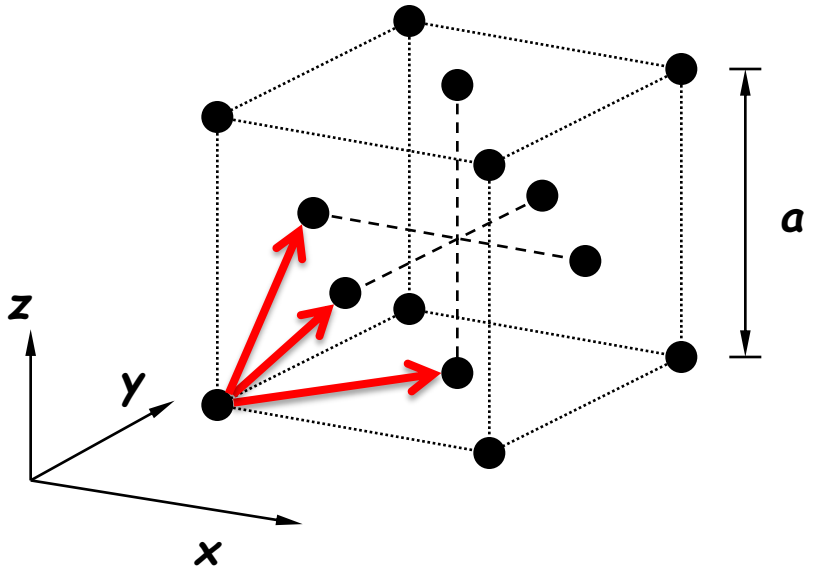
$$\mathbf{a}_3 = \frac{a}{2}\left[\hat{\mathbf{x}} - \hat{\mathbf{y}} + \hat{\mathbf{z}}\right]$$

Body-Centered Cubic Crystal Structure



Face-Centered Cubic Crystal Structure

- Examine the face-centered cubic lattice (fcc):
  - This is formed by adding an additional atom in the center of each face of the simple cubic configuration.
  - This is the most important configuration we will consider.
  - The **primitive vectors** have been written again by using symmetry considerations.

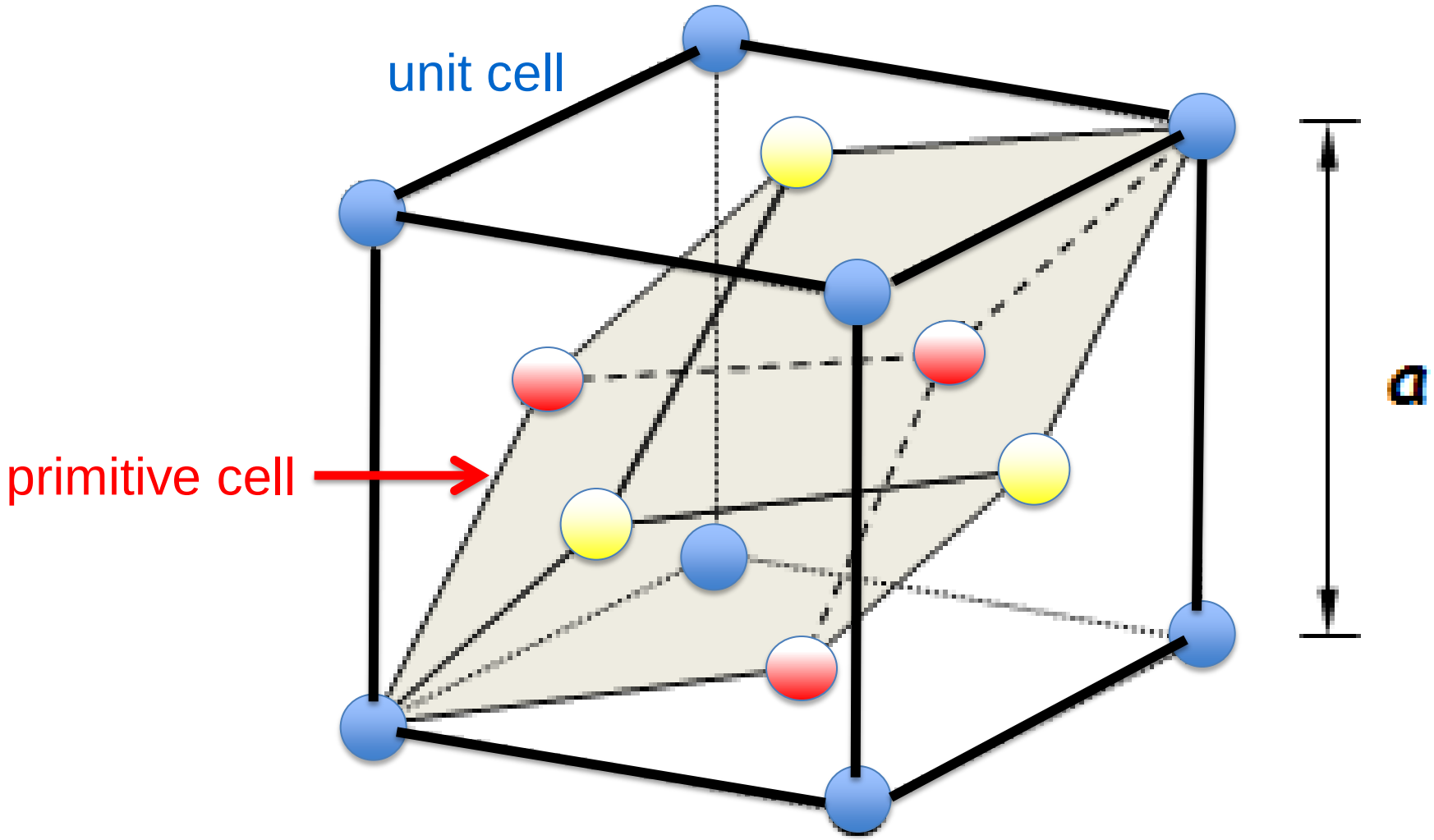


$$\mathbf{a}_1 = \frac{a}{2}[\hat{\mathbf{x}} + \hat{\mathbf{y}}]$$

$$\mathbf{a}_2 = \frac{a}{2}[\hat{\mathbf{y}} + \hat{\mathbf{z}}]$$

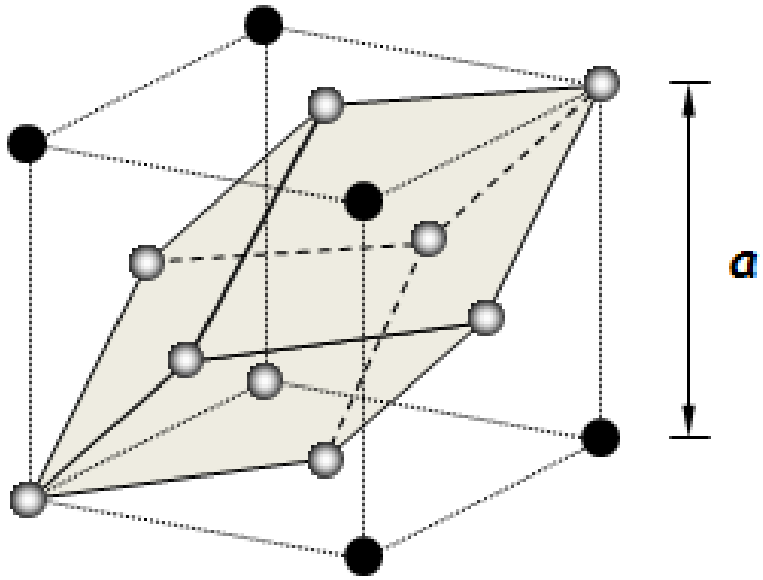
$$\mathbf{a}_3 = \frac{a}{2}[\hat{\mathbf{z}} + \hat{\mathbf{x}}]$$

Faced-Centered Cubic Crystal Structures



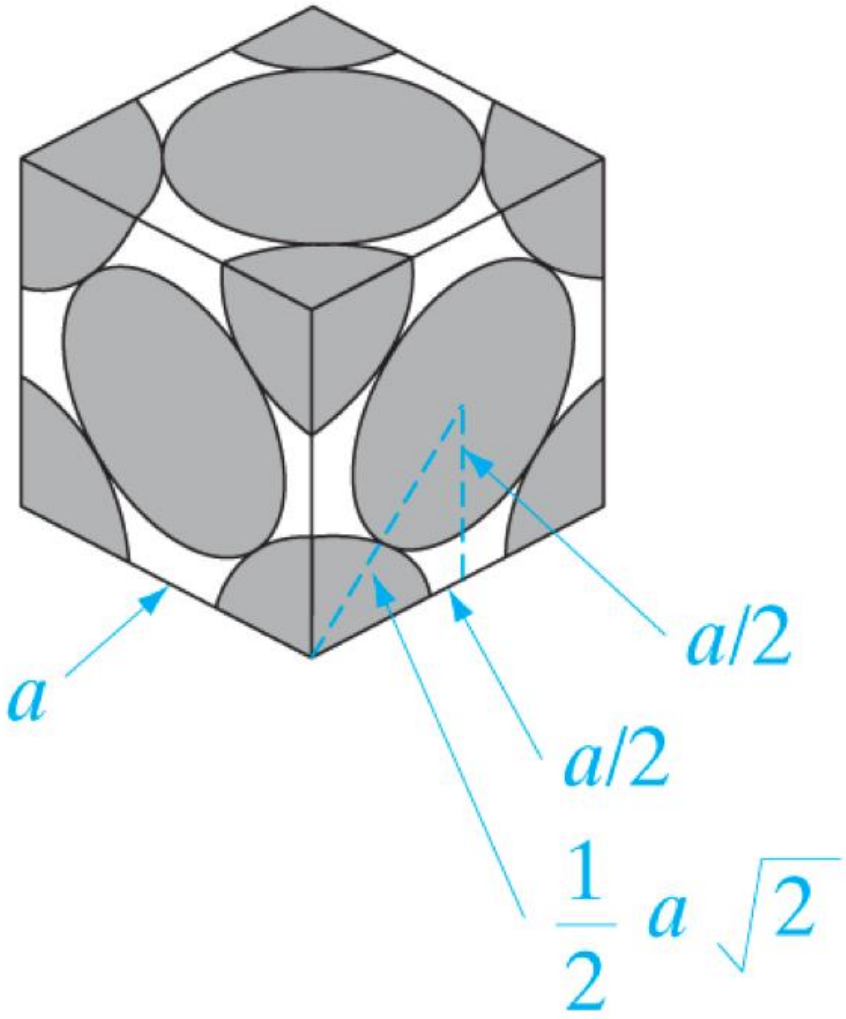
Cubic Crystal Structures

$$V_{primitive} = \frac{a^3}{4}$$



$$V_{unit} = \mathbf{a}_3 \cdot \mathbf{a}_1 \cdot \mathbf{a}_2 = a^3$$

Atomic size from packing of spheres



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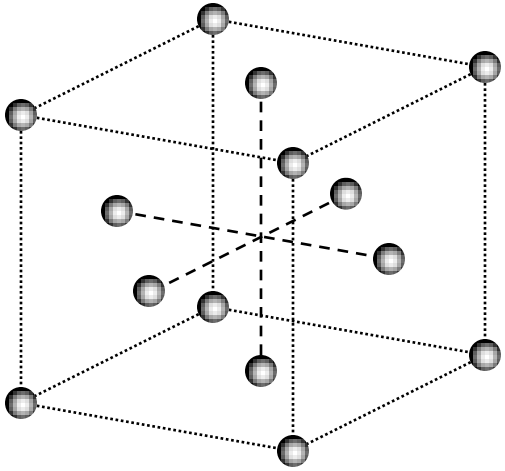
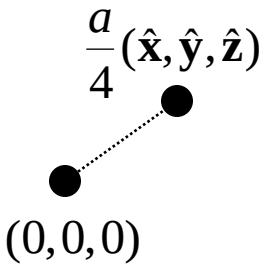
Diamond Lattice

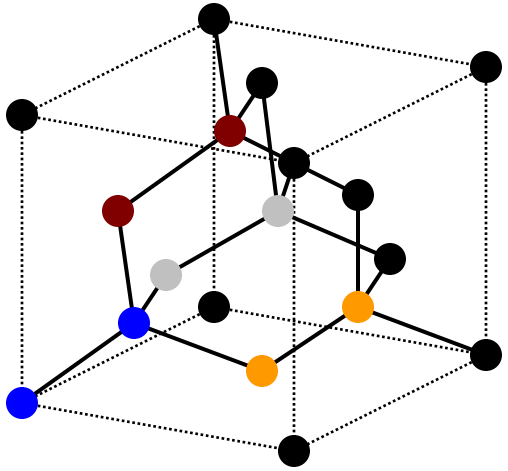
Two interpenetrating fcc lattices



LATTICE



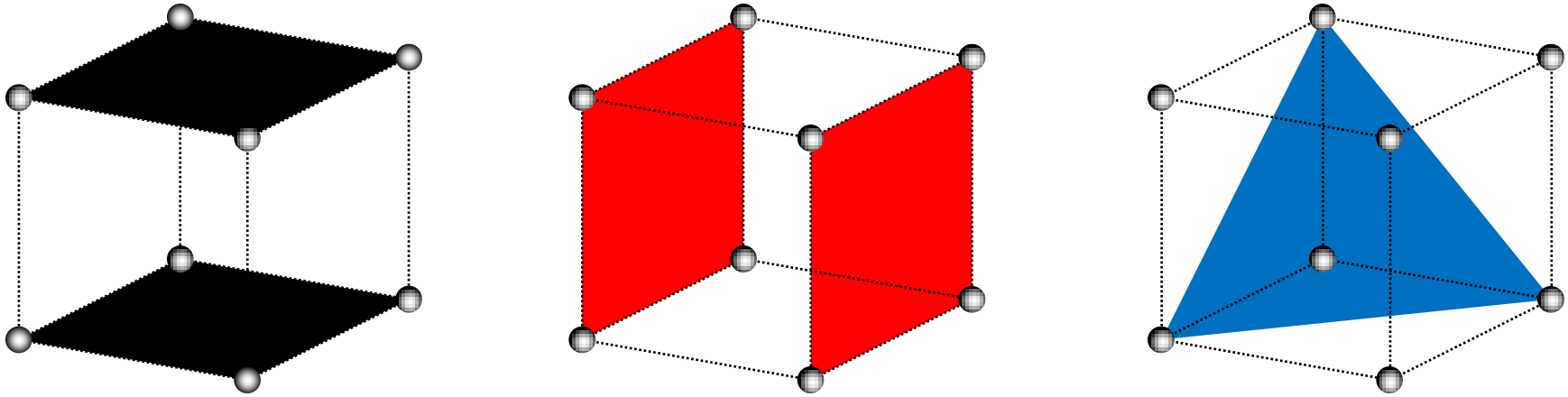
BASIS



UNIT CELL

Miller indices

- For any direction one could define many different equivalent planes.
- For instance, consider the different equivalent crystal planes in a cubic **lattice**.

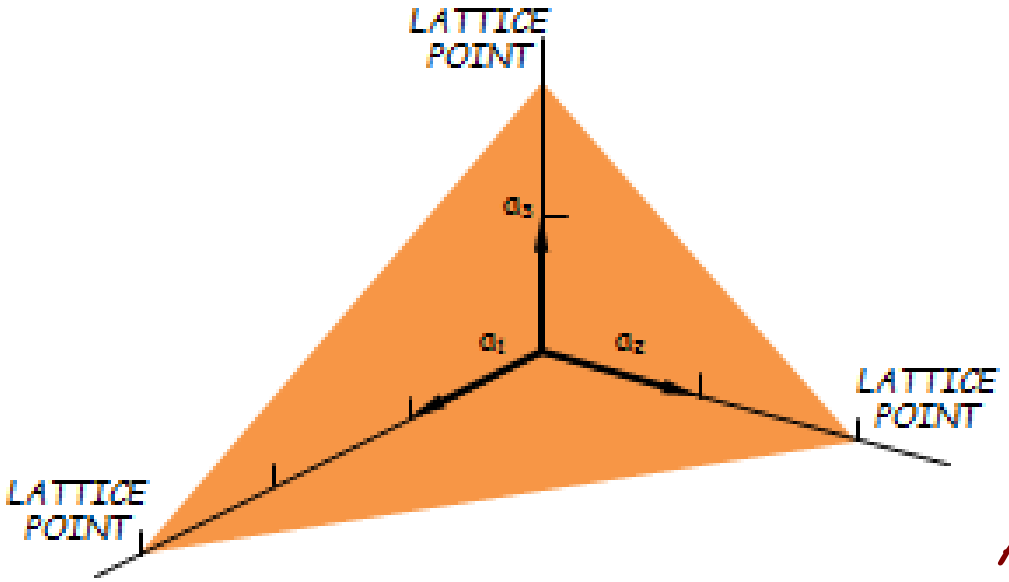


Miller indices

We can classify crystal planes through the use of **Miller Indices**.

1. Start with any arbitrary point in the crystal lattice.
2. Take the three primitive lattice vectors as axes.
3. Next we locate the intercepts of the desired plane with these coordinate axes.
4. Finally, we take the reciprocal of the intercepts and multiply each of these by the smallest factor required to convert them all to integers.
   - **Indices which have no intercept have a Miller Index of zero.**

Miller indices

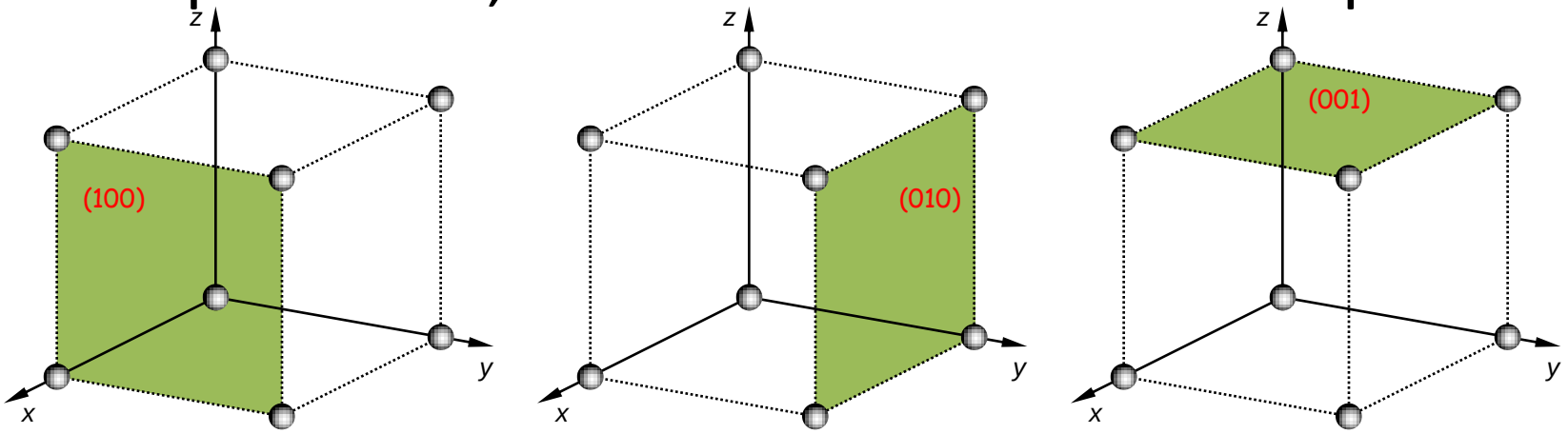


AXIS	INTERCEPT	RECIPROCAL
a_1	3	1/3
a_2	2	1/2
a_3	2	1/2

TO CONVERT THE RECIPROCALS TO INTEGERS WE NEED TO MULTIPLY BY A FACTOR OF SIX THIS YIELDS ***MILLER INDICES (233)***

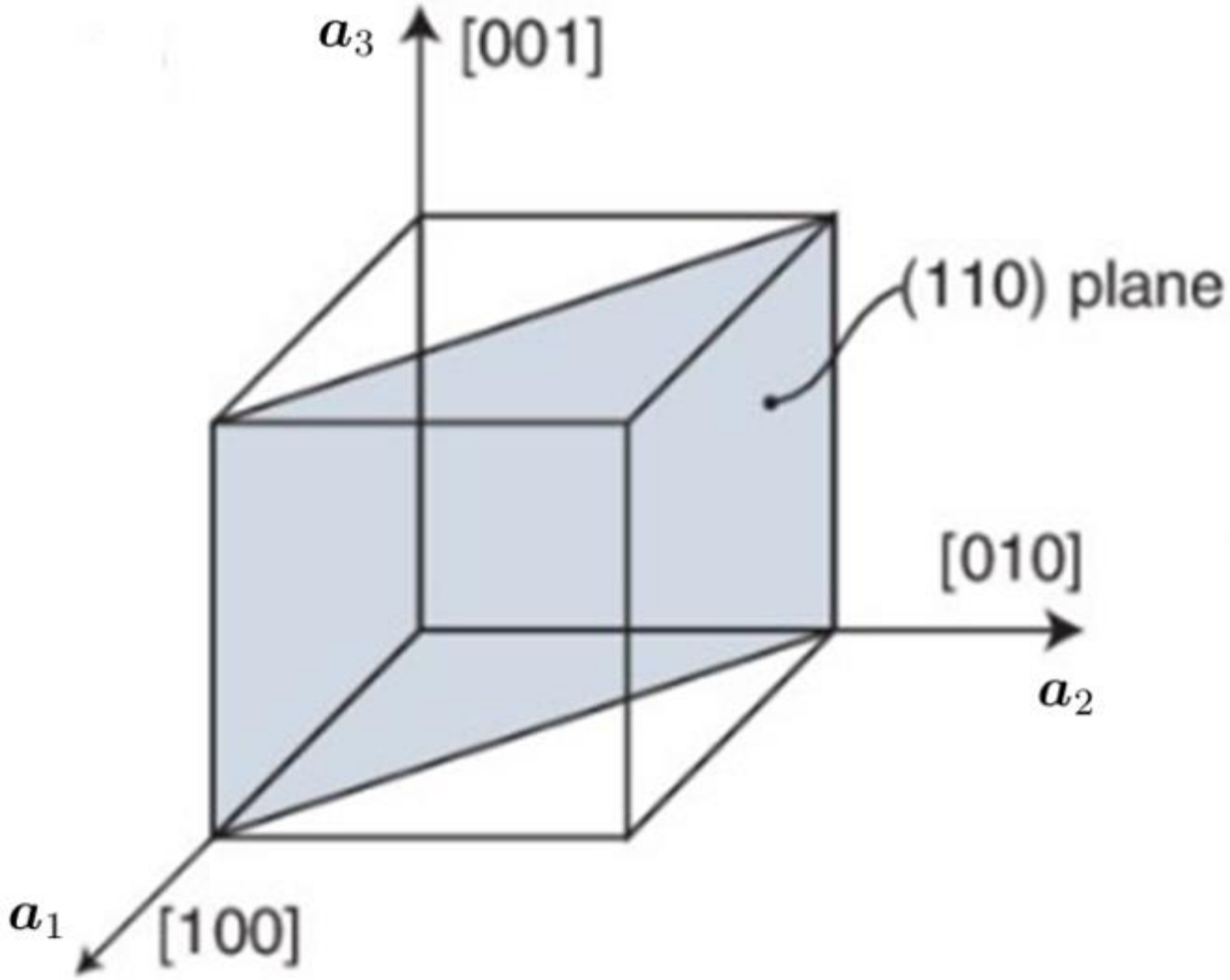
Miller indices

- Since we chose the origin arbitrarily when we began, **Miller indices** define a family of parallel planes.
- To denote crystal planes with the same symmetry, we use **{hkl}**.
- "h" is the x-axis intercept inverse, "k" is the y-axis intercept inverse, and "l" is the z-axis intercept inverse .

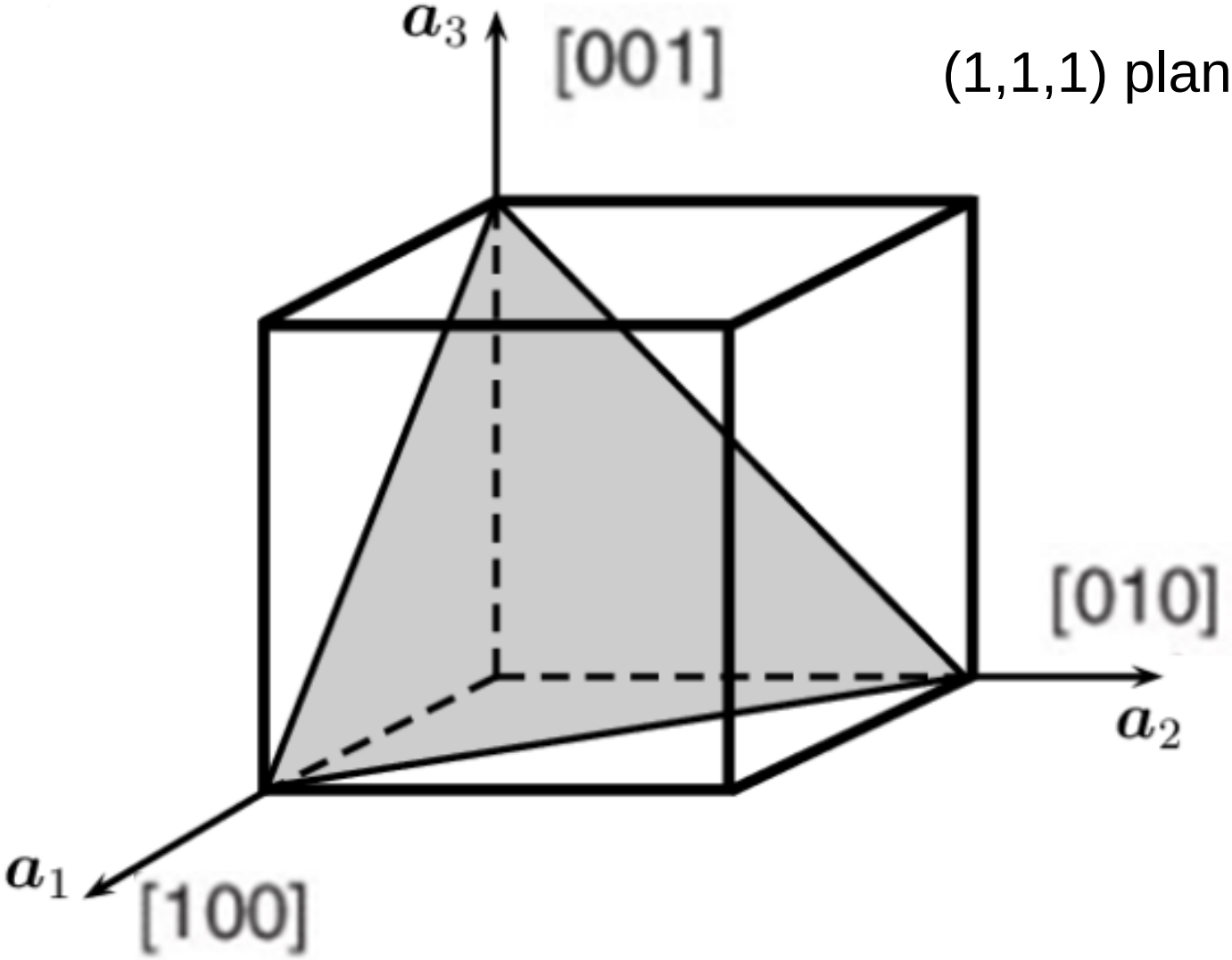


All three planes shown here are related by simple rotations, thus they represent {100} family.

Miller indices



Miller indices



(1,1,1) plane

Miller indices

A crystal plane: **(*hkl*)**

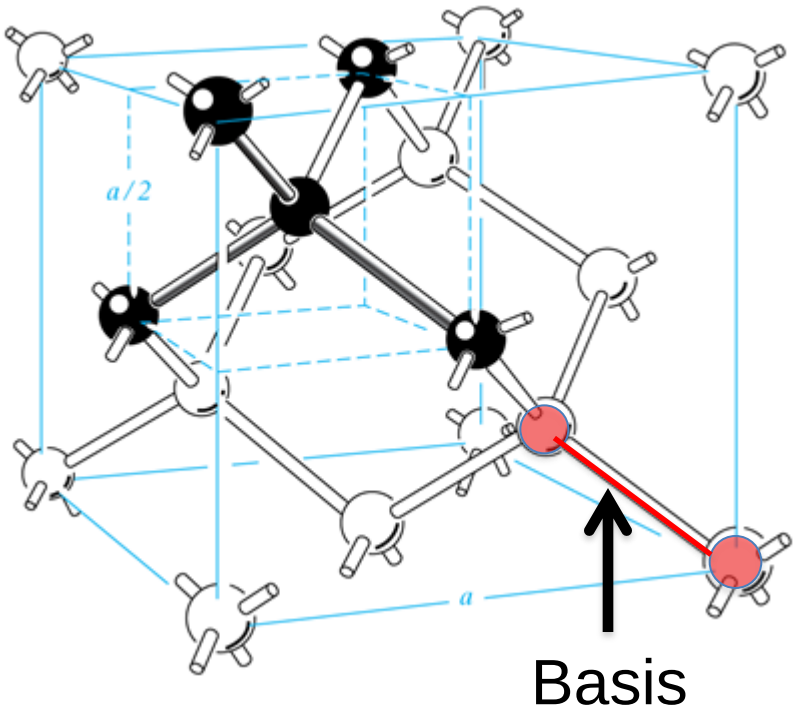
Family of equivalent planes: **{*hkl*}**

Crystal direction: **[*hkl*]**
(normal to plane **(*hkl*)** in a cubic lattice)

Silicon

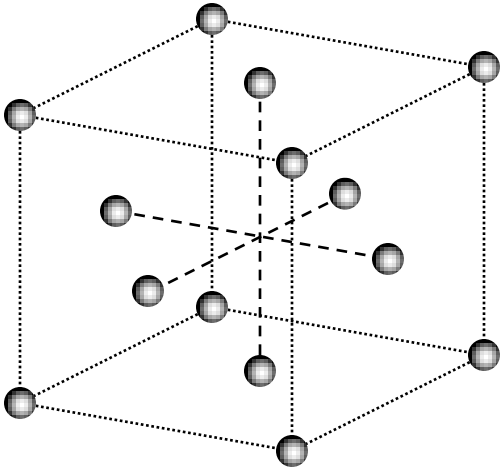
Lattice Constant

a = 5.43 Å



Let’s get to know Silicon better (1)

- How many atoms in the unit cell?
  - Let’s look at the FCC lattice first



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- How many atoms in the unit cell?
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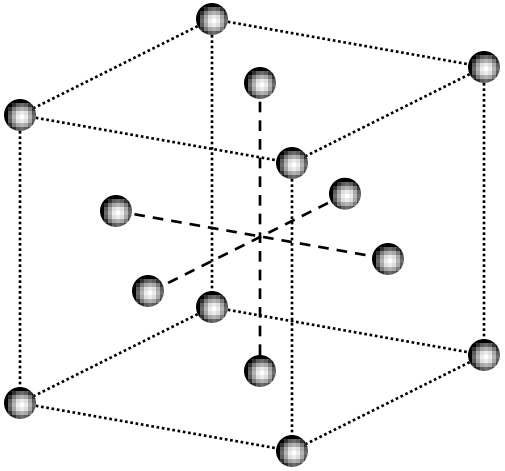
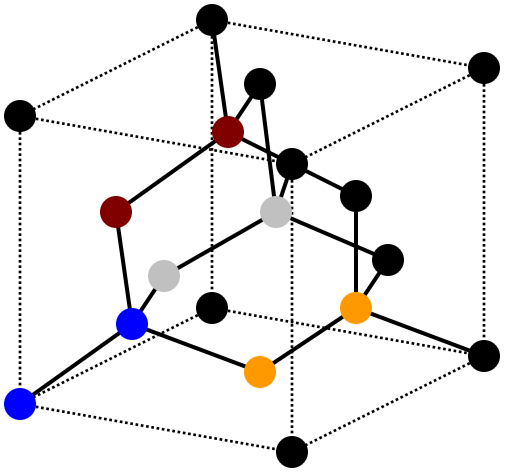
- 4 ATOMS PER CELL



- Now, add the second sub-lattice of the diamond lattice



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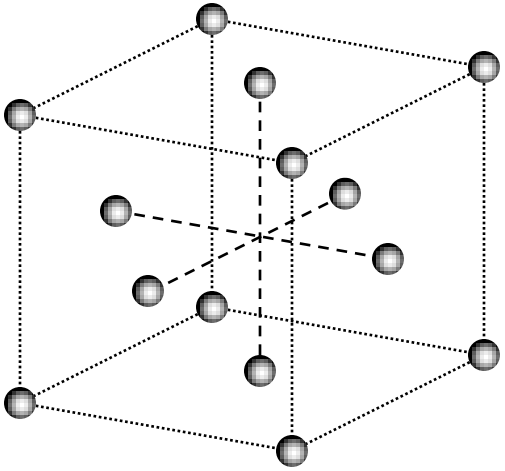
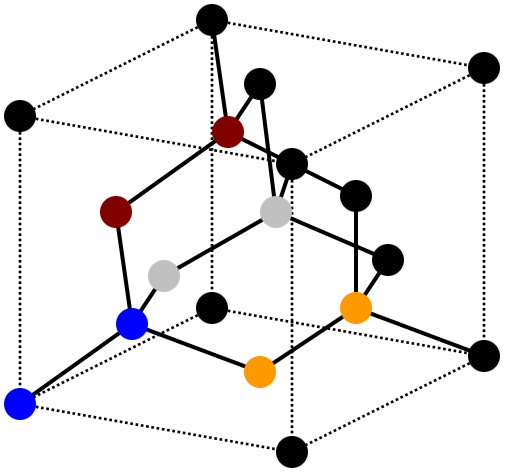
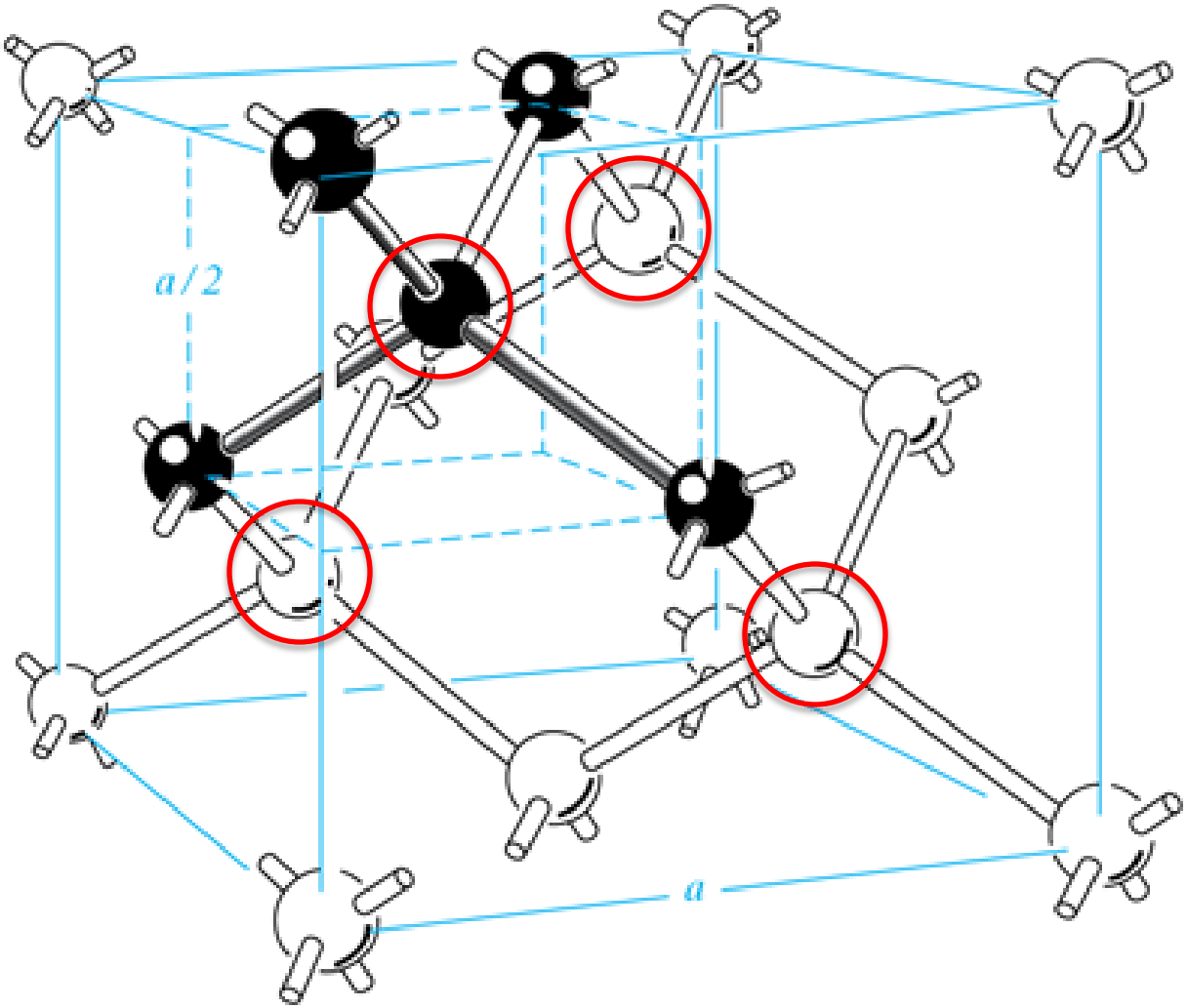


- Now, add the second sub-lattice of the diamond lattice
- 8 ATOMS PER CELL

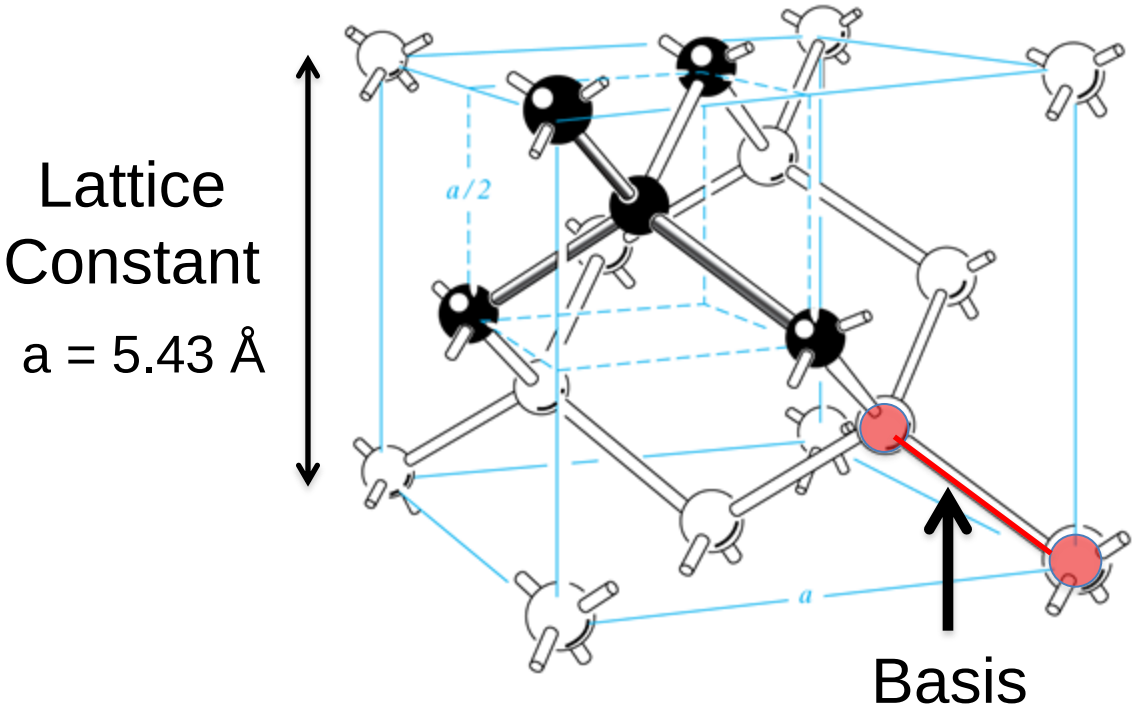


Let’s get to know Silicon better (1)



Let’s get to know Silicon better (2)

- What is the distance between nearest neighbors?



Let's get to know Silicon better (2)

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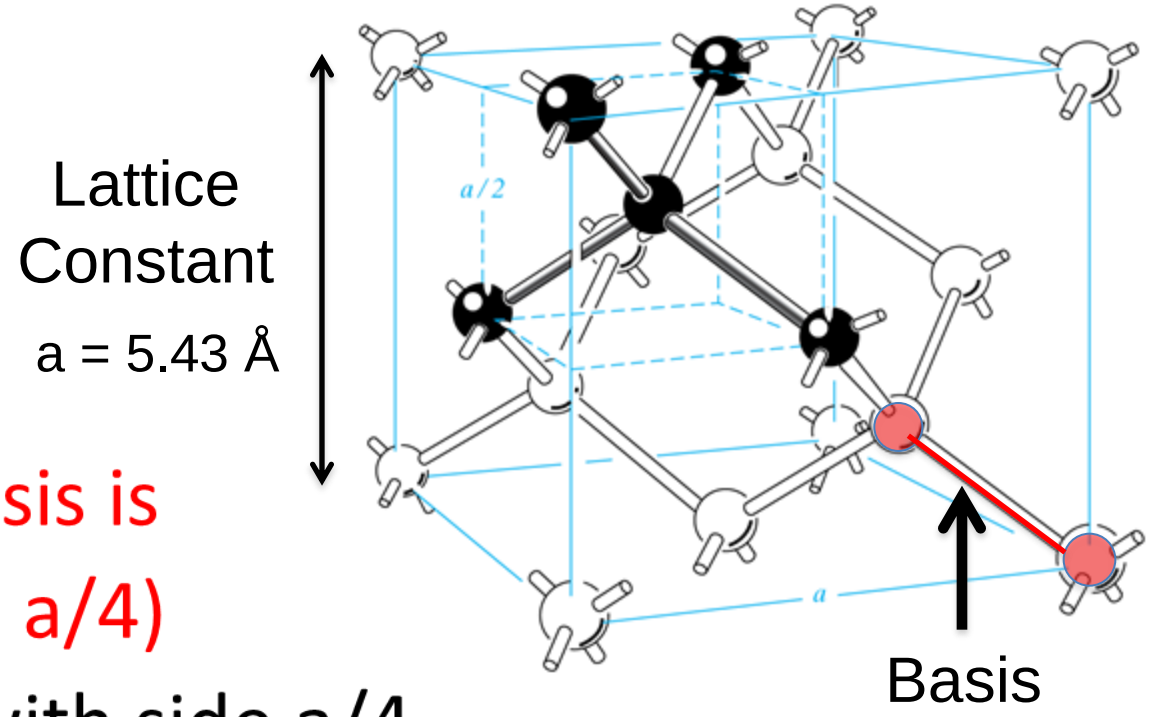


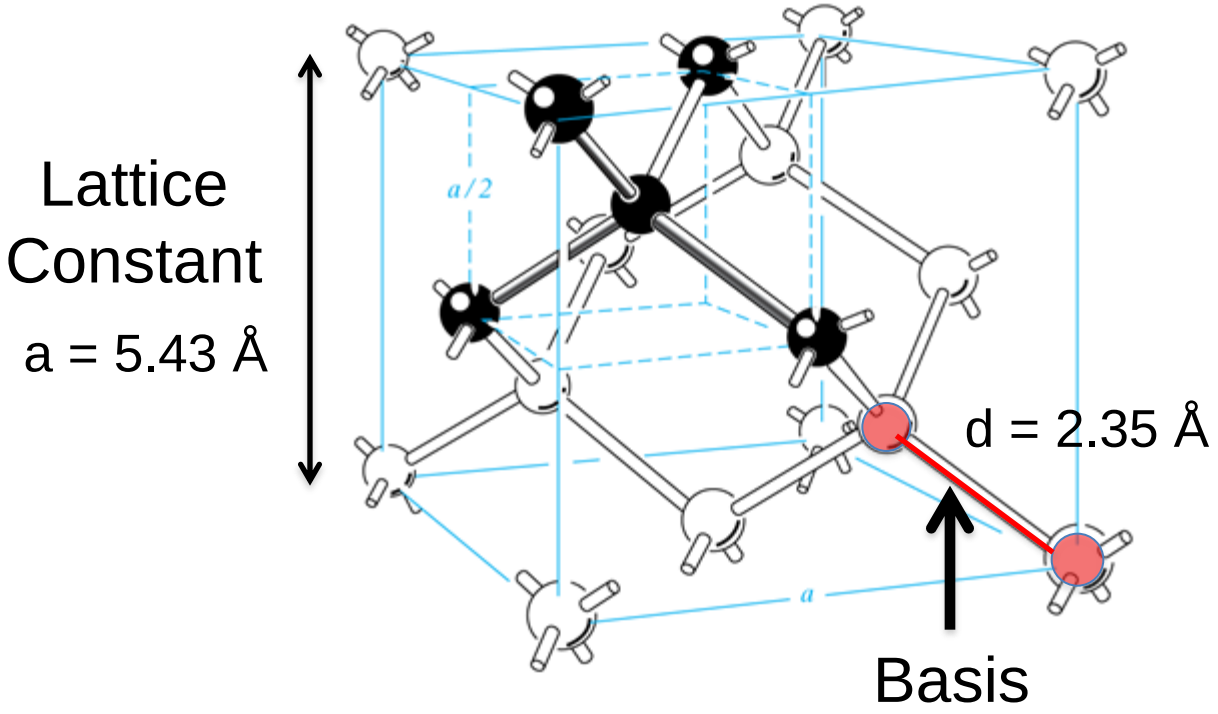
Second atom in basis is offset by (a/4, a/4, a/4)

Diagonal of cube with side a/4

$$d = \frac{\sqrt{3}a}{4} = \frac{1.732 \times 5.43}{4} = 2.35\text{Å}$$

Let’s get to know Silicon better (3)

- What is the packing fraction of Silicon?



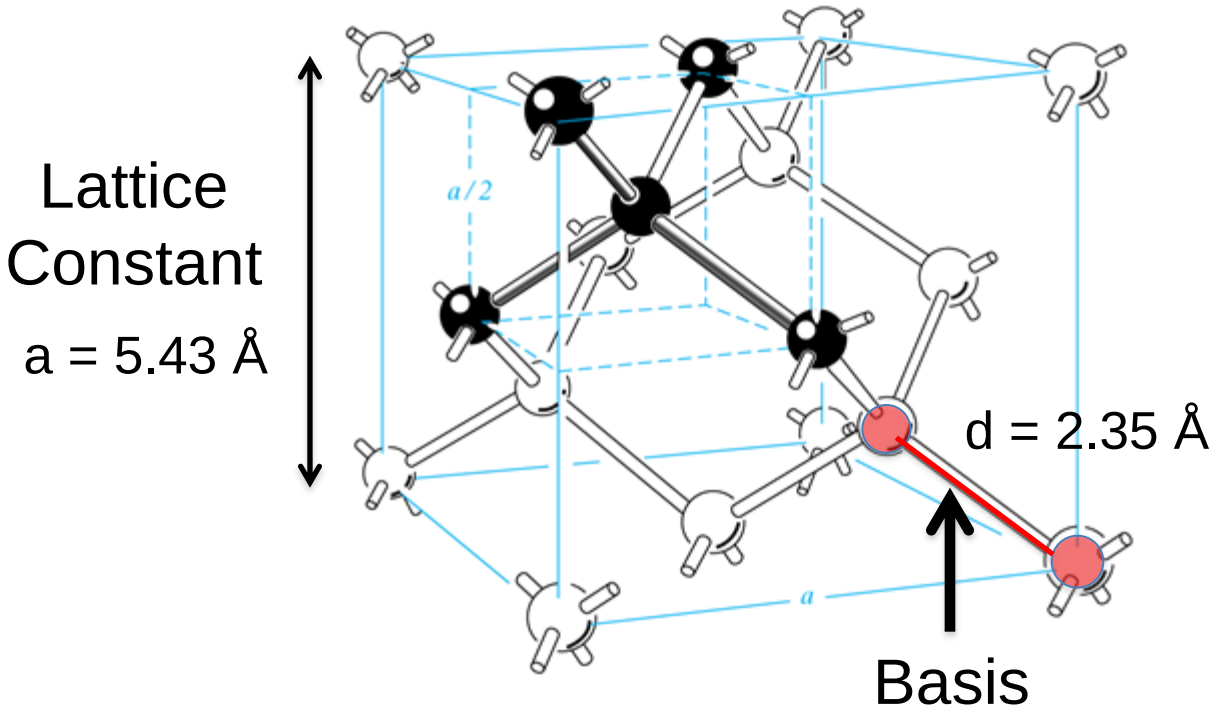
Let's get to know Silicon better (3)

- What is the packing fraction of Silicon?

Volume of unit cell = a^3 = $160.1\ \text{Å}^3$

Volume of atom (assume a sphere)

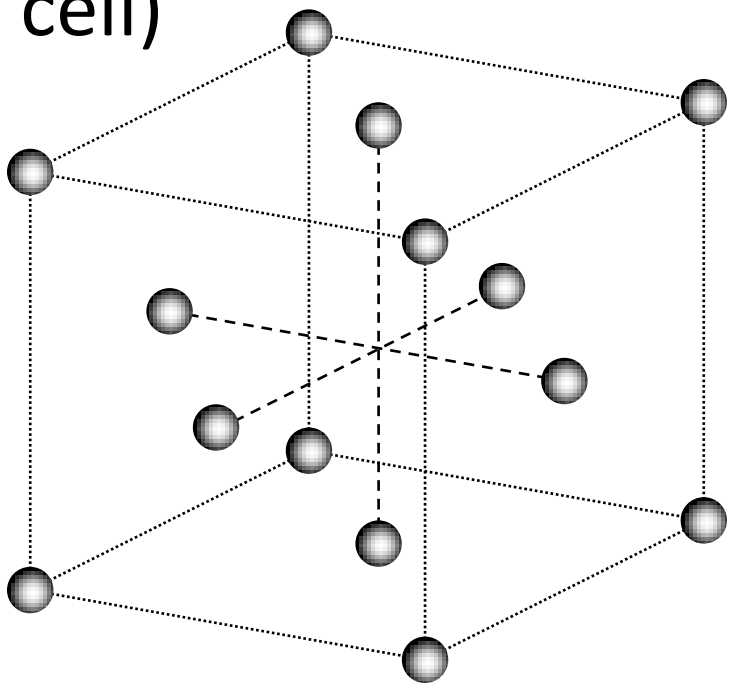
$$\frac{4}{3}\pi\left(\frac{d}{2}\right)^3 = 6.8\ \text{Å}^3$$



Packing fraction = (8 x 6.8)/160.1 = 0.34 = 34%

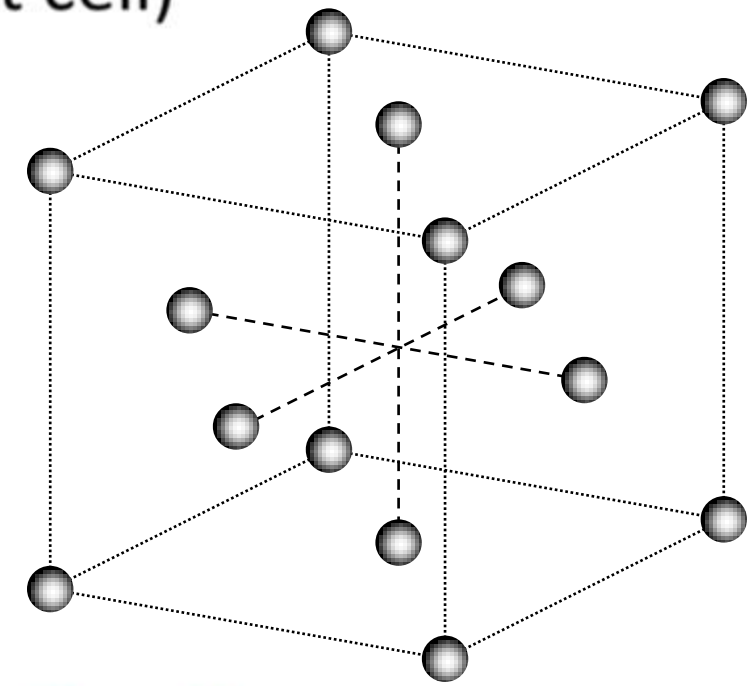
Let’s get to know Silicon better (4)

- What is the packing fraction of a simple fcc lattice? (remember: 4 atoms per unit cell)



Let's get to know Silicon better (4)

- What is the packing fraction of a simple fcc lattice? (remember: 4 atoms per unit cell)



Volume of unit cell = a^3

Nearest neighbor distance =

$$d = \frac{a}{2}\sqrt{2}$$

Volume of atom

$$\frac{4}{3}\pi\left(\frac{a}{4}\sqrt{2}\right)^3 = 0.185\ a^3$$

Packing fraction = (4 x 0.185) a^3 / a^3 = 0.74 = 74%

Interesting… that's more than twice than for diamond lattice.

Packing fractions for cubic lattices

- Face-Centered Cubic

$$\sqrt{2}\frac{\pi}{6} = 0.74$$

- Body-Centered Cubic

$$\sqrt{3}\frac{\pi}{8} = 0.68$$

- Simple Cubic

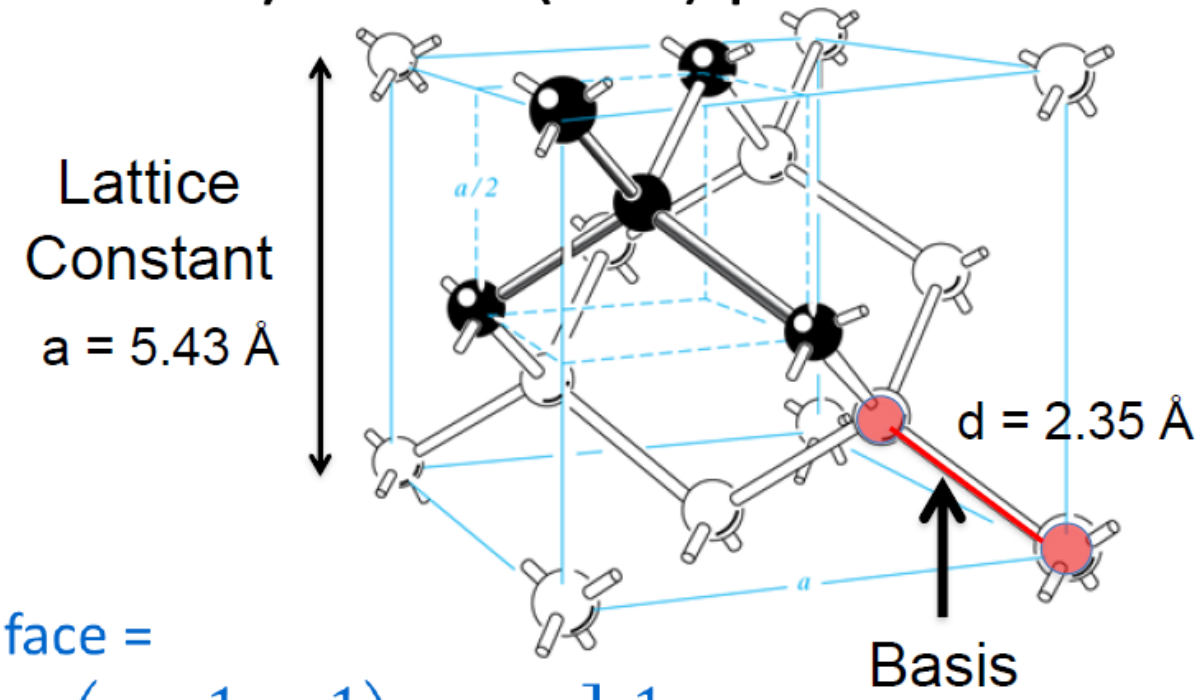
$$\frac{\pi}{6} = 0.52$$

- Diamond Lattice

$$\sqrt{3}\frac{\pi}{16} = 0.34$$

Let's get to know Silicon better (5)

- What is the areal density of the (100) plane?



Areal Density =

= # Atoms on face/ Area face =

$$= \left[\left(4 \times \frac{1}{8} + \frac{1}{2}\right)_{\substack{above \\ surface}} + \left(4 \times \frac{1}{8} + \frac{1}{2}\right)_{\substack{below \\ surface}}\right] \frac{1}{a^2} = 2/a^2$$

$$= 6.78 \times 10^{18} m^{-2} = 6.78 \times 10^{14} cm^{-2}$$

Podcasts on the elements

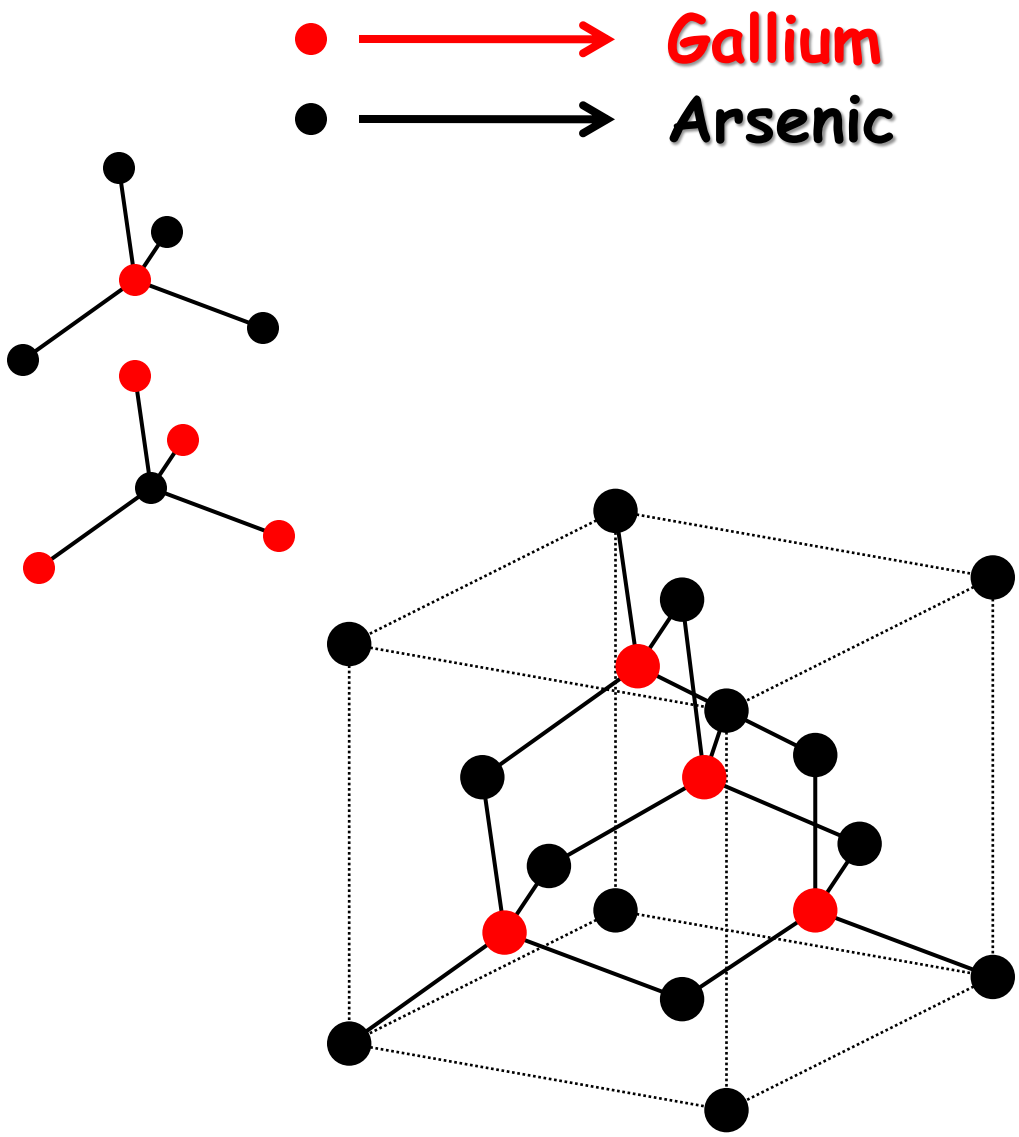
- Do you want to know more about Silicon while relaxing?
  – BBC Radio 4 program (28 minutes):
  https://www.bbc.co.uk/sounds/play/b08rfh05

- **Here is the download page for all BBC podcasts on the Elements:**
  https://www.bbc.co.uk/programmes/p01rcrn6/episodes/downloads

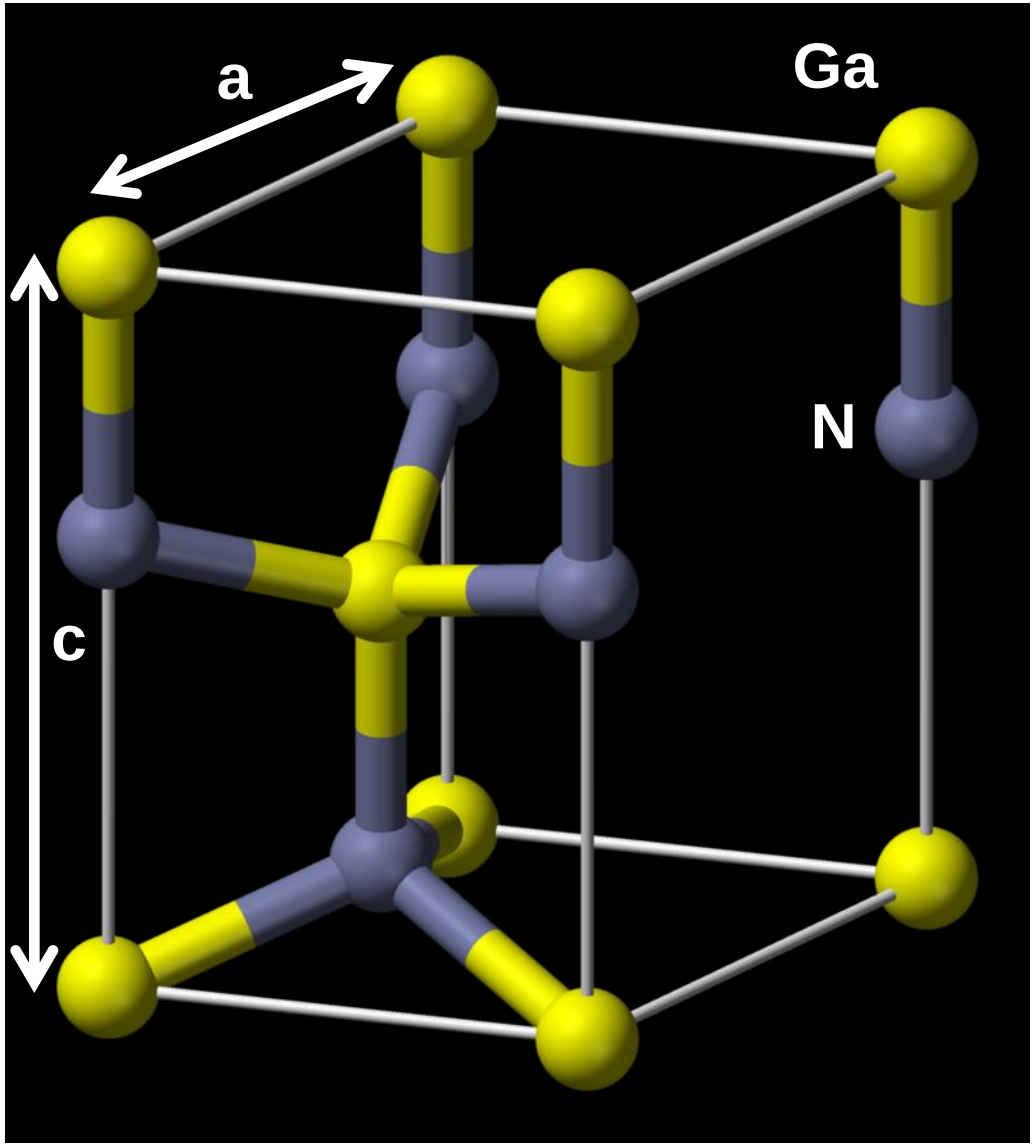
- **Suggested ones directly pertinent to the class:**
  Silicon – chips https://www.bbc.co.uk/programmes/p02rnxxh
  Silicon – solar https://www.bbc.co.uk/programmes/p02rnxvm
  Germanium https://www.bbc.co.uk/programmes/p03mrtq0
  Gallium and Indium https://www.bbc.co.uk/programmes/p02ssjnx

Compound Semiconductors

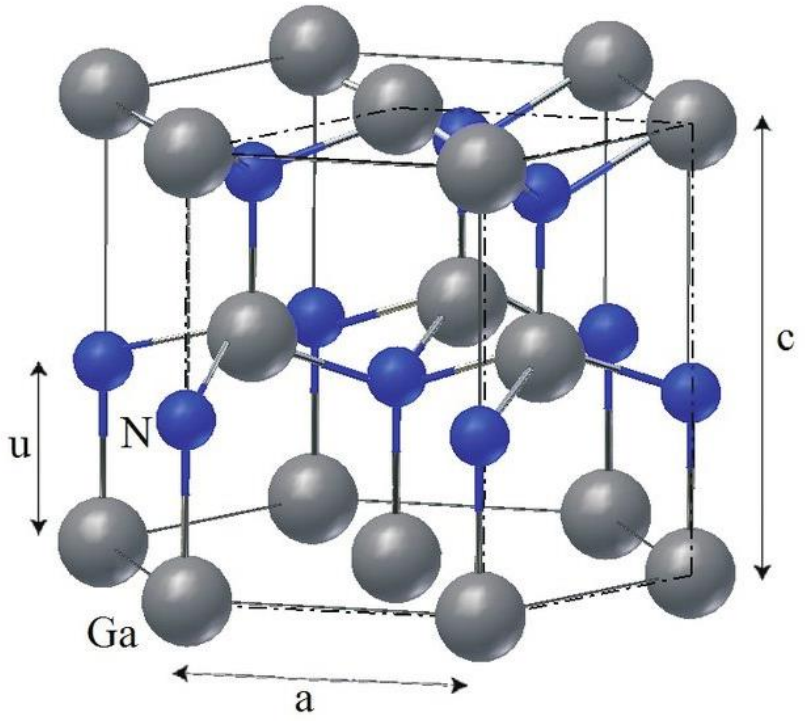
- Many compound semiconductors such as Gallium Arsenide (GaAs) exhibit the **zincblende** crystal structure.
  - The atomic configuration is the same as **diamond**.



Another example: Wurtzite Structure



Hoang et al. (2013)



Adapted from Wikipedia, “Wurtzite”

Important Material Systems