ECE 340
Lecture 3: Semiconductors and Crystal Structure

Class Outline:

- Semiconductor Crystal Lattices
- Semiconductor Crystal Growth
Key Questions

- Why is crystal order important?
- How is a crystal defined?
- What are the most common types of crystal lattices used in semiconductor devices?
Semiconductor Crystal Lattices

What is the crystal structure?

Crystalline | Polycrystalline | Amorphous

• Crystal structures come in three basic kinds
  
  – In the **CRYSTALLINE** state the atoms are ordered into a well-defined lattice that extends over very long distances.
  
  – **POLYCRYSTALLINE** materials consist of small crystallites that are embedded in regions of material.
  
  – In the **AMORPHOUS** state there is little or no evidence for long-range crystalline order.
Semiconductor Crystal Lattices

What does it matter if it is crystalline or not?

- Crystalline
- Amorphous

- We can get a lot of information from the unit cell:
  - Density of atoms
  - Distance between nearest atoms
    - Calculate forces between atoms
  - Perform simple calculations
    - Fraction of atoms filled in volume
    - Density of atoms
Semiconductor Crystal Lattices

Since we care about crystalline lattices, let’s examine the periodic lattice...

- In the periodic lattice:
  - Symmetric array of points is the lattice.
  - We add the atoms to the lattice in an arrangement called a basis.
  - We can define a set of primitive vectors which can be used to trace out the entire crystal structure.
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In this section we consider some of the lattice types that will be important for our discussion of semiconductors...

- Examine the simple cubic structure:
  - All primitive vectors are equal in all three dimensions.
  - Here again, the balls represent the lattice points, but no basis has been added.

\[
\begin{align*}
  \mathbf{a}_1 &= a\mathbf{\hat{x}} & (2.1) \\
  \mathbf{a}_2 &= a\mathbf{\hat{y}} & (2.2) \\
  \mathbf{a}_3 &= a\mathbf{\hat{z}} & (2.3)
\end{align*}
\]
Semiconductor Crystal Lattices

A simple variant on the cubic lattice is the body-centered cubic lattice...

- Examine the body-centered cubic lattice (bcc):
  - Same as simple cubic but with an additional atom at the center of the cell.
  - **Primitive vectors** are written in the more convenient symmetric form but other representations exist.

\[
\begin{align*}
\mathbf{a}_1 &= \frac{a}{2} [\hat{x} + \hat{y} - \hat{z}] \tag{2.4} \\
\mathbf{a}_2 &= \frac{a}{2} [-\hat{x} + \hat{y} + \hat{z}] \tag{2.5} \\
\mathbf{a}_3 &= \frac{a}{2} [\hat{x} - \hat{y} + \hat{z}] \tag{2.6}
\end{align*}
\]
Semiconductor Crystal Lattices

A final variant is the face-centered cubic lattice...

- 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.

\[
\begin{align*}
a_1 &= \frac{a}{2}[\hat{x} + \hat{y}] \quad (2.7) \\
a_2 &= \frac{a}{2}[\hat{y} + \hat{z}] \quad (2.8) \\
a_3 &= \frac{a}{2}[\hat{z} + \hat{x}] \quad (2.9)
\end{align*}
\]
But be careful...

- There is a difference between unit cells and primitive cells.
  - The primitive cell is the volume associated with one lattice point.
  - Often it is more convenient to use a unit cell that is larger than the primitive cell since such a cell illustrates the crystal symmetry in a clearer way.

\[
V_{\text{unit}} = a_3 \cdot a_1 \cdot a_2 = a^3
\]  
\[
V_{\text{primitive}} = a_3 \cdot (a_1 \times a_2) = \frac{a^3}{4}
\]
Now let’s look at the silicon crystal...

- To discuss the crystal structure of different semiconductors we will need to account for the **basis** unit that is added to each **lattice** point.
  - Elemental semiconductors such as silicon and germanium both exhibit the **diamond** structure.
  - Named after one of the two crystalline forms of carbon.

- Here we display the silicon **unit cell**.
  - The balls each represent one silicon atom.
  - The solid lines represent chemical bonds.
  - Note how the bonds form a tetrahedron.
  - How many atoms per unit cell?
Semiconductor Crystal Lattices

Looks confusing, but it’s not so bad...

- It is really just two inter-penetrating fcc lattices with a diatomic basis.
- It looks more complex because we do not show atoms extending beyond the unit cell by convention.
- In the figure below, each different color represents pairs of atoms from the same basis.
- The black balls represent atoms with one atom in their basis outside the unit cell.
Semiconductor Crystal Lattices

What about compound semiconductors?

• Many compound semiconductors such as Gallium Arsenide (GaAs) exhibit the **zincblende** crystal structure.
  - The atomic configuration is the same as **diamond**.
  - The difference lies in that each successive atom is from a different chemical element.

Useful questions to ask:

• How many atoms per unit cell?
• Avogadro’s number: \( N_A = \# \text{ atoms} / \text{mole} \)
• Atomic mass: \( A = \text{grams} / \text{mole} \)
• Atom counting in unit cell: \( \text{atoms} / \text{cm}^3 \)
• How do you calculate density?
Crystal Growth - Silicon

- Seed Crystal
- Silicon Chunks
- Molten Silicon
- Silicon Ingot

Image of a silicon ingot.
Heterojunctions are typically produced by a process known as **MOLECULAR-BEAM EPITAXY**.

- This is performed in an ultra-high vacuum (UHV) evaporation chamber working at pressures of $10^{-11}$ Torr.
- The materials to be grown are provided from heated **KNUDSEN CELLS** in which the individual elements are individually vaporized.

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**A SCHEMATIC DIAGRAM SHOWING THE KEY COMPONENTS OF A MOLECULAR-BEAM EPITAXY SYSTEM**
Careful control of the deposition rates and the substrate temperature are required to realize heterojunctions with well-defined interfaces.

- In order to achieve high uniformity the substrate is heated to approximately 600 °C and is slowly rotated in the vacuum chamber.
- The growth rate of the epitaxial layer is of order several micro \( \text{MICRONS PER HOUR} \), which allows for atomic level resolution in the growth process.
- The growth is monitored in situ using electron diffraction and mass spectroscopy.

TEM IMAGES OF EPITAXIALLY GROWN GaAs/AlGaAs
Example Problem

Treating atoms as rigid spheres with radii equal to $\frac{1}{2}$ the distance between the nearest neighbors, show that the ratio of the volume occupied by atoms to the total available volume in an FCC is 74%.