

Homework #1

The FCC, HCP and BCC Crystal Structures

Due 5pm Monday Oct. 7

Turn in outside of Durand 110 or email to [duerloo at stanford.edu](mailto:duerloo@stanford.edu)

The most common elemental structures are known as face-centered cubic (FCC), hexagonal close packed (HCP), and body-centered cubic (BCC). They serve as the basis for many common alloy systems and for several classes of more complex structures. Simplistic energetic considerations suggest that we can treat individual atoms as “hard spheres”, which are constrained to be in contact (“bonded”) with one another. This problem session is devoted to building hard-sphere models and performing geometrical calculations in order to illustrate some important features of the FCC, HCP, and BCC structures. In this homework, atomic positions are given in terms of the *conventional* unit cell and/or the *primitive* unit cell. Since the unit cells are translated and repeated in three dimensions to generate a macroscopic crystal, it is necessary to describe only a unit cell in order to describe the crystal as a whole.

You may find a web-based crystal visualization application helpful for this homework:

<http://www.dawgSDK.org/crystal/en/library/>

[http://www.chemtube3d.com/solidstate/hcp\(final\).htm](http://www.chemtube3d.com/solidstate/hcp(final).htm)

<http://cst-www.nrl.navy.mil/lattice/index.html>

Optional reference reading for this HW:

First part of Ch 1 in Hammond

Chapter 17 in de Graef and McHenry

Chapter 3 in Kelly and Knowles

1. Face-Centered Cubic (e.g., Al, Cu, Ag, Au, Ni, Pd, Pt, γ -Fe)

Conventional unit cell axes: $a=b=c$ $\alpha=\beta=\gamma=90^\circ$

Atomic positions, relative to conventional unit cell: $(0 \ 0 \ 0)$, $(\frac{1}{2} \ \frac{1}{2} \ 0)$, $(\frac{1}{2} \ 0 \ \frac{1}{2})$, $(0 \ \frac{1}{2} \ \frac{1}{2})$

These parameters are necessary and sufficient to describe the FCC unit cell. The axes of the cell are mutually perpendicular and of equal length. Upon translation in three directions (parallel to a, b, and c), an FCC crystal is produced. Each unit cell, in the shape of a cube, has one atom located at each corner and one at each face center:

Corners: $(0 \ 0 \ 0)$, $(1 \ 0 \ 0)$, $(0 \ 1 \ 0)$, $(0 \ 0 \ 1)$, $(1 \ 1 \ 0)$, $(1 \ 0 \ 1)$, $(0 \ 1 \ 1)$, $(1 \ 1 \ 1)$

Face Centers: $(\frac{1}{2} \ \frac{1}{2} \ 0)$, $(\frac{1}{2} \ 0 \ \frac{1}{2})$, $(\frac{1}{2} \ 0 \ \frac{1}{2})$, $(\frac{1}{2} \ \frac{1}{2} \ 1)$, $(\frac{1}{2} \ 1 \ \frac{1}{2})$, $(1 \ \frac{1}{2} \ \frac{1}{2})$

Using foam spheres or one of the web tools, build a hard-sphere model of the FCC structure.

(a) Identify all the close-packed directions (directions along which spheres are in contact) and all close-packed planes. Draw the arrangements of atoms on the close-packed plane.

(b) How many atoms are there per unit cubic (conventional) cell? Assuming that the hard-spheres touch along the close-packed direction, calculate the fraction of space occupied by the “atoms”.

Homework #1
The FCC, HCP and BCC Crystal Structures

2. Hexagonal Close Packed (e.g., Be, Mg, Zn, Cd, Co, Ti, Zr)

Primitive (and conventional) unit cell axes: $a = b \neq c$ $\alpha = \beta = 90^\circ, \gamma = 120^\circ$

Atomic positions: $(0 \ 0 \ 0), \left(\frac{2}{3} \ \frac{1}{3} \ \frac{1}{2}\right)$

As before, these parameters are necessary and sufficient to describe the unit cell. Like the FCC structure, the HCP structure is based on stacked close-packed planes, although the stacking sequences are different. In the HCP structure, however, one axis, conventionally taken to be the c-axis, is longer than the other two; further, the angle between the two other axes (a and b) is 120° . Thus the unit cell coordinate system is not Cartesian. There is one atom located at each corner of a parallelepiped, and one atom in its interior (but not at the exact center):

Corners: $(0 \ 0 \ 0), (1 \ 0 \ 0), (0 \ 1 \ 0), (0 \ 0 \ 1), (1 \ 1 \ 0), (1 \ 0 \ 1), (0 \ 1 \ 1), (1 \ 1 \ 1)$

Interior: $\left(\frac{2}{3} \ \frac{1}{3} \ \frac{1}{2}\right)$

Build a hard-sphere model of the HCP structure.

- (a) Identify the close-packed directions and all close-packed planes. Draw the arrangements of atoms on the close-packed plane.
- (b) How many atoms are there per unit cell in the complete crystal? Assuming that the hard-spheres touch along the close-packed direction, calculate the fraction of space occupied by the spherical atoms.
- (c) Calculate the ideal c/a ratio assuming contact between adjacent hard spheres.
- (d) How are the close-packed planes and the stacking sequences of the FCC and HCP structures similar, and how are they different? The differences account for the vastly different mechanical properties of these two types of crystals.

Homework #1

The FCC, HCP and BCC Crystal Structures

3. Stacking faults in Close-Packed Structures

- (a) An intrinsic stacking fault in FCC can be considered as a missing close-packed plane, and an extrinsic fault as an additional close-packed plane. Write down the stacking sequences for these two faults.
- (b) How would one convert FCC to HCP by a Shockley partial dislocation mechanism?
- (c) How would one create a twin structure (i.e., mirror image or reverse stacking sequence) from a Shockley partial dislocation mechanism (i.e., ABCABC to CBACBA).
- (d) An intrinsic fault can also be created by the passage of a Shockley partial dislocation on a single close-packed plane. How would an *extrinsic* fault be created by Shockley partials? What local structure is created for the intrinsic fault, and what is created for the extrinsic fault?
- (e) Intrinsic stacking faults in the HCP structure cannot be made simply by removing a plane of atoms since AA stacking is not energetically favorable. However, a related fault can be made by passage of a single Shockley partial dislocation. Derive the stacking sequence for such a stacking fault. What structure is created locally?

Note: Stacking faults in FCC-based materials are also revealed by high resolution TEM. Figure 1 shows an extrinsic stacking fault in ZnTe, with the associated stacking sequence. ZnTe has the sphalerite crystal structure, but only the FCC lattice is revealed in Figure 1 at the resolution available at that time.

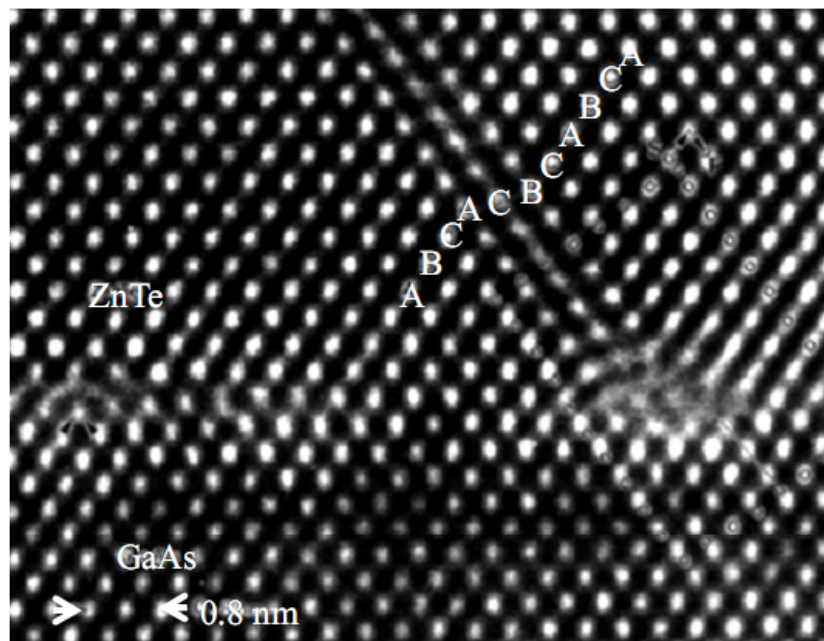


Fig 1. An extrinsic stacking fault at the interface between ZnTe and GaAs
(Courtesy of Schwartzman and Sinclair, 1991)

Homework #1
The FCC, HCP and BCC Crystal Structures

4. Body Centered Cubic (e.g., α -Fe, Li, Na, K, V, Nb, Ta, Cr, Mo, W)

Conventional unit Cell axes: $a=b=c$ $\alpha=\beta=\gamma=90^\circ$

Atomic positions: $(0 \ 0 \ 0), \left(\frac{1}{2} \ \frac{1}{2} \ \frac{1}{2}\right)$

This structure is not close-packed, but the notion of a “closest-packed” plane is still useful. As in FCC crystals, the conventional unit cell is based on a simple cube. There is a single atom located at each corner, and one at the cube center:

Corners: $(0 \ 0 \ 0), (1 \ 0 \ 0), (0 \ 1 \ 0), (0 \ 0 \ 1), (1 \ 1 \ 0), (1 \ 0 \ 1), (0 \ 1 \ 1), (1 \ 1 \ 1)$

Interior: $\left(\frac{1}{2} \ \frac{1}{2} \ \frac{1}{2}\right)$

Build a model of a BCC structure.

(a) Identify the close-packed directions and the closest-packed planes. Draw the arrangements of atoms on the closest-packed plane.

(b) How many atoms are there per cubic unit cell in the complete crystal? Assuming that the hard-spheres touch along the close-packed direction, calculate the fraction of space occupied by the “atoms”.