3.1. The set of {110} planes in an FCC unit cell passes through all corners of the cubic lattice and some face-centered atoms. The {110} set, however, misses the remaining face atoms. Write the Miller indices for a set of planes which is parallel to (110) but passes through all atoms of the FCC lattice.

To be parallel to (110) it is a multiple of (110) in a cubic system. The (220) or the family of planes {220} pass through the remaining face centered atoms. So the planes {110} and {220} pass through all of the atoms in the FCC lattice.

3.4. Calculate the number of atoms for an HCP unit cell.

It depends on how you draw the cell but the way we drew it in class the HCP lattice has 7 atoms in each of the two (0001) planes at the top an bottom and 3 atoms in the (0002) plane. The 3 atoms in the (0002) are not shared by another unit cell so these count totally to the HCP cell. The center atom on the (0001) plane is shared by 2 unit cells and there are two of these for the two (0001) planes so this contributes one atom to the unit cell. Each edge atom is shared by 3 cells above and 3 cells below so 6 cells. There are 12 edge atoms so for the two (0001) planes these contribute 24/(6*2) = 2 atoms. The HCP unit cell has 6 atoms.

3.6. From the information given in Problem 3.5 above, show that the *c/a* ratio for the HCP structure is generally $\sqrt{8/3}$ if the atoms are assumed to be spherical. Compare this result with the experimental *c/a* ratios for Zn, Mg, and Zr.

a is the length of a side in the hexagonal (1000) plane, and c is the height of the HCP lattice. For HCP the c/a ratio should be $\sqrt{(8/3)} \sim 1.633$.

Consider a grouping of three atoms in the hexagonal closest packed plane which make an equilateral triangle with side length a = R for touching spheres. If an atom is placed on top of this to make a pyramid of four atoms, the height from plane of the centers of the lower three spheres to the center of the top sphere is c/2 or one half of the height of the hexagonal cell.

The triangle in the (0001) plane from to the center of the triad is composed of two 30-60-90 triangles with side ratios 1 (opposite 30):2 (opposite 90):$\sqrt{3}$ (opposite 60) so the distance from the side of the three-atom layer to the center is a/(2$\sqrt{3}$) the side is a/2 and the other side is a/$\sqrt{3}$.

This 30:60:90 has a coincident side with a triangle with one corner in the upper atom, a second in the lower plane atom and a third in the center of the lower (0001) plane. The side in the (0001)

plane has length a/√3 since it is coincident with the side described above. The height of this triangle is c/2 and the remaining side has length "a "since it is a closest packed line on a side of the four atom pyramid. The Pythagorean Theorem gives $a^2/3 + c^2/4 = a^2$ or $a/c = \sqrt{(8/3)}$.
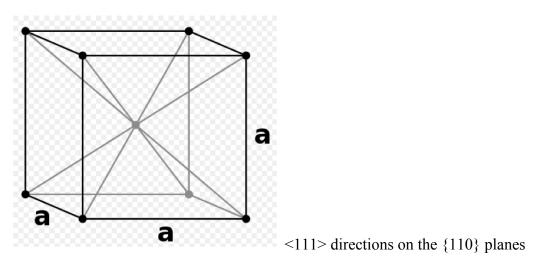
There are other ways to get this answer.

3.7. State the slip plane and the slip direction in a hypothetical simple cubic lattice.

The closest packed plane in simple cubic is {100} and the closest packed direction is <100> so the slip plane system for simple cubic is {100}<100>.

3.8. Show that a ⟨111⟩ direction lies in the (110) plane by sketching the appropriate direction and plane. Which one of the two (direction or plane) are close-packed assuming a BCC crystal structure? Discuss the implications for slip.

The <111> direction is closest packed in the BCC structure. The (110) plane is the densest plane. This is the slip system for BCC which requires some heat to activate since it is not a closest packed plane.

<111> directions on the {110} planes

3.9. Determine (a) the coordination number, (b) the number of each ion per unit cell, and (c) the lattice constant (expressed in ionic radii) for the CsCl and the NaCl crystal structures.

NaCl is a FCC structure so the coordination number is 12 and there are four ions of each type per cell. CsCl is a simple cubic structure so the coordination number is 6 and there is one ion of

each type per unit cell (four corners shared by 4 cells each). In both cases we consider a pair of Na+ and Cl- or Cs+ and Cl- as a lattice repeat unit.

The closest packed directions in CsCl are <111>. In this direction we have a length of $2R_{Cs} + 2R_{Cl}$ for distance. This forms a triangle with a cube side of length "a" and with a [110] line of length $a\sqrt{2}$. By the Pythagorean Theorem we have $a^2 = (2R_{Cs} + 2R_{Cl})^2/3$.

For FCC the closest packed directions are the <110> directions. But in NaCl closest packing occurs in the [100] direction since $2R_{Ns} + 2R_{Cl}$ is larger than $4 R_{Cl}/\sqrt{2}$ (the [100] is also longer than the [111]). So $a = (2R_{Ns} + 2R_{Cl})$.

3.11. Calculate the packing factor for diamond cubic silicon.

Diamond Cubic has an FCC like structure with an atom 1/4 of the way along [111] so that there are 4 extra interior atoms compared to FCC. This allows the carbon atoms to form tetrahedral sp2 bonds. FCC has 8 corners shared by 8 cells each plus 6 sides shared by 2 cells each so diamond cubic has a total of 8 atoms in the unit cell. Another way to look at the lattice is two FCC lattices with one shifted by [1/4,1/4,1/4]. A closest packed arrangement occurs with the corner atom and the atom along the [111] direction 1/4 of the way across. This distance (center to center) is 2R where R is the radius of the atom. The total diagonal distance is $a\sqrt{3}$ so we have $2R = a\sqrt{3}/4$, or the lattice spacing, $a = 8/\sqrt{3}$ R. The unit cell volume is $V = R^3 (8/\sqrt{3})^3$. The occupied volume is $8 * 4/3 \pi R^3$, so the packing factor is $\pi \sqrt{3}/16 \sim 0.34$.

3.14. Calculate the density of copper from its atomic mass. Compare your value with the density given in the Appendix. (The lattice parameter for Cu is $a = 3.6151$ Å.)

Copper has an FCC structure so there are 4 atoms per unit cell. Each atom has a mass of 63.54 g/mole. The unit cell has a volume of a^3 and there are 10^8 Å/cm and Avogadro's number is 6.022 e23/mole. So the density is $(4*63.54 \text{ g/mole}*10^{24}\text{Å}^3/\text{cm}^3)/(6.022\text{e}23/\text{mole}*(3.6151\text{Å})^3) = 8.933$ g/cm^3. The density listed by Google is 8.92 g/cm^3.

3.16. Calculate the distance between two nearest face atoms of the conventional FCC unit cell.

The closest packed directions are <110> in FCC. They are separated by twice the atomic radius 2R. This distance is equal to $a/\sqrt{2}$.

Describe briefly the origin of the smelting of metal ore (Hummel chapter 1). (One paragraph)

Hummel describes a possible origin for the smelting of metal ore, which is mostly oxides and sulfides of metals. The smelting process requires high temperatures, above the melting point for the metal, so on the order of 2500°C, and a highly reducing environment where the

electronegativity of the reducing agent is higher than that of the metal oxide. The conditions of extremely high temperatures and a reducing environment do not occur in normal fires so this technology had to be developed and was developed at many locations around the world independently (apparently). It is believed that the sintering of ceramics from natural clays and the production of glazes from metal oxides lead to the desire for higher temperature kilns. It was probably discovered by accident that in the presence of a reducing environment and at high temperatures ground state metals could be produced from common metal oxide and sulfide ores, particularly those of copper and tin (and perhaps zinc). This lead first to the Copper age and then to the bronze age (bronze is an alloy of copper and tin).

Callister Problems:

3.30 This problem you just need to draw the direction arrows on a Cartesian coordinate system with the lattice superimposed.

3.17 Beryllium has an HCP unit cell for which the ratio of the lattice parameters c/a is 1.568. If the radius of the Be atom is 0.1143 nm, **(a)** determine the unit cell volume, and **(b)** calculate the theoretical density of Be and compare it with the literature value.

For HCP a = 2R = 0.2286 nm. c = 1.568 a = 0.3584 nm. The hexagonal plane is made up of 3 parallograms of base a and height a $\sqrt{3}/2$ so the area of the hexagonal plane is $3*\sqrt{3}$ $a^2/2$. The volume of the unit cell is then, 0.04866 nm^3.

The unit cell contains 6 atoms (see problem 3.4 above), Be has a molar mass of 9.012 g/mole, So the density is (6*9.012 g/mole*10^{21}nm^3/cm^3)/(6.022e23/mole*0.04866 nm^3) = 1.845 g/cm^3. Google lists the density as 1.8477 g/cm^3.

3.5 Show that the atomic packing factor for BCC is 0.68.

The <111> directions are closest packed in BCC so 4R = a $\sqrt{3}$ and the unit cell volume is $64R^3/(3\sqrt{3})$. The BCC cell contains 2 atoms, one for the center atom and one for the corner atoms. The packing factor is $2* 4/3$ π $R^3/(64R^3/(3\sqrt{3})) = \sqrt{3}$ $\pi/8$ = 0.680.

3.6 Show that the atomic packing factor for HCP is 0.74.

The area of the hexagonal plane is $3*\sqrt{3}$ $a^2/2$ from 3.17 and the height is $a\sqrt{(8/3)}$ so the cell volume is $3\sqrt{2}$ a^3. The cell contains 6 atoms from problem 3.4. For the hexagonal cell a = 2R The packing factor is $6*(4/3$ π $a^3/8)/(3\sqrt{2}$ $a^3) = 0.740$.