

Physics 140A-Introduction to Solid State Physics
Winter, 2016
Problem Set 2
Due Friday, February 5th

Crystal structure and symmetry:

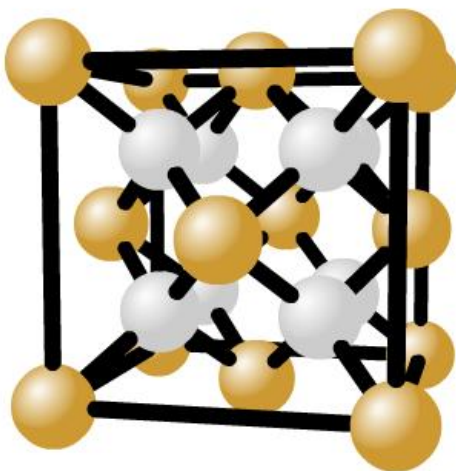
(Problems in Omar from Chapter 1 indicated as 1.x), plus some special problems. Full credit for doing all except those listed as **Optional**.

[1] Problem 1.1. In fact, these are the primitive basis vectors for the fcc crystal structure (that is, the basis vectors leading to a primitive (non-centered) unit cell for fcc)).

[2] Referring to Problem 1, consider now the planes with indices (100) and (001) in the conventional fcc structure. What are the indices of these same planes when expressed in terms of the primitive axes. (Either system is OK, just so we consistently use one or the other!)

[3] Problem 1.2, for Al and Fe only. Compare your answer to measured atomic densities in no./cm^3 , which are 2.70 and 7.87 g/cm^3 .

[4] Consider the crystal structure below, which is called fluorite. Each side of this unit cell has the same length, and all axes are orthogonal. There is no atom in the exact center of the unitcell. Check out this structure also at <http://www.dawgsdk.org/crystal/en/library/fcc#0002>



- (a) To which of the 14 crystal classes does this belong? Why? What is its Bravais lattice?
- (b) What is the simplest formula for a compound with this crystal structure (with no common factor in the subscripts)? Indicate how you arrive at your answer.
- (c) What is one possible atomic basis for this crystal? Indicate all atoms involved clearly, either on the color image or with a separate sketch.
- (d) Show that the yellow atoms in fact are tetrahedrally bonded to the blue atoms, using one of them as an example. The blue atoms are at $(1/4a, 1/4a, 1/4a)$ type locations.
- (e) Sketch the (110) plane for this crystal, and show where all blue and yellow atoms would be located on it.
- (f) There is also a set of (110) planes, denoted $\{110\}$. Sketch the (110) plane lying just in front of the one in (e), and indicate the positions of the atoms on it. What is its perpendicular spacing with respect to its nearest-neighbor planes?

[5] Problem 1.3.

[6] **[Optional only]** Problem 1.4.

[7] Problem 1.7.

[8] **[Optional only]** Problem 1.9. Note here that all symmetry operations mentioned only act on 2 of the 3 coordinates of the object, leaving the one along the fourfold rotation axis unchanged. Then, one way to do this is to let the "object" be a function in 2D, say $f(x,y)$. Then, if we for convenience take the first mirror plane to be along the y axis, it implies that $f(x,y) = f(-x,y)$ for all x and y. Think about what the second rotation axis means in this sense, and then show by the same line of reasoning that the two together imply a clockwise rotation by 90 degrees as well.

[9] Problem 1.10.

[10] Show that, if all of the ions in a NaCl type lattice are spheres touching one another, then the optimum ratio of the radii of the two ions involved must be 0.414. Such considerations lead different ionic crystals to be of NaCl, CsCl, wurzite, or other types, depending on the relative sizes of the ions involved.

[11] Consider some properties of the tight-binding electron wave function for solids that is related to the linear combination of atomic orbitals method for molecules, as introduced in lecture and in Section 5.8 of Omar (or 7.3 of Ibach and Luth):

(a) Show that, if we translate the coordinates in a tight-binding wave function defined over a set of N atoms in a simple non-centered lattice with a basis of one atom,

$$\varphi_{\vec{k}}(\vec{r}) = u_{\vec{k}}(\vec{r}) e^{i\vec{k}\cdot\vec{r}} = C \sum_{\substack{\text{Atoms } A \\ \text{Orbitals } i}}^N e^{i\vec{k}\cdot\vec{R}_A} C_{Ai,\vec{k}} \varphi_{Ai}^{AO}(\vec{r} - \vec{R}_A)$$

by some lattice vector $\vec{R} = n_1\vec{a} + n_2\vec{b} + n_3\vec{c}$, that it still satisfies the condition of being a Bloch wave:

$$u_{\vec{k}}(\vec{r}) e^{i\vec{k}\cdot\vec{r}}, \text{ with } u_{\vec{k}}(\vec{r}) = u_{\vec{k}}(\vec{r} + \vec{R}) \text{ for all } \vec{R}$$

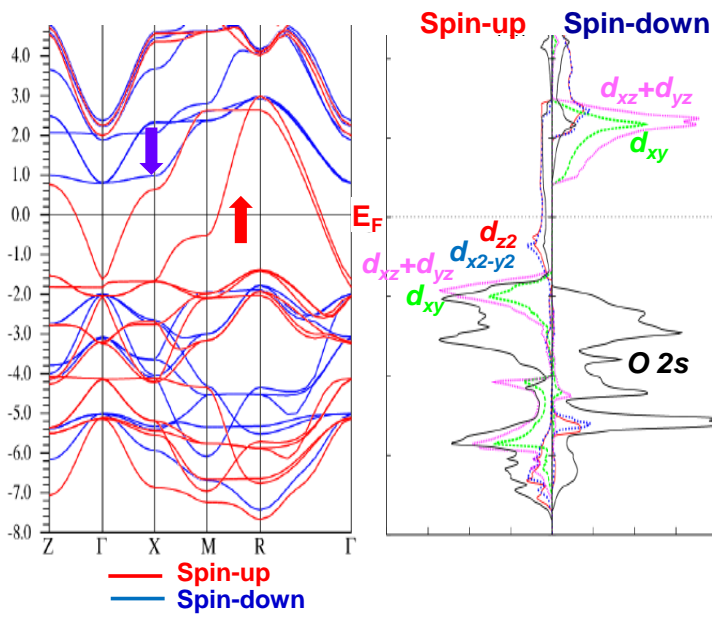
(b) In the limit that there is no overlap between any of the orbitals on different atoms A and B, such that $\langle \varphi_{Ai}^{AO} | \varphi_{Bj}^{AO} \rangle = 0$, and assuming the orbitals on a given atom to be orthonormal

$\langle \varphi_{Ai}^{AO} | \varphi_{Aj}^{AO} \rangle = \delta_{ij}$, work out the normalization constant C above in terms of the coefficients $C_{Ai,k}$.

[12] Below is a band structure calculation for a certain transition-metal oxide, including the densities of states, as calculated for the different atomic-orbital contributions and different spins.

(a) Is this a metal, and insulator, or a semiconductor? Explain your answer.

(b) Is this material magnetic? Again, explain your answer.



(c) What is responsible for the spin-up bands being lower in energy than the corresponding spin-down bands?