CH 410/510: Intro to CrystalMaker and CrystalDiffract Software

In this lab exercise, you will be introduced to CrystalMaker and CrystalDiffract Software, which has been installed on the laboratory computers to enable you to visualize molecular and solid state structures, and to calculate the X-ray diffraction powder patterns for these structures.

1. Turn on computer, and open CrystalMaker.

2. Under "File", choose "Open". Here you will be able to choose to look at structures that are already in the program's library. In the folder labeled "A", there are structures of single elements. By looking at the different structures in this folder, answer the following questions:

First, look at the diamond structure.

a) What is the coordination number and geometry of each carbon atom in diamond? Do the atoms on the corners and faces of the unit cell have a different coordination than the atoms in the middle?

b) In the diamond structure shown in this program, you are looking at atoms that are completely or partly in the unit cell. The unit cell is the smallest unit that contains the symmetry of the structure which, when translated by unit cell dimensions in all directions generates the crystal. To look at a larger number of atoms in the crystal, go to "Transform" and "Set Range". Click on the "expand" button until the number of atoms increases from 18 to 46. Has your answer to the second question in a) changed?

3. Now go to the "Metallic Structures" folder (under File:Open) and select body-centered cubic.

a) What is the coordination number and geometry of each atom in bcc? Do the atoms on the corners of the unit cell have a different coordination than the atom in the middle?

b) Go to "Transform:Set Range" and expand the structure from 9 to 35 atoms. Has your answer to the second question in a) changed?

4. Now look at the ccp structure (under Metallic Structures). Remember (from lecture) what type of unit cell this is?

a) What is the coordination of the atoms in ccp? Is it the same for all atoms?

b) Rotate the structure so that you can see the close-packed layers. Can you see the ABCABC repeat? (You can do the expand using the“Transform:Set Range” option to see it better).

5. Now look at hcp close packing structure. This looks a little different than what we saw in lecture, because the smallest unit cell is actually the unit shown here. Expand this to 24 or more atoms.

a) What is the coordination of the atoms in hcp? Is it the same for all atoms?

b) Can you see the ABAB repeat of close packed layers?

6. Now use File:open to go to the Basic Structure type folder, and go to the AX files. Open the CsCl structure.

a) What is the coordination number and geometry of Cs in this structure?

b) What is the coordination number and geometry of Cl in this structure?

c) Expand the number of atoms. Is your answer to (b) still the same?

7. Open the NaCl structure. What is the coordination of Na and Cl?

8. Using Crystal Maker you can also visualize any structure for which you know the atom positions and unit cell type. Let's make the perovskite structure. Go to File:New Crystal.

Enter these parameters: Space Group: Pm-3m
Lattice Parameter: 4.9 Å

Add these atoms, with these x, y, z coordinates:

Ba	0.5	0.5	0.5	occupancy: 1.0
O	0.5	0.5	0	occupancy: 1.0
Ti	0	0	0	occupancy: 1.0

a) Now look at the structure. How many Ba, Ti and O are there?

b) The formula of this compound is actually $BaTiO_3$. Can you make sense of this?

c) Now let's generate the x-ray diffraction pattern from this compound.
Go to "Transform: Diffraction Pattern". How many peaks do you see?

You will learn how to interpret this pattern in the next week. Go to "Pattern > Show Labels". Now you are seeing the "Miller Indexes" for each peak. You can also select to see"d-spacing" or "2θ" using "Pattern > Label Style". These will all be useful for you when you have superconductor diffraction patterns to analyze next week.

9. Last, let’s look at the $YBa_2Cu_3O_7$ (YBCO) superconductor structure. You’ll find it under Crystal Structures Library File > Other Inorganics > oxides > YBa2Cu3O7.cmdf.

This structure probably looks a little strange to you. This is the polyhedral representation, where each cation and its coordinating oxygens are shown as a polyhedron (a square prism, a cube, or a square plane). To get something more familiar, go to the Model > Ball and Stick.

Still a bit much? Go to Transform > Set Range, and select “single cell”. This is the unit cell of YBCO. This structure is often related to the perovskite structure, as described in your text. Do you see some similarities? We’ll discuss this more in lecture. Note that you can generate the diffraction pattern for this structure as well, and you’ll do that to compare with your experimental data for this lab.

If you have time, look also at the YBa2Cu3O6.cmdf. This oxygen-deficient structure is not superconducting, and it is produced if not enough oxygen is available during firing. Compare this structure with the “O-7” compound. What is the main difference?

You are encouraged to use any time remaining to play with these programs and become familiar with some of the options. They are lots of fun!

Crystal Maker Intro

Name: ___________________

2. a)

2. b)

3. a)

b)

4. a)

b)

5. a)

b)

6. a)

b)

c)

7.

8. (a)

(b)

(c)