3.012 Recitation - Using Mercury software
Tuesday, 1 November 2005

This handout will introduce you to the Mercury software for visualizing atomic structures. Some input files are provided for this class, and instructions for obtaining input files for other materials are at the end of the handout.

Download Software and get Input files

You may want to create a new directory to keep the files for this recitation. To create a directory and change in to it:
$:~> mkdir Hg_recitation; cd Hg_recitation

Download and install the free Mercury software to your own computer from
http://www.ccdc.cam.ac.uk/products/csd_system/mercury/

Copy the supplied .cif files into this directory. (cif = Crystallographic Information File).
$:~/Hg_recitation> add 3.012
$:~/Hg_recitation> cp /mit/3.012/Hg_files/* **.**

To begin Mercury:
$:~/Hg_recitation> add hg
$:~/Hg_recitation> mercury

A series of exercises will introduce you to some features of Mercury. There is often more than one way to accomplish the same thing, so play around a bit to get comfortable with the software.

Visualization of gold (Au)

Open the gold .cif file from the File menu:
File > Open > Au.cif

The screen shows some gold atoms. The change the display of atoms, from the top menu bar
Display > Styles > Ball and stick
or try one of the other styles.

See what happens when you move the mouse with the left, middle, and right mouse buttons and when you hold down the Shift key and Control key with each button.

The conventional Bravais lattice of Au is face centered cubic (FCC) with lattice parameter 4.078 Å (Angstrom = 10^{-10} m).

(1) Can you find the lattice vectors of FCC in the figure on your screen?

To help see this, measure the angles and distances between atoms. To measure the distance between two atoms, select from the scroll-down box
Picking Mode: > Measure Distances
Select two atoms and the distance will appear. Try this for several atom pairs. Below the visualization screen, click the button
More Info > Distances List
Right click on a listed distance and you can change the color to something unique.

To measure the angle created by three atoms, follow the same procedure with
Picking Mode: > Measure Angles
More Info > Angles List

(2) What is the motif of the lattice?

(3) What symmetry elements can you find?

(4) What is the primitive lattice and its motif?

To make the FCC lattice more clear, in the box labeled Display below the visualization screen, click the box for **Packing**. This shows many atoms translated in to three dimensions.

To help clarify the view, you may want to hide some atoms on the screen. From the box above the visualization screen, choose
Picking Mode: Select Atoms
then click on some atoms to hide. Then,
Display > Show/Hide > Atoms…
and click **Hide** to hide atoms or **Toggle** to show the last set of previously hidden atoms

<u>Visualization of gallium arsenide (GaAs)</u>

Let's next open the GaAs.cif file. If Ga and As atoms are the same color on the screen, it will be helpful to change them to different colors. Label the atoms with their names so you can identify them
Display > Label > Label all

Then select the As atoms
Picking Mode: Select Atoms

And change their color
Display > Colours > Atoms… > select colour:

Let's compare the structures of GaAs and Au. It may be helpful to choose the **Packing** feature and hide atoms outside the box showing the cell axes.

(1) What is the Bravais lattice of GaAs?

(2) What is the motif?

(3) What symmetry elements can you find?

For a list of symmetry operations, below the visualization screen, click the button
More Info > Symmetry Operators List…

The space group of GaAs is listed by
More Info > Structure Information…

You'll learn about space groups in the next lecture.

Obtain input file and create a powder diffraction pattern for alumina (Al_2O_3)

The .cif files for many structures are available in the Inorganic Crystal Structure Database (ICSD), which is available at
http://icsdweb.fiz-karlsruhe.de/index.php

Go to the web site in a browser, and you will see many boxes allowing different search criteria. One way to find a compound is to list the elements of the compound in the **Elements** box and the number of elements in the **Element Count** box and press **Search**. Only put spaces between the element names; do not use commas. To find the structure of alumina (Al_2O_3), for example:
Elements: Al O
Element Count: 2

To obtain the .cif file of the material, choose the appropriate entry (Toebbens 2001, for example) and click the **Details** button. Another window appears with the crystallographic information. Click the **Export** button to download the .cif file.

X-ray diffraction (XRD) is a common technique to identify crystalline materials and their properties. XRD was introduced in 3.091, and you'll learn more about the technique in the next few lectures. Here's a quick introduction on how to simulate a powder diffraction pattern of a known material in Mercury.

To obtain the powder diffraction pattern of the material, open the .cif file in Mercury and press the **Powder** button below the visualization screen. Press the **Customize…** button,

and the Powder Diffraction Settings window appears. Adjust the **Start (degrees 2 theta)** and **Stop (degrees 2 theta)** to obtain strongly diffracting peaks. Click **Apply** to see the changes in the diffraction pattern. Moving the cursor over the peaks identifies the (h k l) diffracting plane. Dragging a box the cursor over the low intensity part of the pattern zooms in and shows the more weakly diffracting peaks.