Materials 218/UCSB: Assignment IV

Ram Seshadri (seshadri@mrl.ucsb.edu)

Due date: February 11th 2003

1. Describe (using projections)

   (a) how the ZnS (zinc blende) and the diamond structure are related.

   (b) how the CaF_2 and fcc-Cu structures are related.

   (c) how the CsCl and perovskite structures are related.

2. OsAl has the CsCl structure with $a \sim 3.1$ Å. The structure of $OsAl_2$ is as follows:
   SG = $I4/mmm$ (No. 139) $a = 3.162$ Å $c = 8.302$ Å

Atom	x	y	z
Os[1]	0	0	0
Al[2]	0	0	0.34

[1] (0,0,0) and $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
[2] $\pm$(0,0,0.34) and $\pm(\frac{1}{2},\frac{1}{2},\frac{1}{2}+0.34)$

   This is the structure of many disilicides (including $MoSi_2$).

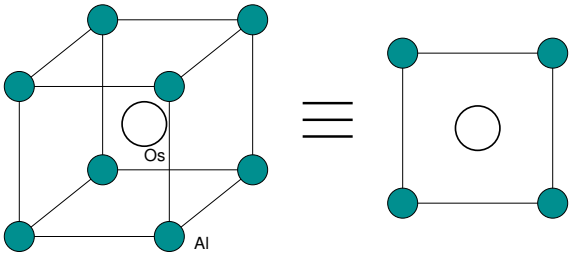
   (a) Sketch the structure of OsAl (the CsCl structure) as projections.

   (b) Sketch the structure of $OsAl_2$ as projections

   (c) What is the Os-Al distance in OsAl

   (d) What are the Os-Al distances in $OsAl_2$ (there are two that are smaller than 3 Å)

   Let the following square (on the right) represent the unit cell of OsAl:



   (e) Use such squares to sketch the structure of $OsAl_2$.[1] In your sketch, distinguish clearly between atoms sitting at $y = 0$ (or 1) and $y = 1/2$, where y is the direction perpendicular to the sheet of paper. I have done this for Al and Os in the sketch above, by using shaded circles for the former, and empty circles for the latter.

   (f) Use the following equation:

$$OsAl + OsAl_2 \longrightarrow Os_2Al_3$$

   to sketch the structure of Os_2Al_3 using the same kinds of squares.

[1] Hint: You should recognize that the structure of $OsAl_2$ is obtained by slicing OsAl slabs and then restacking them with a shift corresponding to body-centering.