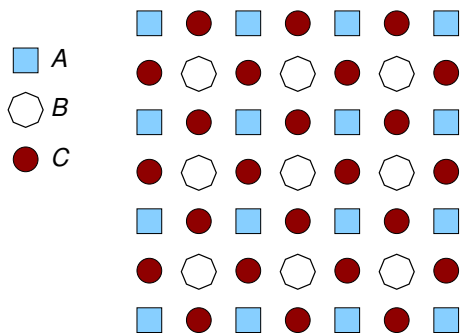


Materials 218/UCSB: Assignment III

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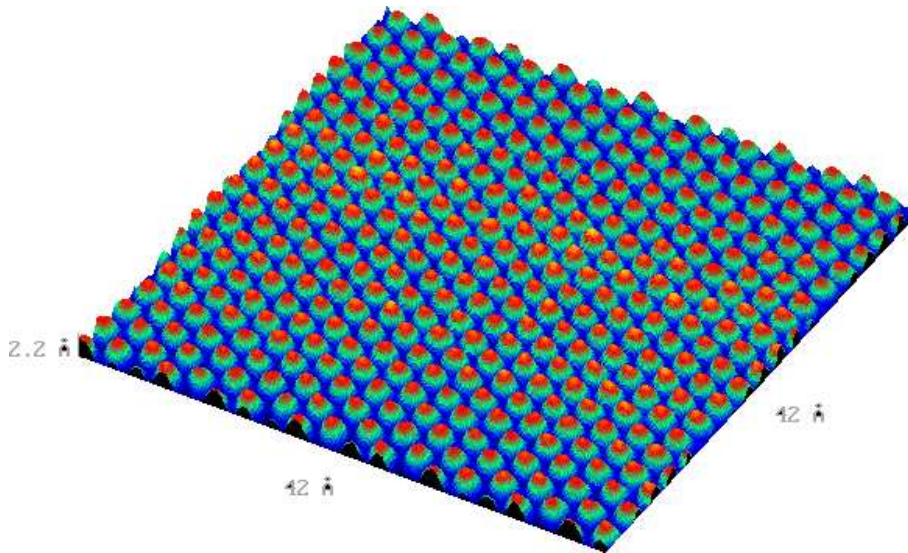
Due date: February 14th 2006

- The accompanying figure shows a two dimensional crystal structure formed by A, B, and C atoms.
 - What is the formula of the compound ?
 - Identify the mirrors and rotation axes at the different atom sites.
 - Outline the unit cell.
 - What is the centering in the crystal ?
 - Can you suggest the name of the plane group.
 - Provide the complete minimal crystal structure description in terms of the plane group, cell parameters and the atom positions.



- The compound OsAl has the following structure: $\text{SG} = Pm\bar{3}m$, $a = 3.00 \text{ \AA}$, Os at $(1/2, 1/2, 1/2)$ and Al at $(0,0,0)$.
 - Sketch the structure as sections, and within a cube.
 - What is this structure type called ?
 - OsAl_2 is formed by successively stacking OsAl cubes, but every new stack is created from the old one by adding $(1/2, 1/2, \approx 1.5)$ Sketch OsAl_2 as sections after generating its coordinates. Is OsAl_2 cubic ? What are the cell parameters.
 - Can you guess the space group of OsAl_2 ?
 - Can you guess how Os_2Al_3 is built up ?
- Sketch the ideal perovskite ABO_3 structure with A atoms at the corners of the cell and the B atom in the middle. What are the coordinates of A, B and O ? Remember to provide the minimal, crystallographic description. How many nearest neighbors do A, B, and O each have ?
- Sketch the perovskite structure as projections and then sketch the rock salt structure as projections. Compare the layers. Are there any structural relationships ? Show that the perovskite structure can be considered as alternate stackings of AO rock salt layers and BO_2 layers.

5. A compound is described with three kinds of atoms in the unit cell, A, B and C. A is in the Wyckoff position $2a$, (for the specific space group) B is in the Wyckoff position $8c$ and C in $24f$. What is the formula of the compound.
6. Given below is an STM image of the surface of a highly oriented graphite crystal. Given what you know about the graphite crystal structure, can you tell what the blimps are? Are they atoms?



The image is from <http://www.physics.louisville.edu/>

7. Carbon nanotubes are formed by rolling up single graphite sheets. Show using a suitable sketch that some carbon nanotubes can possess chiral¹ screw axes along the tube direction.

¹Meaning that there are left and right handed versions such as the screws 6_1 and 6_5