Materials 218/UCSB: Assignment III

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- 1. Sketch the ideal perovskite ABO₃ struture with A atoms at the corners of the cell and the B atom in the middle (as opposed to how it was done in the class). 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 ?
- 2. 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.
- 3. Using the *h*-*c* notation, describe a close packed system with the following stacking sequence ABCB-CACABABCBCACAB. What will the *a*, *b* and *c* parameters of this compound be, assuming the ideal h/a ratio.
- 4. 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.
- 5. You have been told that applying pressure on NaCl crystals converts them to the CsCl crystal structure. How does this fit in with your understanding of the radius ratio rule ?
- 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. Extra points for making a model.

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