MATRL 218: Assignment 3

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1. The compound OsAl has the following structure: SG = \( Pm\bar{3}m \), \( a = 3.00 \text{ Å} \), Os at \((1/2,1/2,1/2)\) and Al at \((0,0,0)\).

   (a) Sketch the structure as sections, and within a cube. Also use VESTA if you wish.

   (b) What is this structure type called?

   (c) OsAl\(_2\) is formed by successively stacking OsAl cubes, but every new stack is created from the old one by adding \((1/2,1/2,\approx1.5)\). Sketch OsAl\(_2\) as sections after generating its coordinates. Is OsAl\(_2\) cubic? What are the cell parameters?

   (d) Can you guess the crystal system and the centering in OsAl\(_2\)?

   (e) Can you guess how Os\(_2\)Al\(_3\) is built up?

2. X-ray studies suggest that mineral Wickmanite (connectivity shown below) has corner-sharing octahedra of MnO\(_6\) and SnO\(_6\) with Mn–O and Sn–O bond lengths of 2.15 Å and 2.02 Å, respectively.

   Using the exponential bond-valence-sum relationship:

   \[
   s = \exp \left( \frac{R_0 - R}{B} \right),
   \]

   and the following values for \( R_0 \) and \( B \) (\( R_0 \) for Mn(II)–O is 1.790 Å; for Sn(IV)–O, it is 1.905 Å, and \( B = 0.37 \text{ Å} \)), calculate the bond valence sums (BVS) for Mn, Sn, and O? What do the BVS tell you about the composition of the compound (hint: is this an oxide)?

3. Use VESTA to sketch the structures of (i) graphite, (ii) diamond, (iii) NaCl, (iv) CsCl, (v) ZnS (wurtzite) and (vi) ZnS (zinc blende).