MATRL 218: Assignment 3

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1. Use VESTA to sketch the structures of (i) NaCl, (ii) CsCl, (iii) ZnS (wurtzite, showing ZnS$_4$ tetrahedra), and (iv) BaZrO$_3$ (showing ZrO$_6$ octahedra).

2. 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, $\approx$1.5) Sketch OsAl$_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?

3. Use VESTA to sketch the structures of CuO and NbO using the provided CIF files that can be directly opened by VESTA. Can you describe how these are derived from the structure of NaCl.