Project 1: Structure of beryllium oxide and its surfaces

Animal studies as well as dissolution experiments suggest that BeO calcined at 773 K (low fired) is more soluble and leads to greater granuloma formation than BeO calcined at 1273K (high fired). More soluble beryllium compounds such as beryllium sulfate led to increased toxicity. Understanding the solubilities of different beryllium compounds is important in determining risk factors for chronic beryllium disease as well as understanding the pathway from inhalation to the disease. Since the mechanism of dissolution depends on the surface structure, characterizing common BeO surfaces and their reactivity is a useful first step. In this first project, you'll consider different possible faces of beryllium oxide and explore their structure using CrystalMaker© a visualization package.

To prepare for this project, you should read the papers by Austerman given to you in our last class. These papers highlight how the method of preparation of beryllium oxide leads to different crystal shapes and different exposed planes. Review the articles on sources of beryllium and choose some beryllium oxide crystal shapes to focus on. Consider what the Abramowski paper says on the Wuff construction. What does this suggest about the surface energy of the different faces in the crystal you are exploring?

During class, I will show you how to use CrystalMaker© to build a beryllium oxide lattice and how to cut the lattice along specific plane directions. You'll repeat this procedure and observe what atoms are exposed with the different plane cuts. Look at all the planes in the crystal shape you chose when reading the Austerman papers. Consider their likely energy ordering of all the surfaces based on a Wuff construction. Can you make a correlation between atomic structure of the surface and energy ordering? Use the second class day devoted to this project to get any other supporting data you might need and start to outline your paper.