Homework #7:

3D Lattices, Point Groups, and Macroscopic Properties of Crystals

Due 5pm Friday Dec. 6
Turn in outside of Durand 110 or email to duerloo *at* stanford.edu

The macroscopic properties of a crystal are often not isotropic but instead are related to the symmetry elements that describe the arrangement of atoms. There are only 32 3D distinct combinations of point symmetry elements - the crystallographic point groups - which are consistent with a three dimensional lattice. A purpose of this homework is to gain some familiarity with these groups and understand the effects they have on macroscopic crystal properties.

1. Determination of 3D lattices

In the orthorhombic crystal system (mutually orthogonal diad axes), four Bravais lattice types are allowed: Primitive (P), body-centered (I), side face centered (C), and all face centered (F). Other crystal systems do not have the these lattice types either because either 1.) the essential symmetry is destroyed (e.g., there can be no C-cubic unit cell), 2). the unit cell can be re-drawn as another type, or 3) the arrangement of points does not constitute a lattice. For each crystal system below, consider each of these four cases (P, I, C, and F) and show which ones are lattices and are unique.

a) Tetragonal
b) Monoclinic
c) Trigonal

2. Crystal Structure Point Groups

The point group is obtained from the space group by converting glide planes to mirrors and screw axes to pure rotations. Look up the space group and hence determine the point group for the following structures – write the name. You can find the set of point group operations for all 3D crystals in the class slides. Using a java viewer, identify the locations of the distinguishing symmetry elements associated with the crystal system to which these structures belong. Note that you may need to consider that some of the distinguishing point symmetry rotations are actually screw axes in the point group, i.e. you will not find a 6-fold rotation in HCP but there is a 6_3 screw axis.

a) FCC
b) HCP
c) Sphalerite
d) Wurtzite

3. Ferroelectricity and pyroelectricity

Using the stereograms for the 3D point groups given in the class slides, determine all possible directions that an electrical polarization can point for each of the 7 crystal classes.

4. Phase changes in $BaTiO_3$

Show that successive changes of symmetry of barium titanate as the temperature is lowered can be explained

by postulating that the cubic crystal first becomes polar along one cube axis, then equally polar along two cube axes together, and finally equally polar along all three cube axes together. $BaTiO_3$ progresses from *m3m* above the Curie temperature (paraelectric phase) to *4mm, mm2* and *3m* as the temperature is lowered.

5. Electrical properties of a monoclinic crystal

Using the method of inspection, calculate the form of the conductivity tensor σ_{ij} in Ohm's law $j_i=\sigma_{ij}E_j$ constrained by the point symmetry of a monoclinic crystal. How many independent measurements are required to completely determine the conductivity properties of this crystal?

6. Electrical properties of graphene

Graphene is of significant interest as a potentially high mobility electronic material.

1) Find the 2D point group of graphene, i.e. assume it is a true 2D material.

2) Using the method of inspection and/or explicit transformation of the tensor, determine the constraints that symmetry places on the electrical conductivity tensor for this material. How many measurements are required to completely determine the electrical conductivity of this material?

3) The 2D nature of graphene makes it amenable to manipulation by MEMS. Suppose you develop a device that can induce a uniaxial strain in one direction in graphene, i.e. the lattice is stretched along one direction. Give the 2D point group of uniaxially strained graphene assuming it is a true 2D material. Assume the strain direction is along an armchair direction. Does it matter in which direction the strain is applied?

4) Determine the electrical conductivity tensor for uniaxially strained graphene. Does it matter in which direction the strain is applied?