MASSACHUSETTS INSTITUTE OF TECHNOLOGY

Applications of Group Theory to the Physics of Solids—6.734J & 8.510J

PROBLEM SET #7

Issued: April 12, 2002 Due: April 19, 2002

1. (a) Find the star of the various types of wave vectors for a two-dimensional triangular lattice $p6mm$, space group #17. For the two-dimensional square lattice (see notes Fig. 13.1 for the case of the two-dimensional square lattice) there are 6 different types of high symmetry points. How many high symmetry points are there for the two-dimensional triangular lattice?

   (b) For each distinct type of k vector of (a), find the symmetry elements in the group of the wave vector for each high symmetry point and identify the corresponding point group.

   (c) Indicate the symmetry subsector of the triangle which contains the minimal set of k vectors that must be used to calculate electron or phonon dispersion relations.

   (d) Find the compatibility relations for the 5 d band basis functions around the symmetry subsector in (c).

2. What are the differences in the electronic basis functions between groups #11 ($p4mm$) and #12 ($p4gm$) at the following k points in the 2D square lattice:

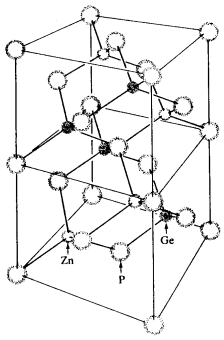
   (a) $k = 0$

   (b) $k = (\kappa, 0)$ for $0 < \kappa < \pi/a$

   (c) $k = (\kappa, \kappa)$ for $0 < \kappa < \pi/\sqrt{2}a$

   (d) $k = (\pi/a, \pi/a)$

3. Consider the ideal chalcopyrite structure for $ZnGeP_2$ where in the limit that all the Zn and Ge lattice sites are occupied by Ga atoms, the zincblende structure is obtained:

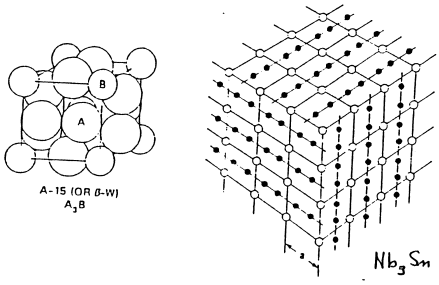


   (a) What is the appropriate space Group? What is the unit cell? What are the site positions for the Zn, Ge and P atoms using the international crystallography tables?

   (b) What is the group of the wave vector for $k = 0$? and for k at the Brillouin zone boundary $k = (\pi/a, 0, 0)$?

   (c) What are the symmetries of the normal modes at $k = 0$ and at the zone boundary in a (100) direction?

4. Consider the crystal structure in the diagram for Nb_3Sn, a prototype superconductor with the A–15 (or β–W) structure. This material is used for high field superconducting magnet applications.



   (a) List the symmetry elements of the space group.

   (b) What is the space group designation? (Use the international crystallography tables.)

   (c) How many lattice modes are there at $k = 0$, what are their symmetries and what are their degeneracies?

   (d) What are the normal mode displacements for each of these lattice modes?

   (e) Which modes are IR active, Raman active? What are the polarizations of the Raman-active modes?