MASSACHUSETTS INSTITUTE OF TECHNOLOGY

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

PROBLEM SET #8

Issued: April 19, 2002 Due: April 26, 2002

1. Tin oxide (SnO_2 with space group #136) is an important electronic material.

   (a) What are the symmetry operations for SnO_2? Give the site locations for the tin and oxygen atoms within the unit cell using the notation in the International Tables for X-ray Crystallography.

   (b) Find the equivalence transformation $\chi_{\text{atom sites}}$ for SnO_2 at the center of the Brillouin zone.

   (c) Find the lattice modes at the zone center $k = 0$, including their symmetries, degeneracies and the normal mode patterns.

   (d) Indicate the IR-activity and Raman activity of these modes.

   (e) What is the mode splitting along the (100) and (001) directions as we move away from $k = 0$?

2. (a) Using the empty lattice, find the energy eigenvalues, degeneracies and symmetry types for the two electronic levels of lowest energy for the fcc lattice at the Γ point ($\vec{k} = 0$). Note that the lowest energy state is a non-degenerate state with Γ_1^+ symmetry.

   (b) Find the appropriate linear combination of plane waves which provide basis functions for the two lowest L-point electronic states for the fcc lattice.

   (c) Which states of the lower and upper energy levels in (a) and (b) are coupled by optical dipole transitions?

   (d) Using compatibility relations, find the symmetries of the energy levels that connect the two Γ-point and two L-point energy levels (see Fig. 16.1).

3. (a) Using $\vec{k}\cdot\vec{p}$ perturbation theory and the results of problem #2, find the form of the $E(\vec{k})$ relations near the L-point in the Brillouin zone for a face centered cubic lattice arising from the lowest levels with L_1 and L_2' symmetry that are doubly degenerate in the free electron model. Which of the non-vanishing $\vec{k}\cdot\vec{p}$ matrix elements at the L-point are equal to each other by symmetry?

   (b) Using the Slater–Koster technique, find the form for $E(\vec{k})$ for the lowest two levels for a face centered cubic lattice.

   (c) Expand your results for (b) about the L-point in a Taylor expansion.

   (d) Compare your results in (c) to those in (a).

   (e) Using $\vec{k}\cdot\vec{p}$ perturbation theory, find the form of $E(k)$ for a non-degenerate band with W_1 symmetry about the W point in the fcc lattice.

4. (a) Using $\vec{k}\cdot\vec{p}$ perturbation theory, find the form of the secular equation for the valence band of Si with Γ_{25}^{+} symmetry.

   (b) Which intermediate states couple to the Γ_{25}^{+} valence band states in second-order $\vec{k}\cdot\vec{p}$ perturbation theory?

   (c) Which matrix elements (listed in Table 17.1) enter the secular equation in (a)?

   (d) What is the form of the secular equation in (a) along a Λ [(000) to (111)] axis?

   (e) Suppose that your silicon sample is a thin film (10 nm thick) grown pseudomorphically on a germanium substrate. What happens to $E(\vec{k})$ for the silicon valence band in the thin film if the germanium substrate is oriented along a (100) direction or if it is oriented along a (110) direction?