PHYS 4000, Fall 2007

Final Exam **9:00-11:00, Friday, 07 December 2007**

NAME: ____

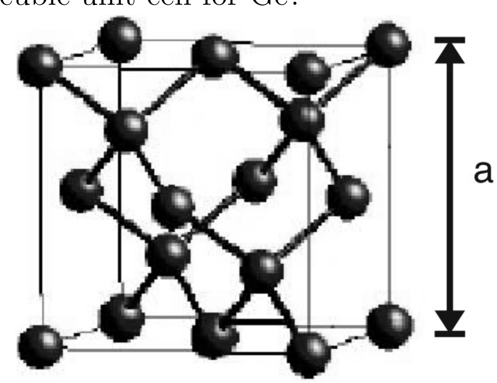
The following pages contain text and figures, followed by questions for you to answer. To receive full credit, you must answer the questions clearly and completely; support your answer with a quantitative relation or formula whenever possible. You have until 11:00 am (approximately 120 minutes from now) to complete this exam.

A CALCULATOR, RULER, AND TWO SHEETS OF FORMULAE (LISTING ANY OF THE NUMBERED EQUATIONS FROM KITTEL (OR ASHCROFT & MERMIN) MAY BE USED. THE SHEET OF FORMULAE MUST BE HANDED IN WITH YOUR ANSWER SHEET.

Total points = 50 (9 pages)

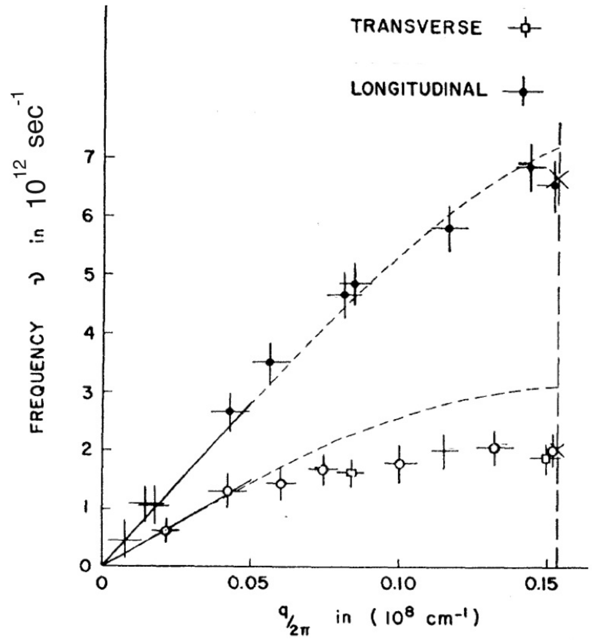
Germanium is a material that adopts a diamond structure, as shown below, with a cubic lattice parameter $a = 5.66$ Å and two atoms in the primitive basis.

(1) [1 point] How many atoms are present it the conventional cubic unit cell for Ge?



(2) [2 points] What is the closest distance between neighbouring (110) planes of Ge atoms?

(3) [4 points] The phonon dispersion curve along the [111] direction of Ge is shown in Figure 1. (Note: In this figure, q denotes wavevector.) Use the data presented in Fig. 1 to estimate the velocity of sound in germanium.



modified from B.N. Brockhouse and P.K. Iyengar, *Phys. Rev.* **108** (1957) 894.

Figure 1. Acoustic branches of the phonon dispersion curve for Ge.

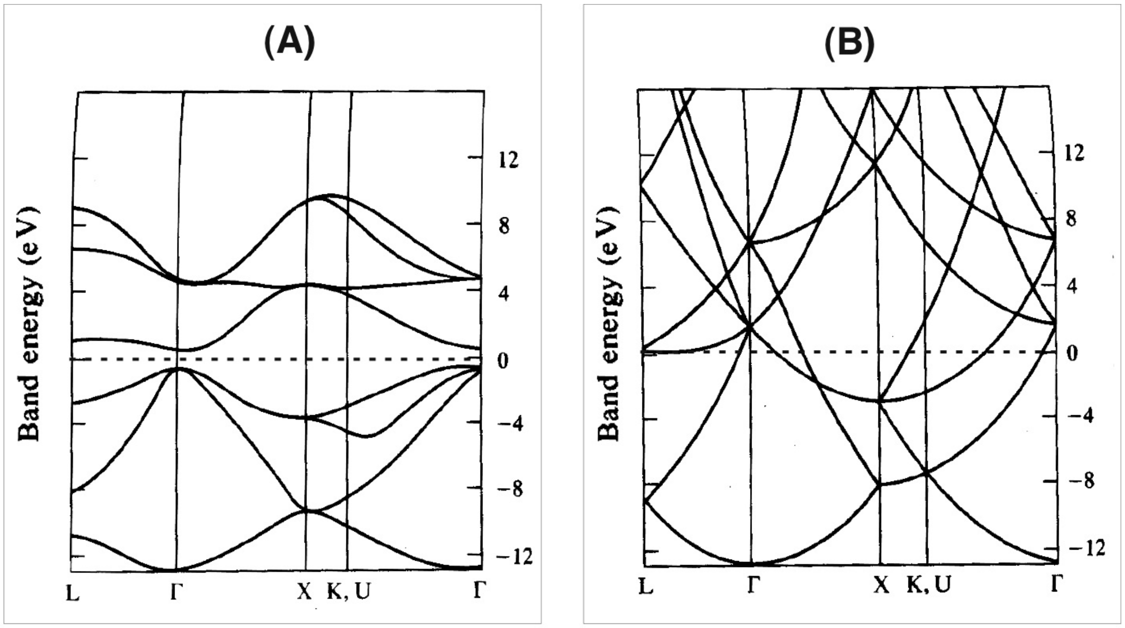
(4) [4 points] Fig. 1 shows the acoustic modes for Ge. In general, under what conditions would you expect to a material to have optical phonon modes? Would you expect Ge to have optical phonon modes? Briefly justify your answer.

(5) [4 points] What is the primary assumption of the Debye model for phonons? Discuss whether it is a better model for acoustic or optical phonons.

(6) [4 points] What is the physical significance of the Debye temperature? What role does it play in the temperature dependence of a material's heat capacity, according to the Debye model?

(7) [3 points] List one experimental technique that can be used to determine a material's phonon dispersion relation, and briefly describe why it yields information about vibrational modes.

(8) [4 points] Figure 2 shows two calculations for the electronic band structure of germanium: one calculated using the free electron model, and the other calculated using the linear-combination of atomic orbitals (LCAO) method. Which diagram, Fig. 2(A) or Fig. 2(B), corresponds to the free electron model? List three characteristics of these plots that led you to your answer.



modified from W.A. Harrison, *Electronic Structure and the Properties of Solids* (1989).

Figure 2. Electronic band structure diagrams calculated for Ge. In both (A) and (B), the Fermi energy is indicated by the dashed line at 0 eV.

(9) [4 points] Germanium has strong covalent bonds. With this information, would you expect the free electron model or the LCAO model to be a more accurate description of the electronic properties of Ge? Justify your answer.

(10) [3 points] Based on your answers to (5) and (6) above, is germanium a metal or semiconductor? Justify your answer.

(11) [4 points] Consider a 3D material that crystallizes in a simple cubic structure (lattice constant 3 Å) with one divalent atom per primitive unit cell. Suppose that the bands for this material can be approximated by nearly-free electron bands that have gaps (magnitude V_G) at the edge of the first Brillouin zone. What is the maximum value of $2V_G$ for which this material will remain metallic?

(12) [4 points] Describe how information from a band structure diagram can be used to determine the group velocities that electrons in the material would have in an applied electric field.

(13) [5 points] Give the definition of a Fermi surface. Then, list one experimental technique that can be used to obtain information about a material's Fermi surface, and briefly describe how it can yield this kind of electronic structure information.

Figure 3 below shows thermal conductivity *vs.* T data for Ge.

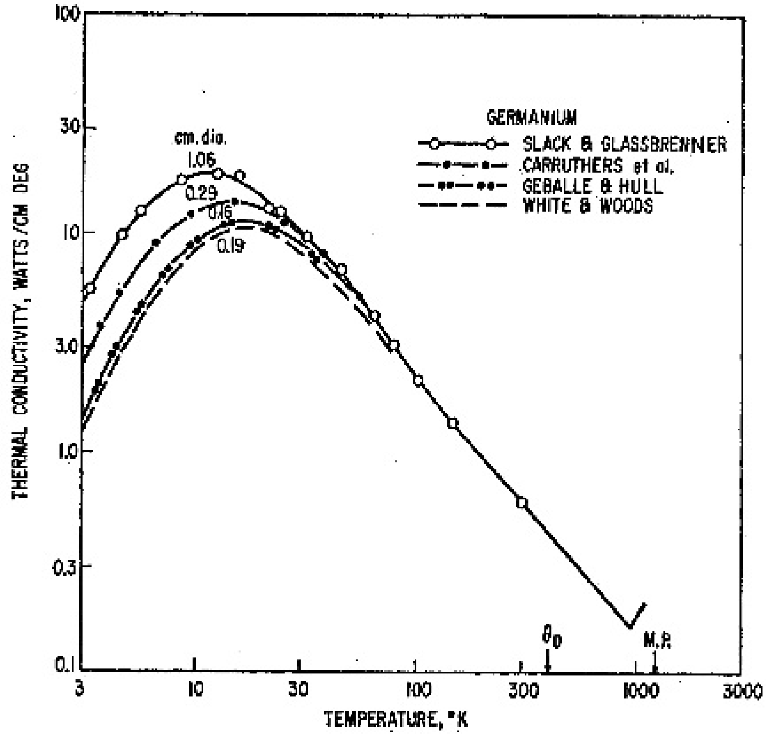


Figure 3. Thermal conductivity data for Ge (Slack and Glassbrenner, Phys. Rev. ***120*** *(1960) 782.)*

(14) [4 points] Describe what scattering mechanisms are dominant at low and high temperatures, and use this information to explain why the thermal conductivity *vs.* T plot for Ge has this shape.