PHYS 4000, Winter 2007

Final Exam **9:00-11:00, Monday, 09 April 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 (approximately 120 minutes from now) to complete this final exam.

A CALCULATOR, RULER, AND UP TO THREE SHEETS OF FORMULAE (LISTING ANY OF THE NUMBERED EQUATIONS FROM SINGLETON OR KITTEL) MAY BE USED. THE SHEETS OF FORMULAE MUST BE HANDED IN WITH YOUR ANSWER SHEET.

Total points = 50 **(10 pages, including this one)**

Figures in this exam were taken from the following journal articles:

E.A. Ekimov *et al.*, *Nature* **428** (2004) 542.

J.M.D. Coey and M. Venkatesan, *Journal of Applied Physics* **91** (2002) 8345.

I.I. Mazin *et al.*, *Physical Review B* **59** (1999) 411.

PART I: Diamond [25 points in 9 questions]

Diamond is composed entirely of carbon atoms and has the same crystal structure as silicon and germanium. The conventional cubic unit cell for diamond is depicted in Figure 1 below.

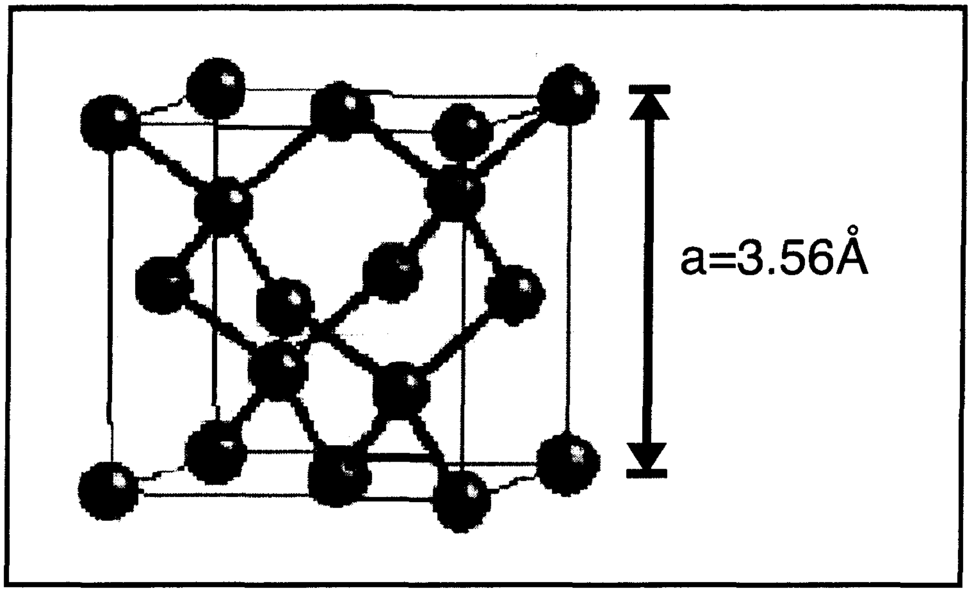


Figure 1

(1) [1 point] What kind of Bravais lattice does diamond have? (Circle the correct answer.)

simple cubic   body-centered cubic   face-centered cubic   hexagonal   none of these

(2) [3 points] Name – and list the Schönflies symbol for - at least three different symmetry elements that are present in the diamond structure.

(3) [2 points] On the bandstructure diagram for diamond shown in Figure 2 below, label the following features:

(i) valence band(s) (ii) conduction band(s)
(iii) heavy hole band (iv) light hole band (v) thermodynamic band gap

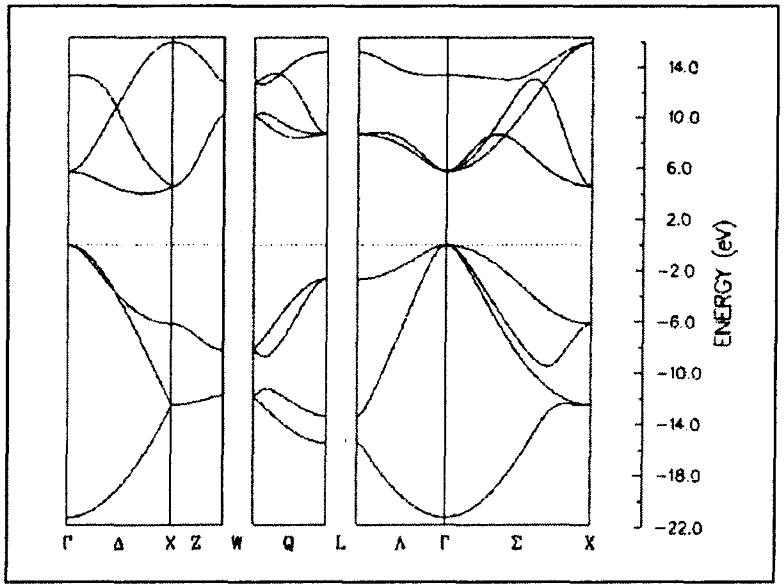


Figure 2

(4) [5 points] The overall shapes and relative positions of the bands in diamond are quite similar to those in silicon and germanium. Briefly describe what factors influence the width (dispersion) and relative (energy) placement of bands, and use this to justify why bands for diamond, silicon, and germanium should look qualitatively similar.

(5) [2 points] Do heavy holes or light holes play a more dominant role in conduction? Provide brief justification for your answer.

(6) [2 points] Is diamond a direct gap material? Briefly explain your reasoning.

(7) [5 points] Can you determine if the band structure shown above for diamond was calculated using the free electron model or the tight-binding model? Briefly justify your answer, and in doing so, list three assumptions of the tight-binding model that differentiate it from the free electron.

(8) [3 points] The density of states plot shown in Figure 3 below was calculated directly from the band structure diagram (Figure 2). In comparison, an experimental determination of the thermodynamic band gap for diamond is 5.5 eV at room temperature. Describe at least two factors that could contribute to the discrepancy between the magnitudes of the theoretical and experimental band gap energies.

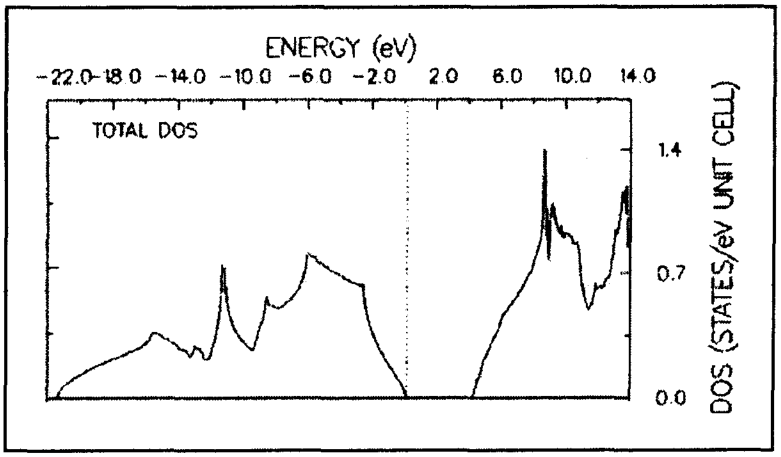
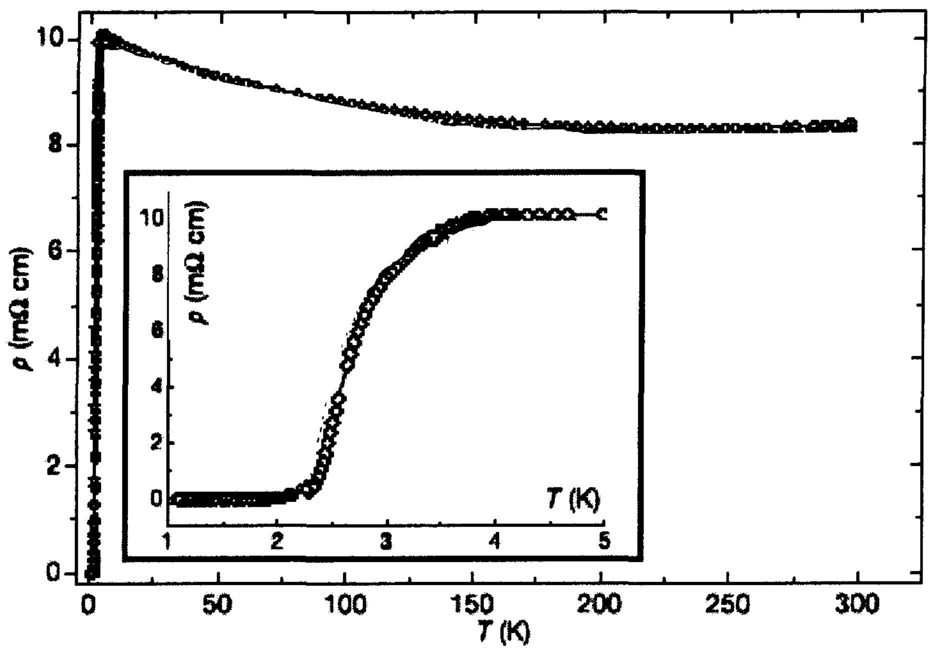


Figure 3

(9) [2 points] Based on what you've learned about diamond in questions (1)-(8), would you classify diamond as a semiconductor or an insulator? Provide brief justification for your answer.

Part II: Special diamond [25 points in 7 questions]

Recent experiments show that diamond can be synthesized – at high temperatures and pressures and with some boron added – to yield very different electrical properties. A plot of electrical resistivity as a function of temperature is shown below for this specially-prepared diamond; the inset emphasizes the low temperature behaviour.



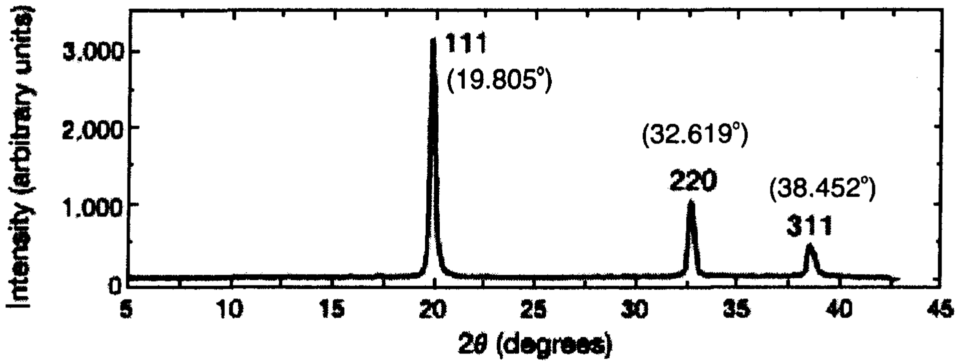
(10) [4 points] Is this specially-prepared diamond a metal, semiconductor, or insulator near room temperature? How does this change at temperatures below 3 K? Support your answers with relevant qualitative and quantitative features of the resistivity plot.

(11) [3 points] Describe the physical basis of Wiedemann-Franz relation and the conditions under which it is typically valid. Would you expect this relation to be valid for the specially-prepared diamond at room temperature? Briefly justify your answer.

(12) [4 points] Give an expression that relates the electrical conductivity of a metal to scattering events. Describe the type(s) of scattering processes that play an important role in the electrical resistivity of metals near room temperature.

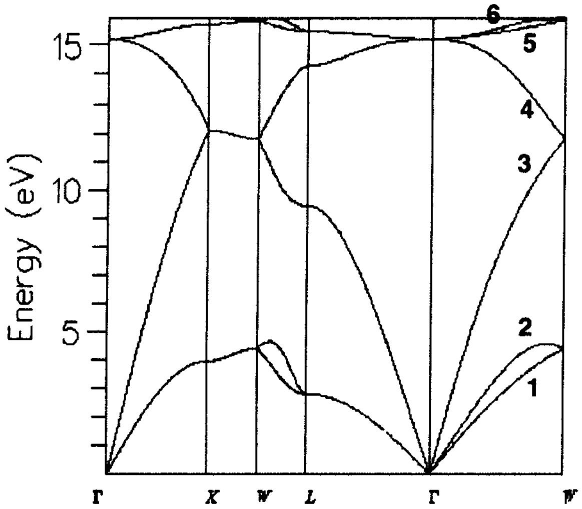
(13) [5 points] Both semiconductors and conventional superconductors show gaps in the density of electronic states near the Fermi energy. Describe the differences in what the gaps mean (in terms of *origins* and *magnitudes* of the gaps) in both classes of materials.

A powder X-ray diffraction pattern for the specially-prepared diamond is shown below.



(14) [4 points] Given the Miller indices and 2θ positions of the Bragg peaks, and assuming incident X-ray radiation with a wavelength of 0.71 Å, what is the (cubic) lattice parameter of this specially-prepared diamond?

A phonon dispersion curve for diamond is shown below.



(15) [1 point] Six branches of the phonon dispersion curve are numbered in the figure above. Which are optical branches?

(16) [4 points] The phonon dispersion curves shown above describe the frequencies associated with normal modes of vibration in diamond. Assume that these vibrational modes can be modeled by the vibrational modes in a one-dimensional system of coupled harmonic mass-and-spring oscillators. What determines how many normal modes are possible? What determines the energy associated with the highest frequency mode? Provide brief justifications for your answers.