

ELEC 4700 Assignment #2

Question 1 (Kasop 4.2) Molecular Orbitals and Atomic Orbitals

Consider a linear chain of four identical atoms representing a hypothetical molecule. Suppose that each atomic wavefunction is 1s wavefunction. This system of identical atoms has a center of symmetry C with respect to the center of the molecule (midway between the second and the third atom), and all molecular wavefunctions must be either symmetric or antisymmetric about C .

- Using LCAO principle, sketch the possible molecular orbitals.
- Sketch the probability distribution $|\psi|^2$
- If more nodes in the wavefunction lead to greater energies, order the energies of the molecular orbitals.

Note: The electron wavefunctions, and the related probability distributions, in a simple potential energy well that are shown in Figure 3.15 can be used as a rough guide towards finding the appropriate molecular wavefunctions in the four-atom symmetric molecule. For example, if we were to smooth the electron potential energy in the four-atom molecule into a constant potential energy, that is, generate a potential energy well, we should be able to modify or distort, without flipping, the molecular orbitals to somewhat resemble ψ_1 to ψ_4 sketched in Figure 3.15. Consider also that the number of nodes increases from none for ψ_1 to three for ψ_4 in Figure 3.15.

Question 2 (Kasop 4.16) Thermoelectric effects and E_F

Consider a thermocouple pair that consists of gold and aluminum. One junction is at 100°C and the other is at 0°C . A voltmeter (with a very large input resistance) is inserted into the aluminum wire. Use the properties of Au and Al in Table 4.3 to estimate the emf registered by the voltmeter and identify the positive end.

Question 3 (Kasop 4.24) Thermal Conductivity

- a. Given that silicon has Young's modulus of about 110 GPa and a density of 2.3 g cm^{-3} , calculate the mean free path of phonons in Si at room temperature.
- b. Diamond has the same crystal structure as Si but has a very large thermal conductivity, about $1000\text{ W m}^{-1}\text{ K}^{-1}$ at room temperature. Given that diamond has a specific heat capacity c_s of $0.50\text{ J K}^{-1}\text{g}^{-1}$, Young's modulus of 830 GPa, and density ρ of 0.35 g cm^{-3} , calculate the mean free path of phonons in diamond.
- c. GaAs has a thermal conductivity of $200\text{ W m}^{-1}\text{ K}^{-1}$ at 100 K and $80\text{ W m}^{-1}\text{ K}^{-1}$ at 200 K. Calculate its thermal conductivity at 25°C and compare with the experimental value of $44\text{ W m}^{-1}\text{ K}^{-1}$. (Hint: Take $\kappa \propto T^{-n}$ in the temperature region of interest; see Figure 4.48)

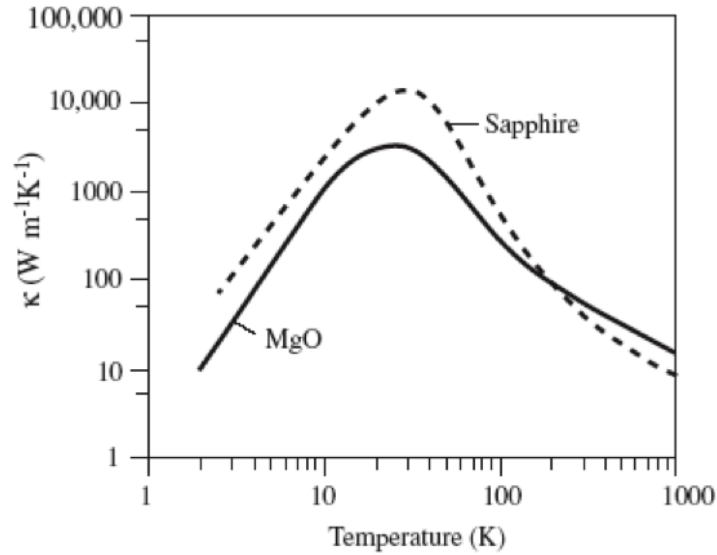


Figure 4.48: Thermal conductivity of sapphire and MgO as a function of temperature

Question 4 (Kasop 5.1) Bandgap and photodetection

- Determine the maximum value of the energy gap that a semiconductor, used as a photoconductor, can have if it is to be sensitive to yellow light (600 nm).
- A photodetector whose area is $5 \times 10^{-2} \text{ cm}^2$ is irradiated with yellow light whose intensity is 2 mW cm^{-2} . Assuming that each photon generates one electron-hole pair, calculate the number of pairs generated per second.
- From the known energy gap of the semiconductor GaAs ($E_g = 1.42 \text{ eV}$), calculate the primary wavelength of photons emitted from this crystal as a result of electron-hole recombination.
- Is the above wavelength visible ?
- Will a silicon photodetector be sensitive to the radiation from a GaAs laser ? Why ?

Question 5 (Kasop 5.13) GaAs

Ga has a valency of III and As has V. When Ga and As atoms are brought together to form the GaAs crystal, as depicted in Figure 5.54, the three valence electrons in each Ga and the five valence electrons in each As are all shared to form four covalent bonds per atom. In the GaAs crystal with some 10^{23} or so equal numbers of Ga and As atoms, we have an average of four valence electrons per atom, whether Ga or As, so we would expect the bonding to be similar to that in the Si crystal: four bonds per atom. The crystal structure, however, is not that of diamond but rather that of zinc blende (Chapter 1).

- What is the average number of valence electrons per atom for a pair of Ga and As atoms and in the GaAs crystal ?
- What will happen if Se or Te, from Group VI, are substituted for an As atom in the GaAs crystal ?
- What will happen if Zn or Cd, from Group II, are substituted for a Ga atom in the GaAs crystal ?
- What will happen if Si, from Group IV, is substituted for an As atom in the GaAs crystal ?
- What will happen if Si, from Group IV, is substituted for a Ga atom in the GaAs crystal ? What do you think **amphoteric dopant** means ?
- Based on the above discussion, what do you think the crystal structures of the III-V compound semiconductors AlAs, GaP, InAs, InP, and InSb will be ?

Figure 5.54 The GaAs crystal structure in two dimensions. Average number of valence electrons per atom is four. Each Ga atom covalently bonds with four neighboring As atoms and vice versa.

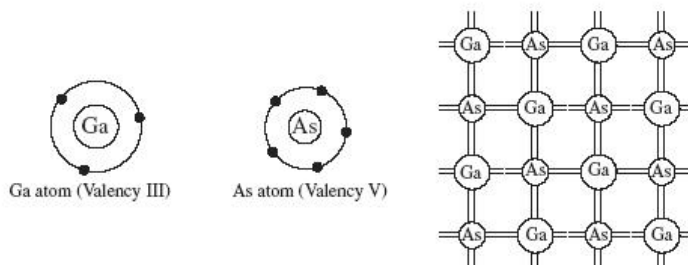


Figure 5.54

Question 6 (Kasap 5.24) Schottky Junction

- a. Consider a Schottky junction diode between Au and n -Si, doped with 10^{16} donors cm^{-3} . The cross-sectional area is 1 mm^2 . Given the work function of Au as 5.1 eV, what is the theoretical barrier height, Φ_B , from the metal to the semiconductor ?
- b. Given that the experimental barrier height Φ_B is about 0.8 eV, what is the reverse saturation current and the current when there is a forward bias of 0.3 V across the diode ? (Use Equation 4.37.)

Question 7 (Kasap 6.15) Ultimate Limits to Device Performance

- a. Consider the speed of operation of an n -channel FET-type device. The time required for an electron to transit from the source to the drain is $\tau_t = L/v_d$, where L is the channel length and v_d is the drift velocity. This transit time can be shortened by shortening L and increasing v_d . As the field increases, the drift velocity eventually saturates at about $v_{dsat} = 10^5 \text{ m s}^{-1}$ when the field in the channel is equal to $E_c \approx 10^6 \text{ V m}^{-1}$. A short τ_t requires a field that is at least E_c .
 1. What is the change in the PE of an electron when it traverses the channel length L from source to drain if the voltage difference is V_{DS} ?
 2. This energy must be greater than the energy due to thermal fluctuations, which is of the order of kT . Otherwise, electrons would be brought in and out of the drain due to thermal fluctuations. Given the minimum field and V_{DS} , what is the minimum channel length and hence the minimum transit time ?
- b. Heisenberg's uncertainty principle relates the energy and the time duration in which that energy is possessed through a relationship of the form (Chapter 3) $\Delta E \Delta t > \hbar$. Given that during the transit of the electron from the source to the drain its energy changes by eV_{DS} , what is the shortest transit time, τ , satisfying Heisenberg's uncertainty principle ? How does it compare with your calculation in part (a) ?
- c. How does electron tunneling limit the thickness of the gate oxide and the channel length in a MOSFET ? What would be typical distances for tunneling to be effective ? (Consider Example 3.10).