

**Problem 1— “DOS for a 2D electron gas” (14 pts)**

For a two-dimensional electron gas confined within a square region of sides  $a$ , we have:

$$E = \frac{h^2}{8m_e a^2} (n_1^2 + n_2^2) \quad (\text{eq.1})$$

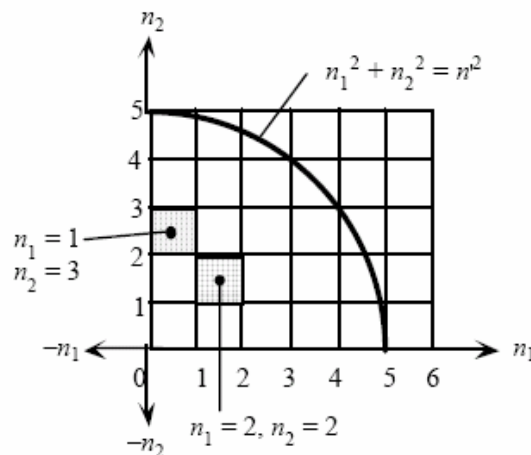
Only positive  $n_1$  and  $n_2$  are allowed. Each  $n_1$  and  $n_2$  combination is an orbital state. Define

a new variable  $n$  as:  $n^2 = n_1^2 + n_2^2$ . Substituting into (eq.1):  $E = \frac{h^2}{8m_e a^2} n^2$  (eq.2)

Let us consider how many states there are with energies less than  $E'$ , where  $E'$

corresponds to  $n \leq n'$ ,  $E' = \frac{h^2}{8m_e a^2} n'^2$  (eq.3)

$$\therefore n' = \sqrt{\frac{8a^2 m_e E'}{h^2}} \quad (\text{eq.4})$$



**Figure 1** Each state, or electron wavefunction in the crystal, can be represented by a box at  $n_1, n_2$ .

Consider Figure 1. All states within the quarter arc defined by  $n'$  have  $E < E'$ . The area of this quarter arc is the total number of orbital states. The total number of states,  $S$ , including spin is twice as many,

$$S = 2\left(\frac{1}{4}\pi n'^2\right) = \frac{1}{2}\pi \frac{8a^2 m_e E'}{h^2} = \frac{4\pi a^2 m_e E'}{h^2} \quad (\text{eq.5})$$

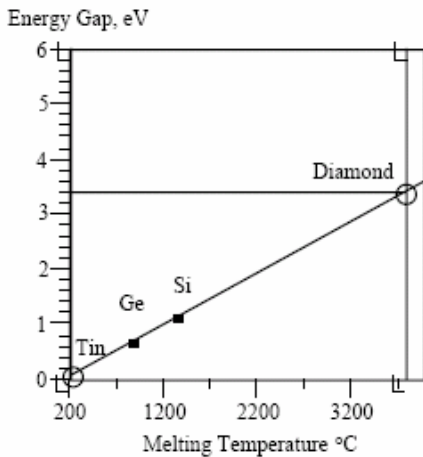
The density of states  $g$  is defined as the number of states per unit area per unit

energy. Therefore, we have  $g = \frac{1}{a^2} \frac{dS}{dE'} = \frac{1}{a^2} \frac{4\pi a^2 m_e}{h^2} = \frac{4\pi m_e}{h^2}$ . (eq.6)

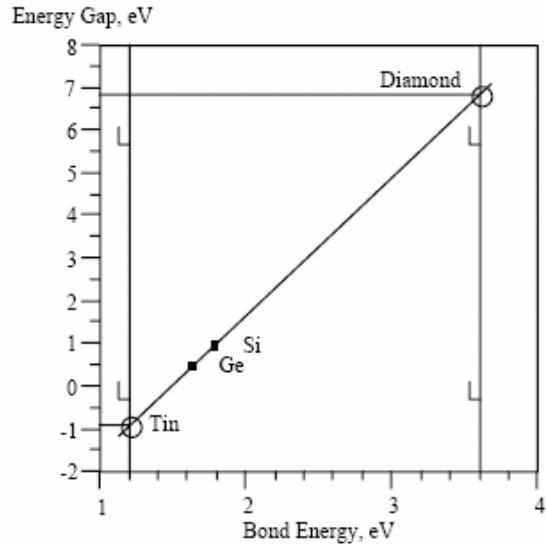
Thus, for a two dimensional gas, the density of states is constant.

**Problem 2— “Diamond and Tin” (14 pts)**

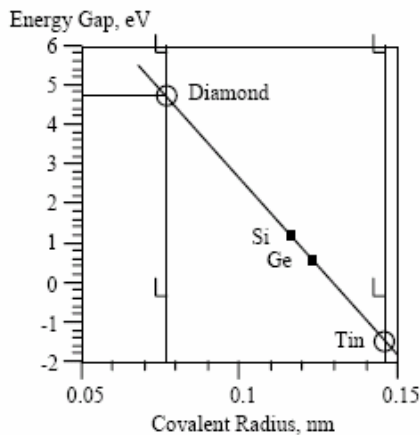
From the properties in the table, we have the following plots:



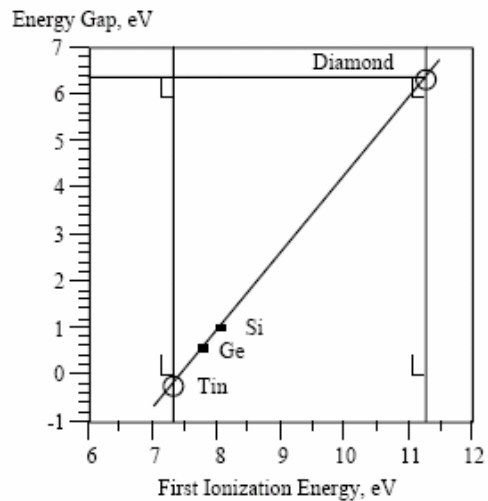
(a) Energy gap versus melting temperature. From the plot, it seems that diamond has an  $E_g = 3.4$  eV and Sn has  $E_g \approx 0$  or is a metal



(b) Energy gap versus bond energy. From the plot, it seems that diamond has an  $E_g = 6.8$  eV and Sn has  $E_g \approx -0.9$  or is a metal



(c) Energy gap versus covalent radius. From the plot, it seems that diamond has an  $E_g = 4.7$  eV and Sn has  $E_g \approx -1.5$  eV or is a metal.



(d) Energy gap versus first ionization energy. From the plot, it seems that diamond has an  $E_g = 6.3$  eV and Sn has  $E_g \approx -0.3$  eV or is a metal.

Each is a plot of the band gap  $E_g$  (or energy gap) vs. some property. The straight in each is drawn to pass through Si and Ge. Diamond and tin points are then located this straight line at the intersections with the vertical lines representing the corresponding properties of diamond and tin. (6 pts)

a) Diamond has an  $E_g$  greater than Si and Ge. Averaging the four  $E_g$  for diamond find 5.3 eV, which is close to the experimental value of 5.5 eV. (3 pts)

b) (i) All the four properties indicate that tin has  $E_g \leq 0$  or is a metal. (2 pts)

(ii) Tin's semiconductivity can be tested by examining its electrical conductivity and optical absorption (see Chapter 5 in the textbook). For example, for metals the conductivity should NOT be thermally activated over a wide temperature range, whereas for semiconductors there will be an Arrhenius temperature dependence over at least some temperature range. Further, semiconductors have an absorption edge that corresponds to  $h\nu > E_g$  (Chapter 5 in the textbook).

As indicated by the trend of band gap energy with covalent radius, one might expect tin to act more like a semiconductor if it were compressed under hydrostatic pressure, so that its interatomic spacing decreased and  $E_g$  increased. (3 pts)

**Problem 3—"Bohr model of the Hydrogen atom" (10 pts)**

The Coulombic force is given as  $F_{Coulomb} = \frac{Z_1 Z_2 e^2}{4\pi\epsilon_0 r_n^2} = \frac{e^2}{4\pi\epsilon_0 r_n^2}$ , (Eq.1)

The centripetal force is  $F_{Centripetal} = \frac{mv_n^2}{r_n}$  (Eq.2)

Balancing the Coulomb and the centripetal forces leads to:  $\frac{e^2}{4\pi\epsilon_0 r_n^2} = \frac{mv_n^2}{r_n}$ . (Eq.3)

From the equations above we have  $v_n^2 = \frac{e^2}{4\pi\epsilon_0 m r_n}$ . (Eq.4)

Also  $2\pi r_n = n\lambda = n \frac{h}{p} = n \frac{h}{mv_n} \Rightarrow r_n (mv_n) = n\hbar$ . (Eq.5)

Substituting in to Eq.4, we have

$$v_n = \frac{e^2}{4\pi\epsilon_0 n\hbar} = \frac{e^2}{2\epsilon_0 n\hbar}, \quad (\text{Eq.6})$$

$$r_n = \frac{n^2 \hbar^2 4\pi\epsilon_0}{me^2} = \frac{n^2 \hbar^2 \epsilon_0}{m\pi e^2}, \quad (\text{Eq.7})$$

and  $E_{total}^n = KE + PE = \frac{mv_n^2}{2} - \frac{4\pi\epsilon_0 e^2}{r_n} = -\frac{mv_n^2}{2}$ . (Eq.8)

Hence, the binding energy  $E_n = -E_{total}^n = \frac{me^4}{32\pi^2 n^2 \epsilon_0^2 \hbar^2} = \frac{me^4}{8n^2 \epsilon_0^2 \hbar^2}$

Plugging in the values for the physical constants we obtain

$$r_1 = 0.0529 \text{ nm}, v_1 = 2.18 \times 10^6 \text{ m/s}, \text{ and } E_1 = 13.58 \text{ eV}.$$

**Problem 4—“Fermi energy and electron concentration” (12 pts)**

Since Cu is in group I, its valency (G) is also 1. The electron concentration  $n$  is then the atomic concentration multiplied by the group number, or,

$$n = G \frac{N_A D}{M_{at}} = (1) \frac{6.022 \times 10^{23} \times 8.96 \times 10^3}{63.55 \times 10^{-3}} = 8.490 \times 10^{28} / m^3$$

Using equation (4.22) in the text,

$$E_{F0} = \frac{h^2}{8qm_e} \left( \frac{3n}{\pi} \right)^{2/3}$$

$$= \frac{(6.626 \times 10^{-34})^2}{8 \times 1.6 \times 10^{-19} \times 9.109 \times 10^{-31}} \left( \frac{3 \times 8.490 \times 10^{28}}{3.1416} \right)^{2/3} = 7.04 \text{ eV}$$

Comparing with experimental value,

$$|\% \text{ difference}| = \left| \frac{7.04 - 6.5}{6.5} \right| \times 100\% = 8.31\%. \quad (4 \text{ pts for each metal})$$

$E_{F0}$  can be calculated for Zn and Al in the same way. The values are summarized in the following table:

**Table Q4.8-2** Summarized values for Fermi energy at absolute zero temperature.

Metal	$n \text{ (m}^{-3}\text{)} (\times 10^{28})$	$E_{F0} \text{ (eV)}$ (calculated)	$E_{F0} \text{ (eV)}$ (experimental)	% Difference
Cu	8.490	7.04	6.5	8.31
Zn	13.15	9.43	11.0	14.3
Al	18.07	11.7	11.8	0.847

It shows that calculated values are close to experimental values.