國立清華大學命題紙

八十四學年度材料科學工程研究所 所 丙 組碩士班研究生入學考試

科目 物理化學(II) 科號 1402 共 5 頁第 1 頁 *請在試卷【答案卷】內作答

1. (10%) Assume that there is one conduction electron per atom in a gold crystal, and the energy levels available to the electrons are those of a cubic box.

(a) Show that the number of electrons per unit volume in an energy range from E to E + dE is given by the density of states function;

$$N(E)dE = \frac{\pi}{2}\left(\frac{8m}{h^2}\right)^{3/2} E^{1/2}\, dE \quad (m = 0.9109 \times 10^{-30}\,\text{kg of e's})$$

(b) Hence, prove the maximum level (Fermi level) occupied by the electrons at 0 K is

$$E_F = \left(\frac{3L}{8\pi V}\right)^{2/3} \frac{h^2}{2m}$$

where L/V is the number of electrons per unit volume occupying energy levels from E = 0 to $E = E_F$

(c) Gold is face centered cubic with 4 atoms per unit cell and unit length a_0 = 0.408 nm. Calculate the Fermi level of gold (in J or in eV as unit).

2. (10%) Suppose that an electron moving in one dimension with a kinetic energy of 9.5 eV meets a barrier of height 10 eV and width 1.0 nm.

(a) Estimate the probability that the electron will tunnel through the barrier. (The penetration probability

$$P = 16\varepsilon(1-\varepsilon)\, e^{-2l/D} \quad \text{where } \varepsilon = \frac{E}{V},\; D = \left[\frac{\hbar^2}{2m(V-E)}\right]^{1/2}$$

e's charge = 1.602×10^{-19}C, exp(-7.24) = 7.17×10^{-4})

(b) This situation is similar to that of an electron tunneling through a thin nonconducting layer at an intermetallic contact. Describe the basic principle of the scanning tunneling microscope (STM).

3. (5%) A simple harmonic oscillator with mass m has a restoring force equal to -kx. Write the Hamiltonian for this system.

4. (10%)

(a) The two-particle rigid rotator undergoes rotation about its center of mass. Write the Hamiltonian for this system using spherical coordinate.

(b) The eigenvalues for the rigid rotator are

$$E_J = \frac{J(J+1)\hbar^2}{2I}$$

where the moment of inertia is given by $I = \mu r^2$. What is the degeneracy of each level?

(c) Prepare a plot of the energy levels expressed in unit of $\hbar^2/2I$.

5.(5%) Identify which of the following functions are eigenfunctions of the operator $\frac{d}{dx}$: (a) e^{ikx}, (b) coskx , (c) K, (d) kx, (e) $d^{-\alpha x^2}$. Give the corresponding eigenvalue where is appropriate.

6. (10%) Explain as simple as possible.

(a) angular momentum

(b) Wien's displacement law of blackbody radiation

(c) quantum

(d) two examples for wave and particle properties for a matter

(e) The uncertainty principle

(f) Born interpretation for the wavefunction

(g) $E_n = \frac{n^2h^2}{8ma^2}$ for a particle in one-dimension box, why is $n \neq 0$?

(h) zero-point energy

(i) spin

(j) degeneracy

7. (10%) Metal M has an fcc structure with a_0 = 0.4220 nm. It's oxide, MO, crystalizes with NaCl structure and a_0 = 0.5016 nm. Calculate the nearest M-M distances in MO and M at 25°C. Comment on the calculated results.

8. (16%) Use band theory to classify solids according to electronic properties into insulator, metal, intrinsic semiconductor, and impurity semiconductor.

9. The reaction $2AO + O_2 \rightarrow 2AO_2$ is tentatively assigned as

$AO + AO$	$\rightarrow$	A_2O_2	k_1	(1)
A_2O_2	$\rightarrow$	$2AO$	k_2	(2)
$A_2O_2 + O_2$	$\rightarrow$	$2AO_2$	k_3	(3)

(a) (5%) Obtain the rate law

$$\frac{d[AO_2]}{dt} = \frac{2k_1k_3[AO]^2[O_2]}{k_2 + k_3[O_2]}$$

by applying the steady state approximation to $[A_2O_2]$

(b) (9%) Suppose a very small fraction of A_2O_2 formed in (1) goes to form products in (3), while most of the A_2O_2 reverts to AO in (2). Given the activation energies are $E_1 = 90$ kJ, $E_2 = 190$ kJ, and $E_3 = 70$ kJ, calculate the overall activation energy.

10. (10%) Briefly describe the operating principle of Laser. Use CO_2 laser as an example.