

## CH448/548 Surface Chemistry 2007

### Midterm Exam

Name : \_\_\_\_\_

Score : \_\_\_\_\_ / 85

**SHOW WORKING WHERE APPROPRIATE TO ENSURE PARTIAL CREDIT**

Possibly useful information :

$$k_0 = 2\pi [E(\text{eV}) / 150]^{1/2} \text{ \AA}^{-1} \quad \lambda = h / mv$$

$$h = 6.626 \times 10^{-34} \text{ J s}$$

$$k = 1.381 \times 10^{-23} \text{ J / K}$$

$$R = 8.314 \text{ J / mol K}$$

$$m_e = 9.109 \times 10^{-31} \text{ kg}$$

$$N_A = 6.022 \times 10^{23}$$

$$1 \text{ atm} = 760 \text{ torr} = 101,325 \text{ Pa}$$

Molecular masses (amu):    H 1.008            C 12.01            O 16.00



0. Circle the most appropriate answer – you might want to answer this after doing the rest of the exam first (circle either answer for 1 pt).

This exam was a Valentine's Day Present / a Valentine's Day Massacre

1. (10 pts) You have finally graduated from OSU (in 2022) with a Ph.D. You go to a job interview with "Surfaces R Us" (President, P.R. Watson, OSU retired). Part of the interview consists in answering the following questions. (2 pts each).

Name a good technique to image the surface of a copolymer.

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Name a good technique to determine the structure of a reconstructed clean surface.

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Name a good technique to determine the adsorption enthalpy of a molecule on a surface.

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Name a good technique to find the geometry of a molecule adsorbed on a surface.

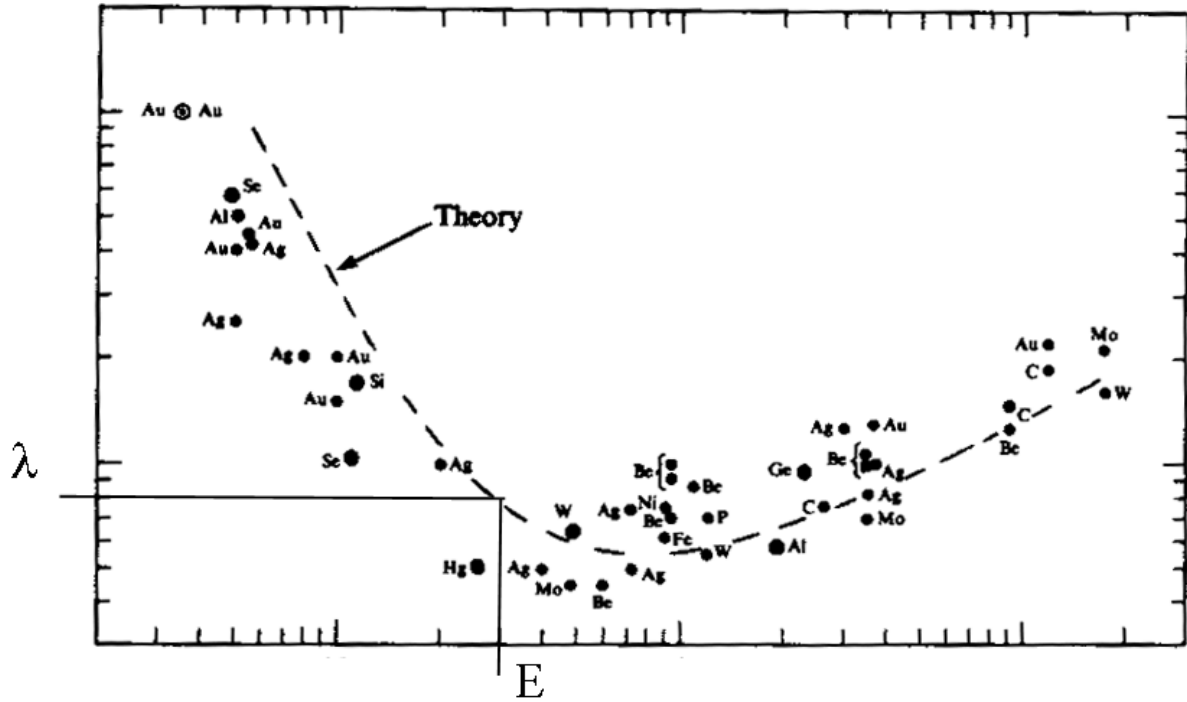
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Name a good technique to measure the size of atomic-size defects on a Si surface.

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2. (4 pts) A surface is prepared from a single crystal of a bcc metal. The surface is perpendicular to the (110) plane, runs parallel to the z-axis and passes through the point (0.5, 1, 0) in the unit cell. What are the Miller indices of this surface?

3. (10 pts) Below is the “Universal Curve” of electron escape depth as a function of electron kinetic energy, but it is missing any numerical axis labels.



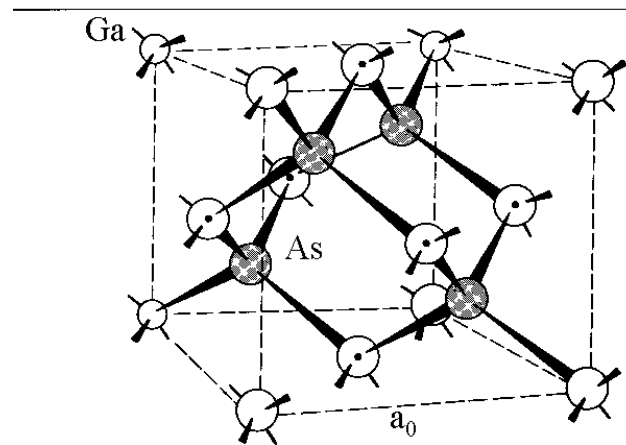
a) Estimate the values of E and  $\lambda$ . (2 pts each)

E = \_\_\_\_\_ eV       $\lambda$  = \_\_\_\_\_ pm

b) Where on this curve is an electron most “surface sensitive”? (2 pts)

c) What is the meaning of “mean free path”? (4 pts)

4. (20 pts) Below is shown the crystal structure of GaAs.



- a) Sketch the unit mesh of the GaAs(110) surface and the atoms present in the plane. Only include atoms that lie in the surface plane, not those that lie a little above or below it. The atoms need not be to scale, but identify which are Ga and which are As. Mark the (a, b) vectors that define the unit mesh. (6 pts)

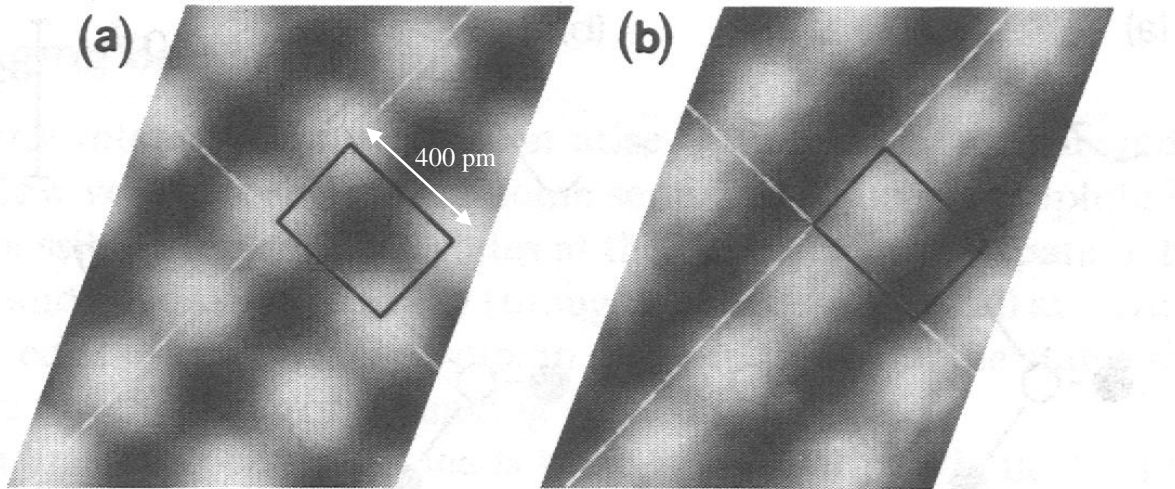
b) What are the lengths of the unit mesh vectors in units of the unit cell parameter  $a_0$ ? (2 pts)

$$|\underline{a}| = \text{_____} a_0 \qquad |\underline{b}| = \text{_____} a_0$$

c) What will be the relative lengths of the reciprocal lattice vectors for this surface? (2 pts)

$$|\underline{a}^*| / |\underline{b}^*| = \text{_____}$$

(d) Below are STM images of the GaAs(110) surface taken at two different tip voltages. The white cross-hairs are centered on the same location in each image and the black rectangle is similarly invariant. The lattice constant of GaAs is 400 pm. You can assume that the sample has not physically moved during the measurement or changed chemically in any way.



i) what does the black rectangle represent? \_\_\_\_\_ (2 pts)

ii) what are the white features in (a)? \_\_\_\_\_ (2 pts)

iii) what are the white features in (b) \_\_\_\_\_ (2 pts)

iv) why do one set of white features show up in each image and not both sets in both images? (4 pts)

5) (25 pts total) a) What do the following formulas describe and what is the significance of the parameters? (5 pts each part)

i)  $r = v_m \theta^m \exp(-\Delta H / RT)$        $m = 1, 2$

Formula describes \_\_\_\_\_

$m =$  \_\_\_\_\_

$v_m =$  \_\_\_\_\_

$\theta^m =$  \_\_\_\_\_

$\Delta H =$  \_\_\_\_\_

ii)  $\theta = (bP)^m / (1 + (bP)^m)$        $m = 0.5, 1$

Formula describes \_\_\_\_\_

$m =$  \_\_\_\_\_

$b =$  \_\_\_\_\_

$\theta =$  \_\_\_\_\_

At high pressures what is the limiting value of  $\theta$ ? \_\_\_\_\_

iii)  $P / V(P^* - P) = 1 / V_m c + (c-1)P / V_m c P^*$

Formula describes \_\_\_\_\_

Name associated with formula \_\_\_\_\_

$V_m =$  \_\_\_\_\_

$c =$  \_\_\_\_\_

$P^* =$  \_\_\_\_\_



b) The activation energy of desorption of an associatively adsorbed molecule  $X_2$  is 108 kJ/mol. If the attempt frequency for desorption is  $10^{13} \text{ s}^{-1}$  what will be the rate of desorption of  $X_2$  at 500K? Take the coverage to be unity and that desorption is first order (5 pts)

c) an experiment studies the adsorption of A(g) and B(g) on metal X. Both A and B adsorb associatively on the same site on the surface. Assuming the adsorptions are Langmuirian with  $b_A = 1 \text{ torr}^{-1}$  and  $b_B = 10 \text{ torr}^{-1}$  what will be the coverages of A and B on the surface when  $P_A = P_B = 100 \text{ torr}$ ? (5 pts)

5. (15 pts) A 50:50 mixture of  $^{12}\text{C}^{16}\text{O}$  and  $^{14}\text{C}^{18}\text{O}$  is exposed to the surface of a metal. The following are experimental observations.

a) TDS data has asymmetric peaks with equal areas for masses 28 and 32, no peak at mass 30 or any other mass.

Asymmetric peaks means \_\_\_\_\_ (1 pt)

Specie(s) desorbing are \_\_\_\_\_ (2 pts)

Equal areas and no peak at mass 30 means

\_\_\_\_\_ (2 pts)

The type of adsorption is \_\_\_\_\_ (1 pt)

Draw a sketch of the adsorbate(s) on the surface: (4 pts)

b) Predict the approximate HREELS spectrum for adsorption on the surface. Label peaks with the type of vibration involved. (5 pts)

