The University of Western Ontario

Name:______________________

Student #:________________________

P9826 Fall 2010

<u>Midterm exam -due November 1, 2010, 6pm</u>

Total - 30 points

<u>Instructions:</u>

Write your student ID on the every page of this exam printout AND any additional page you enclose. Use the additional pages for your answers if needed. Disregard next page (p. 2, it is for marking purposes only).

You are allowed to use calculators, textbooks and lecture notes.

Total there are 8 questions, you have a choice in questions 6, and questions 7-9

Total - 30 points

Good luck!

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1	**2**	**3**	**4**	**5**	**6.1**	**6.2**	**6.3**	**6.4**	**6.5**	**6.6**	**6.7**	**6.8**	**6.9**	**6.10**	**7**	**8**	**9**	**Total**
3	**3**	**2**	**2**	**2**	**2**	**2**	**2**	**2**	**2**	**2**	**2**	**2**	**2**	**2**	**3**	**3**	**3**	**30**

Questions (Total - 30 points):

1. (*3 point*) (a) Sketch a possible real space structure and the LEED pattern for a (3×1) overlayer on the (100) surface of an fcc metal. Use different symbols for LEED diffraction peaks of overlayer and substrate. Indicate the unit cell vectors for the surface and the overlayer, and of the reciprocal lattice.

(b) Are multiple domains of (3×1) symmetry possible on fcc(100)? If so, how is the LEED pattern affected? Show sketches, as appropriate.

(c)What is the surface coverage of an ideal (3×1) atomic overlayer on fcc Ni(100)? Express as fractional coverage in monolayers, and as atoms/cm^2. The nearest neighbor spacing in Ni is 2.49 Å.

2. (*3 points*) The electron emission properties of tungsten are given in the table (see next page). Please do the following calculations.

(a) Plot the data in the form of a Richardson plot, and determine the values of the work function $e\phi$ and pre-exponential factor (B).

(b) Assume the tungsten is covered by tungsten oxide layer, and that the work function increases by 1.55eV. Plot a new Richardson plot for T < 2000K (the range over which the oxygen will remain adsorbed). Assume the same B as above.

(c) Assume that the surface is coated with a low work function BaO/SrO mixture, giving a work function 1.9 eV lower than the value for clean W. Generate a Richardson plot for this surface T < 1400K (the approximate range of stability). Assume the same B as above.

(d) For each of the 3 surfaces, indicate the temperature at which the emission current density is 1×10^{-5} A/cm^2.

Temp. K	Resistivity microhm cm	Electron emission amp./cm^2
300	5.65	—
400	8.06	—
500	10.56	—
600	13.23	—
700	16.09	—
800	19.00	—
900	21.94	—
1000	24.93	1.07×10^{-15}
1100	27.94	1.52×10^{-13}
1200	30.98	9.73×10^{-12}
1300	34.08	3.21×10^{-10}
1400	37.19	6.62×10^{-9}
1500	40.36	9.14×10^{-8}
1600	43.55	9.27×10^{-7}
1700	46.78	7.08×10^{-6}
1800	50.05	4.47×10^{-5}
1900	53.35	2.28×10^{-4}
2000	56.67	1.00×10^{-3}
2100	60.06	3.93×10^{-3}
2200	63.48	1.33×10^{-2}
2300	66.91	4.07×10^{-2}
2400	70.39	1.16×10^{-1}
2500	73.91	2.98×10^{-1}
2600	77.49	7.16×10^{-1}
2700	81.04	1.63
2800	84.70	3.54
2900	88.33	7.31
3000	92.04	1.42×10
3100	95.76	2.64×10

3. (*2 point*) Explain why a scanning tunneling microscope achieves an atomic resolution.

4. (*2 points*) When measuring spherical particles of less than 10 nm on a substrate with an atomic force microscope, an experienced operator uses the height of the sphere to estimate the size of the object. Explain why, instead of using the measured lateral dimension (size) of the sphere, he/she selects to do so.

5. (*2 points*) Explain why phase shift imaging in AFM may be useful in differentiating composite materials. **Hint:** Think about AFM tip as of a forced oscillator.

6. (*12 points*)

Answer 6 of the following 10 questions (*2 points each*). Justify your answer, i.e., show computations, sketch figures, etc., needed to obtain the answer.

6.1 Which has a smaller inelastic mean-free path in most materials, an electron with kinetic energy of 2 eV or 100 eV?

6.2 What is the de Broglie wavelength of an electron with kinetic energy of 75 eV?

6.3 Calculate the pressure necessary to keep a $1cm^2$ Si(001) surface clean for 1 hour at 300K, assuming a sticking coefficient of 1 for all gases, no dissociation of the gas upon adsorption and that “clean” mean <0.01ML of adsorbed impurities.

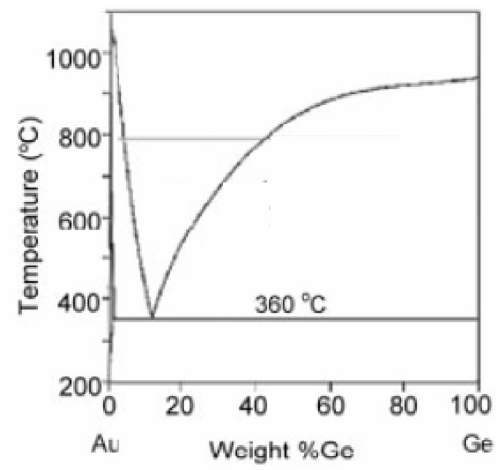
6.4 You are making XPS measurements of Mo $3d_{5/2}$ which has a natural line width (lifetime width) of 1.5eV. If the photon source has a width of 0.75eV, and your analyzer resolution of 0.5eV, what is the measured line width of Mo $3d_{5/2}$?

6.5 A rectangular piece of Ni (ρ=8.9g/cm^3) 1 cm wide, 1 cm deep and 2 cm long is precisely half submerged (long axis vertical) in molten Cu (assume no dissolution of Ni into the Cu; density of molten Cu is 8.5 g/cm^3). If the molten Cu has a surface tension with the ambient of 1500 ergs/cm^2 and a contact angle of 140^o is observed, what forces are required to keep the Ni block stationary? Give a force direction, i.e., lifting or sinking direction. (1 erg = 10^{-7} Joule; gravitational constant g = 9.8 m/s^2)

6.6 If boron is diffused into a thick slice of silicon with no previous boron in it at a temperature of 1100°C for 5 h, what is the depth below the surface at which the concentration is 10^{17} atoms/cm^3 if the surface concentration is 10^{18} atoms/cm^3? D = 4 × 10^{-13} cm^2/s for boron diffusing in silicon at 1100°C.

z	erf z	z	erf z	z	erf z	z	erf z
0	0	0.40	0.4284	0.85	0.7707	1.6	0.9763
0.025	0.0282	0.45	0.4755	0.90	0.7970	1.7	0.9838
0.05	0.0564	0.50	0.5205	0.95	0.8209	1.8	0.9891
0.10	0.1125	0.55	0.5633	1.0	0.8427	1.9	0.9928
0.15	0.1680	0.60	0.6039	1.1	0.8802	2.0	0.9953
0.20	0.2227	0.65	0.6420	1.2	0.9103	2.2	0.9981
0.25	0.2763	0.70	0.6778	1.3	0.9340	2.4	0.9993
0.30	0.3286	0.75	0.7112	1.4	0.9523	2.6	0.9998
0.35	0.3794	0.80	0.7421	1.5	0.9661	2.8	0.9999

6.7 (a) What is the function of Au during the growth of Si or Ge nanowires? (b) Name two general approaches to growth nanowires? (c) Using the phase diagram below describe 4 steps of Ge nanowire growth; (d) What parameters determine nanowire diameter? (e) Name (at least) three ways to terminate the growth process.



6.8 The Ti $2p_{5/2}$ binding energy is 454.0eV in metallic Ti. When Ti is oxidized to TiO_2, a chemical shift ΔE_B of 4.9 eV is observed. What is the sign of the chemical shift (on the binding energy scale), why? If you had an analyzer which could measure it, would you expect the chemical shift of the Ti 1s to be the same, greater or less than 4.9eV? Why?

6.9 Discuss the advantages and disadvantages of using Low Energy Electron Microscope in comparison with Scanning Tunneling Microscope for <u>determining the reconstructions on a single crystal metal surface</u>.

6.10 You are depositing *fcc* Au (d_{Au}=2.88Å) onto the *bcc* Fe(110) surface (d_{Fe}-2.54 Å) What growth mode do you expect in the first monolayer, Nishyama-Wasserman or Kurdjimov-Sachs? Indicate <u>why.</u>

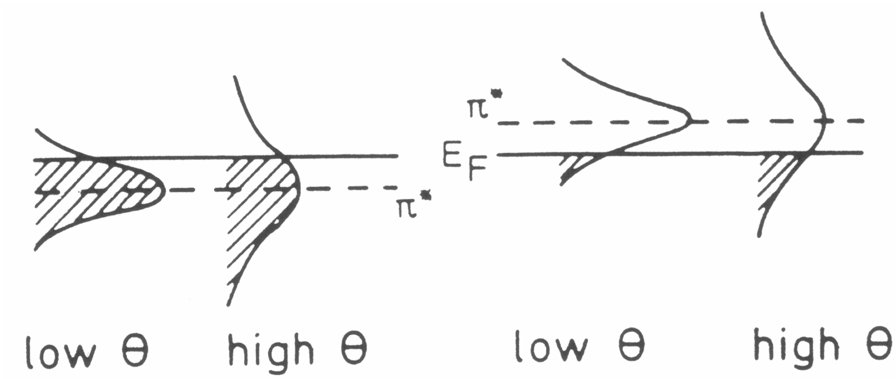
Answer 2 of the following 3 questions (*3 points each*).

7. (*3 points)* Consider a 1D crystal whose *bulk* electron dispersion relation is $\varepsilon(k) = \varepsilon_o - bk^2$, where $b > 0$, so that there is a maximum of this band at k = 0.

Suppose there is a surface state at the surface of this crystal, and that this surface state has an energy $\varepsilon_0 + \Delta$ just above the valence band maximum (*i.e.*, Δ is small and positive). Such a surface state is expected to decay exponentially into the bulk like e^{kx}, where k is the exponential decay constant.

Give a simple argument that allows you to express k in terms of the parameters b and Δ.

8. (*3 points)* For simple diatomic molecule such as CO and NO, the $2\pi^*$ electronic energy level plays a key role in bonding to a metal surface. The molecular orbital is antibonding (that is, bond weakening) with respect to the C-O or N-O bond, respectively. As such, its occupation can influence the strength of this bond. For the isolated CO molecule, this level is the lowest energy unoccupied orbital. For NO, it is the highest occupied orbital. When the molecule approaches a surface of a late transition metal, the 2p orbital will interact with the states near the metal Fermi level, broaden in energy, and can be characterized as partially occupied. Furthermore, owing to interaction with neighboring adsorbed molecules at the surface, the level tends to be narrow for low coverage (low θ) and broadened for high coverage (high θ). As illustrated in figure below (representing NO on the left and CO on the right), this change in level width has very different consequences for an initially filled or initially empty orbital.



Based on the above information and the diagram, describe how you would expect the characteristic frequency of C-O and N-O stretching vibrational modes to behave as a function of molecular coverage on a metal surface. Why do you expect this behavior?

9) (*3points*) An electron is trapped in a two-dimensional infinite potential well with widths $L_x = L_y$.

a) Find the energies of the lowest five possible energy levels for this trapped electron, and construct corresponding energy-level diagram.

b) As a multiple of $\frac{h^2}{8mL^2}$, what is the energy difference between the ground state and the third excited state of the electron?