The University of Western Ontario
Department of Physics and Astronomy

P9826b Winter 2013

January 28, 2013

Homework Assignment #1 (due on February 6, 2013)

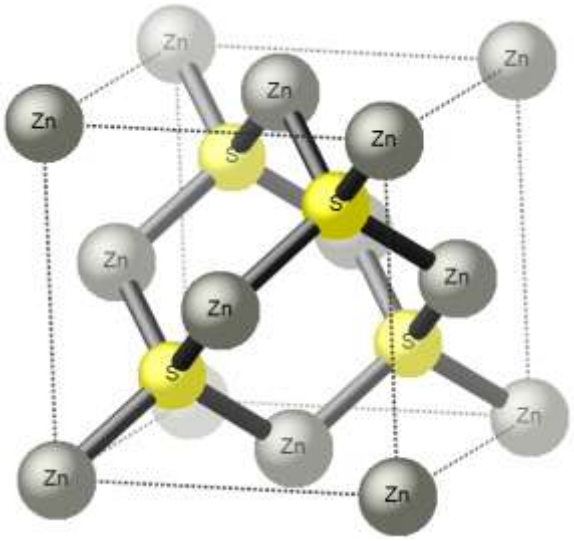
Problems:

1. (4 points) Find the crystallographic structure of one of the materials studied in your research project. If this material is known to have several crystallographic forms, list all of them and select the one with the highest symmetry group. For instance, if you study corrosion of Ni alloys, consider Ni crystal structure. If you project has no connection with crystalline solids, take zincblende crystal structure as shown in the figure below.

(a) Consider the following surfaces: (*i*) (100); (*ii*) (111); (*iii*) (110); (*iv*) (211). Sketch out the ideal surface structure of each. If applicable, identify the ones with the polar termination.

(b) *Order of magnitude estimates of γ.* Estimate how many bonds does one need to break to form (100) and (111) surfaces of this material. Which surface has lower surface energy: (100) or (111)?

(c) Compare your predictions for surface energies with the values from the literature (list your references).



ZnS structure is similar to diamond structure. It has Zn cations at the *fcc* lattice sites and S anions occupy 4 tetrahedral-coordinated vacancy sites.

2. (4 points) Consider that in the pictures (including next page) you are looking down at a surface. The larger circles represent the substrate atom positions and dark dots represent the overlayer atom positions. Overlayer unit cells are shown. For each structure:

(a) Draw the substrate unit cell and vectors, and the primitive overlayer unit cell and unit cell vectors.

(b) Calculate the ideal coverage (in monolayers) of the overlayer.

(c) If the primitive overlayer surface unit cell can be named with Wood's notation, do so. If it cannot, try to identify a nonprimitive cell which can be so named.

(d) Give the matrix notation for the primitive overlayer unit cell.

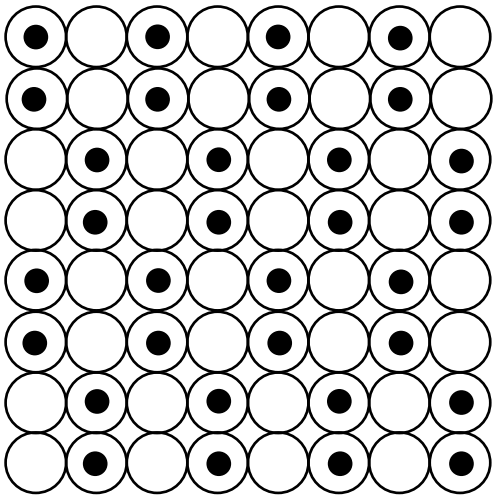
(e) Classify the surface overlayer as simple, coincident or incoherent.

For each real space surface structure provided:

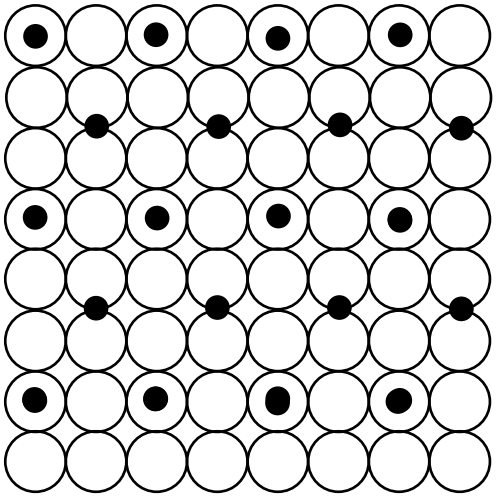
(f) Construct reciprocal unit cells for the substrate and the overlayer (show both the magnitude and the directions of the vectors).

(g) Sketch LEED patterns for each case, using different symbols distinguish the peak positions for the substrate and the overlayer (Hint: don't forget about possible domains!).

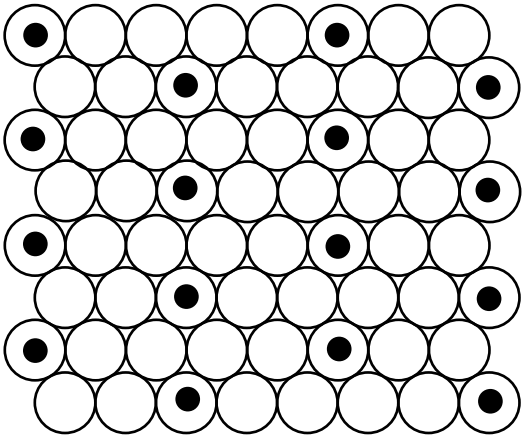
(a)



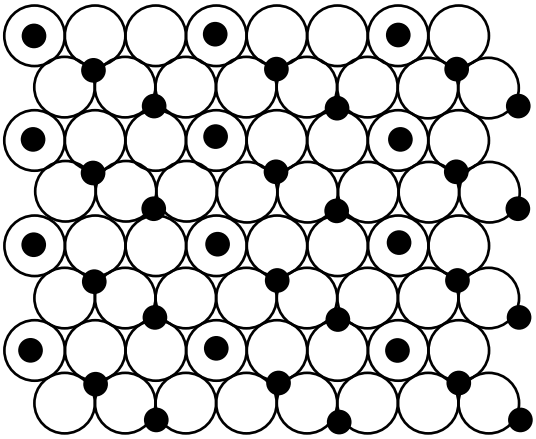
(b)



(c)



(d)



3. (2 points) According to Hertz-Knudsen equation, the flux of molecules hitting unit area of a surface in unit time is

$$Z_W = \frac{p}{(2\pi m k_B T)^{1/2}}$$

where p is pressure, m molecular mass, k_B Bolzmann constant and T temperature. The dissociative sticking coefficient of H_2 on Si (001) is 1×10^{-10} at room temperature. There are 6.8×10^{18} Si atom per m^2 on the Si (100) surface. Estimate the coverage of H atoms that results from exposing a Si (100) surface to 1×10^{-5} Pa of H_2 for 30 min. Justify the use of a constant sticking coefficient.

4. (3 points) When CO binds in sites of progressively higher coordination number on a transition metal surface (on-top ⇒ two-fold bridge ⇒ three-fold hollow ⇒ four-fold hollow) both the π and σ contributions to bonding increase in magnitude.

(a) Predict the trends that are expected in the CO stretching frequency and chemisorption bond energy with change of site.

(b) When the π bonding interaction with the surface is weak, which adsorption site is preferred?

5. (2 points) Consider the oxidation of steel plate in a gas atmosphere at T=927°C. Calculate the time necessary to increase the oxygen content to 0.36 wt% at 0.4 mm below the surface of the plate. Assume the oxygen content at the surface to be 2.0 wt % and that the nominal oxygen content of the steel gear before oxidation is 0.18 wt%. Diffusion coefficient of oxygen in γ iron ay 927°C is $1.28\times10^{-11}m^2/s$.

Use the value of the error function from the table below for a solution. (*Hint:* refer to the second Fick's law of diffusion to solve it).

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