Western University
Department of Physics and Astronomy
Surface Science, Physics 9826b, Winter 2013

Additional Problems for Final Exam

1. (#2.8 K.K.)The dimer unit on a Si(001) surface has a bonding orbital just below E_F and an antibonding orbital just above E_F. Make a prediction about STM images that are taken at positive compared with negative voltages. Do the images look the same and if not how do they differ?

A bonding orbital has enhanced electron density between the nuclei involved in the bond. An antibonding orbital has a node. When imaged below E_F (positive tip bias) the bonding orbital is imaged and an electron cloud extending over the nuclei is expected to have a maximum in the middle. Above E_F (imaging with a negative tip), the antibonding state with a node between the dimer atom is imaged. See picture below as an example
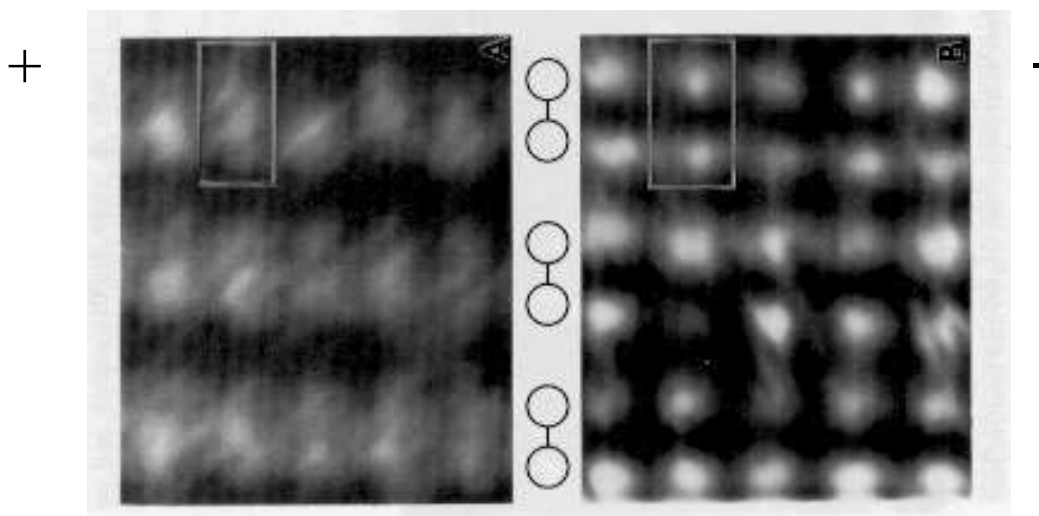
2. (#4.13 K.K.) Many different pressure units are encountered in surface science and conversion are inevitable. Shat that

$$Z_W = 3.51 \times 10^{22} cm^{-2} s^{-1} \frac{p}{\sqrt{MT}}$$

where p is given in torr, M in g mol^{-1} and T in Kelvin. Derive a similar expression that relates the SI units of pressure (Pa), molar mass (kg mol^{-1}) to the flux in m^{-2}s^{-1}.

Note that kg mol^{-1} is the SI unit of molar mass whereas the molecular weight in g mol^{-1} is used in the first expression. The original expression for the impingement rate is $Z_W = \dfrac{p}{(2\pi m k_B T)^{1/2}}$,

where all SI units are used, p is in Pa, m is the particle mass in kg and T is in K.

We can substitute $R=N_A k_B$, $M=N_A m$

$$Z_W = \frac{p}{(2\pi \dfrac{M}{N_A} \dfrac{R}{N_A} T)^{1/2}} = \frac{N_A p}{(2\pi MRT)^{1/2}} = 2.63 \times 10^{24} m^{-2} s^{-1} \frac{p}{(MT)^{1/2}} \; ; \; where \; p \; is \; in \; Pa \; and \; M \; is \; in$$

kg mol^{-1}.

$$Z_W = 2.63 \times 10^{24} m^{-2} s^{-1} \left(\frac{1m^2}{10^4 cm^2} \right) \frac{p}{(M(1000g/1kg)T)^{1/2}} \left(\frac{760torr}{10^5 Pa} \right) = 3.51 \times 10^{22} cm^{-2} s^{-1} \frac{p}{(MT)^{1/2}}$$

Now p is in torr and M is in g mol^{-1}.

3. Calculate the ratio of oxide volume to metal volume (Pilling-Bedworth ratio) for the oxidation of Al to Al_2O_3. The density of Al is 2.7 g/cm^3 and that of aluminum oxide – 3.7 g/cm^3.

What does this ratio tell you?

See your lecture notes

4. (#5.13 K.K.) The dipole moments of O(a) and OH(a) on Pt(111) are 0.035 and 0.05 e Å, respectively. Calculate the shift in the adsorption energy caused by the interaction of the electric field in the double layer with the dipoles when the surface is biased at 1V relatively to the point of zero charge.

The dipole moment of OH(a) is D(OH) = 0.05 e Å, that of O(a) is D(O) = 0.035 e Å. The bias potential at the surface is U=1V. The typical double layer width is 3Å. Hence the electric field in the double layer is

$$E = \frac{U}{d} = \frac{1V}{3\text{Å}} = 0.33 \, V\text{Å}^{-1}$$

The shift in energy of the dipole is given by the product of the electic field and the dipole moment:

OH(a): ΔE(OH)=ED=$0.33 \, V\text{Å}^{-1} \times 0.05 e\text{Å} = 0.017 eV$

O(a): ΔE(O)=ED=$0.33 \, V\text{Å}^{-1} \times 0.035 e\text{Å} = 0.012 eV$

5. (a) Write equation for the secondary ion signal intensity from element m in a SIMS experiment.

(b) Identify and explain the importance of each parameter.

(c) Describe and explain the variation of the Al^+ signal as a function of depth, as a depth profile analysis is performed through an aluminum oxide film on Al.

(d) What are the implications of this observation for quantitative elemental analysis using SIMS?

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6. Cu and TaN are used for metal interconnects in CMOS devices (TaN as a diffusion barrier). You need to characterize a sample with the ultra-thin (~5-7Å) Au, TaN, and Cu layers deposited on Si using Rutherford Backscattering Spectroscopy (RBS). But you don't know exact sequence, whether it is (a) Au/Cu/TaN/Si(001); (b) Cu/Au/TaN/Si(001); (c) TaN /Cu/Au/Si(001)

First you ran a sample using 1MeV He$^+$ incident beam with the detector located at 170° and you got a spectrum, as shown below:

(a) Label all the peaks in the spectrum; *see below*

(b) Two of the elements are not resolved. Suggest at least <u>one</u> way to resolve them, if you can change incident energy in the 100keV-10MeV range, or you can change the incident projectiles (e.g., use H$^+$, or N$^+$ instead of He$^+$) *Kinematic factors for Ta and Au with He$^+$ are 0.915 and 0.92, and, therefore RBS peaks of these elements will be detected at 915keV and 920keV, respectively.The width of the peaks are ~ 15keV (as can be estimated from the figure below). If we use heavier incident ions, for instance N$^+$, kinematic factors will be different: 0.733 for Ta and 0.752 for Au. For the same energy (1MeV) these peaks will be separated enough to be resolved. They will be separated even more at higher incident energy.*

(c) If all three layers are continuous and amorphous, suggest other <u>two</u> techniques/experiments you can use to find out which of the compositions (a), (b) or (c) will represent the multilayered stack. *SIMS, XPS (can detect Cu oxide or Ta oxide)*

(d) Suggest at least <u>two</u> techniques to measure N content in the TaN layer. *SIMS, XPS*