P627 / CHEM 541 F2010
SURFACE / INTERFACE SCIENCE
Midterm Exam
SOLUTIONS

1] a) From geometry of ECS:

$$\gamma_{10} = \gamma_{01} = \gamma_{\bar{1}0} = \gamma_{0\bar{1}} = 200 \text{ erg/cm}$$

$$\gamma_{11} = \gamma_{\bar{1}\bar{1}} = \gamma_{10}/\sqrt{2} = 141.4 \text{ erg/cm}$$

Since there are no facets in the $(1\bar{1})$ or $(\bar{1}1)$ directions we know that

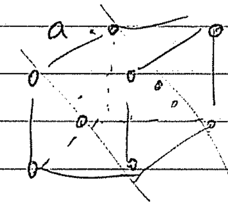
$$\left.\begin{matrix}\gamma_{1\bar{1}} \\ \gamma_{\bar{1}1}\end{matrix}\right\} > \sqrt{2}\,\gamma_{10} = 283 \text{ erg/cm}$$

b) let the length of the (10) face be l. Then $A = 3l^2 \Rightarrow l = \frac{1}{\sqrt{3}}$ cm

$$E_{TOT} = 4l(200 \text{ erg/cm}) + 2\sqrt{2}\,l\,\frac{200}{\sqrt{2}} \text{ erg/cm} = 6l(200 \text{ erg/cm})$$

$$= (6/\sqrt{3})(200 \text{ erg}) = 693 \text{ erg}$$

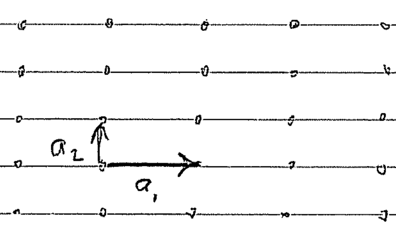
2] Cu(110) $\Rightarrow$ fcc(110)



Note (110) direction is close-packed

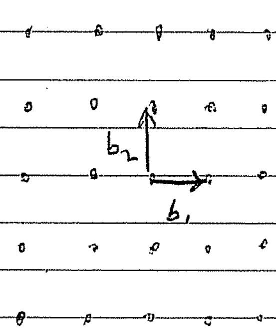
Spacing = a along (100)
= $a/\sqrt{2}$ along (110)

a)



$a_1 = 0.361$ nm
$a_2 = \left(\frac{1}{\sqrt{2}}\right)(0.361 \text{ nm}) = 0.255$ nm

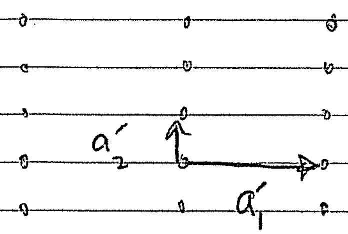
b)



$$b_1 = \frac{2\pi}{a_1} = (2\pi/0.361) \text{ nm}^{-1}$$

$$b_2 = \frac{2\pi}{a_2} = (2\pi/0.255) \text{ nm}^{-1} = \sqrt{2}\,b_1$$

c)

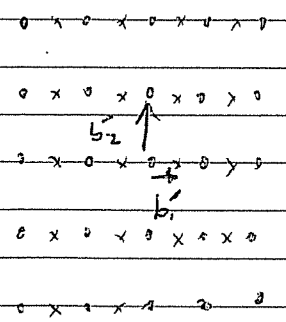


Missing row reconstruction

$a_1' = 2a_1 = 2(0.361\,\text{nm}) = 0.722\,\text{nm}$

$a_2' = a_2 = 0.255\,\text{nm}$

d)



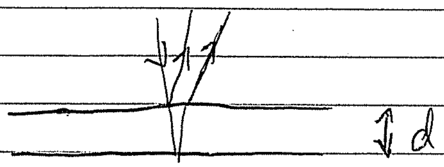
o = Spot exist w/ both bulk terminated and reconstructed surface

x = New spots from reconstruction

$b_1' = b_1/2 = \frac{2\pi}{2a_1} = \frac{2\pi}{a_1'} = (2\pi/0.722)\,\text{nm}^{-1}$

$b_2' = \frac{2\pi}{a_2'} = \frac{2\pi}{a_2} = (2\pi/0.255)\,\text{nm}^{-1}$

e) For free electron $k = \sqrt{\frac{2mE}{\hbar^2}} = 0.51\sqrt{E}$ where E is in eV and k in Å^{-1}



For constructive interference at normal incidence

want $2d = \lambda n \Rightarrow \lambda = \frac{2d}{n}$

for Cu(110), $d = 2.55\,\text{Å}$

or $k = \frac{2\pi}{\lambda} = \frac{\cancel{2}\pi n}{\cancel{2}d} = \frac{n\pi}{d}$

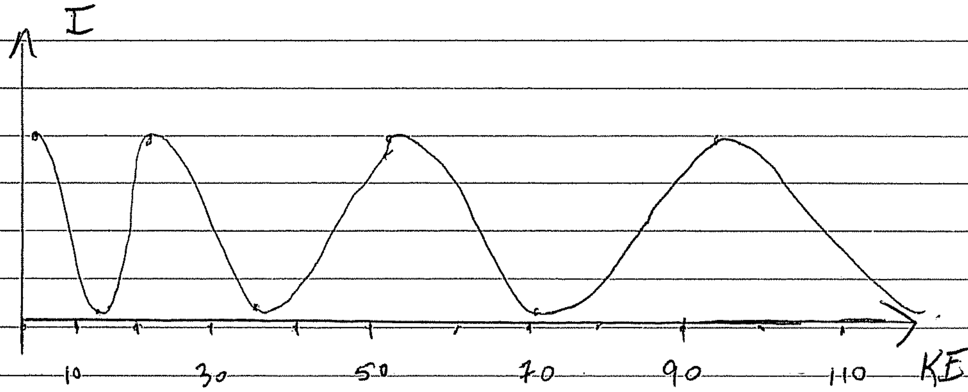
$\Rightarrow$ constructive interference when $E = \left(\frac{1}{0.51}\right)^2\left(\frac{\pi}{2.55}\right)^2 n^2$ eV

$E = (5.84\,\text{eV})\,n^2 \Rightarrow$

E (eV)	n
5.84	1
23.3	2
52.5	3
93.4	4

E (eV)	n
13.1	1
36.5	2
71.5	3
118.2	4

$\Rightarrow$ destructive interference: $k = \frac{2\pi}{\lambda} = \frac{(n+\frac{1}{2})\pi}{d} \Rightarrow E = \left(\frac{1}{0.51}\right)^2\left(\frac{\pi}{2.55}\right)^2(n+\tfrac{1}{2})^2$



Note how energy spacing between peaks is not uniform (obviously because $\lambda \propto E^{-1/2}$)

Also minima NOT midway between maxima (same reason)

3

$$\frac{E_1}{E_0} = \left[\frac{\left[M_2^2 - M_1^2 \sin^2\theta\right]^{1/2} + M_1\cos\theta}{M_1 + M_2}\right]^2$$

$M_W = 184$ $\quad M_{Re} = 186$ $\quad M_p = 1$ $\quad M_\alpha = 4$ $\quad$ Let $\theta = 135^\circ = \frac{3\pi}{4}$

a) $(W-p)$ $\quad \frac{E_1}{E_0} = \left[\frac{\left[(184)^2 - \sin^2\left(\frac{3\pi}{4}\right)\right]^{1/2} + \cos\left(\frac{3\pi}{4}\right)}{185}\right]^2 = 0.981615$

$(Re-p)$ $\quad \frac{E_1}{E_0} = 0.981811$ $\quad$ So with 1 MeV protons:

$E_{1\,(W-P)} = 981,615\ eV$ $\quad$ $E_{1\,(Re-P)} = 981811\ eV$ $\quad$ $\Delta E = 196\ eV$

b) $W-\alpha \Rightarrow E_1 = 928,454\ eV$; $Re-\alpha \Rightarrow E_1 = 929,195\ eV$ $\quad \Delta E = 741\ eV$

Big improvement using α rather than p

3 (c) Backscattering $\Theta = 180^\circ = \pi$

$(W\text{-}p) \Rightarrow E_1 = 978495\ eV$; $(Re\text{-}p) \Rightarrow E_1 = 978724\ eV \Rightarrow \Delta E = 229$

$(W\text{-}\alpha) \Rightarrow E_1 = 916704\ eV$; $(Re\text{-}\alpha) \Rightarrow E_1 = 917562\ eV \Rightarrow \Delta E = 850$

Clearly using α rather than p gives much larger mass separation than increasing backscattered angle from $135^\circ \to 180^\circ$

4) Conductance through apperture:

$$C_A = (11.5)(\pi D^2/4) = 226\ l/s$$

For Tube: $C_{Tube} = \sim 30\ l/s$ from chart

$$\frac{1}{C} = \frac{1}{C_A} + \frac{1}{C_T} = \frac{1}{226} + \frac{1}{30} = 0.0377 \Rightarrow C = 26.5\ l/s$$

$$\frac{1}{S} = \frac{1}{S_p} + \frac{1}{C} \Rightarrow S = C\left[\frac{1}{1 + C/S_p}\right] = 26.5\left[\frac{1}{1 + \frac{26.5}{60}}\right] = 18.4\ l/s$$

For Elbow: $C = (12.5)\left[\frac{D^3}{L_1 + L_2 + \alpha D}\right]$ $\quad \alpha = 1.33\,(\theta/180^\circ)$

here $\theta = 90^\circ \Rightarrow \alpha = 0.665$

$$C_{el} = (12.5)\left[\frac{125}{20+20+(0.665)(5)}\right] = (12.5)(2.89) = 36.1$$

$$\Rightarrow \frac{1}{C} = \frac{1}{C_A} + \frac{1}{C_E} = \frac{1}{226} + \frac{1}{36.1} = 0.0313 \Rightarrow C = 31.13\ l/s$$

$$\Rightarrow S = 31.1\left[\frac{1}{1 + \frac{31.1}{60}}\right] = 20.5\ l/s$$

the elbow wins!

5 (a) The Fowler-Nordheim equation may be written:

$$\frac{J}{V^2} = a \exp\left\{\frac{-b\phi^{3/2}}{cV}\right\}$$ so, plotting $\ln(J/V^2)$ vs $\frac{1}{V}$ gives a linear plot whose slope $\sim \phi^{\frac{3}{2}}$.

$$\Rightarrow \ln\left[\frac{J}{V^2}\right] = \text{const} + \left(\frac{b\,\phi^{3/2}}{c}\right)\left(\frac{1}{V}\right)$$

So, comparing different materials: $\left(\frac{\text{Slope } A}{\text{Slope } B}\right) = \left(\frac{\phi_A}{\phi_B}\right)^{3/2}$

or, taking W(110) as a reference:

$$\phi_{\text{material}} = \phi_{W(110)}\left(\frac{\text{Slope}_{\text{mystery}}}{\text{Slope}_{W(110)}}\right)^{2/3}$$

From diagram, $\text{Slope}_{W(110)} \cong \left[\frac{-18-(-14.5)}{3.5-2.6}\right] = \left[\frac{-3.5}{0.9}\right] = -3.89$

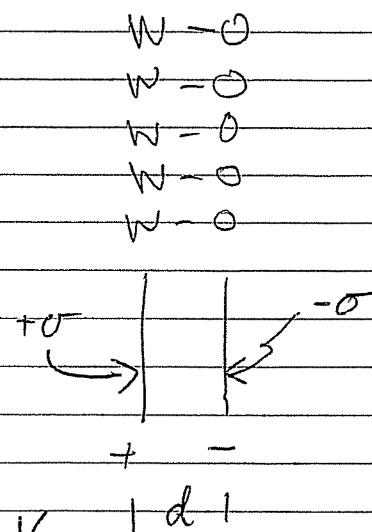
$$\text{Slope}_{\text{mystery}} \cong \left[\frac{-18-(-10)}{4-1.25}\right] = \left[\frac{-8}{2.75}\right] = -2.91$$

So $$\phi_m = (5.70)\left(\frac{-2.91}{-3.89}\right)^{2/3} = (5.70\text{ eV})(0.824) = 4.7\text{eV}$$

(b) So we see that the mystery material would be better than W(110), but worse than the (less stable) W(116) surface. It would be better to have an even lower work function for a field emitter tip

(c) Field emitter sources are preferable because the may be run at a relatively low temperature and thus have a smaller energy spread.

6 | Consider the oxygen–W charge exchange as creating a dipole layer (like a parallel plate capacitor). For a surface charge density σ, the electric field in the gap is $\frac{\sigma}{\epsilon_0}$, and the potential difference is $\frac{\sigma d}{\epsilon_0} = V$



Since W(100) is bcc, we have a square surface net ⇒ one W-O per unit cell. Unit cell area = $(3.17\,\text{Å})^2 = 10.05\,\text{Å}^2$

$$A = 1.005 \times 10^{-19}\ m^2$$

We have $V = 1.5\ V$ and $d = 1\,\text{Å}$, also $\epsilon_0 = 8.85 \times 10^{-12}\ C/V{\cdot}m$

So $\sigma = \frac{\epsilon_0 V}{d} = \frac{(8.85 \times 10^{-12}\ C/V.m)(1.5\ V)}{10^{-10}\ m} = 0.133\ C/m^2$

$= 8.3 \times 10^{17}\ e^-/m^2 \Rightarrow (8.3 \times 10^{17}\ e/m^2)(1 \times 10^{-19}\ m^2/cell)$

$= 8.3 \times 10^{-2}\ e^-/cell$ or approx $0.1\ e^-$ per W-O bond

7] a] For d_{z^2}, at $k=0$ the orbital phase indicates a bonding configuration while at $k=\frac{\pi}{a}$, neighbouring orbitals are antibonding. The strong overlap indicates a large energy difference between $k_{\parallel}=0$ and $k=\frac{\pi}{a}$ so there is a wide band. The d_{xz} + d_{yz} bands are non-bonding at $k=0$ but bonding at $k=\pi/a$, so they disperse downward with increasing k. The overlap is weaker so band width is narrower. These two bands are degenerate. The d_{xy} orbitals go from a weakly bonding to weakly nonbonding and thus disperse upward with increasing k.

b] The d_{xy} orbitals are oriented perpendicular to the dispersion direction and therefore have very little overlap in the dispersion direction. Hence, even as they change phase the overlap changes only slightly so the energy change is small.

c)

Dos: