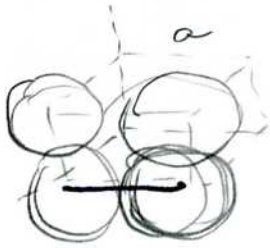


Answers To HW Set #1

1. a) primitive



$$V_{\text{cell}} = a^3$$

$$a = 2r$$

Each sphere lies at a cube corner + touches 8 cubes.

$$V_{\text{spheres}} = 8 \times \frac{1}{8} \left(\frac{4}{3} \pi r^3 \right)$$

$$V_s = \frac{4}{3} \pi \left(\frac{a}{2} \right)^3 = \frac{\pi}{6} a^3$$

$$V_s = 0.52 V_{\text{cell}}$$

b) bcc $\begin{matrix} 0 \cdot 0 \\ 0 \cdot 0 \end{matrix}$ (face)

center sphere lies totally within cube, while spheres on face touch 8 cubes.

major diagonal $4r = \sqrt{3} a$

$$V_{\text{cell}} = a^3 \quad r = \frac{\sqrt{3} a}{4}$$

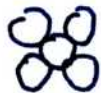
$$V_s = \frac{4}{3} \pi r^3 + \frac{8}{8} \left(\frac{4}{3} \pi r^3 \right)$$

$$= \frac{8}{3} \pi \left\{ \frac{\sqrt{3}}{4} \right\}^3 V_{\text{cell}}$$

$$= \frac{\sqrt{3}}{8} \pi V_{\text{cell}} = 0.68 V_{\text{cell}}$$

c) fcc

$$V_{\text{cell}} = a^3$$



(face)

6 faces. Center atom touches 2 cubes.

$$4r = \sqrt{2} a$$

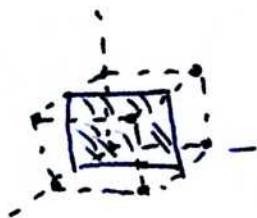
$$r = \frac{\sqrt{2} a}{4}$$

$$V_s = 6 \times \frac{1}{2} \left(\frac{4}{3} \pi r^3 \right) + \frac{8}{8} \left(\frac{4}{3} \pi r^3 \right)$$

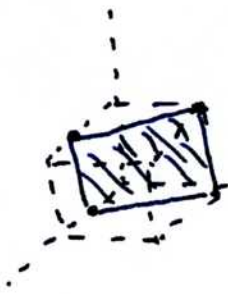
$$V_s = 4 \left(\frac{4}{3} \pi r^3 \right) = 4 \cdot \frac{4}{3} \cdot \frac{2\sqrt{2} \pi a^3}{64}$$

$$V_s = \frac{\pi \sqrt{2}}{6} V_{\text{cell}} = 0.74 V_{\text{cell}}$$

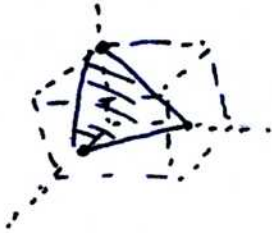
2. simple cubic:



(200) Intercepts: $\frac{1}{2} \infty \infty$

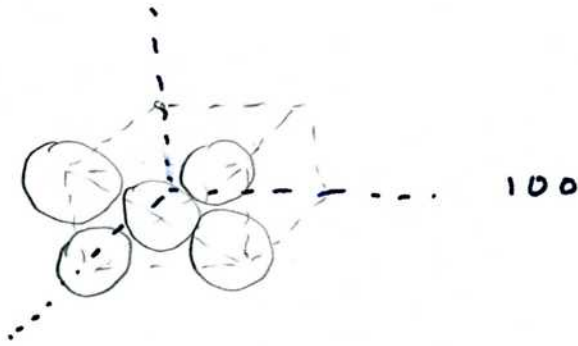


(210) Intercepts = $\frac{1}{2}, 1, \infty$

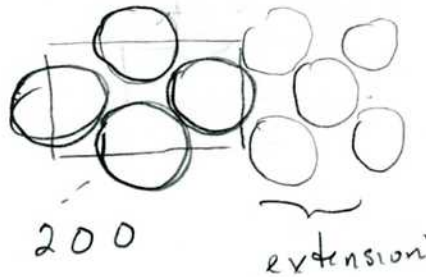
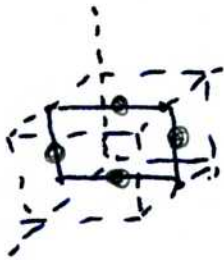


(221) Intercepts = $\frac{1}{2}, \frac{1}{2}, 1$

Face-centered cubic:



100

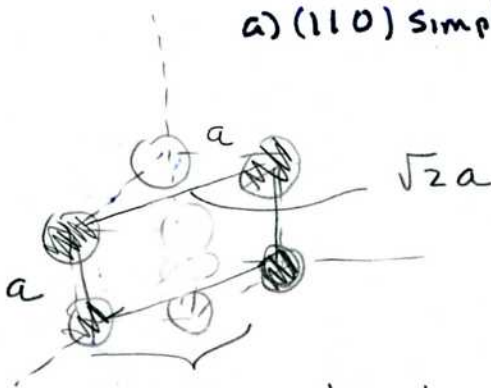


same as 100

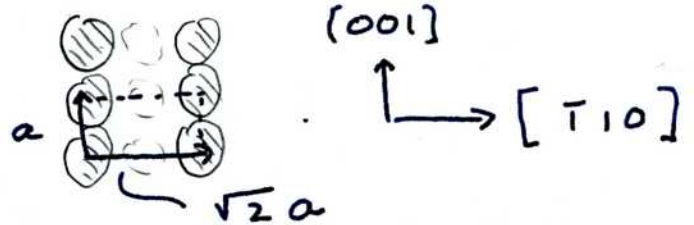
\therefore Label both planes 200

3.

a) (110) simple cubic

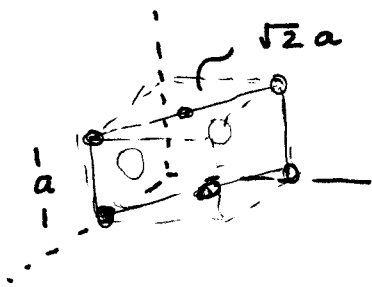


spheres touch vertically
 $2r = a$



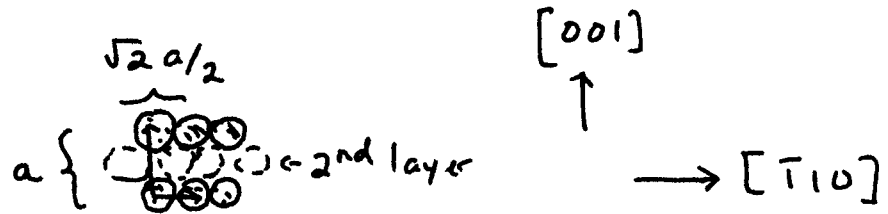
$\sqrt{2} a \times a$ OR $2\sqrt{2} r \times 2r$
2nd row only partially visible

b) (110) fcc



Face diagonal $\odot\odot\odot$
 $4r = \sqrt{2}a$

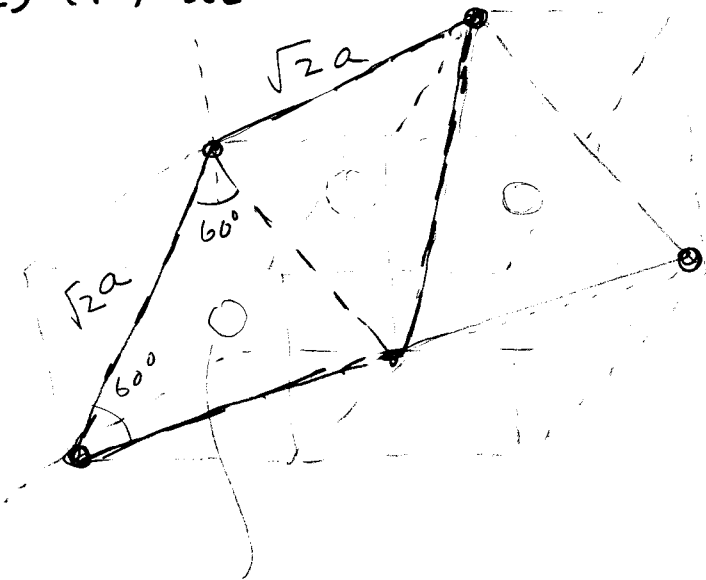
• touch each other



$\frac{\sqrt{2}a}{2} \times a$ OR $2r \times \frac{4r}{\sqrt{2}}$

OR $2r \times 2.83r$

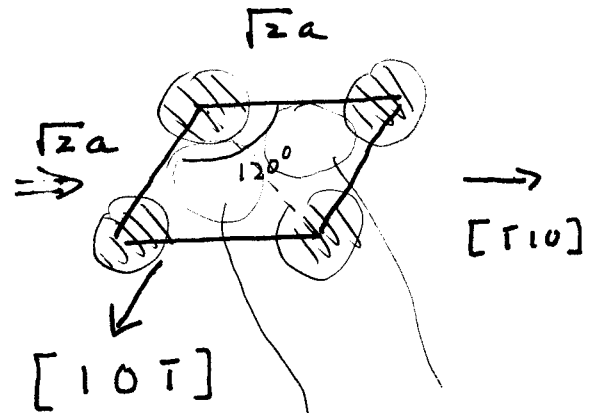
c) (111) bcc



central spheres

$4r = \sqrt{3}a$

$a = 4r/\sqrt{3}$



2nd 3rd layer?
 (central spheres)

$\sqrt{2}a \times \sqrt{2}a$

$4r\sqrt{2/3} \times 4r\sqrt{2/3}$

OR $3.27r \times 3.27r$

4. $s = e^{-E_s/kT}$

$T = 300K$

$E_s = 0.12V \Rightarrow s = 2.09 \times 10^{-2}$
 ($k_B = 8.62 \times 10^{-5} eV$)

\therefore Extra time needed = $\frac{time(100\% sticking)}{s} = 47.85 \times time(100\% sticking)$

From class notes:

$$t' = 47.85 t = 47.85 \frac{Ns}{I} \quad N_s \sim 10^{15} \text{ cm}^{-2}$$

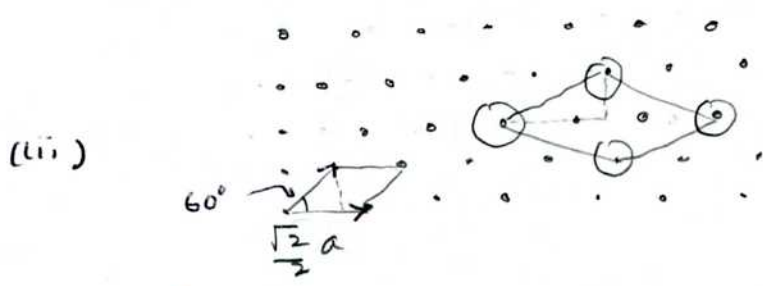
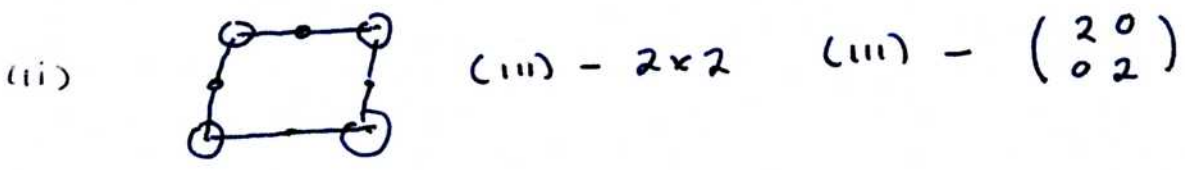
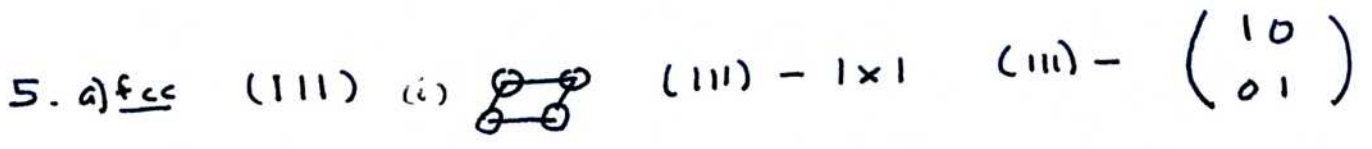
$$I = \frac{P}{\sqrt{2\pi m k T}} \quad m = \frac{10 \text{ amu}}{N_A} \quad k = 1.38066 \times 10^{-16} \text{ erg/K}$$

$$N_A = 6.022 \times 10^{23} \text{ amu/gm}$$

$$P = 1 \text{ atm} = 1.013250 \times 10^6 \text{ dyne/cm}^2$$

$$I = 4.87 \times 10^{23} \text{ molecules/cm}^2 \text{ s}$$

$$t' = 9.8 \times 10^{-8} \text{ s} \quad \text{still fast despite barrier.}$$



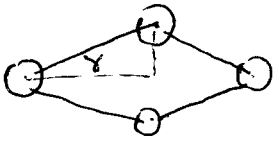
$$\frac{\sqrt{2}}{2} a \sin 60^\circ = \frac{\sqrt{2}}{2} \frac{\sqrt{3}}{2} a$$

$$\text{hypotenuse}^2 = \left(\frac{9 \times 2}{16} + \frac{2 \times 3}{16} \right) a^2$$

$$= \frac{24}{16} a^2 = \frac{3}{2} a^2$$

$$\text{hyp} = \sqrt{3/2} a = \sqrt{3} \frac{a}{\sqrt{2}} = (\sqrt{3}) \left(\frac{\sqrt{2}}{2} a \right)$$

$\therefore \sqrt{3} \times \sqrt{3}$ Now "rotation:"



$$\gamma = \tan^{-1} \frac{\sqrt{6}/4}{3\sqrt{2}/4} = 30^\circ \quad 2\gamma = 60^\circ, \text{ preserved}$$

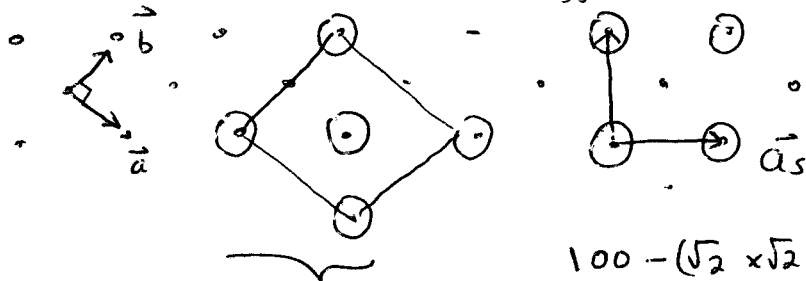
Wood's: (111) - ($\sqrt{3} \times \sqrt{3}$) - $R 30^\circ$

$$\vec{a}_s = \frac{3}{2} \vec{a} - \vec{b} \sin 60^\circ$$

$$\vec{b}_s = \frac{3}{2} \vec{a} + \vec{b} \sin 60^\circ$$

$$G = \begin{pmatrix} 3/2 & -\sqrt{3}/2 \\ 3/2 & \sqrt{3}/2 \end{pmatrix}$$

b) (i) fcc (100)



$$|\vec{a}| = |\vec{b}| = \frac{\sqrt{2}}{2} a$$

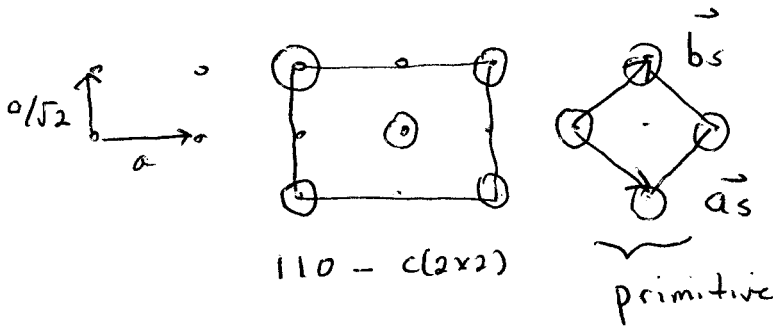
100 - c(2x2)

100 - ($\sqrt{2} \times \sqrt{2}$) - $R 45^\circ$

For primitive cell $\vec{a}_s = \vec{a} + \vec{b}$ $\vec{b}_s = -\vec{a} + \vec{b}$

$$\Rightarrow G = \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \Rightarrow 100 - \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$$

(ii) fcc (110)



110 - c(2x2)

primitive

Matrix Notation For Primitive:

$$\vec{a}_s = \vec{a} - \vec{b} \quad \vec{b}_s = \vec{a} + \vec{b}$$

$$G = \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}$$

c) (i) fcc (100) 100 - (2x2) $G = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$

(ii) fcc (110) 110 - (1x2) $G = \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}$

6. Fermi Temperature $T_F = E_F/k_B$ $k_B = 8.617 \times 10^{-5} \text{ eV/K}$

$$E_F = \frac{\hbar^2}{2m_e} \left(3\pi^2 \rho_{elec} \right)^{2/3} \left(\frac{2m_e E_F}{\hbar^2} \right)^{3/2} = 3\pi^2 \rho$$

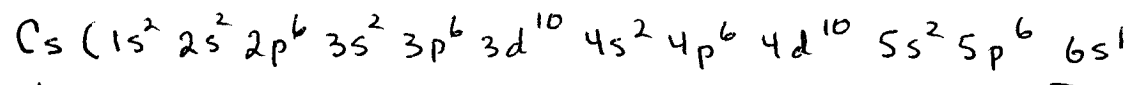
$$\rho_{elec} = \frac{1}{3\pi^2} \left(\frac{2m_e E_F}{\hbar^2} \right)^{3/2}$$

$1 \text{ eV} = 1.602 \times 10^{-12} \text{ erg}$
 $\hbar = 1.0545 \times 10^{-27} \text{ erg-s}$
 $m_e = 9.11 \times 10^{-28} \text{ gm}$
 $1 \text{ \AA} = 10^{-8} \text{ cm}$

$$\frac{\mu(T)}{E_F} = 1 - \frac{\pi^2}{12} \left(\frac{T}{T_F} \right)^2$$

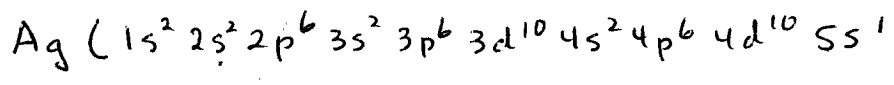
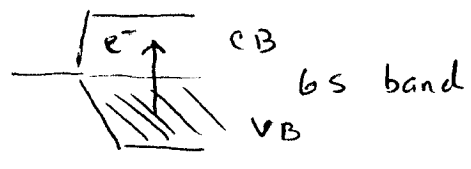
$$\mu(T) - E_F = - E_F \frac{\pi^2}{12} \left(\frac{T}{T_F} \right)^2$$

Species	E_F (eV)	T_F (K)	ρ_{elec} (\AA^{-3})	T_{mp} (K)	$\mu(T_{mp}) - E_F$ (eV)
Cs	1.59	18,450	9.11×10^{-3}	301.4	-3.49×10^{-4}
Ag	5.49	63,700	5.84×10^{-2}	1235	-1.70×10^{-3}
Al	11.7	135,780	0.182	933	-4.54×10^{-4}

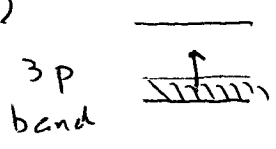
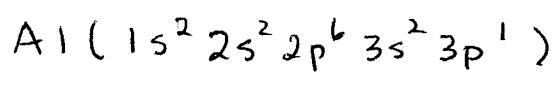
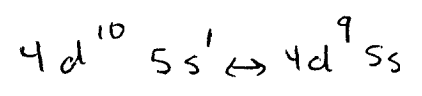
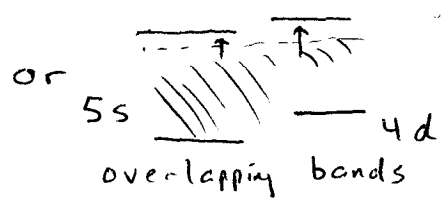
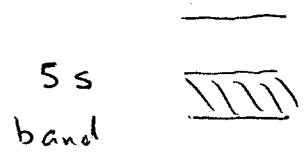


alkali metal

half-filled valence band



noble metal



7. A standard metal has a high delocalized electron density at its surface. Whether or not the electron density can be used in bonding to adsorbates depends upon whether the valence bands are full or partially empty; and whether they are of s character or d character.

Si, in its reconstructed state, has 2 dangling bonds per atom, which can be used to form bonds, such as is the case with H atoms.

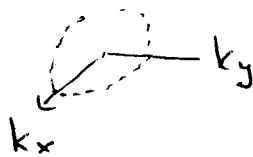
$$8. E_{n_x, n_y} = \frac{\pi^2 \hbar^2}{2mL^2} (n_x^2 + n_y^2) = \frac{\hbar^2}{2} (k_x^2 + k_y^2) = \frac{\hbar^2 k^2}{2}$$

$$k_x = \frac{n_x \pi}{L} \quad k_y = \frac{n_y \pi}{L}$$

$$k^2 = k_x^2 + k_y^2$$

$$A = L^2$$

$$\text{No. States} = 2 \cdot \frac{\pi k_{\max}^2}{(2\pi/L)^2} \quad (0 - E_{\max})$$



$$\text{No. States} = \frac{1}{2\pi} A k_{\max}^2 \quad (0 - E_{\max})$$

$$E_{\max} = \hbar^2 k_{\max}^2 / 2m_e$$

$$k_{\max}^2 = 2m_e E_{\max} / \hbar^2$$

$$\text{No. States} = \frac{A}{2\pi} \frac{2m_e E_{\max}}{\hbar^2} = N_{\text{elec}} \text{ if } E_{\max} = E_F$$

$$N_{\text{elec}} = \frac{A}{\pi \hbar^2} m_e E_F \Rightarrow$$

$$E_F = \frac{\pi \hbar^2}{m_e} \underbrace{\frac{N_e}{A}}_{\rho_s}$$

$$E_F = \frac{\pi \hbar^2}{m_e} \rho_s$$

ρ_s surface density

$$9. \quad q = \sum_{i=0}^{\infty} e^{-E_i/k_B T} \quad E_i = \hbar\omega(i + 1/2) \quad \text{mode}$$

$$q = e^{-\hbar\omega/2k_B T} \underbrace{\sum_{i=0}^{\infty} e^{-i\hbar\omega/k_B T}}_{\text{geometric series}} = e^{-\hbar\omega/2k_B T} \frac{1}{1 - e^{-\hbar\omega/k_B T}}$$

geometric series

$$1 + x + x^2 + \dots = \frac{1}{1-x} \quad x = e^{-\hbar\omega/k_B T}$$

$$\ln q = -\frac{\hbar\omega}{2k_B T} - \ln [1 - e^{-\hbar\omega/k_B T}]$$

$$\frac{\partial \ln q}{\partial T} = \frac{\hbar\omega}{2k_B T^2} + \frac{\hbar\omega/k_B T^2 e^{-\hbar\omega/k_B T}}{1 - e^{-\hbar\omega/k_B T}}$$

$$\langle E \rangle_{\text{mode}} = k_B T^2 \frac{\partial \ln q}{\partial T} = \frac{\hbar\omega}{2} + \frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1}$$