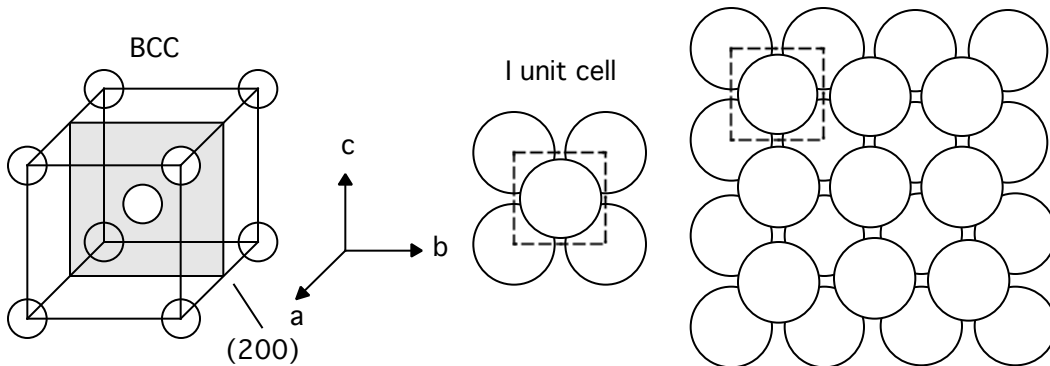


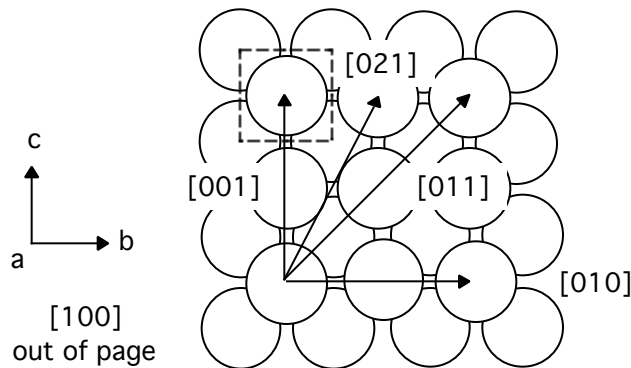
CEM 924 (Spring 2001) - Problem Set #2 (KEY)

- (1) (a) (5 points) Sketch the (tungsten) W(200) surface (as viewed from along the surface normal).

W is BCC. Note that the atoms do not "touch" in this plane!



- (b) (5 points) On your sketch of the surface, label the [100], [010], [001], [011] and [021] directions.

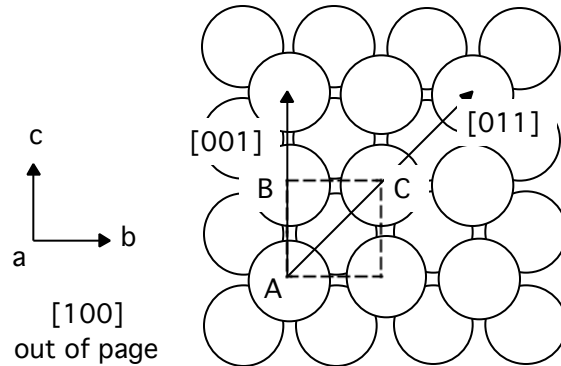


- (c) (5 points) Calculate the absolute surface coverage (in atoms·cm⁻²) for the W(200) surface if the dimension of the tungsten *bulk* unit cell, $a_0 = 3.16 \text{ \AA}$.

Referring to the figure in part (a) above, the separation between atoms in the [001] and [010] directions = a_0 . Therefore, the surface coverage is

$$\begin{aligned} \text{absolute} &= \frac{1}{3.16 \times 10^{-8} \text{ cm}}^2 \\ &= 1.00 \times 10^{15} \text{ cm}^{-2} \end{aligned}$$

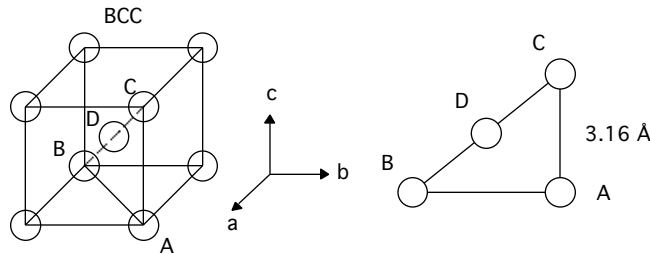
(d) (5 points) What is the distance between the centers of two adjacent W atoms in the [001] and [011] directions?



$$AB = a_0 = 3.16 \text{ \AA}$$

$$AC = \sqrt{2} a_0 = 4.47 \text{ \AA}$$

(e) (5 points) What is the nearest neighbor distance for (*surface* or *bulk*) W?



The nearest neighbor distance for a BCC crystal is actually along the body diagonal (BD or CD).

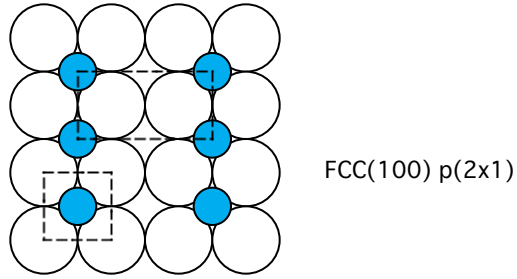
$$AB = \sqrt{2} 3.16 \text{ \AA} = 4.47 \text{ \AA}$$

$$BC = \sqrt{AC^2 + AB^2} = \sqrt{(9.99 + 19.97)} = 5.47 \text{ \AA}$$

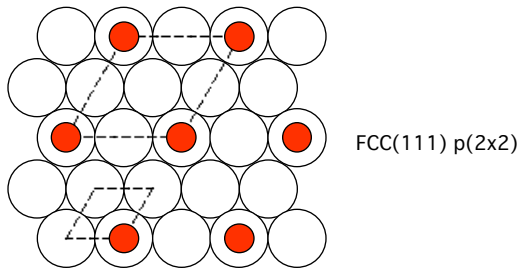
$$BD = BC / 2 = 2.74 \text{ \AA}$$

(2) Sketch the following surface adsorbate structures:

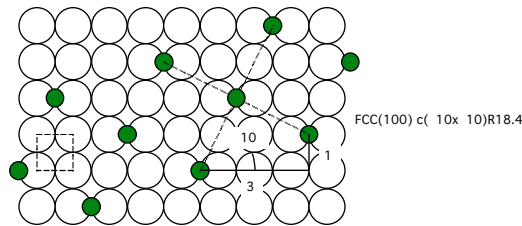
(a) (5 points) FCC(100) p(2x1) - O with O atoms adsorbed in 4-fold hollow sites.



(b) (5 points) FCC(111) p(2x2) - S with S atoms adsorbed in on-top sites.



(c) (5 points) FCC(100) $c(\sqrt{10} \times \sqrt{10})R18.4$ -N with N atoms adsorbed in 2-fold bridge sites.

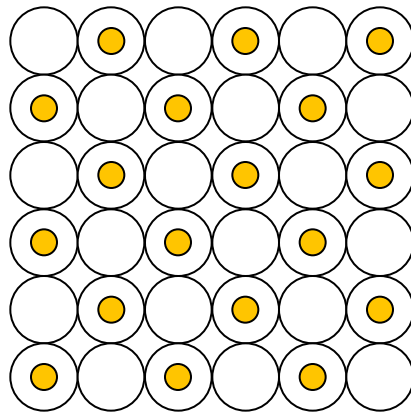


(d) (5 points) Calculate the fractional coverage (adsorbate atoms per surface primitive unit cell) for the structure given in part (c)

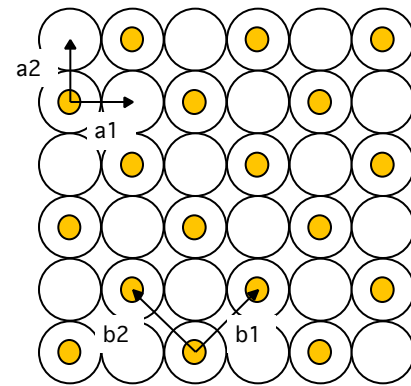
In a single adsorbate mesh there are a total of 2 atoms. The number of surface primitive cells (atoms) in this area is $\sqrt{10} \times \sqrt{10} = 10$. Therefore, coverage is

$$\begin{aligned} \text{frac} &= \frac{\# \text{ adsorbate atoms}}{\# \text{ surface primitive unit cell}} \\ &= \frac{2}{10} \\ &= 0.2 \end{aligned}$$

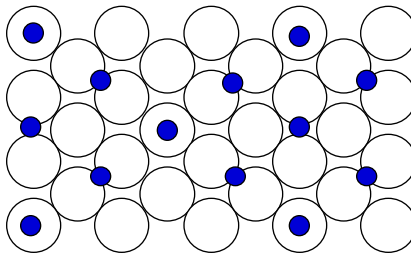
(3) Give the matrix notation for the following adsorbate structures: (Hint: There are several acceptable answers for (c)!)



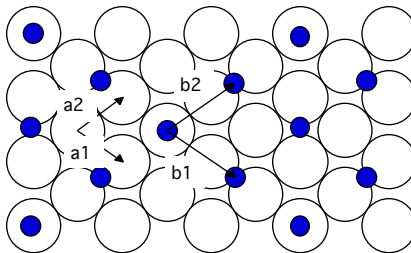
(a) (5 points)



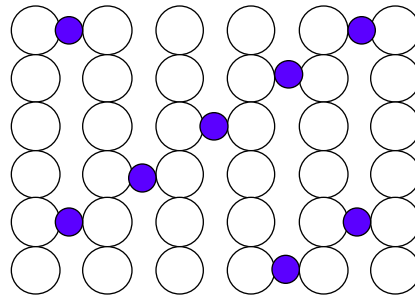
$$\text{FCC}(100) = \begin{pmatrix} 1 & 1 \\ \bar{1} & 1 \end{pmatrix}$$



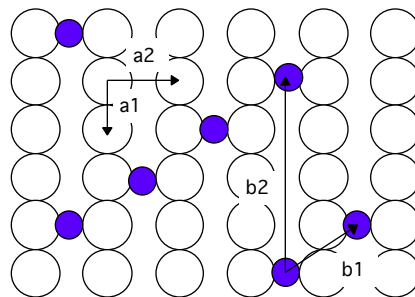
(b) (5 points)



$$\text{BCC}(110) - \begin{matrix} 3/2 & 0 \\ 0 & 3/2 \end{matrix}$$



(c) (5 points)



$$\text{FCC}(110) - \begin{matrix} \bar{1} & 1 \\ 4 & 0 \end{matrix} \quad \text{or} \quad \begin{matrix} \bar{1} & 1 \\ 3 & 1 \end{matrix} \quad \text{or} \quad \begin{matrix} \bar{1} & 1 \\ 2 & 2 \end{matrix}$$

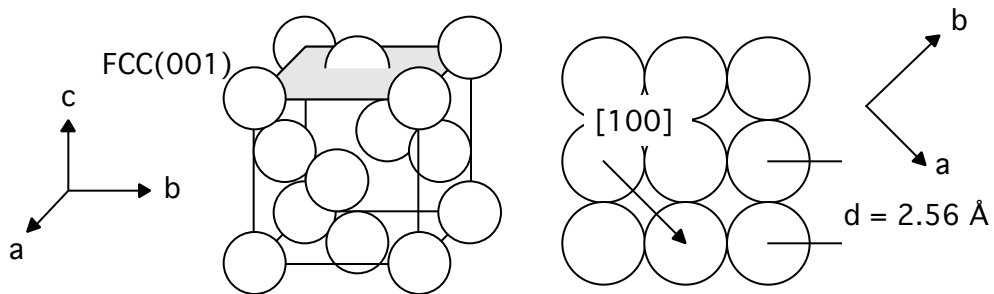
Note that for a structure that has a variety of binding sites (for example, half on-top, half bridge sites) the elements in the matrix can take fractional values.

- (4) (a) (15 points) In a LEED experiment, a 50 eV beam of electrons directed along the surface normal strikes a Cu(001) surface. Copper is a FCC metal with nearest-neighbor distance of 2.56 Å. By drawing an Ewald sphere diagram for surface diffraction, calculate the diffraction angle for the [10] back-scattered (diffracted) beam along the [100] direction.

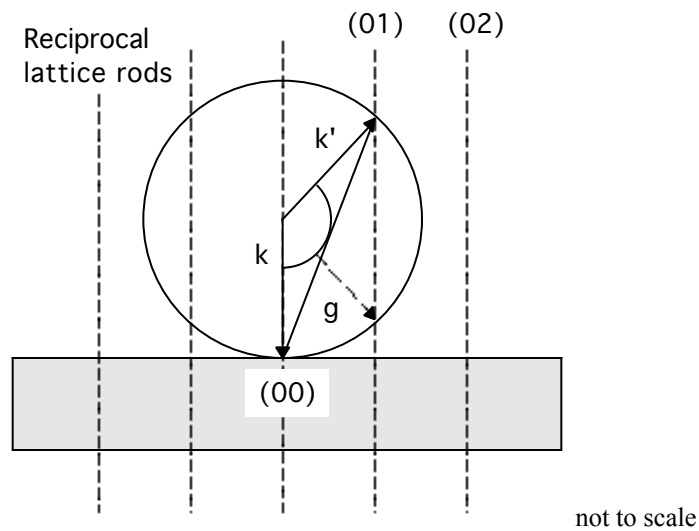
First calculate the wavevector \mathbf{k} , for the incident electrons from the de Broglie relation

$$\begin{aligned}
 &= \frac{h}{p} \quad \text{de Broglie wavelength} \\
 p &= m v = \sqrt{2meV} = 3.82 \times 10^{-24} \text{ kg m s}^{-1} \\
 &= \frac{6.63 \times 10^{-34} \text{ J s}}{3.82 \times 10^{-24} \text{ kg m s}^{-1}} \quad (\text{J} = \text{kg s}^{-2} \text{ m}^2) \\
 &= 1.73 \times 10^{-10} \text{ m} = 1.73 \text{ \AA} \\
 \bar{k} &= \frac{2}{d} = 3.63 \text{ \AA}^{-1}
 \end{aligned}$$

Next calculate the spacing of the reciprocal lattice rods in the [100] direction for a Cu(001) surface



So the reciprocal lattice rods are spaced $2/d = 1.74 \text{ \AA}^{-1}$. Now we can draw the Ewald sphere

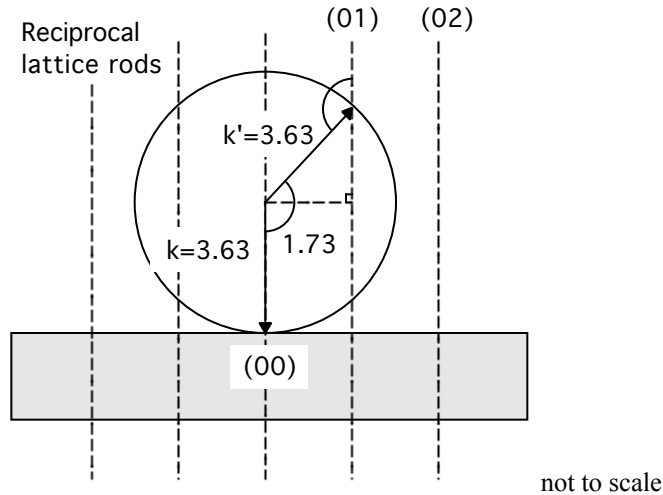


$$d \sin \theta = \sqrt{h^2 + k^2}$$

$$= \sin^{-1} \left(\frac{1.73 \text{ \AA}}{3.62 \text{ \AA}} \right) = 28.5^\circ$$

$$\text{or } = (180^\circ - 28.5^\circ) = 151.5^\circ$$

Note that the diffraction angle can also be calculated by geometry



$$\sin \theta = \frac{1.73 \text{ \AA}^{-1}}{3.63 \text{ \AA}^{-1}} = 0.477$$

$$= 28.5^\circ \text{ (forward -scattered) or } 151.5^\circ \text{ (back -scattered)}$$

(b) (10 points) At what incident beam energy is the back-scattered (02) beam (just) diffracted?

According to the expression for diffraction

$$d \sin \theta = \sqrt{h^2 + k^2}$$

$$= \sin^{-1} \left(\sqrt{h^2 + k^2} \frac{1}{d} \right)$$

there can be no solution for $h = 0$ and $k = 2$ when the $(\sqrt{h^2 + k^2} / d)$ term exceeds 0.5.

Otherwise, we attempt to find the arcsin of a number greater than 1! Hence, the value for $(\sqrt{h^2 + k^2} / d)$ that (just) gives us a value of 0.5 is when $d = 1.81 \text{ \AA}$. This corresponds to a beam energy of

$$\begin{aligned}
&= \frac{h}{p} \\
&= \frac{h}{\sqrt{2 m e V}} \\
V &= \frac{h^2}{2 m e} \\
&= \frac{6.62 \times 10^{-34} \text{ J s}}{1.81 \times 10^{-10} \text{ m}}^2 \frac{1}{2 \cdot 9.11 \times 10^{-31} \text{ kg} \cdot 1.602 \times 10^{-19} \text{ C}} \\
&= 45.8
\end{aligned}$$

The (02) beam just becomes diffracted using a beam energy of 45.8 eV. At lower beam energies, only the (01) beam(s) will be visible.

Total 85 points