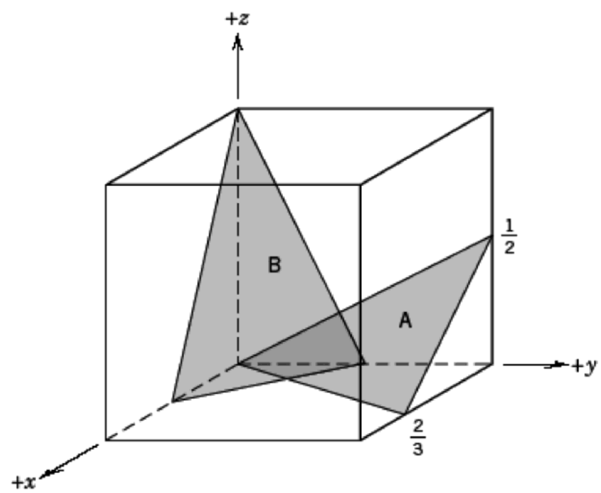
QUESTION 01

a) Sketch a tetragonal unit cell, and within that cell indicate locations of the $\frac{1}{2}\,1\,\frac{1}{2}$ and $\frac{1}{4}\,\frac{1}{2}\,\frac{3}{4}$ point coordinates.

b) Within a cubic unit cell, sketch the following directions:

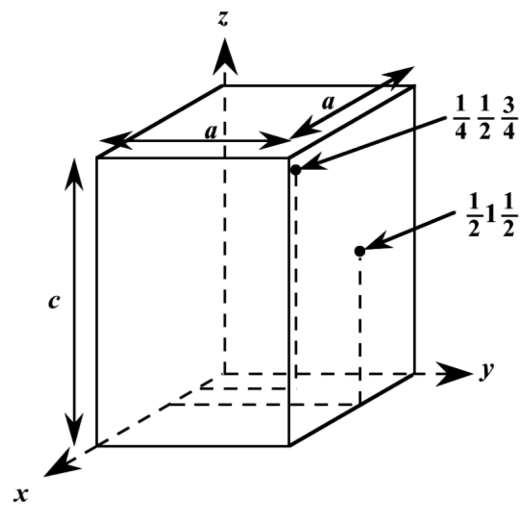
$[\bar{1}10]$, $[\bar{1}\bar{2}1]$, $[0\bar{1}2]$

c) Determine the Miller indices for the planes shown in the following unit cell:

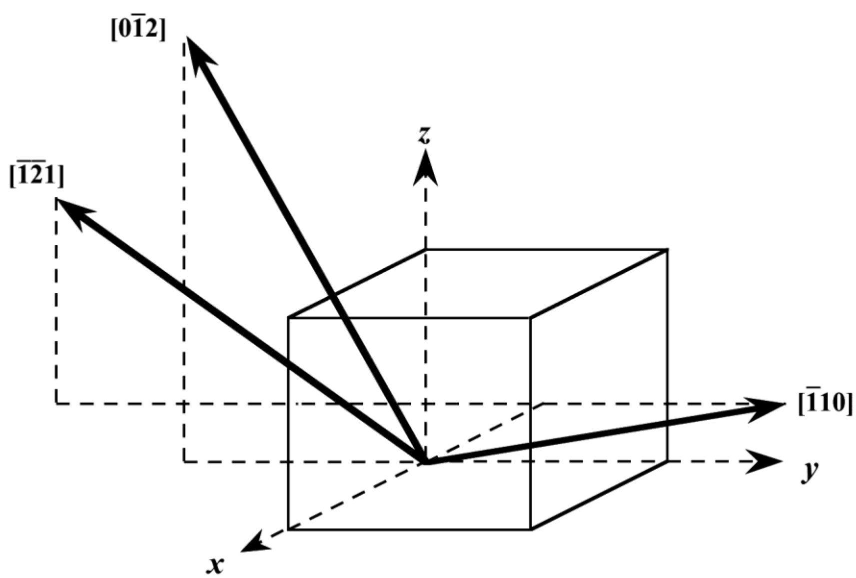


SOLUTION:

a) A tetragonal unit in which are shown the $\frac{1}{2}1\frac{1}{2}$ and $\frac{1}{4}\frac{1}{2}\frac{3}{4}$ point coordinates is presented below.



b) The directions asked for are indicated in the cubic unit cells shown below.



c) For plane A since the plane passes through the origin of the coordinate system as shown, we will move the origin of the coordinate system one unit cell distance to the right along the *y* axis; thus, this is a $(3\bar{2}4)$ plane, as summarized below.

	x	y	z
Intercepts	$\frac{2a}{3}$	$-b$	$\frac{c}{2}$
Intercepts in terms of *a*, *b*, and *c*	$\frac{2}{3}$	-1	$\frac{1}{2}$

Reciprocals of intercepts	$\frac{3}{2}$	– 1	2
Reduction	3	– 2	4
Enclosure		$(3\bar{2}4)$	

For plane B we will leave the origin at the unit cell as shown; this is a (221) plane, as summarized below.

	x	y	z
Intercepts	$\frac{a}{2}$	$\frac{b}{2}$	c
Intercepts in terms of *a*, *b*, and *c*	$\frac{1}{2}$	$\frac{1}{2}$	1
Reciprocals of intercepts	2	2	1
Reduction	not necessary		
Enclosure	(221)		

QUESTION 02

Calculate the radius of a vanadium atom, given that V has a BCC crystal structure, a density of 5.96 g/cm^3, and an atomic weight of 50.9 g/mol.

SOLUTION:

This problem asks for us to calculate the radius of a vanadium atom. For BCC, n = 2 atoms/unit cell, and

$$V_C = \left(\frac{4R}{\sqrt{3}}\right)^3 = \frac{64R^3}{3\sqrt{3}}$$

Since, from Equation of the density.

$$\rho = \frac{nA_V}{V_C N_A} = \frac{nA_V}{\left(\frac{64R^3}{3\sqrt{3}}\right)N_A}$$

And solving for R the previous equation

$$R = \left(\frac{3\sqrt{3}nA_V}{64\rho N_A}\right)^{1/3}$$

and incorporating values of parameters given in the problem statement

$$R = \left[\frac{(3\sqrt{3})(2 \text{ atoms/unit cell})(50.9 \text{ g/mol})}{(64)(5.96 \text{ g/cm}^3)(6.022 \times 10^{23} \text{ atoms/mol})}\right]^{1/3}$$
$$= 1.32 \times 10^{-8} \text{ cm} = 0.132 \text{ nm}$$

QUESTION 03

Determine the expected diffraction angle for the first-order reflection from the (113) set of planes for FCC platinum when monochromatic radiation of wavelength 0.1542 nm is used. R (0.1387 nm)

SOLUTION:

We first calculate the lattice parameter

$$a = 2R\sqrt{2} = (2)(0.1387 \text{ nm})(\sqrt{2}) = 0.3923 \text{ nm}$$

Next, determinate the interplanar spacing for the (113) set of planes

$$d_{113} = \frac{a}{\sqrt{(1)^2 + (1)^2 + (3)^2}} = \frac{0.3923 \text{ nm}}{\sqrt{11}} = 0.1183 \text{ nm}$$

And finally, employment of Equation 3.13 yields the diffraction angle as

$$\sin\theta = \frac{n\lambda}{2d_{113}} = \frac{(1)(0.1542\ \text{nm})}{(2)(0.1183\ \text{nm})} = 0.652$$

Which leads to

$$\theta = \sin^{-1}(0.652) = 40.69°$$

And, finally

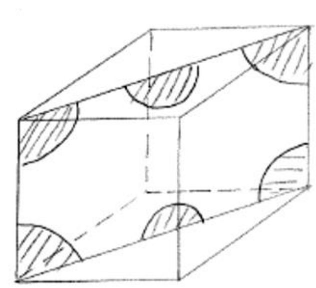
$$2\theta = (2)(40.69°) = 81.38°$$

QUESTION 04

a) Calculate the planar atomic density in atoms per square millimeter for (110) crystal plane in FCC gold, which has the atomic radius of 0.1442 nm.

b) Calculate the linear atomic density in atoms per millimeter for [111] in BCC vanadium, which has an atomic radius of 0.1316 nm.

SOLUTION



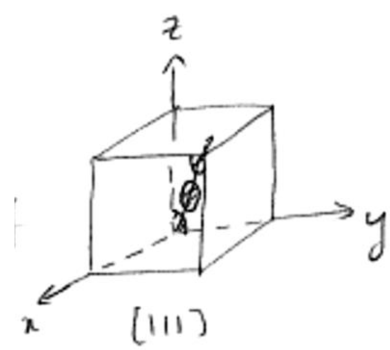
Equation (3.10), planar density: $\rho_p = \frac{number\ of\ atoms\ centered\ on\ a\ plane}{area\ of\ plane}$

a) For FCC unit cell, a_o=4r/$\sqrt{2}$
   4×0.1442=$\sqrt{2}a$ → a= 0.4078 nm
   No of atoms in the plane: 4 corners ×1/4 atom per corner + ½ atoms×2 (in mid position) = 2 atoms

   The area of the plane is ($\sqrt{2}$ a)(a) = $\sqrt{2}$ a^2

$$\rho_p = \frac{2}{\sqrt{2(0.40788 \times 10^{-9})^2}} = 8.5 \times 10^{12}\ atom/mm^2$$

b) Equation (3.8), planar density:



$$\rho_p = \frac{number\ of\ atoms\ centered\ on\ direction\ vector}{length\ of\ direction\ vector}$$

For BCC unit cell, $a_o=4r/\sqrt{3}$

$4\times 0.13162=\sqrt{3}a \rightarrow$ a= 0.3039 nm

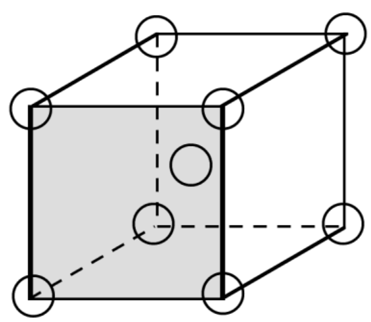
For the [111] direction

$$\rho_l = \frac{2}{\sqrt{3}a} = 3.799 \times 10^6\ atom/mm$$

QUESTION 05

a) Derive planar density expressions for BCC (100) and (110) planes in terms of the atomic radius
b) For a BCC single crystal, would you expect the surface energy for a (100) plane to be greater or less than that for a (110) plane? Why?

Solution:

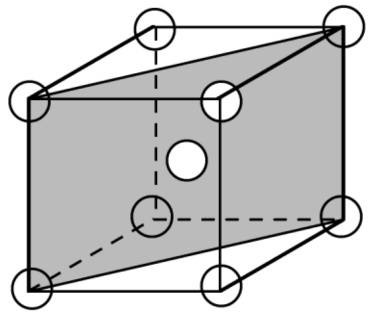


For this (100) plane there is one atom at each of the four cube corners, each of which is shared with four adjacent unit cells. Thus, there is the equivalence of 1 atom associated with this BCC (100) plane. The planar section represented in the above figure is a square, wherein the side lengths are equal to the unit cell edge length, $\frac{4R}{\sqrt{3}}$;

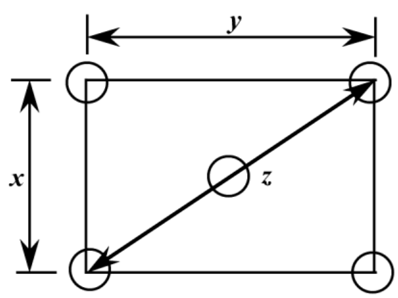
Area of this square is just $\left(\frac{4R}{\sqrt{3}}\right)^2 = \frac{16R^2}{3}$. Hence, the planar density for this (100) plane is just

$$PD_{100} = \frac{\text{number of atoms centered on (100) plane}}{\text{area of (100) plane}}$$

$$= \frac{1 \text{ atom}}{\frac{16\ R^2}{3}} = \frac{3}{16\ R^2}$$



For this (110) plane there is one atom at each of the four cube corners through which it passes, each of which is shared with four adjacent unit cells, while the center atom lies entirely within the unit cell. Thus, there is the equivalence of 2 atoms associated with this BCC (110) plane. The planar section represented in the above figure is a rectangle, as noted in the figure below.



From this figure, the area of the rectangle is the product of *x* and *y*. The length *x* is just the unit cell edge length, which for BCC (Equation 3.3) is $\frac{4R}{\sqrt{3}}$. Now, the diagonal length *z* is equal to 4*R*. For the triangle bounded by the lengths *x*, *y*, and *z*

$$y = \sqrt{z^2 - x^2}$$

Or

$$y = \sqrt{(4R)^2 - \left(\frac{4R}{\sqrt{3}}\right)^2} = \frac{4R\sqrt{2}}{\sqrt{3}}$$

Thus, in terms of *R*, the area of this (110) plane is just

$$\text{Area (110)} = xy = \left(\frac{4R}{\sqrt{3}}\right)\left(\frac{4R\sqrt{2}}{\sqrt{3}}\right) = \frac{16R^2\sqrt{2}}{3}$$

And, finally, the planar density for this (110) plane is just

$$\text{PD}_{110} = \frac{\text{number of atoms centered on (110) plane}}{\text{area of (110) plane}}$$

$$= \frac{2 \text{ atoms}}{\frac{16R^2\sqrt{2}}{3}} = \frac{3}{8R^2\sqrt{2}}$$

The surface energy for a crystallographic plane will depend on its packing density [i.e., the planar density (Section 3.11)]—that is, the higher the packing density, the greater the number of nearest-neighbor atoms, and the more atomic bonds in that plane that are satisfied, and, consequently, the lower the surface energy. From the solution to a), the planar densities for BCC (100) and (110) are $\frac{3}{16R^2}$ and $\frac{3}{8R^2\sqrt{2}}$, respectively—that is $\frac{0.19}{R^2}$ and $\frac{0.27}{R^2}$. Thus, since the planar density for (110) is greater, it will have the lower surface energy.