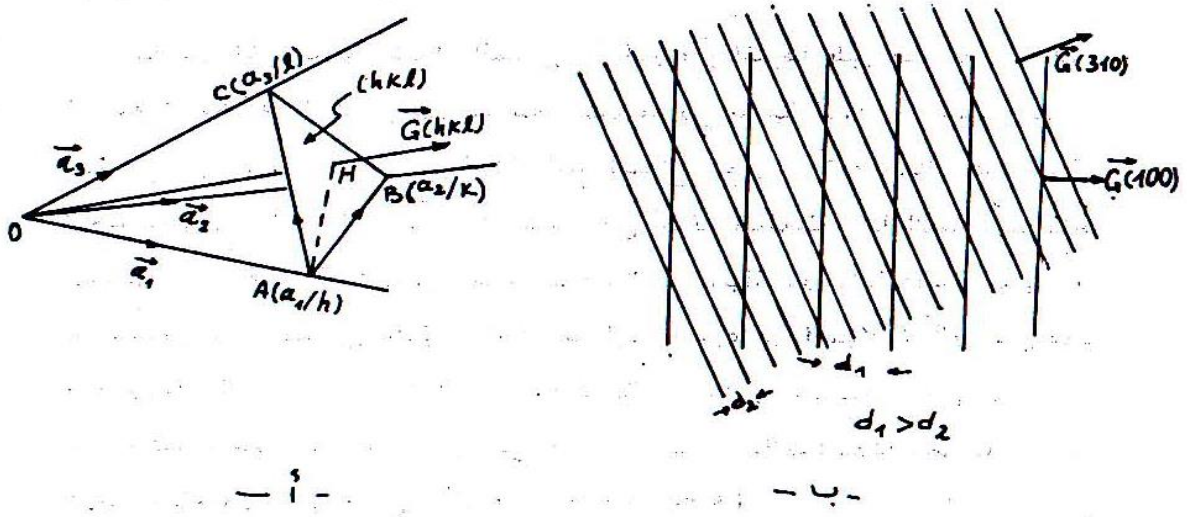
التمرين الأول:

برهن أن شعاع الشبكة المعكوسة $\mathbf{G}_{hkl}$ عمودي على المستوى البلوري (hkl)؟

الحل من كتاب عقيل

ولبرهان هذه الخاصية العامة نأخذ مستويا محددا بقرائن ملر (h k ℓ) يقطع أشعة الانسحاب الاساسية لشبكة برافي $\vec{a_3}$ ، $\vec{a_2}$ ، $\vec{a_1}$ بالنقاط $A(\frac{a_1}{h},0,0)$ ، $B(0,\frac{a_2}{k},0)$ ، $C(0,0,\frac{a_3}{\ell})$ حيث a_3 ، a_2 ، a_1 هي أبعاد الخلية الاساسية، كما في الشكل (2 ـ 7 أ). نأخذ شعاع الشبكة المعكوسة المحدد بالارقام h و k و ℓ:



ـ أ ـ ـ ب ـ

شكل (2 ـ 7)

$$\vec{G}(hk\ell) = h\vec{b}_1 + k\vec{b}_2 + \ell\vec{b}_3 \qquad (25-2)$$

ونأخذ الشعاعان $\vec{AB}$ و $\vec{AC}$ الواقعان في المستوي المدروس $(hk\ell)$:

$$\vec{AB} = \frac{\vec{a}_2}{k} - \frac{\vec{a}_1}{h} \quad , \quad \vec{AC} = \frac{\vec{a}_3}{\ell} - \frac{\vec{a}_1}{h}$$

والآن نبرهن أن الشعاع $\vec{G}(hk\ell)$ عمودي على الشعاعين $\vec{AB}$ و $\vec{AC}$:

$$\vec{G}\cdot\vec{AB} = (h\vec{b}_1 + k\vec{b}_2 + \ell\vec{b}_3)\cdot\left(\frac{\vec{a}_2}{k} - \frac{\vec{a}_1}{h}\right) = 0$$

$$\vec{G}\cdot\vec{AC} = (h\vec{b}_1 + k\vec{b}_2 + \ell\vec{b}_3)\cdot\left(\frac{\vec{a}_3}{\ell} - \frac{\vec{a}_1}{h}\right) = 0$$

وذلك لان $\vec{a}_i \cdot \vec{b}_j = 2\pi\,\delta_{ij}$. معنى هذا أن الشعاع $\vec{G}(hk\ell)$ عمودي على المستوي $(hk\ell)$ " لان المستقيم العمودي على مستقيمين في مستوي يكون عموديا على المستوي نفسه ".

التمرين الثاني:

برهن أن طويلة الشعاع في الشبكة المعكوسة $\mathbf{G}_{hkl}$ يتناسب مع مقلوب البعد العمودي بين المستويات البلورية (hkl)؟

الحل

البرهان: نعود للشكل (2 ـ 7 أ) فنقول بأن أحد المستويات المتوازية $(hk\ell)$ يمر بالمركز " 0 " (معادلته $hx + ky + \ell z = 0$) والمستوي الموازي والأقرب له هو المبين في الشكل (ومعادلته $hx + ky + \ell z = 1$). ونفرض أن الفاصلة بين مجموعة المستويات المتوازية هذه تساوي $d_{hk\ell}$ وتساوي البعد OH حيث $\vec{G}$ وبالتالي (OH) عمودي على المستويات $(hk\ell)$. ويمكن اعتبار البعد OH كمسقط للشعاع $\vec{OA}$ على الشعاع $\vec{G}$ ، أي أن :

$$\vec{G}(hk\ell)\cdot\vec{OA} = |\vec{G}|\,d_{hk\ell}$$

$$(h\vec{b}_1 + k\vec{b}_2 + \ell\vec{b}_3)\cdot\frac{\vec{a}_1}{h} = |\vec{G}|\cdot d_{hk\ell}$$

ومنه نجد أن:

$$d_{hk\ell} = \frac{2\pi}{|\vec{G}(hk\ell)|} \qquad (27-2)$$

أي أن الفاصلة بين المستويات الشبكية المتوازية $(hk\ell)$ تتناسب عكسيا مع قيمة شعاع الشبكة المعكوسة العمودي عليها ، وهذه الأخيرة معتمدة على قيم h ، k ، ℓ (المعادلة 2 ـ 25). معنى هذا أن الفاصلة بين المستويات البلورية ذات القرائن الكبيرة تكون صغيرة بالنسبة للفاصلة بين المستويات ذات القرائن الصغيرة، وهذه النتيجة تبدو واضحة في الشكل (2 ـ 7 ب).

التمرين رقم 3:

برهن ان الكثافة العقدية السطحية للمستويات البلورية المتوازية (hkl) تساوي $\delta=d_{hkl}/v$ بحيث v هو حجم الخلية الأساسية و d_{hkl} هو البعد العمودي بين المستويات؟

الحل : (أ) ندرس داخل الشبكة مكعب طول ضلعه 1 متر، قاعدتان منه تعـــود لمجموعة المستويات المتوازية $(hkl)^{(*)}$. يحتوي هذا المكعب على n عقـــدة أي أن الكثافة العقدية الحجمية n. وكذلك يحتوي هذا المكعب على $\frac{1}{d}$ (حيث d بالمتر) مستويا متوازيـا من المجموعة (hkl). وعدد العقد في كل مستوي (داخـل المكعب) هي الكثافة العقدية السطحية σ . لذلك فان العدد الكلي للعقد داخـل الحجم $1م^3$ (n) يسـاوي $\sigma \times \frac{1}{d}$ أي أن $n = \sigma \left(\frac{1}{d}\right)$. وبما أن $n\nu = 1$ حيث ν - حجم الخلية الأساسية للشبكة المبـاشرة (انظر الفقرة 3 من الفصل الاول)

اذن :

$$(1)\quad \sigma_{hkl} = \frac{d_{hkl}}{\nu}$$

وبما أن $d_{hkl} = \frac{2\pi}{|\vec{G}(hkl)|}$ اذن:

$$(2)\quad \sigma_{hkl} = \frac{2\pi}{\nu\,|\vec{G}(hkl)|}$$

التمرين رقم 4:

بالاعتماد على التمرين رقم 3 برهن ان الكثافة العقدية السطحية تكون اكبر ما يمكن للمستويات المتوازية (111) في البلورة المكعبة الممركزة السطوح، و للمستويات (110) للبلورة المكعبة الممركزة الجسم؟

الحل

بما أن $\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$ تحدد كل عقد الشبكة حيث $\vec{R}$ محدد بالاشعة الاساسية لذلك نحسب σ (الذي يمثل عدد العقد) بالنسبة للمستوي (HKL) ثم نحسب $(hk\ell)$ من معادلات التحويل وليس العكس.

(ب) الشبكة المكعبة fcc : حجم الخلية الأساسية $v = a^3/4$. الأشعة الاساسية للشبكة المعكوسة هي :

$$\vec{b}_1 = \frac{2\pi}{a}(-\vec{i}+\vec{j}+\vec{k}) \;,\; \vec{b}_2 = \frac{2\pi}{a}(\vec{i}-\vec{j}+\vec{k}) \;,\; \vec{b}_3 = \frac{2\pi}{a}(\vec{i}+\vec{j}-\vec{k})$$

وشعاع الانسحاب الاساسي للشبكة المعكوسة :

$\vec{G} = H\vec{b}_1 + K\vec{b}_2 + L\vec{b}_3$ عمودي على المستوي ذو القرائن (HKL) المحسوبة بالنسبة للمحاور الاساسية $\vec{a}_1, \vec{a}_2, \vec{a}_3$. أذن :

$$\vec{G}(HKL) = \frac{2\pi}{a}\{(-H+K+L)\vec{i} + (H-K+L)\vec{j} + (H+K-L)\vec{k}\}$$

$$|\vec{G}(HKL)| = \frac{2\pi}{a}\{3(H^2+K^2+L^2) - 2(HK+HL+KL)\}^{1/2}$$

والكثافة السطحية للشبكة fcc تساوي :

$$(3)\quad \sigma(HKL) = \frac{4}{a^2}\,\frac{1}{\{3(H^2+K^2+L^2) - 2(HK+HL+KL)\}^{1/2}}$$

والتناسب العكسي بين (H,K,L) و σ يسمح لنا باختيار قيم قليلة للقرائن للحصول على σ عالية :

$hk\ell$		HKL	σ
100	$\begin{pmatrix} 0 & 1/2 & 1/2 \\ 1/2 & 0 & 1/2 \\ 1/2 & 1/2 & 0 \end{pmatrix}$	011	$2/a^2$
110		112	$1,4/a^2$
111		111	$2,3/a^2$ ←

التمرين رقم 5:

Draw the following direction vectors in cubic unit cells:

a. [100] and [110]
b. [112]
c. [$\bar{1}$10]
d. [$\bar{3}\bar{2}\bar{1}$]
e. Find the angle between [100] and [$\bar{1}$10]
f. Find the angle between [112] and [$\bar{1}$10]

■ Solution

a. The position coordinates for the [100] direction are (1, 0, 0) (Fig. EP3.4*a*). The position coordinates for the [110] direction are (1, 1, 0) (Fig. EP3.4*a*).

b. The position coordinates for the [112] direction are obtained by dividing the direction indices by 2 so that they will lie within the unit cube. Thus, they are $(\frac{1}{2}, \frac{1}{2}, 1)$ (Fig. EP3.4*b*).

c. The position coordinates for the $[\bar{1}10]$ direction are (−1, 1, 0) (Fig. EP3.4*c*). Note that the origin for the direction vector must be moved to the lower-left front corner of the cube.

d. The position coordinates for the $[\bar{3}2\bar{1}]$ direction are obtained by first dividing all the indices by 3, the largest index. This gives $-1, \frac{2}{3}, -\frac{1}{3}$ for the position coordinates of the exit point of the direction $[\bar{3}2\bar{1}]$, which are shown in Figure EP3.4*d*.

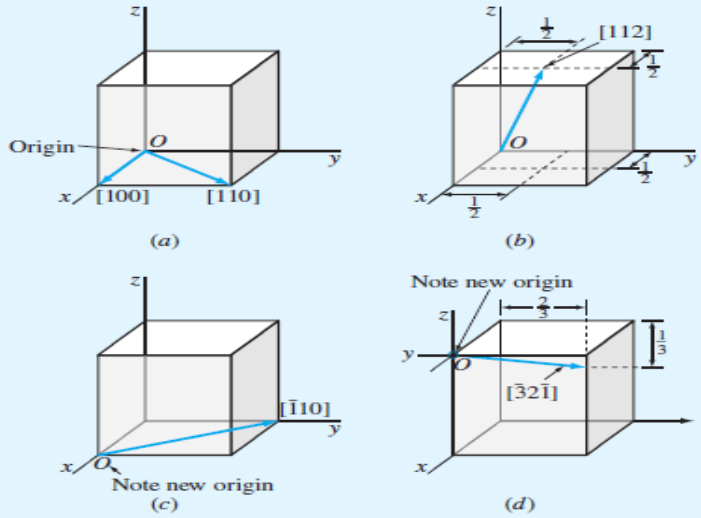


Figure EP3.4
Direction vectors in cubic unit cells.

e. The angle between directions [100] and [110] can be determined using Eq. 3.4 as follows:

$$\| \boldsymbol{A} \| = \sqrt{1^2 + 0^2 + 0^2} = 1$$

$$\| \boldsymbol{B} \| = \sqrt{1^2 + 1^2 + 0^2} = \sqrt{2}$$

$$\cos\theta = \frac{a_x b_x + a_y b_y + a_z b_z}{\| \boldsymbol{A} \| \, \| \boldsymbol{B} \|} = \frac{(1)(1) + (0)(1) + (0)(0)}{(1)(\sqrt{2})} = \frac{1}{\sqrt{2}}$$

$$\theta = 45°$$

f. The angle between directions [112] and $[\bar{1}10]$ can be determined using Eq. 3.4 as follows:

$$\| \boldsymbol{A} \| = \sqrt{1^2 + 1^2 + 2^2} = \sqrt{6}$$

$$\| \boldsymbol{B} \| = \sqrt{-1^2 + 1^2 + 0^2} = \sqrt{2}$$

$$\cos\theta = \frac{a_x b_x + a_y b_y + a_z b_z}{\| \boldsymbol{A} \| \, \| \boldsymbol{B} \|} = \frac{(1)(-1) + (1)(1) + (2)(0)}{(\sqrt{6})(\sqrt{2})} = \frac{0}{\sqrt{12}}$$

$$\theta = 90°$$

التمرين رقم 6:

Determine the direction indices of the cubic direction shown in Figure EP3.5*a*.

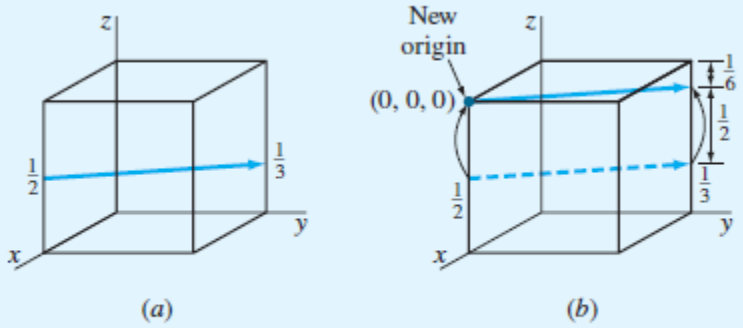


Figure EP3.5

■ **Solution**

Parallel directions have the same direction indices, and so we move the direction vector in a parallel manner until its tail reaches the nearest corner of the cube, still keeping the vector within the cube. Thus, in this case, the upper-left front corner becomes the new origin for the direction vector (Fig. EP3.5*b*). We can now determine the position coordinates where the direction vector leaves the unit cube. These are $x = -1$, $y = +1$, and $z = -\frac{1}{6}$. The position coordinates of the direction where it leaves the unit cube are thus $(-1, +1, -\frac{1}{6})$. The direction indices for this direction are, after clearing the fraction $6x$, $(-1, +1, -\frac{1}{6})$, or $[\bar{6}\bar{6}1]$.

التمرين رقم 7:

Determine the direction indices of the cubic direction between the position coordinates $\left(\frac{3}{4}, 0, \frac{1}{4}\right)$ and $\left(\frac{1}{4}, \frac{1}{2}, \frac{1}{2}\right)$.

■ **Solution**

First we locate the origin and termination points of the direction vector in a unit cube, as shown in Figure EP3.6. The fraction vector components for this direction are

$$x = -\left(\frac{3}{4} - \frac{1}{4}\right) = -\frac{1}{2}$$

$$y = \left(\frac{1}{2} - 0\right) = \frac{1}{2}$$

$$= \left(\frac{1}{2} - \frac{1}{4}\right) = \frac{1}{4}$$

Thus, the vector direction has fractional vector components of $-\frac{1}{2}, \frac{1}{2}, \frac{1}{4}$. The direction indices will be in the same ratio as their fractional components. By multiplying the fraction vector components by 4, we obtain $[\bar{2}21]$ for the direction indices of this vector direction.

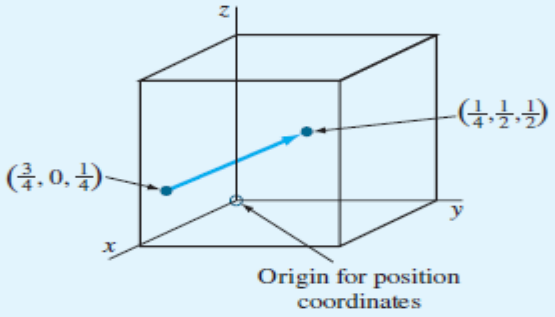


Figure EP3.6

التمرين رقم 8:

Draw the following crystallographic planes in cubic unit cells:

a. (101)
b. $(1\bar{1}0)$
c. (221)
d. Draw a (110) plane in a BCC atomic-site unit cell, and list the position coordinates of the atoms whose centers are intersected by this plane.

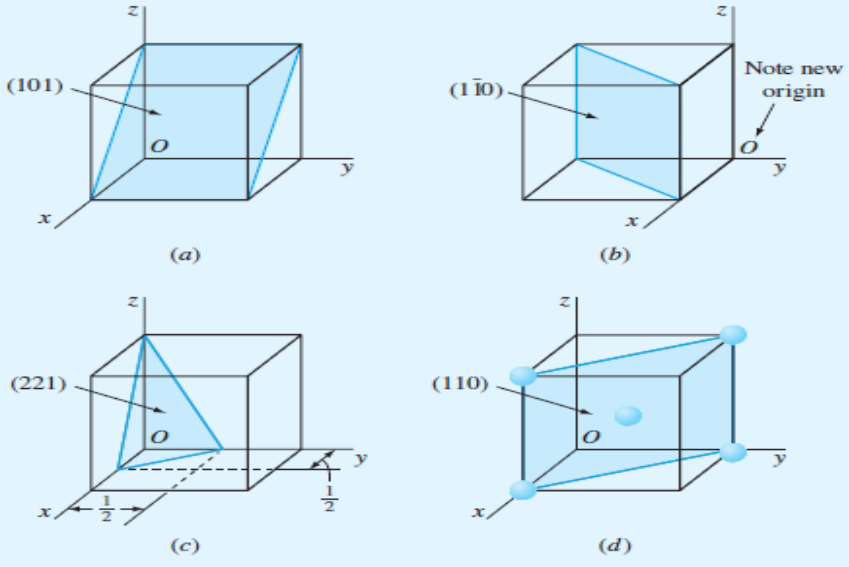


Figure EP3.7
Various important cubic crystal planes.

■ **Solution**

a. First determine the reciprocals of the Miller indices of the (101) plane. These are 1, ∞, 1. The (101) plane must pass through a unit cube at intercepts $x = 1$ and $z = 1$ and be parallel to the y axis (Fig. EP3.7*a*).

b. First determine the reciprocals of the Miller indices of the $(1\bar{1}0)$ plane. These are1, −1, ∞. The $(1\bar{1}0)$ plane must pass through a unit cube at intercepts $x = 1$ and $y = -1$ and be parallel to the z axis. Note that the origin of axes must be moved to the lower-right back side of the cube (Fig. EP3.7*b*).

c. First determine the reciprocals of the Miller indices of the (221) plane. These are $\frac{1}{2}, \frac{1}{2}$, 1. The (221) plane must pass through a unit cube at intercepts $x = \frac{1}{2}$, $y = \frac{1}{2}$, and $z = 1$ (Fig. EP3.7*c*).

d. Atom positions whose centers are intersected by the (110) plane are (1, 0, 0), (0, 1, 0), (1, 0, 1), (0, 1, 1), and $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. These positions are indicated by the solid circles (Fig. EP3.7*d*).

التمرين رقم 9:

Determine the Miller indices of the cubic crystallographic plane shown in Figure EP3.8*a*.

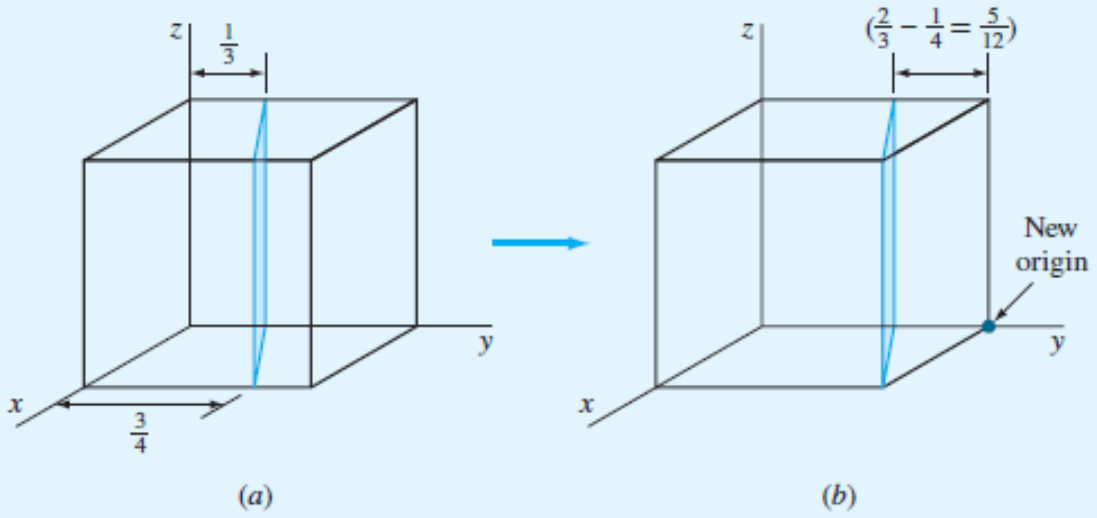


Figure EP3.8

Determine the Miller indices of the cubic crystal plane that intersects the position coordinates $(1, \frac{1}{4}, 0)$, $(1, 1, \frac{1}{2})$, $(\frac{3}{4}, 1, \frac{1}{4})$, and all coordinate axes.

■ **Solution**

First, we locate the three position coordinates as indicated in Figure EP3.9 at *A*, *B*, and *C*. Next, we join *A* and *B*, extend *AB* to *D*, and then join *A* and *C*. Finally, we join *A* to *C* to complete plane *ACD*. The origin for this plane in the cube can be chosen at *E*, which gives

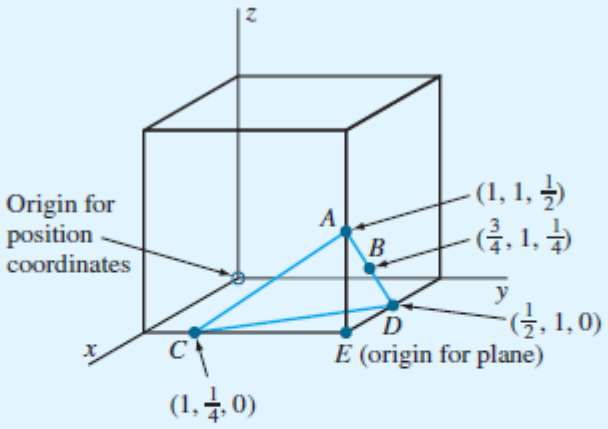


Figure EP3.9

axial intercepts for plane *ACD* at $x = -\frac{1}{2}$, $y = -\frac{3}{4}$, and $z = \frac{1}{2}$. The reciprocals of these axial intercepts are -2, $-\frac{4}{3}$, and 2. Multiplying these intercepts by 3 clears the fraction, giving Miller indices for the plane of $(\overline{6}46)$.

التمرين رقم 10:

Copper has an FCC crystal structure and a unit cell with a lattice constant of 0.361 nm. What is its interplanar spacing d_{220}?

■ **Solution**

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} = \frac{0.361 \text{ nm}}{\sqrt{(2)^2 + (2)^2 + (0)^2}} = 0.128 \text{ nm} \blacktriangleleft$$

التمرين رقم 11:

Copper has an FCC crystal structure and an atomic radius of 0.1278 nm. Assuming the atoms to be hard spheres that touch each other along the face diagonals of the FCC unit cell as shown in Figure 3.7, calculate a theoretical value for the density of copper in mega-grams per cubic meter. The atomic mass of copper is 63.54 g/mol.

■ **Solution**

For the FCC unit cell, $1\sqrt{2}a = 4R$, where a is the lattice constant of the unit cell, and R is the atomic radius of the copper atom. Thus,

$$a = \frac{4R}{\sqrt{2}} = \frac{(4)(0.1278 \text{ nm})}{\sqrt{2}} = 0.3615 \text{ nm}$$

$$\text{Volume density of copper} = \rho_v = \frac{\text{mass/unit cell}}{\text{volume/unit cell}} \tag{3.6}$$

In the FCC unit cell, there are four atoms/unit cell. Each copper atom has a mass of (63.54 g/mol) $(6.02 \times 10^{23}$ atoms/mol). Thus, the mass m of Cu atoms in the FCC unit cell is

$$m = \frac{(4 \text{ atoms})(63.54 \text{ g/mol})}{6.022 \times 10^{23} \text{ atoms/mol}} \left(\frac{10^{-6} \text{ Mg}}{\text{g}} \right) = 4.220 \times 10^{-28} \text{ Mg}$$

The volume V of the Cu unit cell is

$$V = a^3 = \left(0.361 \text{ nm} \times \frac{10^{-9} \text{ m}}{\text{nm}} \right)^3 = 4.724 \times 10^{-29} \text{m}^3$$

Thus, the theoretical density of copper is

$$\rho_v = \frac{m}{V} = \frac{4.220 \times 10^{-28} \text{ Mg}}{4.724 \times 10^{-29} \text{m}^3} = 8.933 \text{ Mg/m}^3 (8.933 \text{ g/cm}^3) \blacktriangleleft$$

التمرين رقم 12:

Calculate the planar atomic density ρ_p on the (110) plane of the α iron BCC lattice in atoms per square millimeter. The lattice constant of α iron is 0.287 nm.

■ **Solution**

$$\rho_P = \frac{\text{equiv. no. of atoms whose centers are intersected by selected area}}{\text{selected area}} \tag{3.7}$$

The equivalent number of atoms intersected by the (110) plane in terms of the surface area inside the BCC unit cell is shown in Figure 3.22 and is

$$1 \text{ atom at center} + 4 \times \frac{1}{4} \text{atoms at four corners of plane} = 2 \text{ atoms}$$

The area intersected by the (110) plane inside the unit cell (selected area) is

$$(\sqrt{2}a)(a) = \sqrt{2}a^2$$

Thus, the planar atomic density is

$$\rho_P = \frac{2 \text{ atoms}}{\sqrt{2}(0.287 \text{ nm})^2} = \frac{17.2 \text{ atoms}}{\text{nm}^2}$$

$$= \frac{17.2 \text{ atoms}}{\text{nm}^2} \times \frac{10^{12} \text{ nm}^2}{\text{mm}^2}$$

$$= 1.72 \times 10^{13} \text{ atoms/mm}^2 \blacktriangleleft$$

التمرين رقم 13:

Calculate the linear atomic density ρ_l in the [110] direction in the copper crystal lattice in atoms per millimeter. Copper is FCC and has a lattice constant of 0.361 nm.

■ **Solution**

The atoms whose centers the [110] direction intersects are shown in Figure EP3.13. We shall select the length of the line to be the length of the face diagonal of the FCC unit cell, which is $\sqrt{2}\,a$. The number of atomic diameters intersected by this length of line are $\frac{1}{2} + 1 + \frac{1}{2} = 2$ atoms. Thus using Eq. 3.8, the linear atomic density is

$$\rho_l = \frac{2 \text{ atoms}}{\sqrt{2}\,a} = \frac{2 \text{ atoms}}{\sqrt{2}(0.361 \text{ nm})} = \frac{3.92 \text{ atoms}}{\text{nm}}$$

$$= \frac{3.92 \text{ atoms}}{\text{nm}} \times \frac{10^6 \text{ nm}}{\text{mm}}$$

$$= 3.92 \times 10^6 \text{ atoms/mm} \blacktriangleleft$$

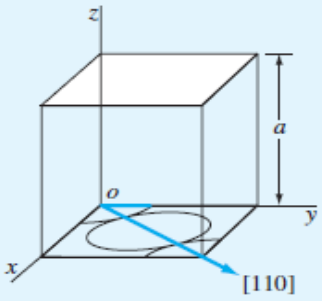


Figure EP3.13
Diagram for calculating the linear atomic density in the [110] direction in an FCC unit cell.

التمرين رقم 12:

Calculate the theoretical volume change accompanying a polymorphic transformation in a pure metal from the FCC to BCC crystal structure. Assume the hard-sphere atomic model and that there is no change in atomic volume before and after the transformation.

■ **Solution**

In the FCC crystal structure unit cell, the atoms are in contact along the face diagonal of the unit cell, as shown in Figure 3.7. Hence,

$$\sqrt{2}a = 4R \quad \text{or} \quad a = \frac{4R}{\sqrt{2}} \tag{3.3}$$

In the BCC crystal structure unit cell, the atoms are in contact along the body diagonal of the unit cell as shown in Figure 3.5. Hence,

$$\sqrt{3}a = 4R \quad \text{or} \quad a = \frac{4R}{\sqrt{3}} \tag{3.1}$$

The volume per atom for the FCC crystal lattice, since it has four atoms per unit cell, is

$$V_{FCC} = \frac{a^3}{4} = \left(\frac{4R}{\sqrt{2}}\right)^3 \left(\frac{1}{4}\right) = 5.66R^3$$

The volume per atom for the BCC crystal lattice, since it has two atoms per unit cell, is

$$V_{BCC} = \frac{a^3}{2} = \left(\frac{4R}{\sqrt{3}}\right)^3 \left(\frac{1}{2}\right) = 6.16R^3$$

The change in volume associated with the transformation from the FCC to BCC crystal structure, assuming no change in atomic radius, is

$$\frac{\Delta V}{V_{FCC}} = \frac{V_{BCC} - V_{FCC}}{V_{FCC}}$$

$$= \left(\frac{6.16R^3 - 5.66R^3}{5.66R^3}\right) 100\% = +8.83\% \blacktriangleleft$$

Chapter 3, Problem 11

Niobium at 20°C is BCC and has an atomic radius of 0.143 nm. Calculate a value for its lattice constant a in nanometers.

Chapter 3, Solution 11

For a BCC unit cell having an edge length a and containing niobium atoms,

$$\sqrt{3}a = 4R \quad \text{or} \quad a = \frac{4}{\sqrt{3}}R = \frac{4}{\sqrt{3}}(0.143 \text{ nm}) = \mathbf{0.330\ nm}$$

Chapter 3, Problem 12

Lithium at 20°C is BCC and has a lattice constant of 0.35092 nm. Calculate a value for the atomic radius of a lithium atom in nanometers.

Chapter 3, Solution 12

For the lithium BCC structure, which has a lattice constant of a = 0.35092 nm, the atomic radius is,

$$R = \frac{\sqrt{3}}{4}a = \frac{\sqrt{3}}{4}(0.35092 \text{ nm}) = \mathbf{0.152\ nm}$$

Chapter 3, Problem 13

Sodium at 20°C is BCC and has a lattice constant of 0.42906 nm. Calculate a value for the atomic radius of a sodium atom in nanometers.

Chapter 3, Solution 13

For the sodium BCC structure, with a lattice constant of a = 0.42906 nm, the atomic radius is,

$$R = \frac{\sqrt{3}}{4}a = \frac{\sqrt{3}}{4}(0.42906 \text{ nm}) = \mathbf{0.186\ nm}$$

Chapter 3, Problem 14

How many atoms per unit cell are there in the FCC crystal structure?

Chapter 3, Solution 14

Each unit cell of the FCC crystal structure contains **four** atoms.

Chapter 3, Problem 15

What is the coordination number for the atoms in the FCC crystal structure?

Chapter 3, Solution 15

The FCC crystal structure has a coordination number of **twelve**.

Chapter 3, Problem 16

Gold is FCC and has a lattice constant of 0.40788 nm. Calculate a value for the atomic radius of a gold atom in nanometers.

Chapter 3, Solution 16

For the gold FCC structure, which has a lattice constant of a = 0.40788 nm, the atomic radius is,

$$R = \frac{\sqrt{2}}{4}a = \frac{\sqrt{2}}{4}(0.40788\text{ nm}) = \mathbf{0.144\,nm}$$

Chapter 3, Problem 17

Platinum is FCC and has a lattice constant of 0.39239 nm. Calculate a value for the atomic radius of a platinum atom in nanometers.

Chapter 3, Solution 17

For the platinum FCC structure, with a lattice constant of a = 0.39239 nm, the atomic radius is,

$$R = \frac{\sqrt{2}}{4}a = \frac{\sqrt{2}}{4}(0.39239\text{ nm}) = \mathbf{0.139\,nm}$$

Chapter 3, Problem 18

Palladium is FCC and has an atomic radius of 0.137 nm. Calculate a value for its lattice constant a in nanometers.

Chapter 3, Solution 18

Letting a represent the FCC unit cell edge length and R the palladium atomic radius,

$$\sqrt{2}a = 4R \quad \text{or} \quad a = \frac{4}{\sqrt{2}}R = \frac{4}{\sqrt{2}}(0.137\text{ nm}) = \mathbf{0.387\,nm}$$

Chapter 3, Problem 19

Strontium is FCC and has an atomic radius of 0.215 nm. Calculate a value for its lattice constant *a* in nanometers.

Chapter 3, Solution 19

For an FCC unit cell having an edge length *a* an containing strontium atoms,

$$\sqrt{2}a = 4R \quad \text{or} \quad a = \frac{4}{\sqrt{2}}R = \frac{4}{\sqrt{2}}(0.215 \text{ nm}) = \mathbf{0.608\,nm}$$

Chapter 3, Problem 20

Calculate the atomic packing factor for the FCC structure.

Chapter 3, Solution 20

By definition, the atomic packing factor is given as:

$$\text{Atomic packing factor} = \frac{\text{volume of atoms in FCC unit cell}}{\text{volume of the FCC unit cell}}$$

These volumes, associated with the four-atom FCC unit cell, are

$$V_{atoms} = 4\left[\frac{4}{3}\pi R^3\right] = \frac{16}{3}\pi R^3 \quad \text{and} \quad V_{\text{unit cell}} = a^3$$

where *a* represents the lattice constant. Substituting $a = \frac{4R}{\sqrt{2}}$,

$$V_{\text{unit cell}} = a^3 = \frac{64R^3}{2\sqrt{2}}$$

The atomic packing factor then becomes,

$$\text{APF (FCC unit cell)} = \left(\frac{16\pi R^3}{3}\right)\left(\frac{1\sqrt{2}}{32R^3}\right) = \frac{\pi\sqrt{2}}{6} = \mathbf{0.74}$$

Chapter 3, Problem 21

How many atoms per unit cell are there in the HCP crystal structure?

Chapter 3, Solution 21

The hexagonal prism contains **six** atoms.

Chapter 3, Problem 22

What is the coordination number for the atoms in the HCP crystal structure?

Chapter 3, Solution 22

The coordination number associated with the HCP crystal structure is **twelve**.

Chapter 3, Problem 23

What is the ideal *c/a* ratio for HCP metals?

Chapter 3, Solution 23

The ideal *c/a* ratio for HCP metals is **1.633**; however, the actual ratios may deviate significantly from this value.

Chapter 3, Problem 24

Of the following HCP metals, which have higher or lower *c/a* ratios than the ideal ratio: Zr, Ti, Zn, Mg, Co, Cd, and Be?

Chapter 3, Solution 24

Cadmium and zinc have significantly higher *c/a* ratios while zirconium, titanium, magnesium, cobalt and beryllium have slightly lower ratios.

Chapter 3, Problem 25

Calculate the volume in cubic nanometers of the titanium crystal structure unit cell. Titanium is HCP at 20°C with a = 0.29504 nm and c = 0.46833 nm.

Chapter 3, Solution 25

For a hexagonal prism, of height c and side length a, the volume is given by:

$$V = (\text{Area of Base})(\text{Height}) = [(6 \times \text{Equilateral Triangle Area})(\text{Height})]$$

$$= (3a^2 \sin 60^o)(c)$$

$$= 3(0.29504\ \text{nm})^2 (\sin 60^o)(0.46833\ \text{nm})$$

$$= \mathbf{0.106\ nm^3}$$

Chapter 3, Problem 26

Rhenium at 20°C is HCP. The height *c* of its unit cell is 0.44583 nm and its *c/a* ratio is 1.633. Calculate a value for its lattice constant *a* in nanometers.

Chapter 3, Solution 26

The rhenium lattice constant *a* is calculated as,

$$a = \frac{c}{c/a} = \frac{0.44583 \text{ nm}}{1.633} = \mathbf{0.273\ nm}$$

Chapter 3, Problem 27

Osmium at 20°C is HCP. Using a value of 0.135 nm for the atom radius of osmium atoms, calculate a value for its unit-cell volume. Assume a packing factor of 0.74.

Chapter 3, Solution 27

From the definition of the atomic packing factor,

$$\text{HCP unit cell volume} = \frac{\text{volume of atoms in HCP unit cell}}{\text{APF}}$$

Since there are six atoms in the HCP unit cell, the volume of atoms is:

$$V_{\text{atoms}} = 6\left(\frac{4}{3}\pi R^3\right) = 8\pi(0.135)^3 = 0.0618 \text{ nm}^3$$

The unit cell volume thus becomes,

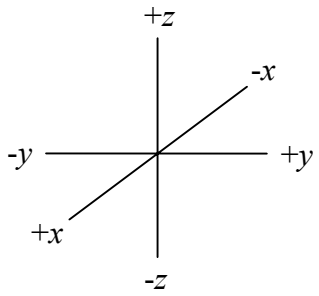
$$\text{HCP unit cell volume} = \frac{0.0618 \text{ nm}^3}{0.74} = \mathbf{0.084\ nm^3}$$

Chapter 3, Problem 28

How are atomic positions located in cubic unit cells?

Chapter 3, Solution 28

Atomic positions are located in cubic unit cells using rectangular x, y, and z axes and unit distances along the respective axes. The directions of these axes are shown below.



Chapter 3, Problem 29

List the atom positions for the eight corner and six face-centered atoms of the FCC unit cell.

Chapter 3, Solution 29

The atom positions at the corners of an FCC unit cell are:
(0, 0, 0), (1, 0, 0), (1, 1, 0), (0, 1, 0), (0, 0, 1), (1, 0, 1), (1, 1, 1), (0, 1, 1)

On the faces of the FCC unit cell, atoms are located at:
(½, ½, 0), (½, 0, ½), (0, ½, ½), (½, ½, 1), (1, ½, ½), (½, 1, ½)

Chapter 3, Problem 30

How are the indices for a crystallographic direction in a cubic unit cell determined?

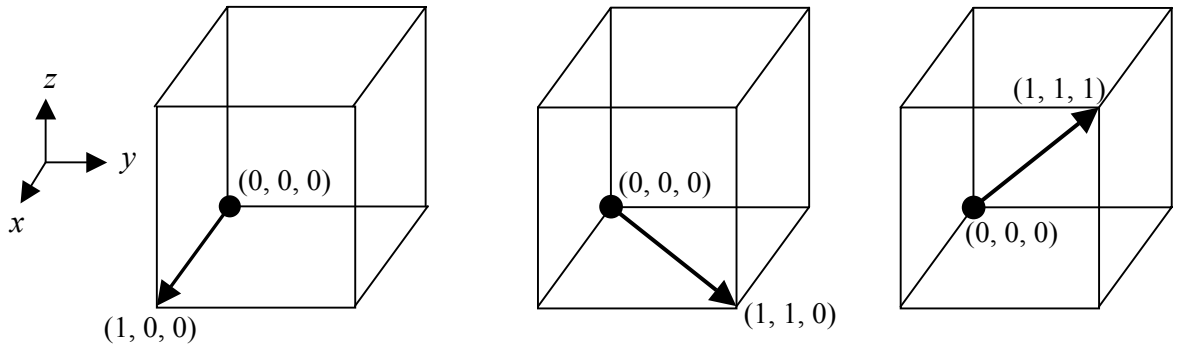
Chapter 3, Solution 30

For cubic crystals, the crystallographic direction indices are the components of the direction vector, resolved along each of the coordinate axes and reduced to the smallest integers. These indices are designated as [uvw].

Chapter 3, Problem 31

Draw the following directions in a BCC unit cell and list the position coordinates of the atoms whose centers are intersected by the direction vector:
(*a*) [100](*b*) [110](*c*) [111]

Chapter 3, Solution 31



(a) Position Coordinates: (0, 0, 0), (1, 0, 0)

(b) Position Coordinates: (0, 0, 0), (1, 1, 0)

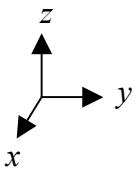
(c) Position Coordinates: (0, 0, 0), (1, 1, 1)

Chapter 3, Problem 32

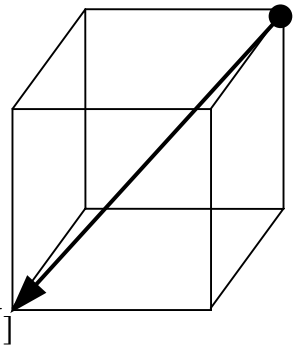
Draw direction vectors in unit cells for the following cubic directions:

(*a*) $[1\,\bar{1}\,\bar{1}]$ (*b*) $[1\,\bar{1}0]$ (*c*) $[\bar{1}2\,\bar{1}]$ (*d*) $[\bar{1}\,\bar{1}3]$

Chapter 3, Solution 32



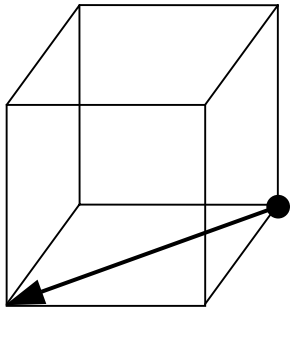
(a)



$x = +1$
$y = -1$
$z = -1$

$[1\,\bar{1}\,\bar{1}]$

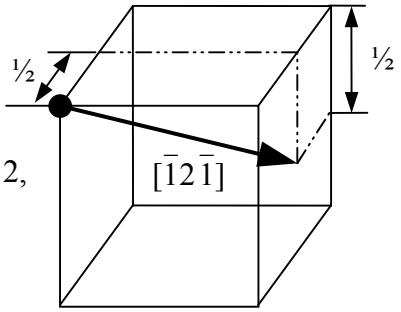
(b)



$x = +1$
$y = -1$
$z = 0$

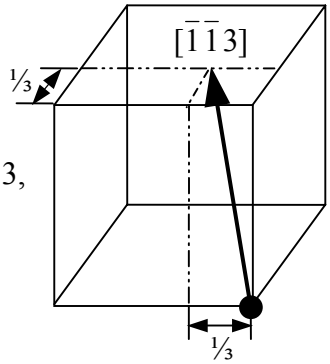
$[1\,\bar{1}\,0]$

(c)



Dividing by 2,
$x = -½$
$y = 1$
$z = -½$

(d)



Dividing by 3,
$x = -⅓$
$y = -⅓$
$z = 1$

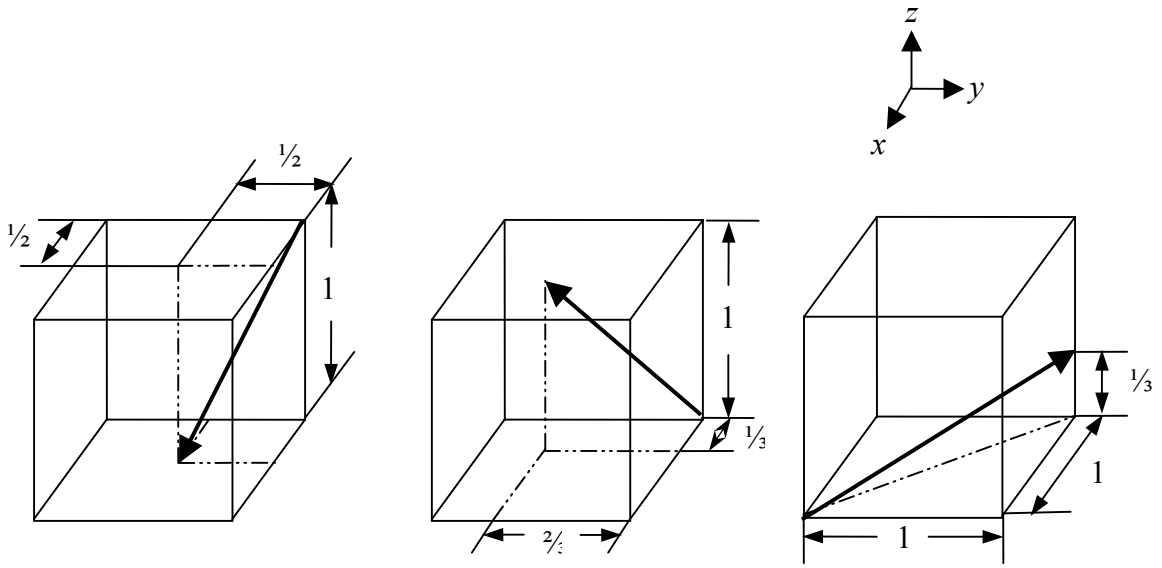
Chapter 3, Problem 33

Draw direction vectors in unit cells for the following cubic directions:

(*a*) $[1\,\bar{1}\,\bar{2}]$ (*c*) $[\bar{3}31]$ (*e*) $[2\,\bar{1}2]$ (*g*) $[\bar{1}01]$ (*i*) $[321]$ (*k*) $[1\bar{2}\bar{2}]$

(*b*) $[1\bar{2}3]$ (*d*) $[0\bar{2}1]$ (*f*) $[2\bar{3}3]$ (*h*) $[12\,\bar{1}]$ (*j*) $[10\bar{3}]$ (*l*) $[\bar{2}\bar{2}3]$

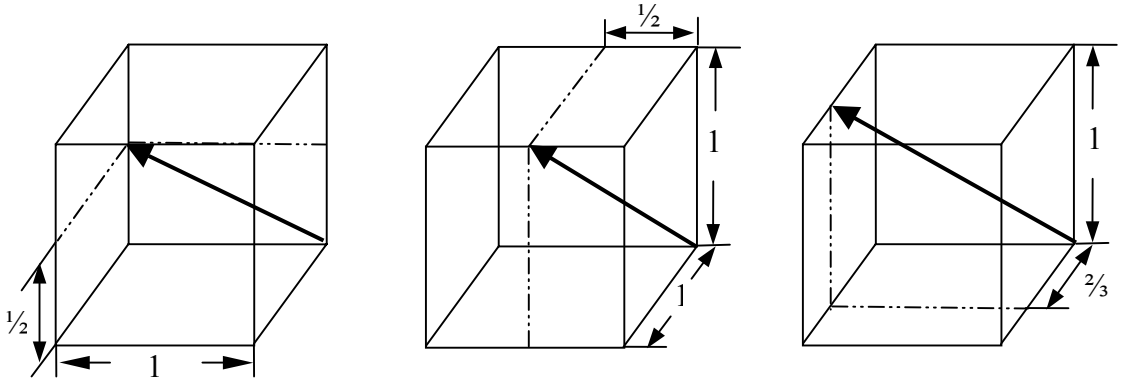
Chapter 3, Solution 33



(a) Dividing $[1\bar{1}\bar{2}]$ by 2,

$$x = \frac{1}{2},\ y = -\frac{1}{2},\ z = -1$$

$$\left(\frac{1}{4}, 1, \frac{1}{4} \right) \qquad [3\ 2\ 1]$$



(d) Dividing $[0\bar{2}1]$ by 2,

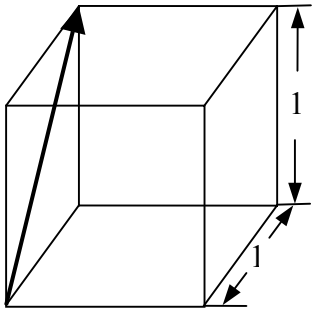
$$x = 0,\ y = -1,\ z = \frac{1}{2}$$

(e) Dividing $[2\,\bar{1}\,2]$ by 2,

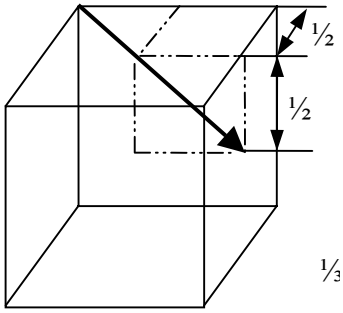
$$x = 1,\ y = -\frac{1}{2},\ z = 1$$

(f) Dividing $[2\bar{3}3]$ by 3,

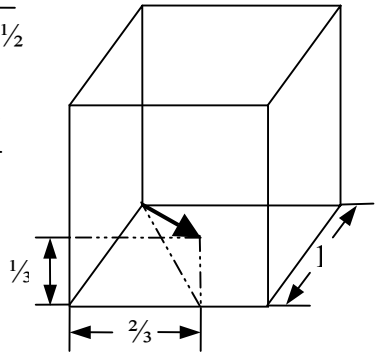
$$x = \frac{2}{3},\ y = -1,\ z = 1$$



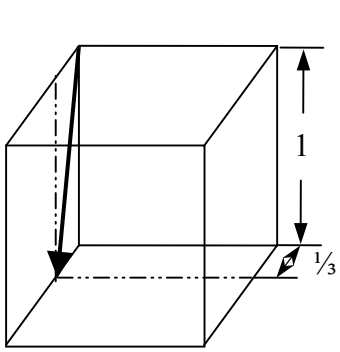
(g) For $[\bar{1}01]$,
$x=-1, y=0, z=1$



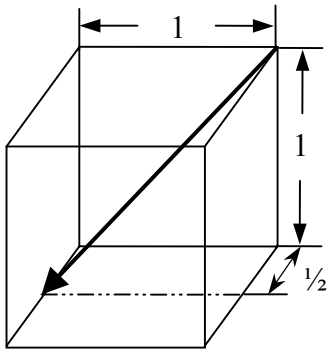
(h) Dividing $[12\bar{1}]$ by 2,
$x=\frac{1}{2}, y=1, z=-\frac{1}{2}$



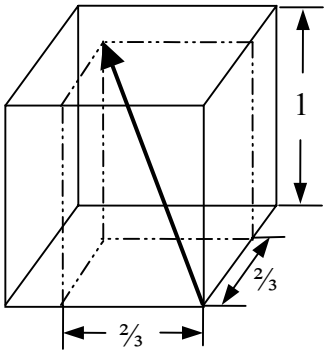
(i) Dividing [321] by 3,
$x=1, y=\frac{2}{3}, z=\frac{1}{3}$



(j) Dividing $[10\bar{3}]$ by 3,
$x=\frac{1}{3}, y=0, z=-1$



(k) Dividing $[1\bar{2}\bar{2}]$ by 2,
$x=\frac{1}{2}, y=-1, z=-1$



(l) Dividing $[\bar{2}\bar{2}3]$ by 3,
$x=-\frac{2}{3}, y=-\frac{2}{3}, z=1$

Chapter 3, Problem 34

What are the indices of the directions shown in the unit cubes of Fig. P3.34?

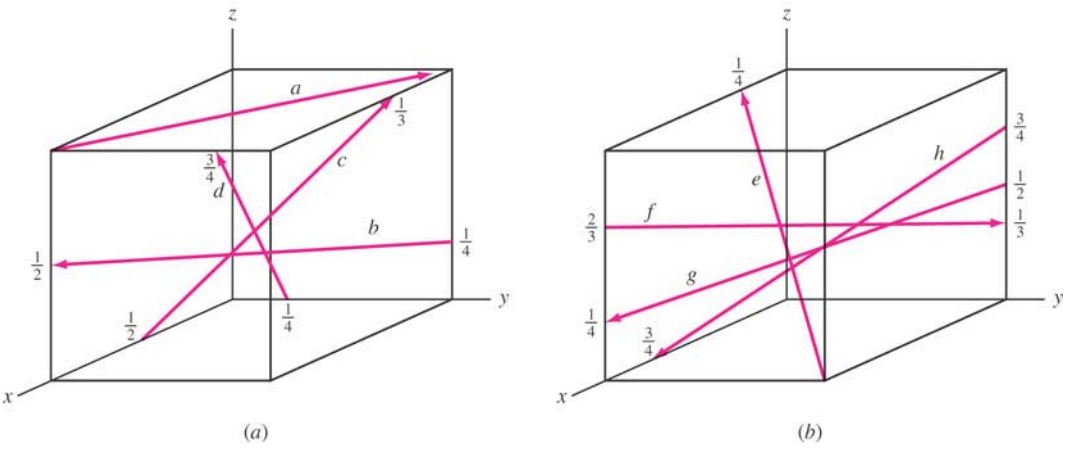
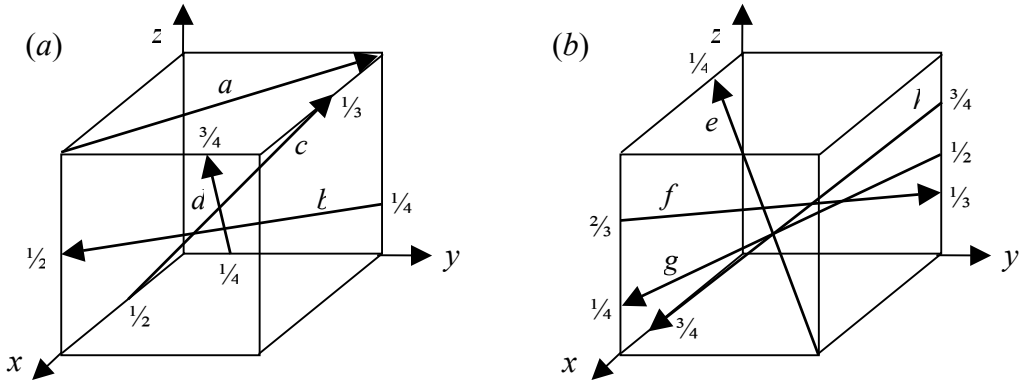
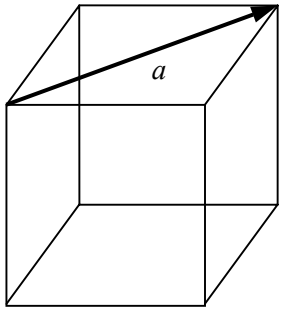


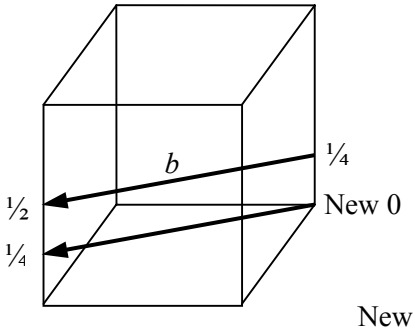
Figure P3.34

Chapter 3, Solution 34

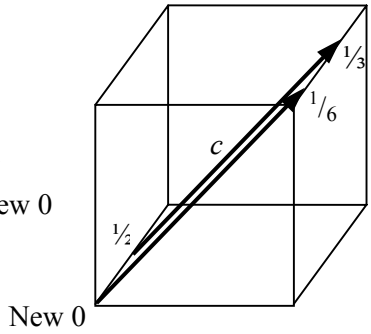




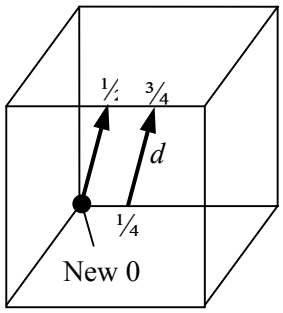
a. Vector components:
$x = -1,\ y = 1,\ z = 0$
Direction indices: $[\bar{1}10]$



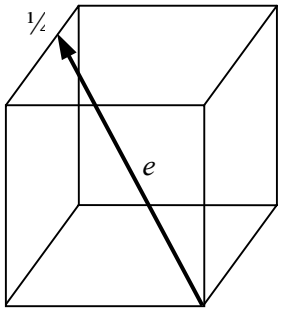
b. Moving direction vector down ¼ , vector components are: $x = 1,\ y = -1,\ z = ¼$
Direction indices: $[4\bar{4}1]$



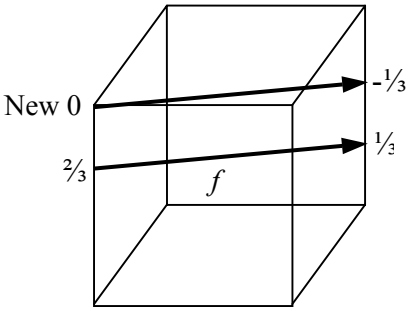
c. Moving direction vector forward ½, vector components are: $x = -1/6,\ y = 1,\ z = 1$
Direction indices: $[\bar{1}66]$



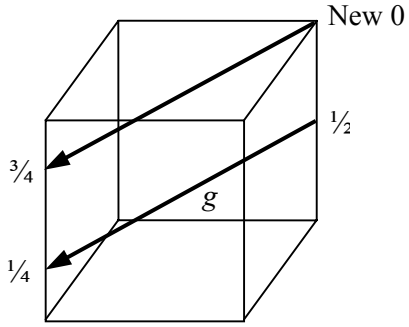
d. Moving direction vector left ¼, vector components are: $x = 1,\ y = ½,\ z = 1$
Direction indices: [212]



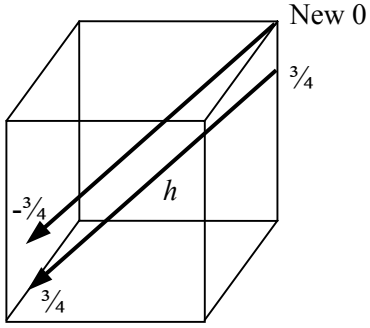
e. Vector components are:
$x = -¾,\ y = -1,\ z = 1$
Direction indices: $[\bar{3}\bar{4}4]$



f. Moving direction vector up ⅓, vector components are:
$x = -1,\ y = 1,\ z = -⅓$
Direction indices: $[\bar{3}31]$



g. Moving direction vector up ½, vector components are: $x = 1, y = -1, z = -¼$
Direction indices: $[4\bar{4}\bar{1}]$



h. Moving direction vector up ¼, vector components are: $x = ¾,\ y = -1, z = -¾$
Direction indices: $[3\bar{4}\bar{3}]$

Chapter 3, Problem 35

A direction vector passes through a unit cube from the $\left(\frac{3}{4}, 0, \frac{1}{4}\right)$ to the $\left(\frac{1}{2}, 1, 0\right)$ positions. What are its direction indices?

Chapter 3, Solution 35

The starting point coordinates, subtracted from the end point, give the vector components:

$$x = \frac{1}{2} - \frac{3}{4} = -\frac{1}{4} \qquad y = 1 - 0 = 1 \qquad z = 0 - \frac{1}{4} = -\frac{1}{4}$$

The fractions can then be cleared through multiplication by 4, giving $x = -1$, $y = 4$, $z = -1$. The direction indices are therefore $\mathbf{[\bar{1}\,4\,\bar{1}]}$.

Chapter 3, Problem 36

A direction vector passes through a unit cube from the $\left(1, 0, \frac{3}{4}\right)$ to the $\left(\frac{1}{4}, 1, \frac{1}{4}\right)$ positions. What are its direction indices?

Chapter 3, Solution 36

Subtracting coordinates, the vector components are:

$$x = \frac{1}{4} - 1 = -\frac{3}{4} \qquad y = 1 - 0 = 1 \qquad z = \frac{1}{4} - \frac{3}{4} = -\frac{1}{2}$$

Clearing fractions through multiplication by 4, gives $x = -3$, $y = 4$, $z = -2$.
The direction indices are therefore $\mathbf{[\bar{3}\,4\,\bar{2}]}$.

Chapter 3, Problem 37

What are the crystallographic directions of a family or form? What generalized notation is used to indicate them?

Chapter 3, Solution 37

A family or form has equivalent crystallographic directions; the atom spacing along each direction is identical. These directions are indicated by $\langle uvw \rangle$.

Chapter 3, Problem 38

What are the directions of the $\left[10\bar{3}\right]$ family or form for a unit cube?

Chapter 3, Solution 38

$$[100],\ [010],\ [001],\ [\bar{1}00],\ [0\bar{1}0],\ [00\bar{1}]$$

Chapter 3, Problem 39

What are the directions of the $\langle 111 \rangle$ family or form for a unit cube?

Chapter 3, Solution 39

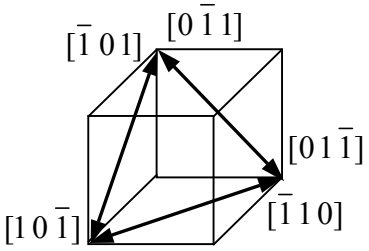
$$[111],\ [\bar{1}\bar{1}\bar{1}],\ [1\bar{1}1],\ [\bar{1}1\bar{1}],$$
$$[\bar{1}11],\ [1\bar{1}\bar{1}],\ [11\bar{1}],\ [\bar{1}\bar{1}1]$$

Chapter 3, Problem 40

What $\langle 110 \rangle$-type directions lie on the (111) plane of a cubic unit cell?

Chapter 3, Solution 40

$$[0\bar{1}1],\ [01\bar{1}],\ [\bar{1}10],\ [1\bar{1}0],\ [\bar{1}01],\ [10\bar{1}]$$

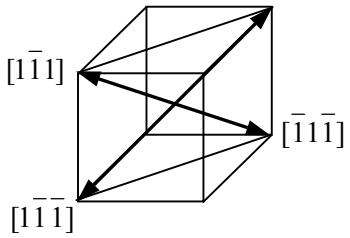


Chapter 3, Problem 41

What $\langle 1\,1\,1 \rangle$-type directions lie on the (110) plane of a cubic unit cell?

Chapter 3, Solution 41

$[1\bar{1}1]$, $[\bar{1}11]$, $[1\bar{1}\bar{1}]$, $[\bar{1}1\bar{1}]$



Chapter 3, Problem 42

How are the Miller indices for a crystallographic plane in a cubic unit cell determined? What generalized notation is used to indicate them?

Chapter 3, Solution 42

The Miller indices are determined by first identifying the fractional intercepts which the plane makes with the crystallographic *x*, *y*, and *z* axes of the cubic unit cell. Then all fractions must be cleared such that the smallest set of whole numbers is attained. The general notation used to indicate these indices is (*hkl*), where *h*, *k*, and *l* correspond to the *x*, *y* and *z* axes, respectively.

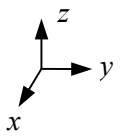
Chapter 3, Problem 43

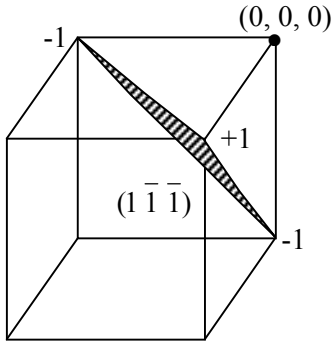
Draw in unit cubes the crystal planes that have the following Miller indices:

(*a*) $(1\,\bar{1}\,\bar{1})$ (*c*) $(1\bar{2}\,\bar{1})$ (*e*) $(3\bar{2}1)$ (*g*) $(20\,\bar{1})$ (*i*) $(\bar{2}32)$ (*k*) $(3\,\bar{1}2)$

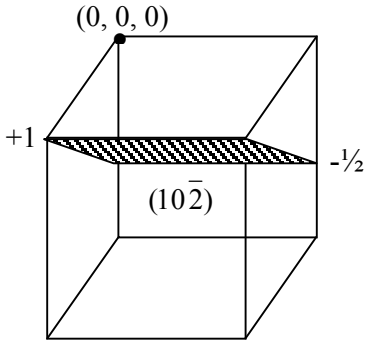
(*b*) $(10\bar{2})$ (*d*) $(21\bar{3})$ (*f*) $(30\bar{2})$ (*h*) $(\bar{2}1\bar{2})$ (*j*) $(13\bar{3})$ (*l*) $(\bar{3}3\,\bar{1})$

Chapter 3, Solution 43

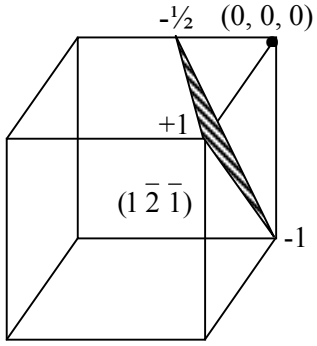




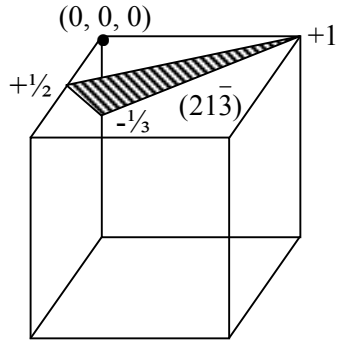
a. For $(1\,\bar{1}\,\bar{1})$ reciprocals are: $x = 1,\ y = -1,\ z = -1$



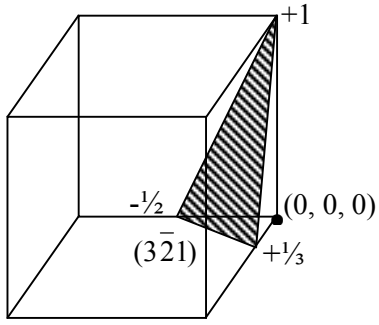
b. For $(10\bar{2})$ reciprocals are: $x = 1,\ y = \infty,\ z = -½$



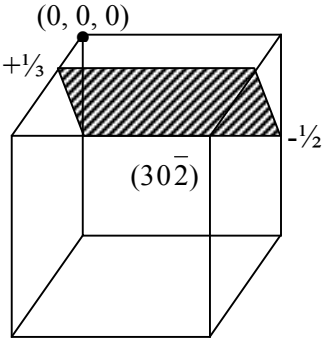
c. For $(1\,\bar{2}\,\bar{1})$ reciprocals are: $x = 1,\ y = -½,\ z = -1$



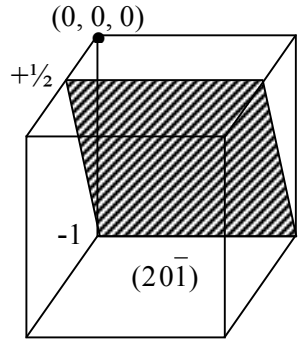
d. For $(21\bar{3})$ reciprocals are: $x = ½,\ y = 1,\ z = -⅓$



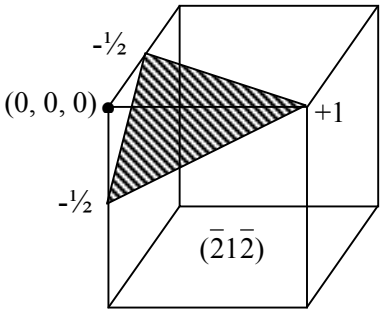
e. For $(3\bar{2}1)$ reciprocals are: $x = ⅓,\ y = -½,\ z = 1$



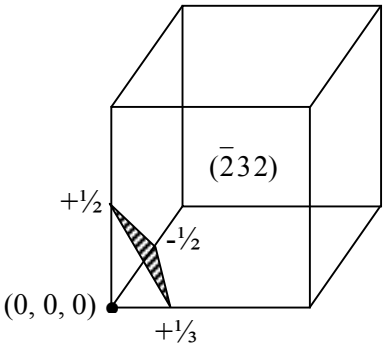
f. For $(30\bar{2})$ reciprocals are: $x = ⅓,\ y = \infty,\ z = -½$



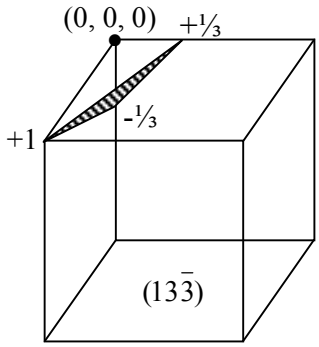
g. For $(20\bar{1})$ reciprocals are: $x = ½$, $y = \infty$, $z = -1$



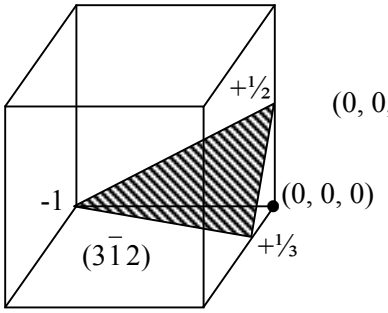
h. For $(\bar{2}1\bar{2})$ reciprocals are: $x = -½$, $y = 1$, $z = -½$



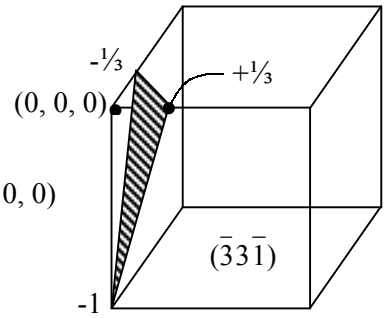
i. For $(\bar{2}32)$ reciprocals are: $x = -½$, $y = ⅓$, $z = ½$



j. For $(13\bar{3})$ reciprocals are: $x = 1$, $y = ⅓$, $z = -⅓$



k. For $(3\bar{1}2)$ reciprocals are: $x = ⅓$, $y = -1$, $z = ½$

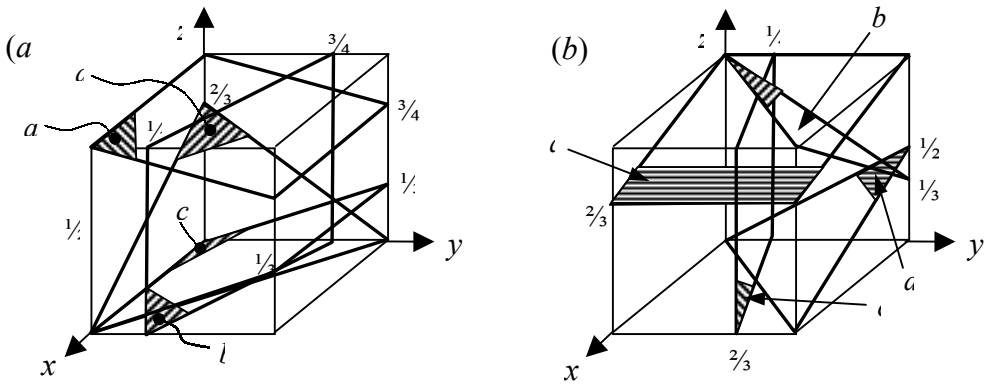


k. For $(\bar{3}3\bar{1})$ reciprocals are: $x = -⅓$, $y = ⅓$, $z = -1$

Chapter 3, Problem 44

What are the Miller indices of the cubic cyrsyallographic planes shown in Fig. P3.44?

Chapter 3, Solution 44



Miller Indices for Figure P3.44(a)

Plane *a* based on (0, 1, 1) as origin		**Plane *b* based on (1, 1, 0) as origin**	
Planar Intercepts	Reciprocals of Intercepts	Planar Intercepts	Reciprocals of Intercepts
$x = \infty$	$\frac{1}{x} = 0$	$x = -1$	$\frac{1}{x} = -1$
$y = -1$	$\frac{1}{y} = -1$	$y = \frac{-5}{12}$	$\frac{1}{y} = \frac{-12}{5}$
$z = -\frac{1}{4}$	$\frac{1}{z} = -4$	$z = \infty$	$\frac{1}{z} = 0$
The Miller indices of plane *a* are **(0 $\bar{1}$ $\bar{4}$)**.		The Miller indices of plane *b* are **($\bar{5}$ $\bar{12}$ 0)**.	
Plane *c* based on (1, 1, 0) as origin		**Plane *d* based on (0, 0, 0) as origin**	
Planar Intercepts	Reciprocals of Intercepts	Planar Intercepts	Reciprocals of Intercepts
$x = \infty$	$\frac{1}{x} = 0$	$x = 1$	$\frac{1}{x} = 1$
$y = -1$	$\frac{1}{y} = -1$	$y = 1$	$\frac{1}{y} = 1$
$z = \frac{1}{3}$	$\frac{1}{z} = 3$	$z = \frac{2}{3}$	$\frac{1}{z} = \frac{3}{2}$
The Miller indices of plane *c* are **(0 $\bar{1}$ 3)**.		The Miller indices of plane *d* are **(2 2 3)**.	

Miller Indices for Figure P3.44(b)

Plane *a* based on (1, 0, 1) as origin

Planar Intercepts	Reciprocals of Intercepts
$x = -1$	$\frac{1}{x} = -1$
$y = \infty$	$\frac{1}{y} = 0$
$z = -\frac{1}{3}$	$\frac{1}{z} = -3$

The Miller indices of plane *a* are $(\bar{1}\ 0\ \bar{3})$.

Plane *b* based on (0, 1, 1) as origin

Planar Intercepts	Reciprocals of Intercepts
$x = 1$	$\frac{1}{x} = 1$
$y = -1$	$\frac{1}{y} = -1$
$z = -\frac{2}{3}$	$\frac{1}{z} = -\frac{3}{2}$

The Miller indices of plane *b* are $(2\ \bar{2}\ \bar{3})$.

Plane *c* based on (0, 1, 0) as origin

Planar Intercepts	Reciprocals of Intercepts
$x = 1$	$\frac{1}{x} = 1$
$y = \frac{-5}{12}$	$\frac{1}{y} = \frac{-12}{5}$
$z = \infty$	$\frac{1}{z} = 0$

The Miller indices of plane *c* are $(5\ \bar{12}\ 0)$.

Plane *d* based on (0, 1, 0) as origin

Planar Intercepts	Reciprocals of Intercepts
$x = 1$	$\frac{1}{x} = 1$
$y = -1$	$\frac{1}{y} = -1$
$z = \frac{1}{2}$	$\frac{1}{z} = 2$

The Miller indices of plane *d* are $(1\ \bar{1}\ \bar{2})$.

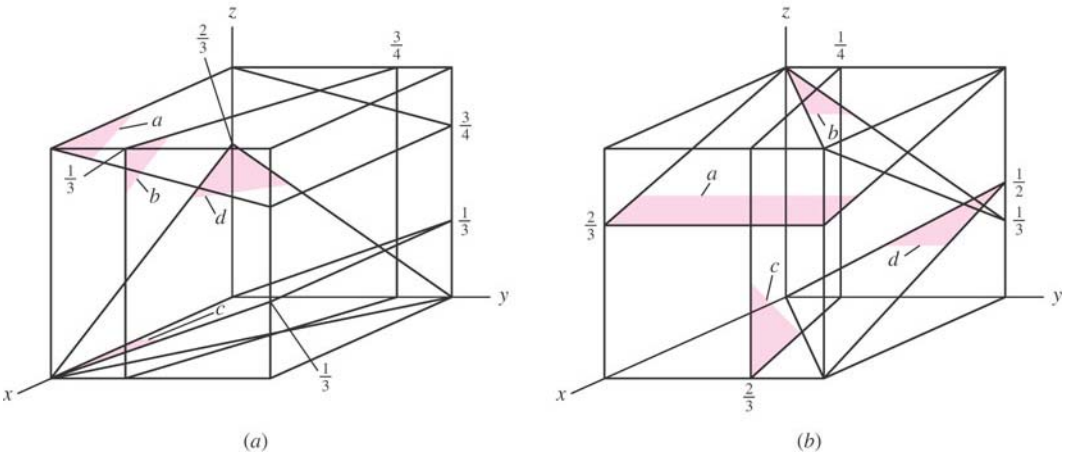


Figure P3.44

Chapter 3, Problem 45

What is the notation used to indicate a family or form of cubic crystallographic planes?

Chapter 3, Solution 45

A family or form of a cubic crystallographic plane is indicated using the notation $\{hkl\}$.

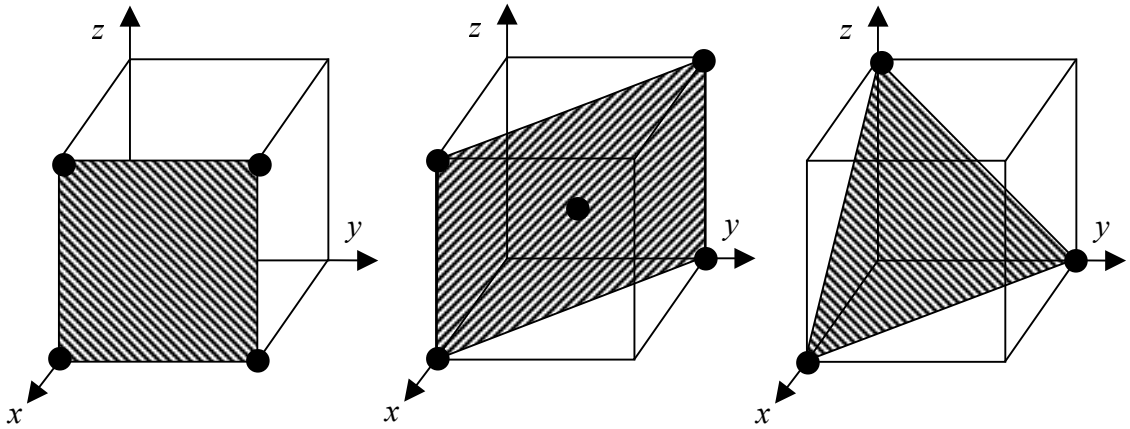
Chapter 3, Problem 46
What are the {100} family of planes of the cubic system?
Chapter 3, Solution 46

$$(100), (010), (001), (\bar{1}00), (0\bar{1}0), (00\bar{1})$$

Chapter 3, Problem 47

Draw the following crystallographic planes in a BCC unit cell and list the position of the atoms whose centers are intersected by each of the planes:
(*a*) (100)(*b*) (110)(*c*) (111)

Chapter 3, Solution 47



a. (1, 0, 0), (1, 0, 1), (1, 1, 0), (1, 1, 1)

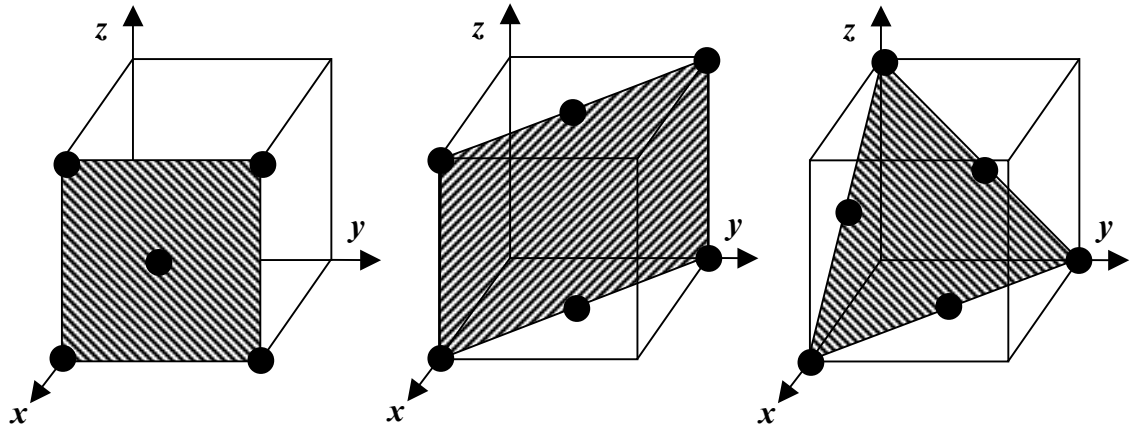
b. (1, 0, 0), (1, 0, 1), (0, 1, 0), (0, 1, 1), (½, ½, ½)

c. (1, 0, 0), (0, 0, 1), (0, 1, 0)

Chapter 3, Problem 48

Draw the following crystallographic planes in an FCC unit cell and list the position coordinates of the atoms whose centers are intersected by each of the planes:
(*a*) (100)(*b*) (110)(*c*) (111)

Chapter 3, Solution 48



a. (1, 0, 0), (1, 0, 1), (1, 1, 0), (1, 1, 1) (1, ½, ½)

b. (1, 0, 0), (1, 0, 1), (0, 1, 0), (0, 1, 1), (½, ½, 0), (½, ½, 1)

c. (1, 0, 0), (0, 0, 1), (0, 1, 0), (½, 0, ½) (½, ½, 0), (0, ½, ½)

Chapter 3, Problem 49

A cubic plane has the following axial intercepts: $a = \frac{1}{3},\ b = -\frac{2}{3},\ c = \frac{1}{2}$. What are the Miller indices of this plane?

Chapter 3, Solution 49

Given the axial intercepts of (⅓, -⅔, ½), the reciprocal intercepts are: $\frac{1}{x} = 3,\quad \frac{1}{y} = -\frac{3}{2},\quad \frac{1}{z} = 2.$ Multiplying by 2 to clear the fraction, the Miller indices are $\mathbf{(6\,\bar{3}\,4)}$.

Chapter 3, Problem 50

A cubic plane has the following axial intercepts: $a = -\frac{1}{2},\ b = -\frac{1}{2},\ c = \frac{2}{3}$. What are the Miller indices of this plane?

Chapter 3, Solution 50

Given the axial intercepts of (-½, -½, ⅔), the reciprocal intercepts are: $\frac{1}{x} = -2,\quad \frac{1}{y} = -2,\quad \frac{1}{z} = \frac{3}{2}.$ Multiplying by 2, the Miller indices are $\mathbf{(\bar{4}\,\bar{4}\,3)}$.

Chapter 3, Problem 51

A cubic plane has the following axial intercepts: $a = 1,\ b = \frac{2}{3},\ c = -\frac{1}{2}$. What are the Miller indices of this plane?

Chapter 3, Solution 51

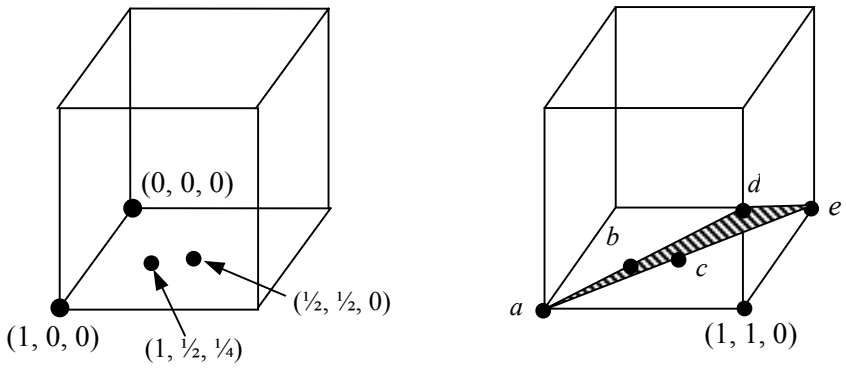
Given the axial intercepts of (1, ⅔, -½), the reciprocal intercepts are: $\frac{1}{x} = 1,\quad \frac{1}{y} = \frac{3}{2},\quad \frac{1}{z} = -2.$ Multiplying by 2, the Miller indices are $\mathbf{(2\ 3\ \bar{4})}$.

Chapter 3, Problem 52

Determine the Miller indices of the cubic crystal plane that intersects the following position coordinates:
$(1, 0, 0);\ (1, \frac{1}{2}, \frac{1}{4});\ (\frac{1}{2}, \frac{1}{2}, 0).$

Chapter 3, Solution 52

First locate the three position coordinates as shown. Next, connect points *a* and *b,* extending the line to point *d* and connect *a* to *c* and extend to *e*. Complete the plane by connecting point *d* to *e*. Using (1, 1, 0) as the plane origin, *x* = -1, *y* = -1 and *z* = ½. The intercept reciprocals are thus $\frac{1}{x} = -1,\ \frac{1}{y} = -1,\ \frac{1}{z} = 2.$ The Miller indices are $\mathbf{(\bar{1}\ \bar{1}\ 2)}$.

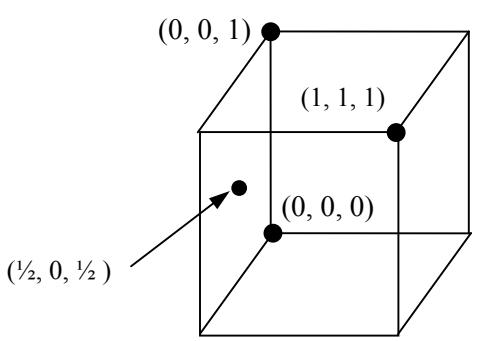


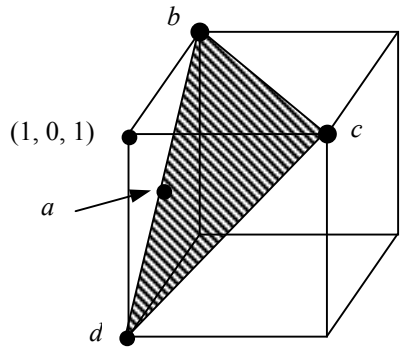
Chapter 3, Problem 53

Determine the Miller indices of the cubic crystal plane that intersects the following position coordinates:
$(\frac{1}{2}, 0, \frac{1}{2})$; (0,0,1); (1,1,1).

Chapter 3, Solution 53

First locate the three position coordinates as shown. Next, connect points *a* and *b* and extend the line to point *d*. Complete the plane by connecting point *d* to *c* and point *c* to *b*. Using (1, 0, 1) as the plane origin, $x = -1$, $y = 1$ and $z = -1$. The intercept reciprocals are thus $\frac{1}{x} = -1,\ \frac{1}{y} = 1,\ \frac{1}{z} = -1$. The Miller indices are $\mathbf{(\bar{1}\,1\,\bar{1})}$.



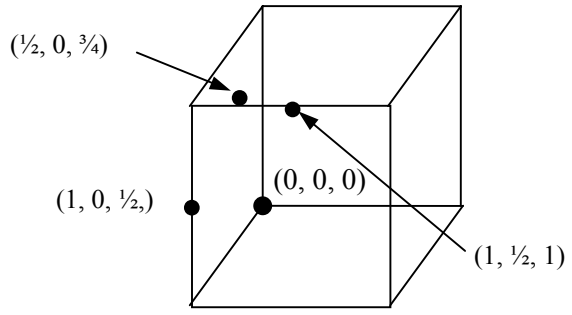


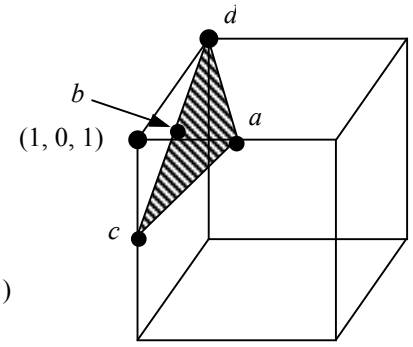
Chapter 3, Problem 54

Determine the Miller indices of the cubic crystal plane that intersects the following position coordinates:
$(1, \frac{1}{2}, 1)$; $(\frac{1}{2}, 0, \frac{3}{4})$; $(1, 0, \frac{1}{2})$.

Chapter 3, Solution 54

After locating the three position coordinates, connect points *b* and *c* and extend the line to point *d*. Complete the plane by connecting point *d* to *a* and *a* to *c*. Using
(1, 0, 1) as the plane origin, $x = -1$, $y = ½$ and $z = -½$. The intercept reciprocals then become
$\frac{1}{x} = -1,\ \frac{1}{y} = 2,\ \frac{1}{z} = -2$. The Miller indices are $\mathbf{(\bar{1}\,2\,\bar{2})}$.





Chapter 3, Problem 55

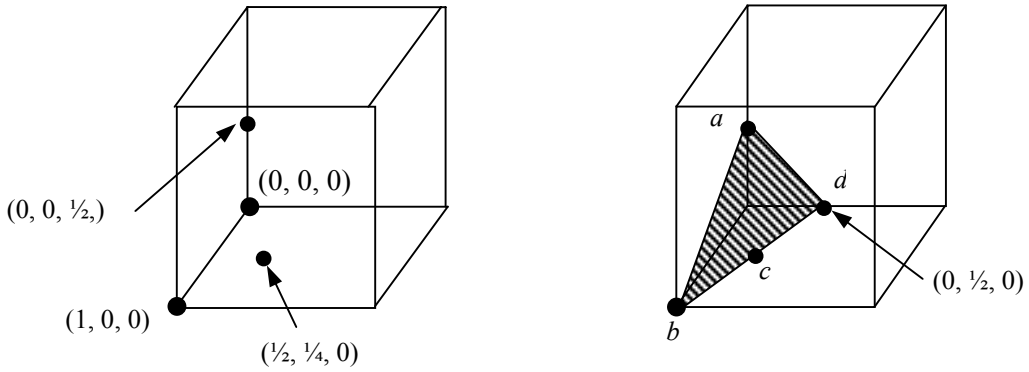
Determine the Miller indices of the cubic crystal plane that intersects the following position coordinates:
$(0,\ 0,\ \frac{1}{2});\ (1,0,0);\ (\frac{1}{2},\frac{1}{4},0)$.

Chapter 3, Solution 55

After locating the three position coordinates, connect points *b* and *c* and extend the line to point *d*. Complete the plane by connecting point *d* to *a* and *a* to *b*. Using

(0, 0, 0) as the plane origin, $x = 1$, $y = ½$ and $z = ½$. The intercept reciprocals are thus $\frac{1}{x} = 1,\ \frac{1}{y} = 2,\ \frac{1}{z} = 2.$

The Miller indices are therefore **(1 2 2)**.



Chapter 3, Problem 56

Rodium is FCC and has a lattice constant *a* of 0.38044 nm. Calculate the following interplanar spacings:
(*a*) d_{111} (*b*) d_{200} (*c*) d_{220}

Chapter 3, Solution 56

(a) $$d_{111} = \frac{0.38044\ \text{nm}}{\sqrt{1^2+1^2+1^2}} = \frac{0.38044\ \text{nm}}{\sqrt{3}} = \mathbf{0.220\ nm}$$

(b) $$d_{200} = \frac{0.38044\ \text{nm}}{\sqrt{2^2+0^2+0^2}} = \frac{0.38044\ \text{nm}}{\sqrt{4}} = \mathbf{0.190\ nm}$$

(c) $$d_{220} = \frac{0.38044\ \text{nm}}{\sqrt{2^2+2^2+0^2}} = \frac{0.38044\ \text{nm}}{\sqrt{8}} = \mathbf{0.135\ nm}$$

Chapter 3, Problem 57

Tungsten is BCC and has a lattice constant a of 0.31648 nm. Calculate the following interplanar spacings: (*a*) d_{110} (*b*) d_{220} (*c*) d_{310}

Chapter 3, Solution 57

(a) $$d_{110} = \frac{0.31648 \text{ nm}}{\sqrt{1^2 + 1^2 + 0^2}} = \frac{0.31648 \text{ nm}}{\sqrt{2}} = \mathbf{0.224\ nm}$$

(b) $$d_{220} = \frac{0.31648 \text{ nm}}{\sqrt{2^2 + 2^2 + 0^2}} = \frac{0.31648 \text{ nm}}{\sqrt{8}} = \mathbf{0.112\ nm}$$

(c) $$d_{310} = \frac{0.31648 \text{ nm}}{\sqrt{3^2 + 1^2 + 0^2}} = \frac{0.31648 \text{ nm}}{\sqrt{10}} = \mathbf{0.100\ nm}$$

Chapter 3, Problem 58

The d_{310} interplanar spacing in a BCC element is 0.1587 nm. (*a*) What is its lattice constant a? (*b*) What is the atomic radius of the element? (*c*) What could this element be?

Chapter 3, Solution 58

(a) $$a = d_{310}\sqrt{h^2 + k^2 + l^2} = (0.1587 \text{ nm})\sqrt{3^2 + 1^2 + 0^2} = \mathbf{0.502\ nm}$$

(b) $$R = \frac{\sqrt{3}a}{4} = \frac{\sqrt{3}(0.502 \text{ nm})}{4} = \mathbf{0.217\ nm}$$

(c) The element is **barium (Ba)**.

Chapter 3, Problem 59

The d_{422} interplanar spacing in an FCC metal is 0.083397 nm. (*a*) What is its lattice constant *a*? (*b*) What is the atomic radius of the metal? (*c*) What could this metal be?

Chapter 3, Solution 58

(a) $a = d_{310}\sqrt{h^2 + k^2 + l^2} = (0.1587 \text{ nm})\sqrt{3^2 + 1^2 + 0^2} = \mathbf{0.502\ nm}$

(b) $R = \dfrac{\sqrt{3}a}{4} = \dfrac{\sqrt{3}(0.502 \text{ nm})}{4} = \mathbf{0.217\ nm}$

(c) The element is **barium (Ba)**.

Chapter 3, Problem 60

How are crystallographic planes indicated in HCP unit cells?

Chapter 3, Solution 60

In HCP unit cells, crystallographic planes are indicated using four indices which correspond to four axes: three basal axes of the unit cell, a_1, a_2, and a_3 , which are separated by 120º; and the vertical *c* axis.

Chapter 3, Problem 61

What notation is used to describe HCP crystal planes?

Chapter 3, Solution 61

HCP crystal planes are described using the Miller-Bravais indices, (*hkil*).

Chapter 3, Problem 62

Draw the hexagonal crystal planes whose Miller-Bravais indices are:

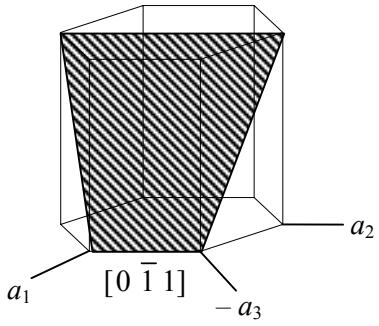
(*a*) $(10\bar{1}1)$ (*d*) $(1\bar{2}12)$ (*g*) $(\bar{1}2\bar{1}2)$ (*j*) $(\bar{1}100)$

(*b*) $(01\bar{1}1)$ (*e*) $(21\bar{1}1)$ (*h*) $(2\bar{2}00)$ (*k*) $(\bar{2}111)$

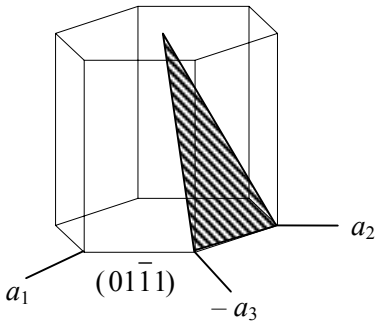
(*c*) $(\bar{1}2\bar{1}0)$ (*f*) $(1\bar{1}01)$ (*i*) $(10\bar{1}2)$ (*l*) $(\bar{1}012)$

Chapter 3, Solution 62

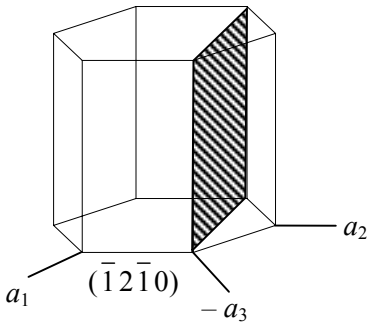
The reciprocals of the indices provided give the intercepts for the plane (a_1, a_2, a_3, and c).



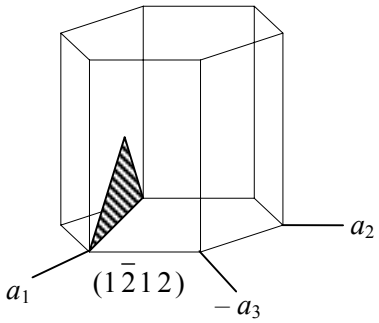
a. $a_1 = 1,\ a_2 = \infty,$
$a_3 = -1,\ c = 1$



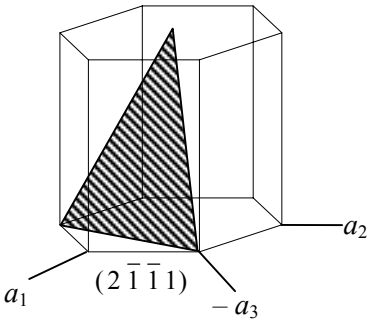
b. $a_1 = \infty,\ a_2 = 1,$
$a_3 = -1,\ c = 1$



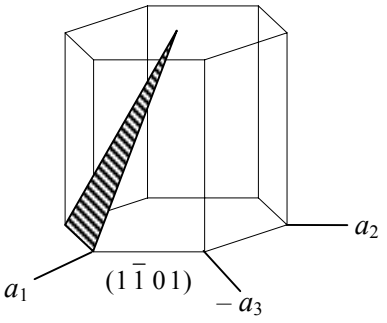
c. $a_1 = 1,\ a_2 = -\frac{1}{2},$
$a_3 = -1,\ c = \infty$



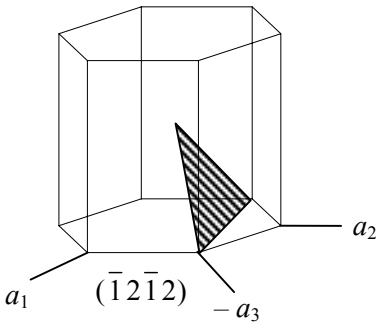
d. $a_1 = 1,\ a_2 = -\frac{1}{2},$
$a_3 = 1,\ c = \frac{1}{2}$



e. $a_1 = \frac{1}{2},\ a_2 = 1,$
$a_3 = -1,\ c = 1$

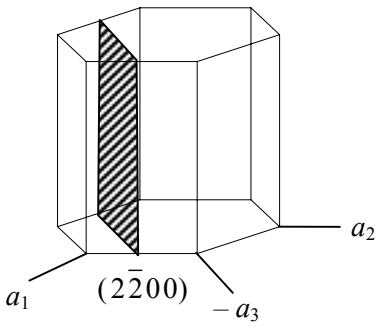


f. $a_1 = 1,\ a_2 = -1,$
$a_3 = \infty,\ c = 1$



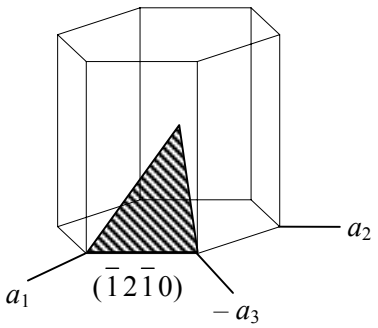
g. $a_1 = -1,\ a_2 = \dfrac{1}{2},$

$a_3 = -1,\ c = \dfrac{1}{2}$



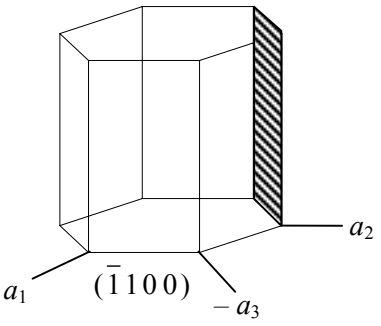
h. $a_1 = \dfrac{1}{2},\ a_2 = -\dfrac{1}{2},$

$a_3 = \infty,\ c = \infty$



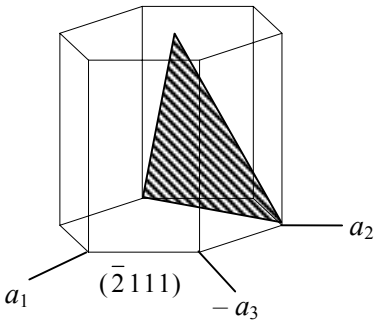
i. $a_1 = 1,\ a_2 = \infty,$

$a_3 = -1,\ c = \dfrac{1}{2}$



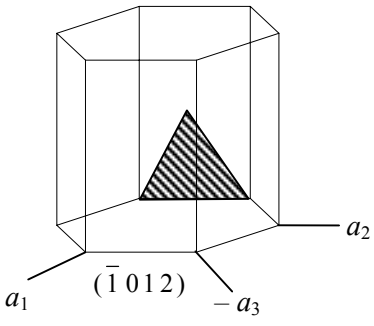
j. $a_1 = -1,\ a_2 = 1,$

$a_3 = \infty,\ c = \infty$



k. $a_1 = -\dfrac{1}{2},\ a_2 = 1,$

$a_3 = 1,\ c = 1$



l. $a_1 = -1,\ a_2 = \infty,$

$a_3 = 1,\ c = \dfrac{1}{2}$

Chapter 3, Problem 63

Determine the Miller-Bravais indices of the hexagonal crystal planes in Fig. P3.63.

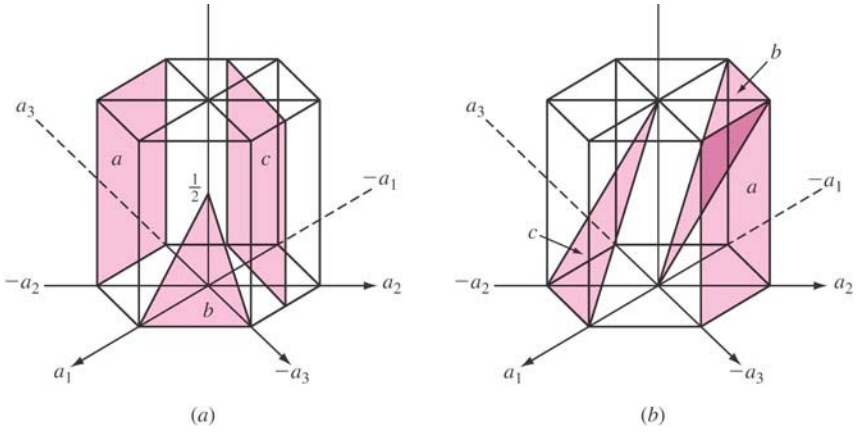


Figure P3.63

Chapter 3, Solution 63

Miller-Bravais Indices for Planes Shown in Figure P3.63(a)

Plane *a*		**Plane *b***		**Plane *c***	
Planar Intercepts	Reciprocals of Intercepts	Planar Intercepts	Reciprocals of Intercepts	Planar Intercepts	Reciprocals of Intercepts
$a_1 = \infty$	$\frac{1}{a_1} = 0$	$a_1 = 1$	$\frac{1}{a_1} = 1$	$a_1 = -½$	$\frac{1}{a_1} = -2$
$a_2 = -1$	$\frac{1}{a_2} = -1$	$a_2 = \infty$	$\frac{1}{a_2} = 0$	$a_2 = ½$	$\frac{1}{a_2} = 2$
$a_3 = 1$	$\frac{1}{a_3} = 1$	$a_3 = -1$	$\frac{1}{a_3} = -1$	$a_3 = \infty$	$\frac{1}{a_3} = 0$
Planar Intercepts	Reciprocals of Intercepts	Planar Intercepts	Reciprocals of Intercepts	Planar Intercepts	Reciprocals of Intercepts
$c = \infty$	$\frac{1}{c} = 0$	$c = ½$	2	$c = \infty$	$\frac{1}{c} = 0$
The Miller indices of plane *a* are $\mathbf{(0\ \bar{1}\ 1\ 0)}$.		The Miller indices of plane *b* are $\mathbf{(1\ 0\ \bar{1}\ 2)}$.		The Miller indices of plane *c* are $\mathbf{(\bar{2}\ 2\ 0\ 0)}$.	

Miller-Bravais Indices for the Planes Shown in Figure P3.63(b)

Plane *a*		**Plane *b***		**Plane *c***	
Planar Intercepts	Reciprocals of Intercepts	Planar Intercepts	Reciprocals of Intercepts	Planar Intercepts	Reciprocals of Intercepts
$a_1 = \infty$	$\frac{1}{a_1} = 0$	$a_1 = 1$	$\frac{1}{a_1} = 1$	$a_1 = 1$	$\frac{1}{a_1} = 1$
$a_2 = 1$	$\frac{1}{a_2} = 1$	$a_2 = -1$	$\frac{1}{a_2} = -1$	$a_2 = -1$	$\frac{1}{a_2} = -1$
$a_3 = -1$	$\frac{1}{a_3} = -1$	$a_3 = \infty$	$\frac{1}{a_3} = 0$	$a_3 = \infty$	$\frac{1}{a_3} = 0$
$c = \infty$	$\frac{1}{c} = 0$	$c = 1$	$\left(\frac{1}{2}, 1, 0\right)$	$c = 1$	$\frac{1}{c} = 1$
The Miller indices of plane *a* are $\mathbf{(0\ 1\ \bar{1}\ 0)}$.		The Miller indices of plane *b* are $\mathbf{(1\ \bar{1}\ 0\ 1)}$.		The Miller indices of plane *c* are $\mathbf{(1\ \bar{1}\ 0\ 1)}$.	

Chapter 3, Problem 64

Determine the Miller-Bravais direction indices of the $-a_1$, $-a_2$, and $-a_3$ directions.

Chapter 3, Solution 64

The Miller-Bravais direction indices corresponding to the $-a_1$, $-a_2$ and $-a_3$ directions are respectively,

$$\left(\frac{1}{4}, 1, \frac{1}{4} \right)$$

Chapter 3, Problem 65

Determine the Miller-Bravais direction indices of the vectors originating at the center of the lower basal plane and ending at the endpoints of the upper basal plane as indicated in Fig. 3.18*d*.

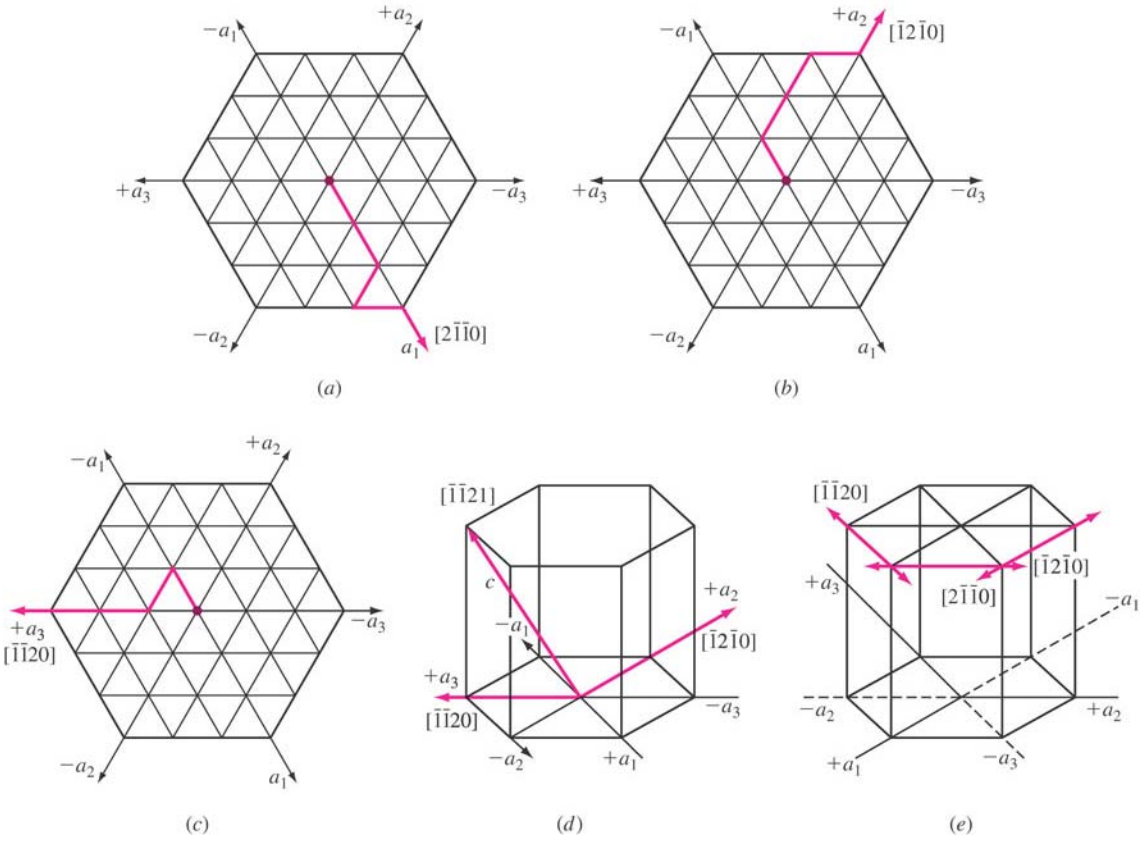
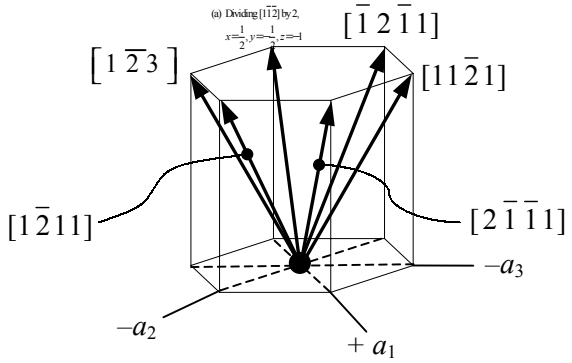


Figure 3.18

Chapter 3, Solution 65

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

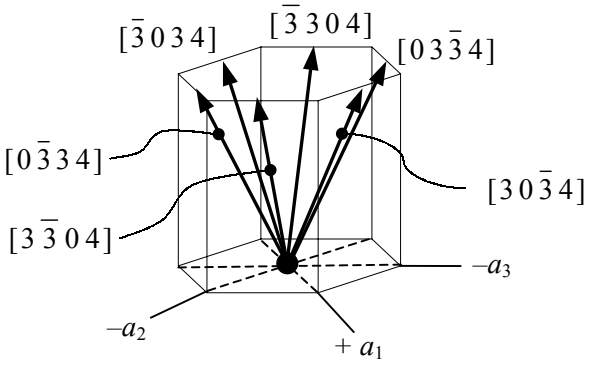


Chapter 3, Problem 66

Determine the Miller-Bravais direction indices of the basal plane of the vectors originating at the center of the lower basal plane and exiting at the midpoints between the principal planar axes.

Chapter 3, Solution 66

$[\bar{3}\,0\,3\,4], [\bar{3}\,3\,0\,4], [0\,3\,\bar{3}\,4],$
$[3\,0\,\bar{3}\,4], [3\,\bar{3}\,0\,4], [0\,\bar{3}\,3\,4]$



Chapter 3, Problem 67

Determine the Miller-Bravais direction indices of the directions indicated in Fig. P3.67.

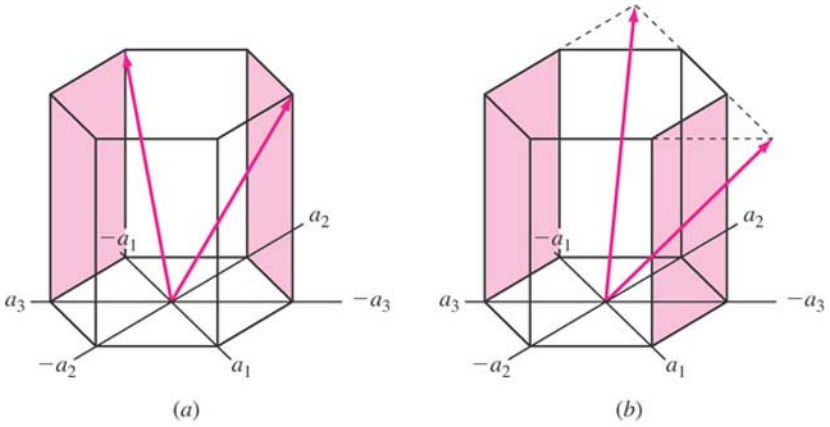
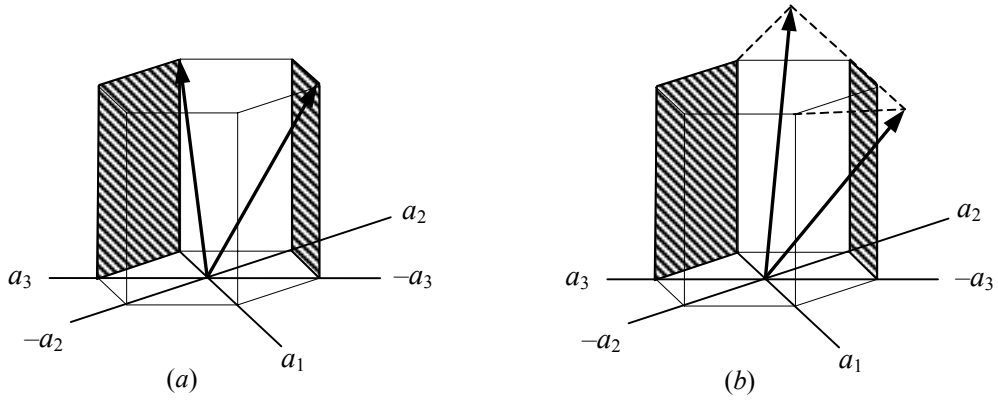


Figure P3.67

Chapter 3, Solution 67



For Fig. P3.67(*a*), the Miller-Bravais direction indices indicated are $[\bar{2}\,1\,1\,1]$ and $[1\,1\,\bar{2}\,1]$. Those associated with Fig. P3.67(*b*) are $[\bar{1}\,1\,0\,1]$ and $[1\,0\,\bar{1}\,1]$.

Chapter 3, Problem 68

What is the difference in the stacking arrangement of close-packed planes in (*a*) the HCP crystal structure and (*b*) the FCC crystal structure?

Chapter 3, Solution 68

Although the FCC and HCP are both close-packed lattices with APF = 0.74, the structures differ in the three dimensional stacking of their planes:

(a) the stacking order of HCP planes is ABAB… ;
(b) the FCC planes have an ABCABC… stacking sequence.

Chapter 3, Problem 69

What are the densest-packed directions in (*a*) the FCC structure and (*b*) the HCP structure?

Chapter 3, Solution 69

(a) The most densely packed planes of the FCC lattice are the **{1 1 1}** planes.
(b) The most densely packed planes of the HCP structure are the **{0 0 0 1}** planes.

Chapter 3, Problem 70

What are the closest-packed directions in (*a*) the FCC structure and (*b*) the HCP structure?

Chapter 3, Solution 70

(a) The closest-packed directions in the FCC lattice are the $\langle \mathbf{1\,\bar{1}\,0} \rangle$ directions.

(b) The closest-packed directions in the HCP lattice are the $\langle \mathbf{1\,1\,\bar{2}\,0} \rangle$ directions.

Chapter 3, Problem 71

The lattice constant for BCC tantalum at 20°C is 0.33026 nm and its density is 16.6 g/cm^3. Calculate a value for its atomic mass.

Chapter 3, Solution 71

The atomic mass can be assessed based upon the mass of tantalum in a unit BCC cell:

$$\begin{aligned}\text{mass/unit cell} &= \rho_v(\text{volume/unit cell}) = \rho_v a^3 \\ &= (16.6\ \text{g/cm}^3)(10^6\ \text{cm}^3/\text{m}^3)(0.33026\times10^{-9}\ \text{m})^3 \\ &= 5.98\times10^{-22}\ \text{g/u.c.}\end{aligned}$$

Since there are two atoms in a BCC unit cell, the atomic mass is:

$$\begin{aligned}\text{Atomic mass} &= \frac{(5.98\times10^{-22}\ \text{g/unit cell})(6.023\times10^{23}\ \text{atoms/mol})}{2\ \text{atoms/unit cell}} \\ &= \mathbf{180.09\ g/mol}\end{aligned}$$

Chapter 3, Problem 72

Calculate a value for the density of FCC platinum in grams per cubic centimeter from its lattice constant *a* of 0.39239 nm and its atomic mass of 195.09 g/mol.

Chapter 3, Solution 72

First calculate the mass per unit cell based on the atomic mass and the number of atoms per unit cell of the FCC structure,

$$\text{mass/unit cell} = \frac{(4\ \text{atoms/unit cell})(195.09\ \text{g/mol})}{6.023\times10^{23}\ \text{atoms/mol}} = 1.296\times10^{-21}\text{g/unit cell}$$

The density is then found as,

$$\rho_v = \frac{\text{mass/unit cell}}{\text{volume/unit cell}} = \frac{\text{mass/unit cell}}{\text{a}^3} = \frac{1.296\times10^{-21}\ \text{g/unit cell}}{[(0.39239\times10^{-9}\ \text{m})^3]/\text{unit cell}}$$

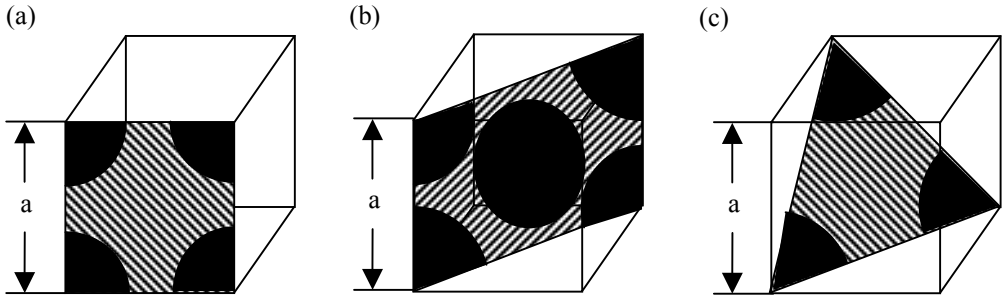
$$= 21,445,113\ \text{g/m}^3\left(\frac{\text{m}}{100\ \text{cm}}\right)^3 = \mathbf{21.45\ g/cm^3}$$

Chapter 3, Problem 73

Calculate the planar atomic density in atoms per square millimeter for the following crystal planes in BCC chromium, which has a lattice constant of 0.28846 nm: (*a*) (100), (*b*) (110), (*c*) (111).

Chapter 3, Solution 73

(Solution C is on the next page.)



To calculate the density, the planar area and the number of atoms contained in that area must first be determined.

(a) The area intersected by the (1 0 0) plane inside the cubic unit cell is a^2 while the number of atoms contained is: (4 corners)× (¼ atom per corner) = 1 atom. The density is,

$$\rho_p = \frac{\text{equiv. no. of atoms whose centers are intersected by selected area}}{\text{selected area}}$$

$$= \frac{1 \text{ atom}}{(0.28846\times10^{-9}\text{ m})^2} = (1.202\times10^{19}\text{atoms/m}^2)\left(\frac{\text{m}}{1000\text{ mm}}\right)^2$$

$$= \mathbf{1.202\times10^{13}\ atoms/mm^2}$$

(b) For the more densely packed (1 1 0) plane, there are:

1 atom at center + (4 corners) × (¼ atom per corner) = 2 atoms

And the area is given as $(\sqrt{2}a)(a) = \sqrt{2}a^2$. The density is thus,

$$\rho_p = \frac{2 \text{ atoms}}{\sqrt{2}(0.28846\times10^{-9}\text{ m})^2} = (1.699\times10^{19}\text{atoms/m}^2)(10^{-6}\text{ m}^2/\text{mm}^2)$$

$$= \mathbf{1.699\times10^{13}\ atoms/mm^2}$$

(c) The triangular (1 1 1) plane contains: (3 corners) × ($^1/_6$ atom per corner) = ½ atom.

The area is equal to $= \frac{1}{2}bh = \frac{1}{2}(\sqrt{2}a)\left(\frac{\sqrt{3}}{2}a\right) = \frac{\sqrt{6}}{4}a^2$. The density is thus,

$$\rho_p = \frac{1/2 \text{ atom}}{\frac{\sqrt{6}}{4}(0.28846\times10^{-9}\text{ m})^2} = (9.813\times10^{18}\text{atoms/m}^2)(10^{-6}\text{ m}^2/\text{mm}^2)$$

$$= \mathbf{9.813\times10^{12}\ atoms/mm^2}$$

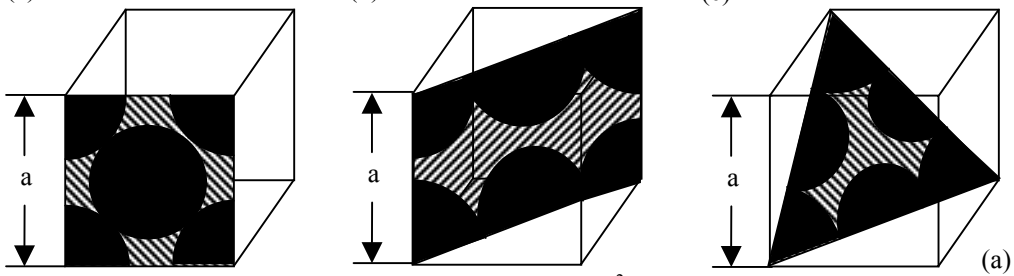
Chapter 3, Problem 74

Calculate the planar atomic density in atoms per square millimeter for the following crystal planes in FCC gold, which has a lattice constant of 0.40788 nm: (*a*) (100), (*b*) (110), (*c*) (111).

Chapter 3, Solution 74

(Solutions B and C are on the next page.)

(a) (b) (c)



(a) The area intersected by the (1 0 0) plane and the FCC unit cell is a^2 while the number of atoms contained is:

1 atom at center + (4 corners) × (¼ atom per corner) = 2 atoms

The density is therefore,

$$\rho_p = \frac{\text{equiv. no. of atoms whose centers are intersected by selected area}}{\text{selected area}}$$

$$= \frac{2 \text{ atoms}}{(0.40788\times10^{-9}\text{ m})^2} = (1.202\times10^{19}\text{atoms/m}^2)\left(\frac{\text{m}}{1000\text{ mm}}\right)^2$$

$$= \mathbf{1.20\times10^{13}\ atoms/mm^2}$$

(b) For the more densely packed (1 1 0) plane, there are:

(2 face atoms) × (½ atom) + (4 corners) × (¼ atom per corner) = 2 atoms

And the area is given as $(\sqrt{2}a)(a) = \sqrt{2}a^2$. The density is thus,

$$[\ \bar{1}\quad 1\quad \bar{1}\ ]$$

(c) The triangular (1 1 1) plane contains:

(3 face atoms × ⅓ atom) + (3 corners) × ($^1/_6$ atom per corner) = 2 atoms

The area is equal to: $= \frac{1}{2}bh = \frac{1}{2}(\sqrt{2}a)\left(\frac{\sqrt{3}}{2}a\right) = \frac{\sqrt{6}}{4}a^2$. The density is therefore,

$$\rho_p = \frac{2 \text{ atoms}}{\frac{\sqrt{6}}{4}(0.40788\times10^{-9}\ \text{m})^2} = (1.963\times10^{19}\text{atoms/m}^2)(10^{-6}\ \text{m}^2/\text{mm}^2)$$

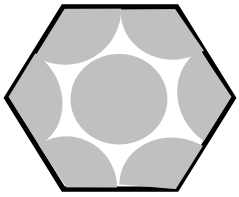
$$= \mathbf{1.963\times10^{13}\ atoms/mm^2}$$

Chapter 3, Problem 75

Calculate the planar atomic density in atoms per square millimeter for the (0001) plane in HCP beryllium, which has a lattice constant a = 0.22856 nm and a c constant of 0.35832 nm.

Chapter 3, Solution 75

The area intersected by the (0 0 0 1) plane and the HCP unit cell is simply the basal area, shown in the sketch to the right:



$$\text{Selected Area} = (6 \text{ triangles}) \times (\text{equilateral triangle area}) = 6\left(\frac{1}{2}a\right)\left(\frac{\sqrt{3}}{2}a\right) = \frac{3\sqrt{3}}{2}a^2$$

While the number of atoms contained is:

1 atom at center + (6 corners) × (⅓ atom per corner) = 3 atoms

The density is therefore,

$$\rho_p = \frac{\text{equiv. no. of atoms whose centers are intersected by selected area}}{\text{selected area}}$$

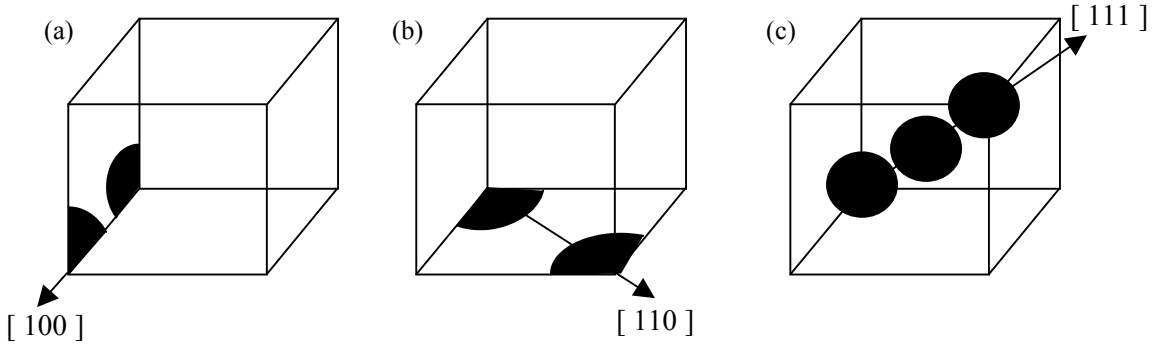
$$= \frac{3 \text{ atoms}}{\frac{3\sqrt{3}}{2}(0.22856 \times 10^{-9} \text{ m})^2} = (2.201 \times 10^{19} \text{atoms/m}^2)\left(\frac{\text{m}}{1000 \text{ mm}}\right)^2$$

$$= \mathbf{2.21 \times 10^{13} \text{ atoms/mm}^2}$$

Chapter 3, Problem 76

Calculate the linear atomic density in atoms per millimeter for the following directions in BCC vanadium, which has a lattice constant of 0.3039 nm: (*a*) [100], (*b*) [110], (*c*) [111].

Chapter 3, Solution 76



In general, the linear atomic density is derived from:

$$\rho_l = \frac{\text{no. of atomic diam. intersected by selected length of direction line}}{\text{selected length of line}}$$

(a) For the [100] direction of BCC vanadium,

$$\rho_l = \frac{\text{no. atom dia.}}{\text{a}} = \frac{1 \text{ atom}}{(0.3039 \text{ nm})(10^{-9} \text{ m/nm})(10^{3} \text{ mm/m})} = \mathbf{3.29 \times 10^{6} \text{ mm}}$$

(b) For the [110] direction of BCC vanadium,

$$\rho_l = \frac{\text{no. atom dia.}}{\sqrt{2}a} = \frac{1 \text{ atom}}{\sqrt{2}(0.3039 \text{ nm})(10^{-6} \text{ mm/nm})} = \mathbf{2.33 \times 10^{6} \text{ mm}}$$

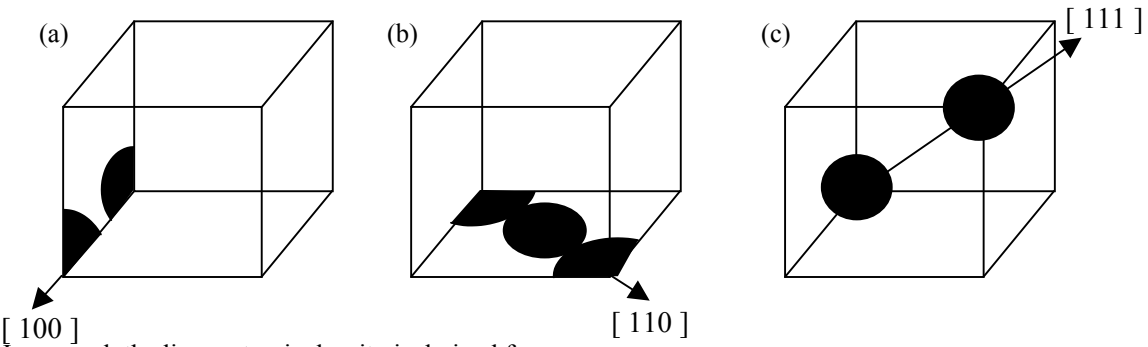
(c) For the [111] direction of BCC vanadium,

$$\rho_l = \frac{\text{no. atom dia.}}{\sqrt{3}a} = \frac{2 \text{ atoms}}{\sqrt{3}(0.3039 \text{ nm})(10^{-6} \text{ mm/nm})} = \mathbf{3.80 \times 10^{6} \text{ mm}}$$

Chapter 3, Problem 77

Calculate the linear atomic density in atoms per millimeter for the following directions in FCC iridium, which has a lattice constant of 0.38389 nm: (*a*) [100], (*b*) [110], (*c*) [111].

Chapter 3, Solution 77



In general, the linear atomic density is derived from:

$$\rho_l = \frac{\text{no. of atomic diam. intersected by selected length of direction line}}{\text{selected length of line}}$$

(a) For the [100] direction of FCC iridium,

$$\rho_l = \frac{\text{no. atom dia.}}{\text{a}} = \frac{1 \text{ atom}}{(0.38389 \text{ nm})(10^{-6} \text{ mm/nm})} = \mathbf{2.60 \times 10^6 \text{ mm}}$$

(b) For the [110] direction of FCC iridium,

$$\rho_l = \frac{\text{no. atom dia.}}{\sqrt{2}a} = \frac{2 \text{ atoms}}{\sqrt{2}(0.38389 \text{ nm})(10^{-6} \text{ mm/nm})} = \mathbf{3.68 \times 10^6 \text{ mm}}$$

(c) For the [111] direction of FCC iridium,

$$\rho_l = \frac{\text{no. atom dia.}}{\sqrt{3}a} = \frac{1 \text{ atom}}{\sqrt{3}(0.38389 \text{ nm})(10^{-6} \text{ mm/nm})} = \mathbf{1.50 \times 10^6 \text{ mm}}$$

Chapter 3, Problem 78

What is polymorphism with respect to metals?

Chapter 3, Solution 78

A metal is considered polymorphic if it can exist in more than one crystalline form under different conditions of temperature and pressure.

Chapter 3, Problem 79

Titanium goes through a polymorphic change from BCC to HCP crystal structure upon cooling through 332°C. Calculate the percentage change in volume when the crystal structure changes from BCC to HCP. The lattice constant a of the BCC unit cell at 882°C is 0.332 nm, and the HCP unit cell has a = 0.2950 nm and c = 0.4683 nm.

Chapter 3, Solution 79

To determine the volume change, the individual volumes per atom for the BCC and HCP structures must be calculated:

$$V_{BCC} = \frac{a^3 \text{ nm}^3/\text{unit cell}}{2 \text{ atoms/unit cell}} = \frac{(0.332 \text{ nm})^3}{2 \text{ atoms}} = 0.0183 \text{ nm}^3/\text{atom}$$

$$V_{HCP} = \frac{(3a^2\text{c})(\sin 60^\text{o}) \text{ nm}^3/\text{unit cell}}{6 \text{ atoms/unit cell}} = \frac{(3)(0.2950 \text{ nm})^2(0.4683 \text{ nm})(\sin 60^\text{o})}{6 \text{ atoms}}$$

$$= 0.01765 \text{ nm}^3/\text{atom}$$

Thus the change in volume due to titanium's allotropic transformation is,

$$\% \text{ Volume change} = \frac{V_{HCP} - V_{BCC}}{V_{BCC}}(100\%)$$

$$= \frac{0.01765 \text{ nm}^3/\text{atom} - 0.0183 \text{ nm}^3/\text{atom}}{0.0183 \text{ nm}^3/\text{atom}}(100\%) = \mathbf{-3.55\%}$$

Chapter 3, Problem 80

Pure iron goes through a polymorphic change from BCC to FCC upon heating through 912°C. Calculate the volume change associated with the change in crystal structure from BCC to FCC if at 912°C the BCC unit cell has a lattice constant a = 0.293 nm and the FCC unit cell a = 0.363 nm.

Chapter 3, Solution 80

First determine the individual volumes per atom for the iron BCC and FCC crystal structures:

$$V_{BCC} = \frac{a^3 \text{ nm}^3/\text{unit cell}}{2 \text{ atoms/unit cell}} = \frac{(0.293 \text{ nm})^3}{2 \text{ atoms}} = 0.01258 \text{ nm}^3/\text{atom}$$

$$V_{FCC} = \frac{a^3 \text{ nm}^3/\text{unit cell}}{4 \text{ atoms/unit cell}} = \frac{(0.363 \text{ nm})^3}{4 \text{ atoms}} = 0.01196 \text{ nm}^3/\text{atom}$$

Thus the change in volume due to iron's allotropic transformation is,

$$\% \text{ Volume change} = \frac{V_{FCC} - V_{BCC}}{V_{BCC}}(100\%) = \frac{0.01196 \text{ nm}^3/\text{atom} - 0.01258 \text{ nm}^3/\text{atom}}{0.01258 \text{ nm}^3/\text{atom}}(100\%)$$

$$= \mathbf{-4.94\%}$$