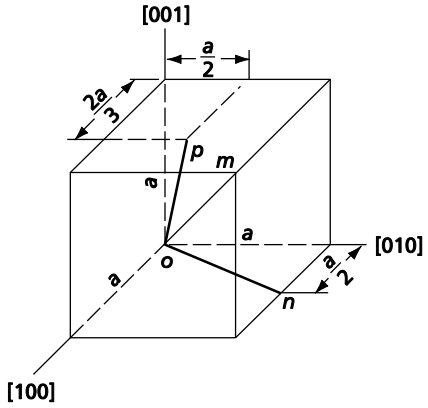
CHAPTER 1 THE STRUCTURE OF METALS

1.1 Determine the direction indices for (a) line *om*, (b) line *on*, and (c) line *op* in the accompanying drawing of a cubic unit cell.



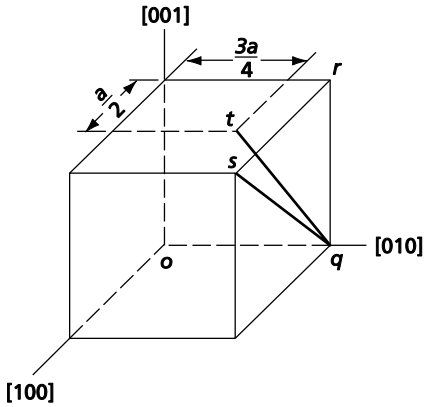
Solution:

(a) The direction indices for line *om* are [111].

(b) The vector components of line *on*, in units of $a = 1$, are $\frac{1}{2}$, 1 and 0 along the x, y and z axes respectively. The corresponding direction indices are accordingly [120].

(c) The components of line *op* are $\frac{2}{3}$, $\frac{1}{2}$, and $\frac{1}{1}$. Thus the indices are [436].

1.2 Determine the direction indices of lines (a) *qr*, (b) *qs*, and (c) *qt*.



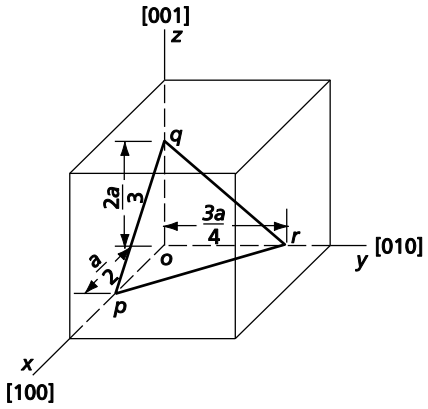
Solution:

(a) The direction indices of line *qr* are [001].

(b) The direction indices of line *qs* are [101].

(c) The direction indices of line *qt* along the x, y and z axes are $\frac{1}{2}$, $\frac{1}{4}$, and $\frac{1}{1}$, yielding the indices $[2\bar{1}4]$.

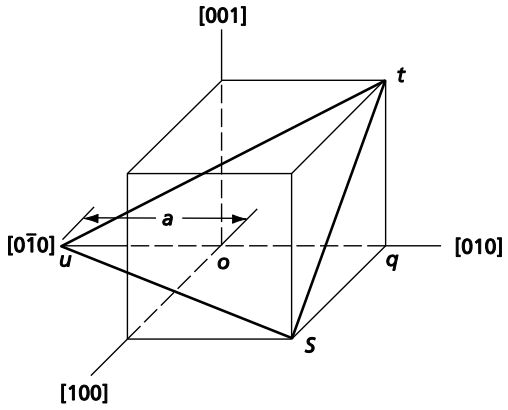
1.3 In this figure, plane *pqr* intercepts the x, y, and x axes as indicated. What are the Miller indices of this plane?



Solution:

The intercepts of plane *pqr* with the three axes are $\frac{1}{2}$, $\frac{3}{4}$, and $\frac{2}{3}$ with the reciprocals $\frac{1}{\frac{1}{2}}$, $\frac{1}{\frac{3}{4}}$, and $\frac{1}{\frac{1}{3}}$, so that the Miller indices of the plane are (12 8 9).

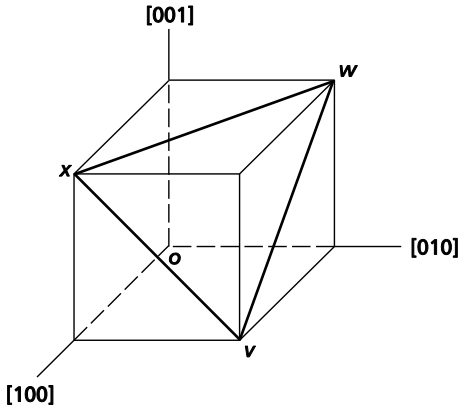
1.4 What are the Miller Indices of plane *stu*?



Solution:

This plane has intercepts $\frac{1}{2}$, -1 and $\frac{1}{2}$, so that the Miller idices are $[2\bar{1}2]$.

1.5 Write the Miller indices for plane *vwx*.



Solution:

On the assumption that parallel planes can be described by the same set of Miller indices, this plane should have the same indices as plane (C) of Fig. 1.16, which are (111).

1.6 Linear density in a given crystallogrphic direction represents the fraction of a line length that is occupied by atoms. Similarly, planar density is the fraction of a crystallographic plane occupied by atsom. The fraction of the volume occupied in a unit cell, on the other hand, is called the

atomic packing factor. The latter should not be confused with bulk densirt, which represents weight per unit volume.

(a) Calculate the linear density in the [100], [110], and [111] directions in body-ccentered cubic (bcc) and face-centered cubic (fcc) structures.

(b) Calculate planar densities in (100), (110), and (111) planes in bcc and fcc structires.

(c) Show that atomic packing factors for bcc, fcc, and hexagonal close-packed (hcp) structures are 0.68, 0.74, and 0.74, respectively.

Solution:

(a) Refering to the hard ball model of BCC structure shown in Fig 1.1c, it can be seen that the atoms touch each other along the diagonal, [111] direction, of the unit cell. Taking R as radius of the atom, its length is equal to 4R. The lattic parameter, is therefore $a = \frac{4R}{\sqrt{3}}$. The edge of the unit cell, [100], is occupied by two half atoms. The linear density in [100] direction is:

$$LD_{[100]} = \frac{2R}{4R/\sqrt{3}} = 0.866$$

For the [110] direction, the length of the diagonal of the cube face is $\sqrt{2}\,a$, which is again occupied by two half atoms.

$$LD_{[110]} = \frac{2R}{\sqrt{2}\,a} = \frac{2R}{\sqrt{2}\times 4R/\sqrt{3}} = 0.612$$

The linear density along [111] direction of BCC is obviously 1.

For FCC unit cell, the atoms touch each other along [110] direction, as can be seen in Fig 1.2B. The lattice parameter is therefore $a = 4R/\sqrt{2}$, and the unit cell diagonal is $\sqrt{3}a = \frac{4\sqrt{3}R}{\sqrt{2}}$. Therefore:

$$LD_{[100]} = \frac{2R}{4R/\sqrt{2}} = 0.707$$

$$LD_{[110]} = 1$$

$$LD_{[111]} = \frac{2R}{4\sqrt{3}R/\sqrt{2}} = 0.408$$

(b) The (100) face of the BCC unit cell, with an area of a^2, is occupied by 4 quarter circle areas. Therefore:

$$PD_{[100]} = \frac{4\,x\frac{1}{4}x\,\pi R^2}{a^2} = \frac{\pi R^2}{(4R/\sqrt{3})^2} = 0.589$$

The [110] plane of BCC has an area of $\sqrt{2}\,a^2$. This plane is occupied by two circles (4 quarter circles + 1). Therefore:

$$PD_{[110]} = \frac{2\pi R^2}{\sqrt{2}(4R/\sqrt{3})^2} = 0.833$$

For FCC structure, the [100] face is occupied by 2 circles (4 quarter circles + 1).

$$PD_{[100]} = \frac{2\pi R^2}{a^2} = \frac{2\pi R^2}{(4R/\sqrt{2})^2} = 0.785$$

The [110] plane of FCC again has 2 circles (4 quarter circles + 2 half circles). It's planar density is therefore:

$$PD_{[110]} = \frac{2\pi R^2}{a \times \sqrt{2}a} = \frac{2\pi R^2}{\sqrt{2}(4R/\sqrt{2})^2} = 0.555$$

(c) The volume of a BCC unit cell is $a^3 = (4R/\sqrt{3})^3 = \frac{64R^3}{3\sqrt{3}}$. The unit cell contains 2 atoms (1 center atom + 8 quarter corner atoms). The packing factor is therefore:

$$PF_{[BCC]} = \frac{2 \times 4/3\,\pi R^3}{64R^3/3\sqrt{3}} = 0.68$$

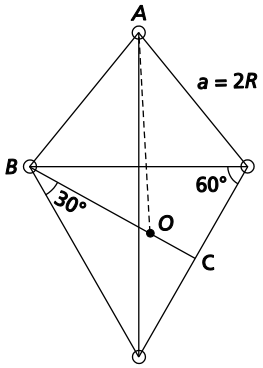
The unit cell of FCC structure contains 4 atoms (8 quarter atoms in corners + 6 half atoms at the center of the faces).

$$PF_{[FCC]} = \frac{4 \times 4/3\,\pi R^3}{a^3} = \frac{4 \times 4/3\,\pi R^3}{(4R/\sqrt{2})^3} = 0.74$$

Since HCP has the same packaging as FCC, its packafing factor is also 0.74. this can also be calculated following Problem 1.7, by calculating the volume of the unit cell and considering that

each unit cell contains 6 atoms (3 central atoms + 2 half atoms at the center of each base + 12 one sixth atoms on the corners).

1.7 Consider the three central atoms with the one at the center of the top plane in Fig 1.16. These four atoms, which all touch each other, form an equilateral tethedron with edges equal to 2R.



Solution:

$$BC = a \sin 60 = {\sqrt{3}\,a}/{a}$$

$$BO = {2}/{3}\,BC = {\sqrt{3}\,a}/{3}$$

$$AO = \sqrt{AB^2 - AO^2} = \sqrt{{2}/{3}}\,a$$

$$C = 2\,AO = 2\sqrt{{2}/{3}}\,a$$

$${C}/{a} = 2\sqrt{{2}/{3}} = 1.63$$

1.8 Iron has a bcc structure at room temperature. When heated, it transforms from bcc to fcc at 1185/K. The atomic radii of iron atoms at this temperature are 0.126 and 0.129 nm for bcc and fcc, respectively. What is the percentage volume change upon transformation from bcc to fcc?

Solution:

Each unit cell of BCC iron contains 2 atoms. The volume of the unit cell is $a^3 = \left(\frac{4R}{\sqrt{3}}\right)^3$. The volume occupied by each atom is therefore $a^3/2 = \frac{1}{2}\left(\frac{4R}{\sqrt{3}}\right)^3$. Substituting 0.126 nm for R results in:

Volume occupied per atom in BCC = 0.01232 $\mathbf{nm^3}$

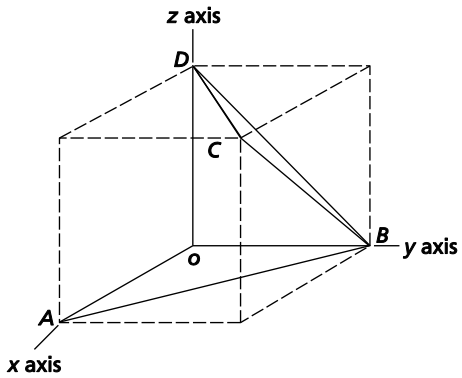
In FCC, the lattice parameter is equal to $4R/\sqrt{2}$, and each unit cell contains four atoms. Therefore:

$$\text{Volume occupied per atom in FCC} = \frac{a^3}{4} = 0.01214\ \mathbf{nm^3}$$

$$\%\text{ volume change} = \frac{(0.0121 - 0.0123)100}{0.0123} = -1.4\%$$

Iron shrinks by 1.4% as it transforms from BCC to FCC at 1185 K.

1.9 This diagram shows the Thompson Tetrahedron, which is a geometrical figure formed by the four cubic {111} planes. It has special significance with regard to plastic deformation in face-centered cubic metals. The corners of the tetrahedron are marked with the letters A, B, C, and D. The four surfaces of the tetrahedron are defined by the triangles ABC, ABD, ACD, and BCD. Assume that the cube in the above figure corresponds to a face-centered cubic unit cell and indentify the planes, corresponding to each of the four surfaces, in terms of their proper Miller indices.



Solution:

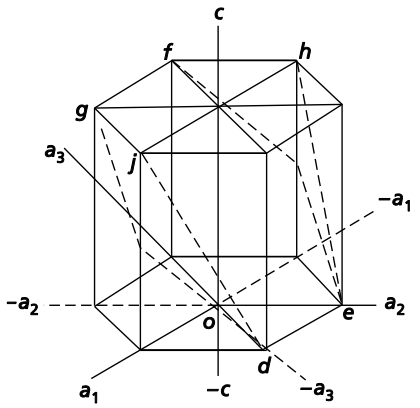
(a) The indices of plane ABD are (111).

(b) The indices of plane ABC are $(1\bar{1}\bar{1})$.

(c) The indices of plane ADC are $(1\bar{1}1)$.

(d) The indices of plane BCD are $(\bar{1}11)$.

1.10 The figure accompanying this problem is normally used to represent the unit cell of a close-packed hexagonal metal. Determine Miller indices for the two planes *defg* and *dehj*, that are outlined in this drawing

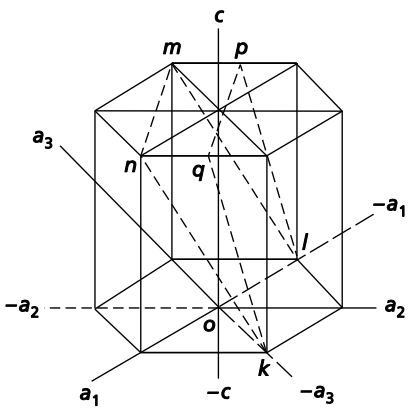


Solution:

(a) Plane *dehj* is parallel to the a_1 axis and may be assumed to intercept it at infinity. It intercepts the a_2 axis at + 1, the a_3 at – 1 and the c axis at + 1. This conforms to the Miller indices $\mathbf{[01\bar{1}1]}$.

(b) Plane *defg* makes indentical intercepts with a_1, a_2, and a_3. However, it intercepts the c axis at $+\frac{1}{2}$. The Miller indices for this latter plane are accordingly $\mathbf{[01\bar{1}2]}$.

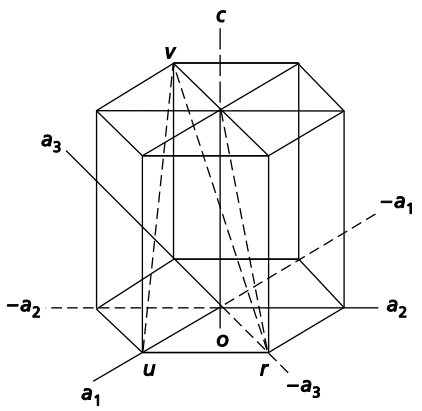
1.11 Two other hexagonal close-paced planes are indicated in this sketch. What are their Miller indices?



Solution:

Both plane *klmn* and *klpq* have basal plane intercepts; a_1 at – 1, a_2 at $\frac{1}{2}$, and a_3 at – 1, while their *c* axis intercepts are + 1 for *klpq* and + $\frac{1}{2}$ for *klmn*. Thus, the indices are $[\bar{1}2\bar{1}1]$ and $[\bar{1}2\bar{1}2]$ respectively.

1.12 Determine the hexagonal close-packed lattice directions of the lines *rt*, *ut*, and *uv* in the figure for this problem. To do this, first determine the vector projection of a line in the basal plane and then add it to the *c* axis projection of the line. Note that the direction indices of the *c* axis are [0001], and that if [0001] is considered a vector its magnitude will equal the height of the unit cell. A unit distance along a diagonal axis of Type I, such as the distance *or*, equals one third of the length of $[2\bar{1}\bar{1}0]$ in Fig. 1.20. The magnitude of this unit is thus equal to $\frac{1}{3[2\bar{1}\bar{1}0]}$. Combine these two quantities to obtain the direction indices of each of the lines.



Solution:

(a) Consider line *rt*. The basal plane projection of this line equals $\frac{1}{3}[\bar{1}\bar{1}20]$ while its c axis projection is [0001]. Adding these two components yeilds:

$$\frac{1}{3}[\bar{1}\bar{1}20] + [0001] = \frac{1}{3}[\bar{1}\bar{1}23].$$

(b) In the case of line *ut* we have:

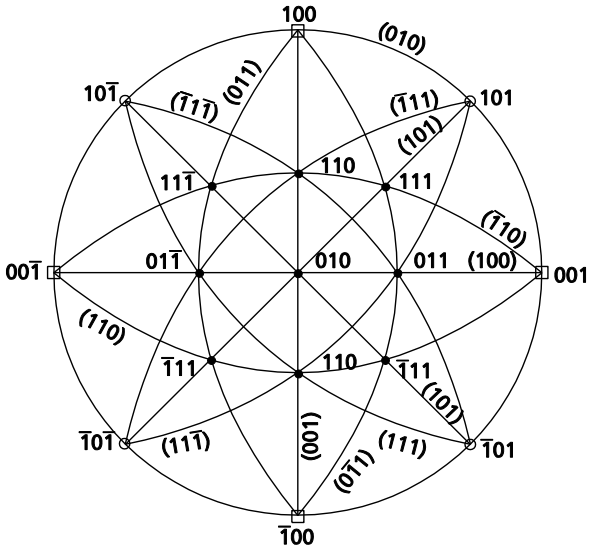
$$\frac{1}{3}[2\bar{1}\bar{1}0] + [0001] = \frac{1}{3}[2\bar{1}\bar{1}3].$$

(c) Finally for line *uv*, the basal plane projectio for this line equals $[1010]$ the addition of this vector to the *c* axis projection is:

$$[\bar{1}010] + [0001] = [\bar{1}011].$$

1.13 Place a piece of tracing paper over the Wulff net as described above, and draw an index mark on the tracing paper over the north pole of the Wulff net. Then draw on the tracing paper the proper symbols that identify the three <100> cube poles, the six <110> poles, and the four <111> octahedral poles as in Fig. 1.33. On the assumption that the basic circle is the [010] plane and that the north pole is [100], mark on the tracing paper the correct Miller indices of all of the <100>, <110>, and <111> poles. Draw in the great circles corresponding to the planes of the plotted poles (see Fig. 1.33). Finally, indentify these planes with their Miller indices.

Solution:

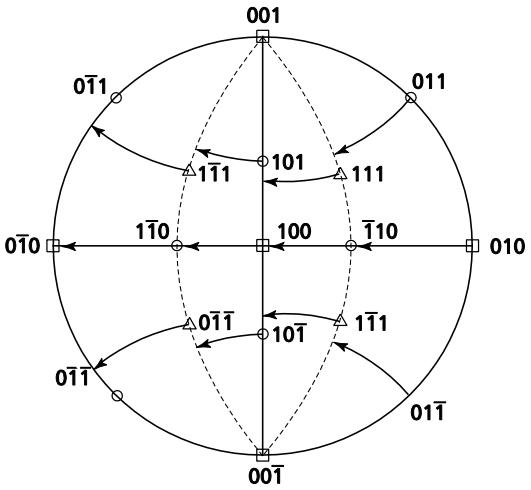


1.14 Place a piece fo tracing paper over the Wulff net and draw on it the index mark at the north pole of the net as well as the basic circle. Mark on this tracing paper all of the poles shown in order to obtain a 100 standard projection. Now rotate this standard projection about the north-south polar axis by 45°, so that the [110] pole moves to the center of the stereographic projection. In this rotation all of the other poles should also be moved through 45° alond the small circles, of the Wulff net, on which they lie. This type of rotation is facillitated by placing a second sheet of tracing paper over the first, and by plotting the rotated data on this sheet. This

exercise shows one of the basic rotations that can be made with a stereographic projection. The other primary rotation involves a simple rotation of the tracing paper around the pin passing through the centeres of both the tracing paper and the Wulff net.

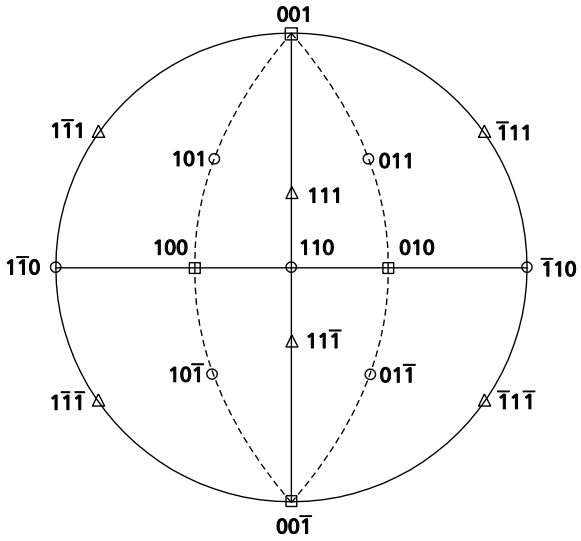
Solution:

Part I



In the above figure, the 45° rotation of the poles along the small circles of the Wulff net are shown.

Part II



The resulting orientations of the poles, after the 45° rotation, are plotted in this stereographic projection.