Example: Copper has an atomic radius of 0.128 nm, an FCC crystal structure, and an atomic weight of 63.5 g/mol. Compute its theoretical density and compare the answer with its measured density.

Solution

Equation 3.5 is employed in the solution of this problem. Since the crystal structure is FCC, *n*, the number of atoms per unit cell, is 4. Furthermore, the atomic weight is given as 63.5 g/mol.The unit cell volume for FCC was determined in Example Problem 3.1 as where *R*, the atomic radius, is 0.128 nm.

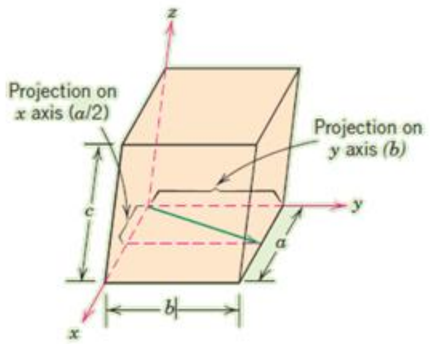
$$\rho = \frac{nA_{Cu}}{V_C N_A} = \frac{nA_{Cu}}{(16R^3\sqrt{2})N_A}$$

$$= \frac{(4\ \text{atoms/unit cell})(63.5\ \text{g/mol})}{[16\sqrt{2}(1.28 \times 10^{-8}\ \text{cm})^3/\text{unit cell}](6.023 \times 10^{23}\ \text{atoms/mol})}$$

$$= 8.89\ \text{g/cm}^3$$

Substitution for the various parameters into Equation 3.5 yields The literature value for the density of copper is 8.94 g/cm3, which is in very close agreement with the foregoing result.

Example: Determine the indices for the direction shown in the accompanying figure.



Solution

The vector, as drawn, passes through the origin of the coordinate system, and therefore no translation is necessary. Projections of this vector onto the *x*, *y*, and *z* axes are, respectively, *a*/2, *b*, and 0*c*, which become $\frac{1}{2}$, 1, and 0 in terms of the unit cell parameters (i.e., when the *a*, *b*, and *c* are dropped). Reduction of these numbers to the lowest set of integers is accompanied by multiplication of each by the factor 2. This yields the integers 1, 2, and 0, which are then enclosed in brackets as [120].

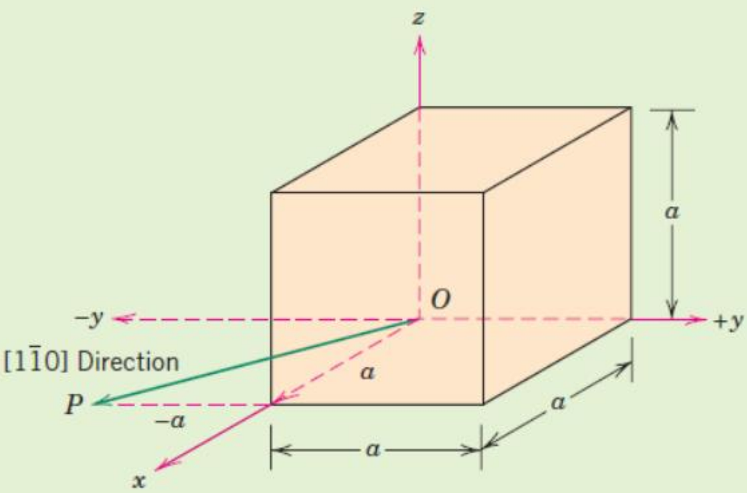
This procedure may be summarized as follows:

	x	y	z
Projections	$a/2$	b	$0c$
Projections (in terms of a, b, and c)	$\frac{1}{2}$	1	0
Reduction	1	2	0
Enclosure		[120]	

Draw a $[1\bar{1}0]$ direction within a cubic unit cell.

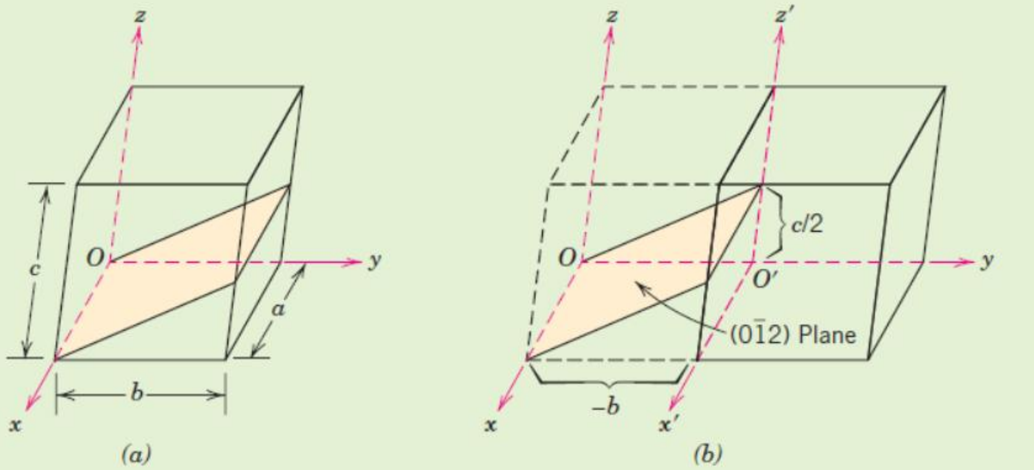
Solution

First construct an appropriate unit cell and coordinate axes system. In the accompanying figure the unit cell is cubic, and the origin of the coordinate system, point O, is located at one of the cube corners.



This problem is solved by reversing the procedure of the preceding example. For this $[1\bar{1}0]$ direction, the projections along the x, y, and z axes are a, $-a$, and $0a$, respectively. This direction is defined by a vector passing from the origin to point P, which is located by first moving along the x axis a units, and from this position, parallel to the y axis $-a$ units, as indicated in the figure. There is no z component to the vector, since the z projection is zero.

Determine the Miller indices for the plane shown in the accompanying sketch (*a*).

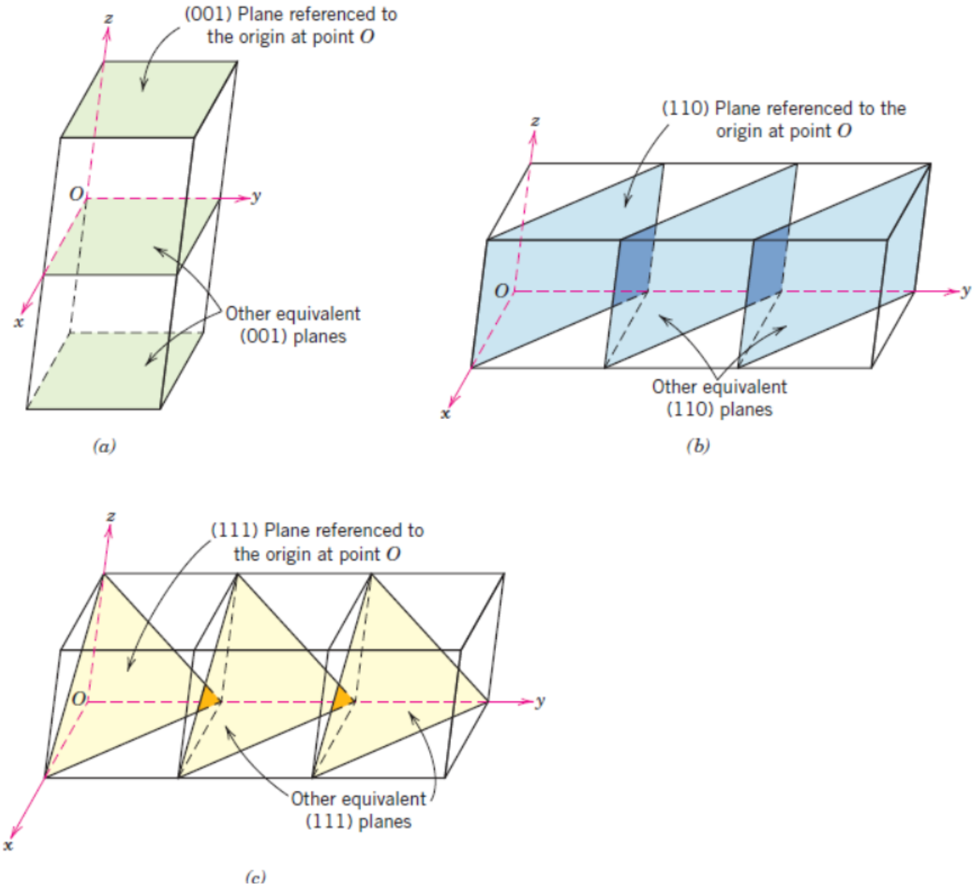


Solution

Since the plane passes through the selected origin O, a new origin must be chosen at the corner of an adjacent unit cell, taken as O' and shown in sketch (*b*). This plane is parallel to the x axis, and the intercept may be taken as ∞a. The y and z axes intersections, referenced to the new origin O', are $-b$ and $c/2$, respectively. Thus, in terms of the lattice parameters a, b, and c, these intersections are ∞, -1, and $\frac{1}{2}$. The reciprocals of these numbers are 0, −1, and 2; and since all are integers, no further reduction is necessary. Finally, enclosure in parentheses yields $(0\bar{1}2)$.

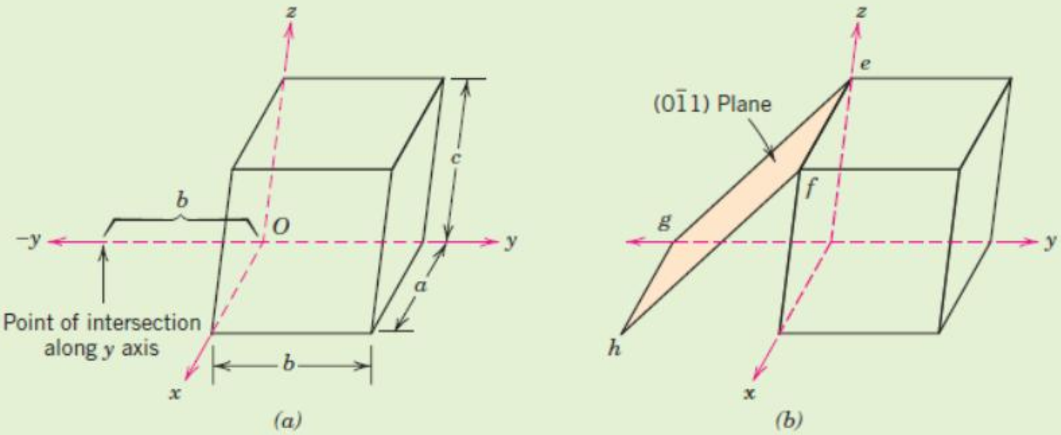
These steps are briefly summarized below:

	x	y	z
Intercepts	∞a	$-b$	$c/2$
Intercepts (in terms of lattice parameters)	∞	-1	$\frac{1}{2}$
Reciprocals	0	-1	2
Reductions (unnecessary)			
Enclosure		$(0\bar{1}2)$	



Representations of a series each of (*a*) (001), (*b*) (110), and (*c*) (111) crystallographic planes

Construct a $(0\bar{1}1)$ plane within a cubic unit cell.



Solution

To solve this problem, carry out the procedure used in the preceding example in reverse order. To begin, the indices are removed from the parentheses, and reciprocals are taken, which yields ∞, -1, and 1. This means that the particular plane parallels the x axis while intersecting the y and z axes at $-b$ and c, respectively, as indicated in the accompanying sketch (*a*). This plane has been drawn in sketch (*b*). A plane is indicated by lines representing its intersections with the planes that constitute the faces of the unit cell or their extensions. For example, in this figure, line *ef* is the intersection between the $(0\bar{1}1)$ plane and the top face of the unit cell; also, line *gh* represents the intersection between this same $(0\bar{1}1)$ plane and the plane of the bottom unit cell face extended. Similarly, lines *eg* and *fh* are the intersections between $(0\bar{1}1)$ and back and front cell faces, respectively.