Material Science
The Structure of Solids:
Crystal Planes, Crystal Defects (Weeks 7)

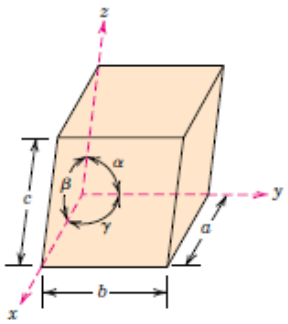
Presented by

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3.10 CRYSTALLOGRAPHIC PLANES

The orientations of planes for a crystal structure are represented in a similar manner as in crystallographic directions. Again, the unit cell is the basis, with the three-axis coordinate system as represented in Figure 3.5. In all but the hexagonal crystal system, crystallographic planes are specified by three Miller indices as (hkl). Any two planes parallel to each other are equivalent and have identical indices. The procedure used to determine the h, k, and l index numbers is as follows:

Figure 3.5 A unit cell with x, y, and z coordinate axes, showing axial lengths (a, b, and c) and interaxial angles (α, β, and γ).



1. If the plane passes through the selected origin, either another parallel plane must be constructed within the unit cell by an appropriate translation, or a new origin must be established at the corner of another unit cell. See note 6

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Note 6: When selecting a new origin, the following procedure is suggested: If the crystallographic plane that intersects the origin lies in one of the unit cell faces, move the origin one unit cell distance parallel to the axis that intersects this plane.

If the crystallographic plane that intersects the origin passes through one of the unit cell axes, move the origin one unit cell distance parallel to either of the two other axes.

For all other cases, move the origin one-unit cell distance parallel to any of the three-unit cell axes.

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2. At this point, the crystallographic plane either intersects or parallels each of the three axes. The coordinate for the intersection of the crystallographic plane with each of the axes is determined (referenced to the origin of the coordinate system). These intercepts for the x, y, and z axes will be designed by A, B, and C, respectively.

3. The reciprocals of these numbers are taken. A plane that parallels an axis is considered to have an infinite intercept and therefore a zero index.

4. The reciprocals of the intercepts are then normalized in terms of (i.e., multiplied by) their respective a, b, and c lattice parameters. That is,

$$\frac{a}{A} \quad \frac{b}{B} \quad \frac{c}{C}$$

5. If necessary, these three numbers are changed to the set of smallest integers by multiplication or by division by a common factor. See note 7.

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Note 7: On occasion, index reduction is not carried; for example, (002) is not reduced to (001). In addition, for ceramic materials, the ionic arrangement for a reduced-index plane may be different from that for a non-reduced one.

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6. Finally, the integer indices, not separated by commas, are enclosed within parentheses, thus: (hkl). The h, k, and l integers correspond to the normalized intercept reciprocals referenced to the x, y, and z axes, respectively.

In summary, the h, k, and l indices may be determined using the following equations:

$$h = \frac{na}{A} \qquad (3.14a)$$

$$k = \frac{nb}{B} \qquad (3.14b)$$

$$l = \frac{nc}{C} \qquad (3.14c)$$

In these expressions, n is the factor that may be required to reduce h, k, and l to integers. An intercept on the negative side of the origin is indicated by a bar or minus sign positioned over the appropriate index. Furthermore, reversing the directions of all indices specifies another plane parallel to, on the opposite side of, and equidistant from the origin. Several low-index planes are represented in Figure 3.11.

One interesting and unique characteristic of cubic crystals is that planes and directions having the same indices are perpendicular to one another.

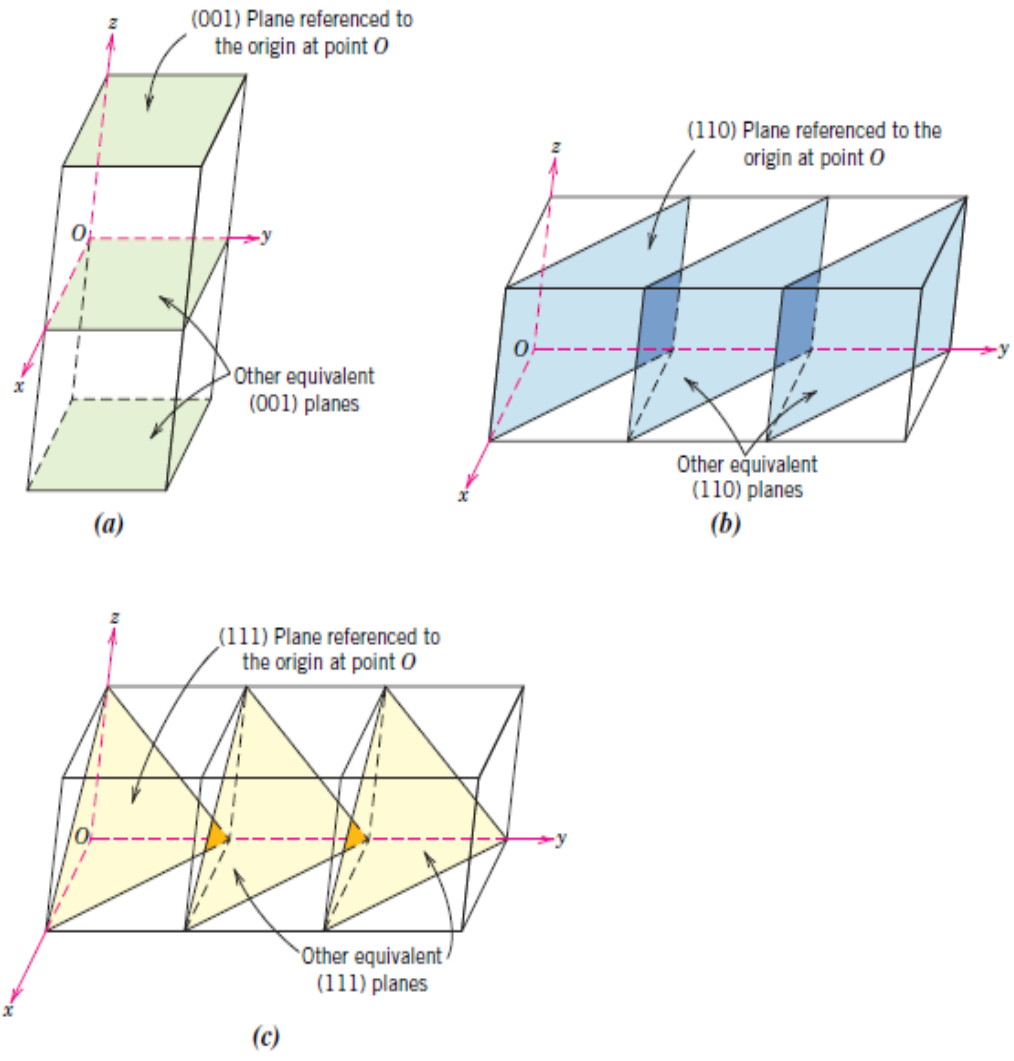
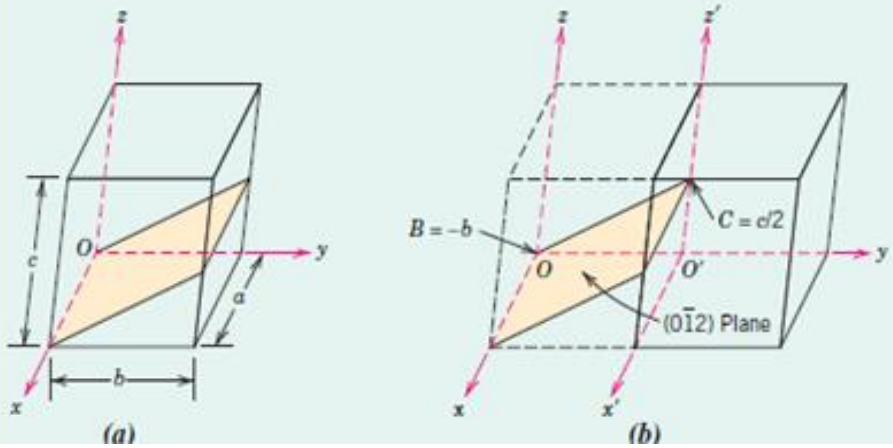


Figure 3.11 Representations of a series each of the (*a*) (001), (*b*) (110), and (*c*) (111) crystallographic planes.

EXAMPLE PROBLEM 3.11

Determination of Planar (Miller) Indices

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



Solution

Because the plane passes through the selected origin O, a new origin must be chosen at the corner of an adjacent unit cell. In choosing this new unit cell, we move one unit-cell distance parallel to the y-axis, as shown in sketch (*b*). Thus x'-y-z' is the new coordinate axis system having its origin located at O'. Because this plane is parallel to the x' axis its intercept is ∞a—that is, $A = \infty a$. Furthermore, from illustration (*b*), intersections with the y and z' axes are as follows:

$$B = -b \qquad C = c/2$$

It is now possible to use Equations 3.14a–3.14c to determine values of h, k, and l. At this point, let us choose a value of 1 for n. Thus,

$$h = \frac{na}{A} = \frac{1a}{\infty a} = 0$$

$$k = \frac{nb}{B} = \frac{1b}{-b} = -1$$

$$l = \frac{nc}{C} = \frac{1c}{c/2} = 2$$

And finally, enclosure of the 0, −1, and 2 indices in parentheses leads to (0$\bar{1}$2) as the designation for this direction.[8]

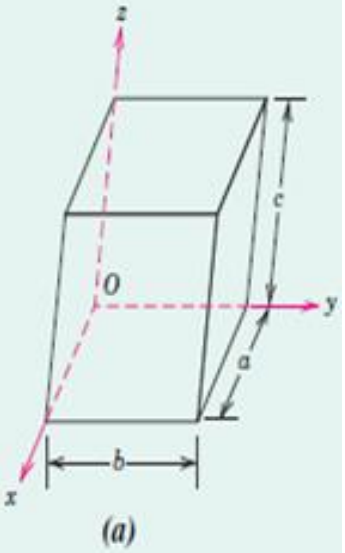
This procedure is summarized as follows:

	x	*y*	*z*
Intercepts (A, B, C)	∞a	$-b$	$c/2$
Calculated values of h, k, and l (Equations 3.14a–3.14c)	$h = 0$	$k = -1$	$l = 2$
Enclosure		(0$\bar{1}$2)	

EXAMPLE PROBLEM 3.12

Construction of a Specified Crystallographic Plane

Construct a (101) plane within the following unit cell.



(a)

Solution

To solve this problem, carry out the procedure used in the preceding example in reverse order. For this (101) direction,

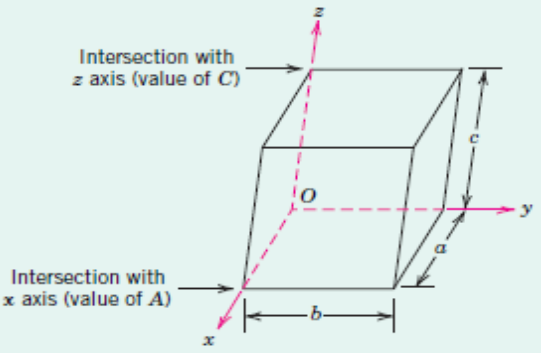
$$h = 1$$
$$k = 0$$
$$l = 1$$

Using these h, k, and l indices, we want to solve for the values of A, B, and C using rearranged forms of Equations 3.14a–3.14c. Taking the value of n to be 1—because these three Miller indices are all integers—leads to the following:

$$A = \frac{na}{h} = \frac{(1)(a)}{1} = a$$

$$B = \frac{nb}{k} = \frac{(1)(b)}{0} = \infty b$$

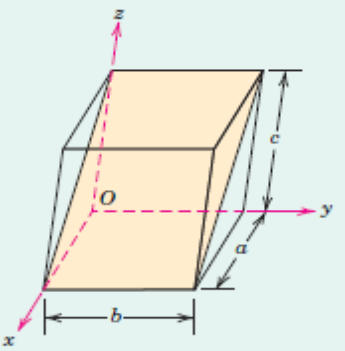
$$C = \frac{nc}{l} = \frac{(1)(c)}{1} = c$$



(b)

Thus, this (101) plane intersects the x axis at a (because $A = a$), it parallels the y axis (because $B = \infty b$), and intersects the z axis at c. On the unit cell shown next are noted the locations of the intersections for this plane.

The only plane that parallels the y axis and intersects the x and z axes at axial a and c coordinates, respectively, is shown next.



(c)

Note that the representation of a crystallographic plane referenced to a unit cell is by lines drawn to indicate intersections of this plane with unit cell faces (or extensions of these faces). The following guides are helpful with representing crystallographic planes:

- If two of the h, k, and l indices are zeros [as with (100)], the plane will parallel one of the unit cell faces (per Figure 3.11*a*).
- If one of the indices is a zero [as with (110)], the plane will be a parallelogram, having two sides that coincide with opposing unit cell edges (or edges of adjacent unit cells) (per Figure 3.11*b*).
- If none of the indices is zero [as with (111)], all intersections will pass through unit cell faces (per Figure 3.11*c*).

CRYSTAL DEFECTS

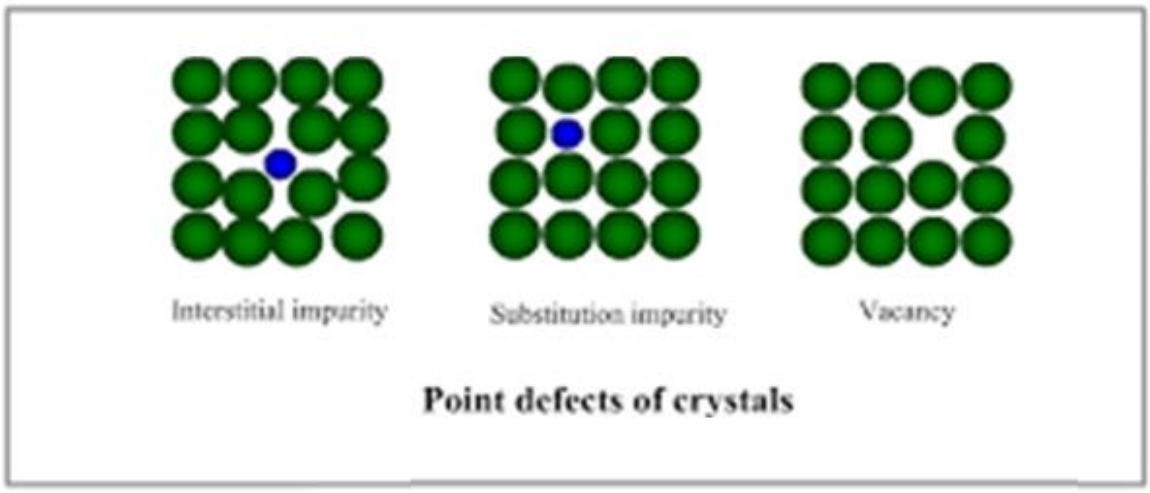
These are imperfection in the regular geometrical arrangement of the atoms in a crystalline solid. These imperfections result from deformation of the solid, rapid cooling from high temperature, or high-energy radiation (X-rays or neutrons) striking the solid. Located at single points, along lines, or on whole surfaces in the solid, these defects influence its mechanical, electrical, and optical behaviour.

Impurity defects are a type of single point defects, which are foreign atoms that replace some of the atoms making up the solid or that squeeze into the interstices; they are important in the electrical behaviour of semiconductors, which are materials used in computer chips and other electronic devices.

Interstitial impurity defect is a type of point defect. It is very small and can be fixed into a tetrahedral or octahedral hole in a lattice. For example: Carbon atoms with steel that contain iron are attached to interstitial impurities.

If a foreign atom displaces or substitutes a host atom which forms lattice and occupies its lattice site, the defect is called substitutional impurity. Such defects can alter the density of the crystal depending upon the mass of the replacing atom relative to replaced atom.

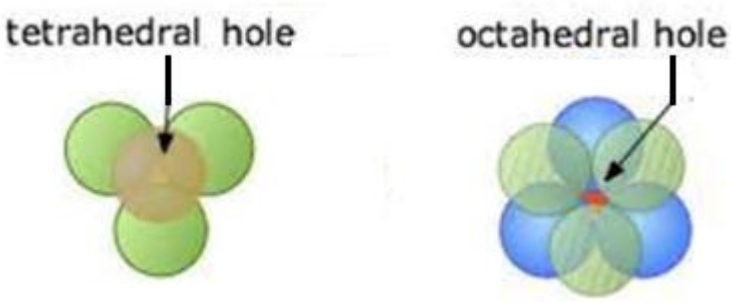
Vacancy defect in crystallography is a type of point defect in a crystal where an atom is missing from one of the lattice sites. Crystals inherently possess imperfections, sometimes referred to as crystalline defects. Vacancies occur naturally in all crystalline materials



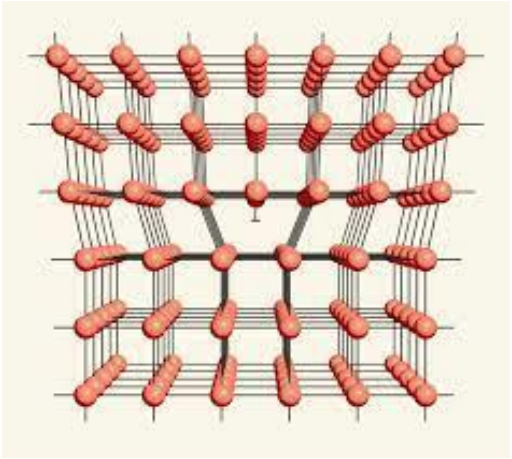
Point defects of crystals

What is octahedral and tetrahedral holes?

If you are in an empty space with 4 atoms as closest neighbours, it is a tetrahedral hole. If 6 atoms a close by, instead, it is a octahedral hole.



Line defects, or dislocations, are lines along which whole rows of atoms in a solid are arranged anomalously. The resulting irregularity in spacing is most severe along a line called the line of dislocation. Line defects can weaken or strengthen solids.



Line Defect (Dislocation)

Surface defects may arise at the boundary between two grains, or small crystals, within a larger crystal. The rows of atoms in two different grains may run in slightly different directions, leading to a mismatch across the grain boundary. Or the boundaries or planes that separate a material into regions, with each region having the same crystalline structure but a different orientation.

