Appendix B

The Miller Indices of a Cubic Crystal

A *crystal* consists of an orderly arrangement of atoms or molecules extending indefinitely in all directions. This arrangement is periodic in the sense that the same patterns of atoms or molecules reappear at regular intervals along certain axes. One can imagine the crystal consisting of a large number of submicroscopic building blocks called *unit cells*. In the case of crystals belonging to the cubic system, the unit cells are tiny cubes that stack in rows and columns to create a rectilinear crystal lattice (Figure B.1). As the illustration suggests, the resulting crystal is not always cubic in shape. In every case, the underlying periodic structure of the crystal remains invariant regardless of its external form or dimensions.

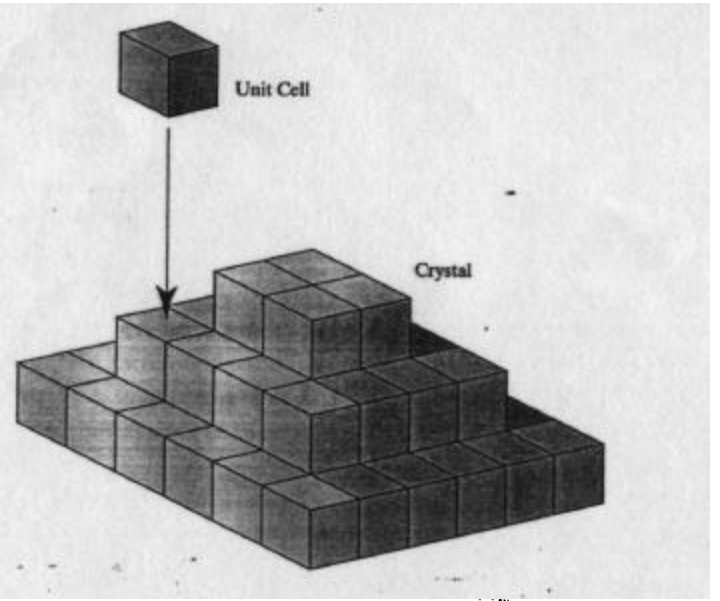

FIGURE B.1 Relationship between a cubic crystal and its unit cell.

A silicon ingot is a single cubic crystal, and each wafer cut from the ingot constitutes a slice cut from this crystal. The properties of the wafer depend on the angle of the cut relative to the axes of the crystal lattice. A set of numbers called *Miller indices* are useful for labeling various cuts of silicon and for labeling directions on the surface of a wafer. This appendix discusses the system of Miller indices used for cubic crystals, including those of silicon and germanium.

A plane intersecting a cubic crystal can be assigned a set of three Miller indices that together specify its orientation relative to the crystal axes. In order to compute these indices, one must first identify the three crystal axes. These lie orthogonal to one another and correspond to the X-, Y-, and Z-axes of the Cartesian coordinate system. The cubic unit cells stack in neat rows and columns aligning to these three axes. The location of any point can be given in terms of multiples of the width of the unit cell along each of the three crystal axes. A plane intersecting the lattice can now be described in terms of its X, Y, and Z intercepts. For example, the intercepts of the plane of Figure B.2A are X = 1, Y = 3, Z = 3. Similarly, the intercepts of the plane of Figure B.2B are X = 3, Y = 2, Z = 2.

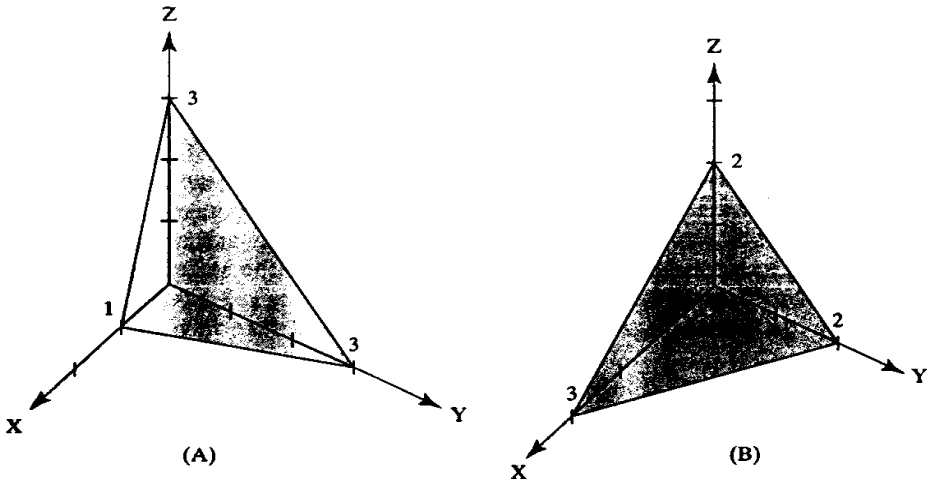

FIGURE B.2 Examples of two planes that intersect a cubic lattice. The tick marks represent multiples of the unit cell dimension.

A crystal plane may lie parallel to one or more of the crystal axes, in which case its intercepts with those planes lie at infinity. For example, the intercepts of a horizontal plane are X = ∞, Y = ∞, Z = 1. Miller indices avoid infinite entries by using the reciprocals of the intercepts rather than the intercepts themselves. For example, the reciprocal intercepts of the horizontal plane are X = 0, Y = 0, Z = 1. A set of Miller indices consists of three integer numbers corresponding to the reciprocal intercepts for the X, Y, and Z axes, respectively. These three reciprocal intercepts are always expressed in terms of the smallest possible integer values and are enclosed in parentheses. For example, the Miller indices of the horizontal plane are (001). The Miller indices of any arbitrary plane can be computed using the following rules:

1. Determine the X, Y, and Z intercepts of the plane. The intercepts of the plane of Figure B.2A are X = 1, Y = 3, Z = 3.
2. Take the reciprocals of the three intercepts. If one or more of the intercepts are infinite, assume that their reciprocals equal zero. The reciprocal intercepts for the plane of Figure B.2A are X = 1, Y = 1/3, Z = 1/3.
3. Multiply the reciprocal intercepts by their lowest common denominator to obtain three integers. The lowest common denominator for the reciprocal

intercepts of the plane of Figure B.2A is three, so the new reciprocal intercepts are X = 3, Y = 1, Z = 1.

4. Enclose the resulting reciprocal intercepts in parentheses to form the Miller indices. The Miller indices for the plane of Figure B.2A are (311). Those for the plane of Figure B.2B are (233). If one or more of the numbers happens to be negative, then a bar is placed over this number in the Miller indices.

Planes whose Miller indices are permutations of one another are said to be *equivalent.* For example, the (001), (010), and (100) planes are all equivalent. This does not mean that these are all one and the same plane; in fact these three planes lie at right angles to one another. Rather, it means that all three of these planes have identical crystallographic properties, which also implies that they have identical chemical, mechanical, and electrical properties. Equivalent planes are denoted by a trio of Miller indices enclosed in braces. Thus, the set of equivalent planes {100} includes the (001), (010), and (100) planes. Remember that Miller indices enclosed in braces refer to a set of planes, and not to any one specific plane. There is no such thing as a {100} wafer—the surface of the wafer might be a (001) plane or a (010) plane or a (100) plane, but it cannot be all three at the same time!

Miller indices can also be used to describe directions relative to the crystal lattice. The line passing perpendicularly through the plane (ABC) has the Miller indices [ABC]. The Miller indices for the X, Y, and Z axes are [100], [010], and [001], respectively. Directions whose Miller indices are permutations of one another are also said to be equivalent. For example, the directions [100], [010], and [001] are equivalent to one another. Equivalent directions are denoted by a trio of Miller indices placed in angle brackets. For example, the set of equivalent directions <100> includes the [100], [010], and [001] directions. Since an axis actually aligns to two direction vectors—that point in opposite directions—the Miller indices for an axis should be enclosed in angle brackets.