

Basic Crystallographic Definitions and Properties of Si, SiGe, and Ge

Stephen H. Jones, Michael H. Jones
June 2002

Virginia Semiconductor, Inc.
1501 Powhatan Street, Fredericksburg, VA 22401
(540) 373-2900, FAX (540) 371-0371
www.virginiasemi.com, shjones@virginiasemi.com

A. Introduction

Two of the more fundamental parameters characterizing Si, SiGe, and Ge substrates are the crystallographic orientation of the wafer surface, and the crystallographic direction perpendicular to the wafer flat. In this article we describe the basic nomenclature, equations, diagrams, and graphs that are used to describe crystallographic orientation. Different orientation wafers are typically used to produce performance advantages within electronic devices, as well as, to illuminate critical anisotropic etch and growth characteristics during device and circuit processing. This is particularly true in the case of micromachined Si devices used in MicroElectroMechanical Systems (MEMS). The general lattice characteristics of Si, SiGe, and Ge are effectively identically with the only difference being the lattice constant or spacing. Therefore the discussion, lattice diagrams, and stereographic projections provided below are applicable to all three material systems.

B. Basic Lattice Structure

Single-crystal Si, SiGe, and Ge used in the microelectronics industry are all members of the simplest three-dimensional lattice system referred to as the cubic lattice system. Any lattice system having a cubic volume as a unit cell belongs to the cubic family. For example the common simple-cubic (sc), body-centered cubic (bcc), and face-centered cubic (fcc) are all cubic lattice systems. The length dimension of the unit cell defines the lattice constant (a). Si, SiGe, and Ge have a cubic lattice structure known as the diamond lattice structure, and the unit cell is actually two interpenetrating fcc lattices separated by $a/4$ along each axis of the cell. Figure 1 shows the unit cell, diamond structure, lattice constant, and the four nearest neighbor atoms bonding the Si lattice.

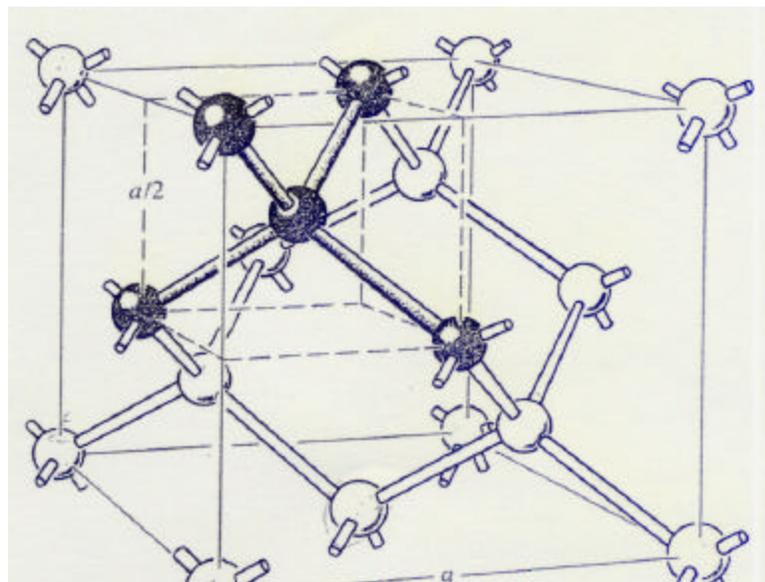


Figure 1. The unit cell and diamond lattice structure for Si, SiGe, and Ge [1].

The lattice constant for Si is 5.43 Å, and the lattice constant for Ge is 5.66 Å. For SiGe, the lattice constant can be approximated using a simple linear interpolation as a function of composition. Bulk Si is an ideal lattice comprised of an infinite number of repetitive unit cells and an infinite number of cross-sectional planes and lattice directions. However, there are several primary planes and lattice directions that are associated with the unit cell of Figure 1. These primary planes are those that form the sides and diagonals of the unit cell.

C. (h,k,l) Miller Indices

All lattice planes and lattice directions are described by their associated Miller Indices. This mathematic description allows the specification, investigation, and discussion of specific planes and directions at the surface or within the bulk of the crystal. For the cubic lattice system, the direction [hkl] defines a vector direction normal to surface of a particular plane or facet. The Miller Indices h,k,l are defined accordingly:

1. Place the unit cell of Figure 1 on an x,y,z Cartesian coordinate system with a lower corner atom at the origin.
2. To define the (hkl) plane, first identify the three intercepts of the plane with the crystal axes (x,y,z). Each separation of one lattice constant, a, is given the value of 1. Planes beyond the unit cell being associated with integers greater than 1. Positive and negative integers are appropriately defined.
3. Take the reciprocal of the three intercept integer values (1/x,1/y,1/z).
4. Reduce these fractions to the smallest set of common integers (h,k,l)

For example, the top of the unit cell shown in Figure 1 defines the (001) plane, while the bottom surface is the (100) plane. Diagonals include the (111) and (110) planes. The set of {100}, {111}, and {110} form the primary planes. Surfaces tipped small angles from the primary planes are considered vicinal surfaces, while planes such as (511) and (711) are high index planes. For example the plane having the intercepts 3,1,1 is the (133) surface, and the direction normal to this surface is the [133]. While, the plane having the intercepts -1,-1,-1 is the (-1,-1,-1) surface. Typically, and regularly, the minus sign is placed above the miller index. Si, SiGe, and Ge wafers are commonly manufactured with the (100), (110) or (111) surface or flat orientations.

Inspection of the unit cell shows 6 identical and symmetric {100} planes that form the sides of the cubic structure. Similarly there are identical {111} and {110} surfaces within the cell. Although these surfaces are different relative to each other mathematically, they are indistinguishable in reality, and are physically and chemically

equivalent. Therefore, the following guidelines [1] are used to define planes and directions.

1. Use the $[\]$ notation to identify a specific direction (ie $[1,0,-1]$).
2. Use the $\langle \rangle$ notation to identify a family of equivalent directions (ie $\langle 110 \rangle$).
3. Use the $()$ notation to identify a specific plane (ie (113)).
4. Use the $\{ \}$ notation to identify a family of equivalent planes (ie $\{311\}$).

D. Basic Surfaces and Planes

In Figure 2 we show several cross-sections that ideal portray the surfaces and two-dimensional-lattice nature for several common crystal planes and directions. The precise configuration of the surface is difficult to describe and in reality complicated, but the general nature of the lattice in a particular crystallographic direction is extremely regular,

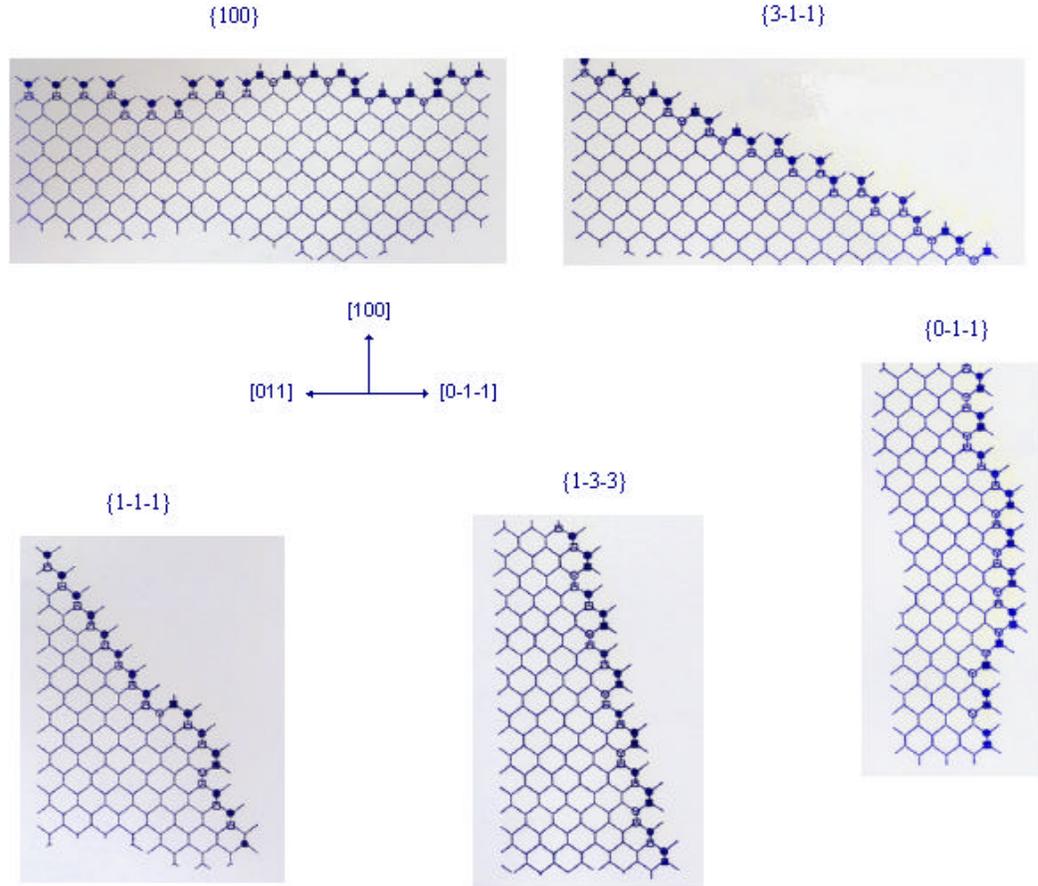


Figure 2. The surface and lattice structure for (100), (3-1-1), (1-1-1), (1-3-3), and (0-1-1) planes.

The angle between any two planes (theta), defined using the appropriate Miller Indices, can be calculated using the following equation,

$$\cos(\theta) = \frac{(hH + kK + lL)}{\sqrt{(HH + KK + LL)(hh + kk + ll)}}$$

where (hkl) defines the first plane and (HKL) defines the second plane.

The angles (in degrees) between several common planes are given in the Table 1. Refer to Figure 3 as needed when considering values in Table 1.

ANGLE	100	110	010	001	101
100	0	45	90	90	45
011	90	60	45	45	60
111	54.7	35.3	54.7	54.7	35.3
211	35.2	30	65.9	65.9	30
311	25.2	31.4	72.4	72.4	31.4
511	15.8	35.2	78.9	78.9	35.2
711	11.4	37.6	81.9	81.9	37.6

Table 1. The angles in degrees between planes for several common combinations.

E. Stereographic Projections

Crystallographic planes and directions are most easily and commonly identified and specified using a stereographic projection (see Figures 3-6). The stereographic projection is a simple mathematical translation that projects the head of every unit vector (which defines all possible crystal directions) $\langle h,k,l \rangle$ onto a two-dimensional graph. Consider the infinite set of unit vectors taken from the origin of the spherical coordinate system and forming a hemisphere. Now project the head of each vector, which is on the surface of the hemisphere, into the plane of the hemisphere. This projection is the stereographic projection. The orientation of the plane at the zenith becomes a point at the center of the graph. All points on the edge of the graph are planes perpendicular to the plane represented by the point in the center of the graph. The {100}, {110}, and {111}, {211} stereographic projections for Si, SiGe, and Ge are given below.

Stereographic Projection <110>

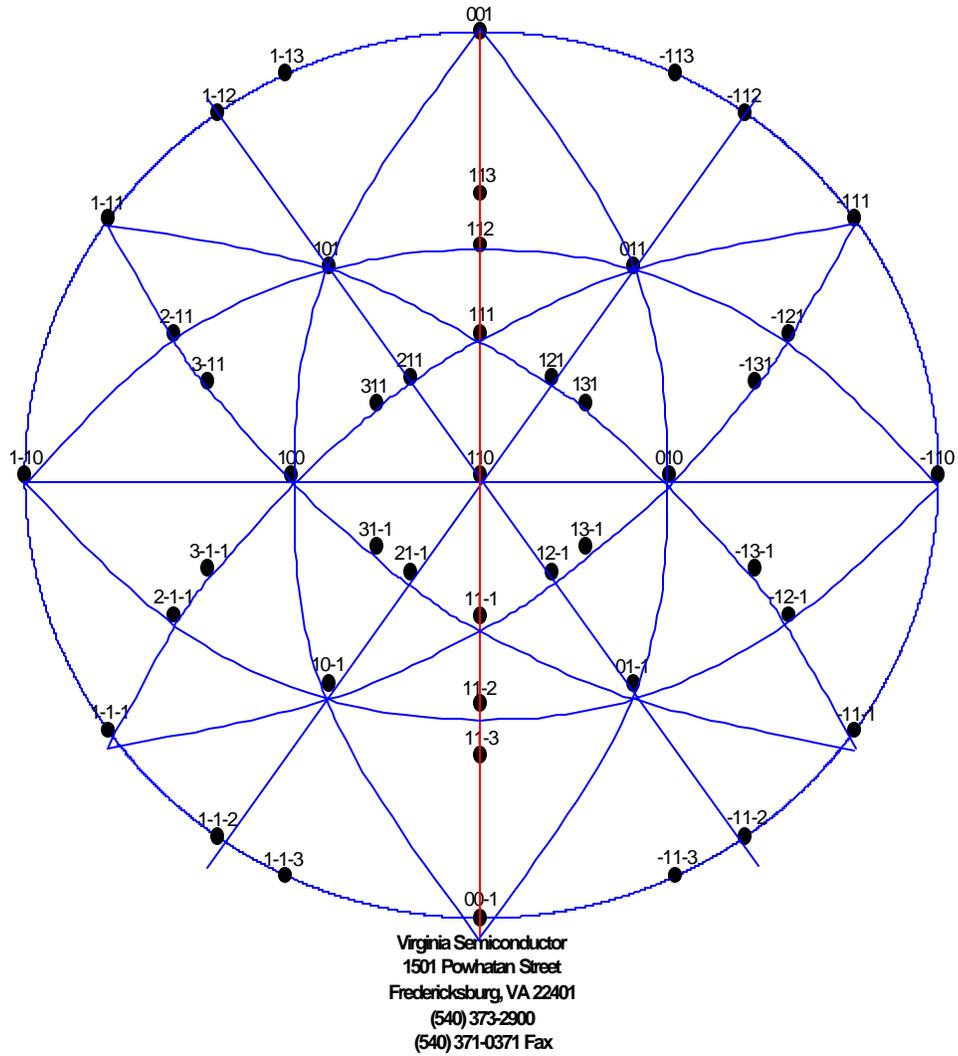


Figure 4. (110) Stereographic Projection for Si, SiGe, and Ge.

Stereographic Projection <111>

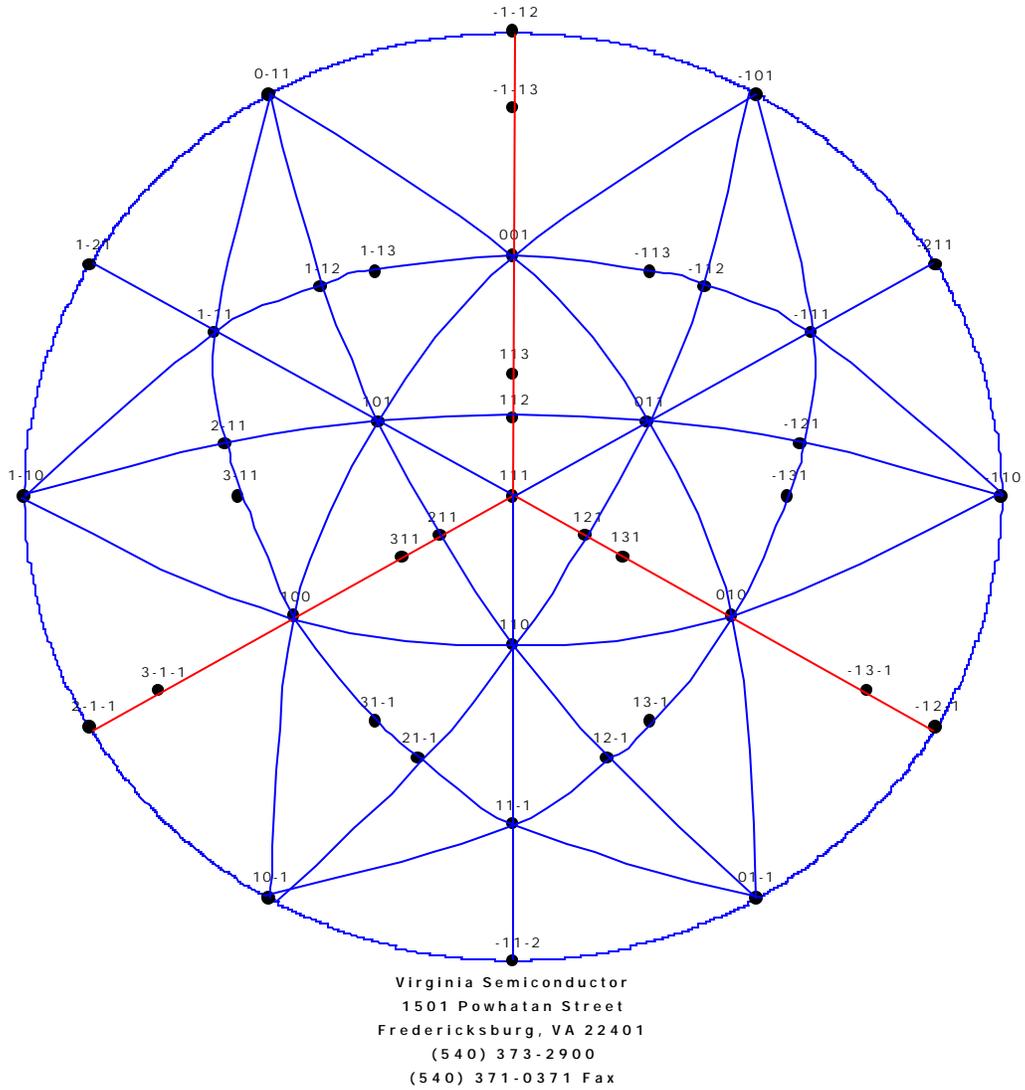


Figure 5. (111) Stereographic Projection for Si, SiGe, and Ge.

G. References

[1] B.G. Streetman, Solid State Electronics, Third Edition, Chapter 1, Prentice Hall, 1990, ISBN 0-13-822941-4