## Miller Indices

Miller Indices are a notation system in crystallography for planes and directions in crystal lattices. Before describing the notation and use of Miller indices, let us briefly go over semiconductors, crystalline solids and the crystal lattice.

Semiconductors are ubiquitous in electronics. The electrical and optical properties of semiconductor materials enabled the advancement in electronic devices (e.g., IC chips). The energy band gap and purity/impurity (doping) of the material are two very important properties that distinguish semiconductors from other solids. The energy band gap determines what wavelengths of light or energy can be absorbed or emitted by the semi-conductor. The energy gap can be increased or decreased by adding or removing impurities from the semiconductor material. This process is known as doping. Slight changes to the purity of the material can have dramatic changes or impurities to the atomic arrangement of the material can have huge changes or effects on the electrical properties. In order to fully understand these properties, it is necessary to learn and understand and describe the atomic arrangement of the semiconductor material.

Semiconductors like Silicon are crystalline solids. What distinguishes crystalline solids from other solids is the arrangement of the atoms making up the crystal are arranged periodically. In other words, unlike amorphous and polycrystalline solids, the atoms in a crystalline solid are not random and can be found to be the same throughout the crystal. The pattern that is repeated, or the crystal's periodicity is defined by a symmetric array of points called the lattice. A crystal can be formed from the lattice when atoms are added to each lattice point.



A volume that fills the space inside the lattice and is found repeating throughout the crystal can represent the lattice. The smallest of such repeating arrangements is called the primitive cell. Vectors can be defined such that the primitive cell can be translated by integral multiples of these vectors. Primitive cells only have lattice points in the corner. Sometimes a unit cell is easier to work with than a primitive cell. The unit cell is used when one wants to study the properties of a crystal by studying a small volume of the crystal rather than the entire crystal itself. Knowing the unit cell, the distances can be calculated between atoms can be calculated and the force holding the lattice can also be calculated. This is important since the force holding the lattice determines which electrons can participate in the conduction process.



(Figures from left to right: Primitive cell, Unit cell)

When observing crystals, its helpful to be able to refer to directions and planes or a set of planes with the lattice. This is done using three integers. Before finding the integers, an xyz coordinate system is setup within the lattice with the axes lined up with the edges of the cell. The three integers can be found by using the following three steps:

- 1. Find the intercepts of the plane with the crystal axes. Express these numbers as integer multiples of the basis vectors.
- 2. Take the reciprocals of the three integers and reduce to the smallest set of integers h,k, and l.
- 3. Label the plane (hkl).

These three integers are called the Miller indices and are the standard method or notation used to describe the orientation of planes within a lattice in relation to a unit cell. It was developed and named after William Hallowes Miller. Miller indices are useful in explaining physical phenomena including the shape of the crystal.



A (214) crystal plane.

## References

- CRYSTAL STRUCTURE PART II. (n.d.).*http://www.ocf.berkeley.edu/*. Retrieved September 13, 2011, from <u>www.ocf.berkeley.edu/~mwg/lab/Miller.pdf</u>
- DoITPoMS TLP Library Lattice Planes and Miller Indices. (n.d.). *Dissemination of IT for the Promotion of Materials Science (DoITPoMS)*. Retrieved September 13, 2011, from <u>http://www.doitpoms.ac.uk/tlplib/miller\_indices/index.php</u>
- Ferry, D., Vasieska, D., & Klimeck, G. (n.d.). Crystal Directions, Wave Propagation and Miller Indices. *nanohub*. Retrieved September 13, 2011, from nanohub.org/resources/9137/download
- Solids / Crystal Structure and Solution. (n.d.). *Chemconnections.org*. Retrieved September 13, 2011, from chemconnections.org/crystals/pdf/crys-solids.pdf
- Streetman, B. G., & Banerjee, S. K. (2006). *Solid State Electronic Devices* (6a. ed.). Upper Saddle River, New Jersey: Prentice-Hall.