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# The Miller Index Activity

## Crystallography Overview Learning Module

### Participant Guide

The *purpose of this learning module* is to introduce the science of crystallography and its importance to microtechnology. Activities provide additional exploration into crystallography and its applications.

#### Description and Estimated Time to Complete

In this activity you explore crystal planes by learning how to identify and notate them using The Miller Index also referred to as Miller Indices. By the end of this activity, you should be able to denote basic crystal planes using Miller indices notation as well as create a three-dimensional model of various planes.

#### Estimated Time to Complete

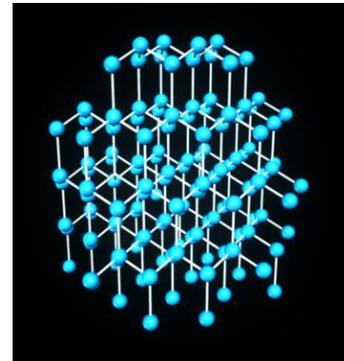
Allow at least 30 minutes to complete this activity.

#### Introduction

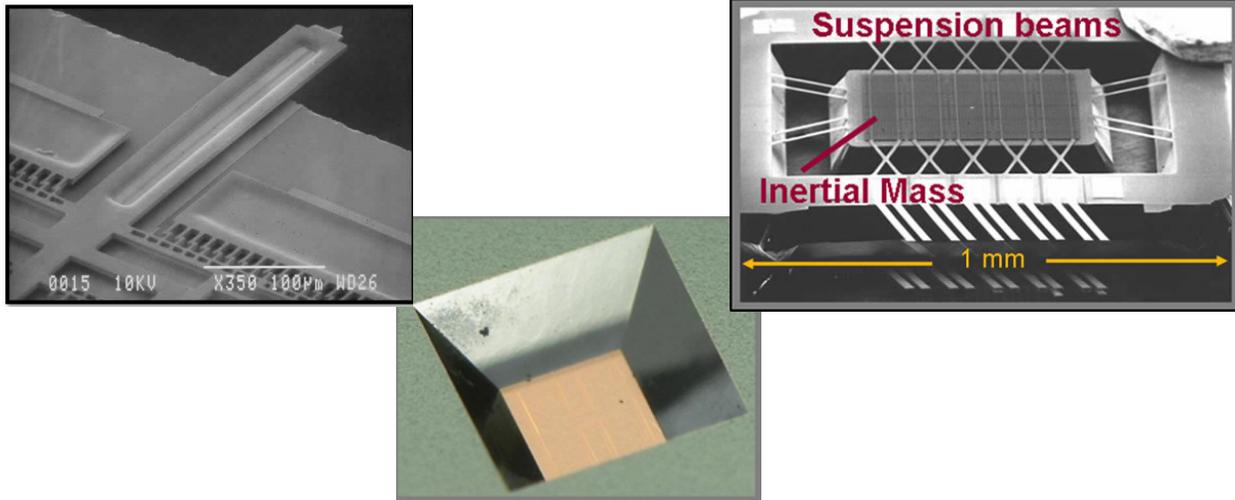
By definition a crystal or a crystalline solid is a solid material consisting of atoms or molecules arranged in a repeating pattern. This pattern forms a lattice structure of stacked planes that extend in all three spatial dimensions. The well-ordered, repeatable bonds between atoms or molecules are typically very strong.

The repeatability and predictability of the bonds and atomic structure of a crystal make it an ideal substrate for MEMS fabrication. Knowing the atomic structure of a substrate enables the design and fabrication of many simple and complex microdevices.

Typical crystalline substrates used in the fabrication of microdevices include silicon, polysilicon, and gallium arsenide<sup>1</sup>.



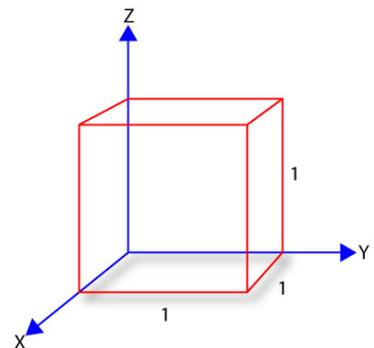
Choosing a crystalline substrate with a specific crystal orientation provides a desired structural effect on a micro-scale. Below are several micro-components that are formed along one or more planes of a crystal substrate. The first component is a microcantilever with a combdrive used to move the cantilever back and forth. The second image is a reference pressure chamber on the backside of a micro-pressure sensor. The third image is an out-of-plane accelerometer that shows an inertial mass and suspension beams fabricated within a crystal substrate. Components in all three of these images were designed and fabricated using specific planes of silicon crystal.



[Cantilever image on the left courtesy of Sandia National Laboratories, Pressure sensor chamber courtesy of the MTTIC / University of New Mexico, Accelerometer courtesy of the University of Michigan]

**How do we identify the many planes and vectors in a crystal structure?**

Miller index notation is a roadmap or directional compass for identifying the crystal planes and directions (vectors) within crystals. Miller indices are three digit notations that indicate planes and vectors within a crystal. These notations are based on the Cartesian coordinate system of x, y, and z. The Cartesian coordinate system is illustrated using the three vectors (axes) x, y, and z. Other coordinate systems are used for more complex crystal structures.



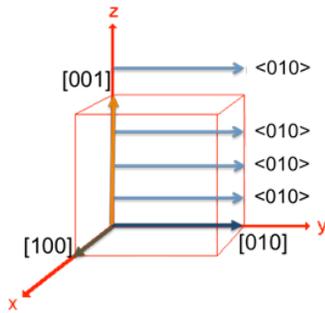
**Vector Notation**

Referring to the graphic “Cartesian Coordinates”, the

- x-axis vector direction is denoted [1,0,0] or [100]
- y-axis vector direction is denoted [0,1,0] or [010]
- z-axis vector direction is denoted [0,0,1] or [001]

(Think of the "1" as being "1 unit" or “1 unit cell” out from the origin or 0,0,0.)

Here is another way to look at it. Let’s look at the [100] vector. If you were to start at the origin (the intersection of the three axes) and take one step (1 unit) down the x-axis and no steps in the directions of the y and z axes, you would be on the [100] vector.



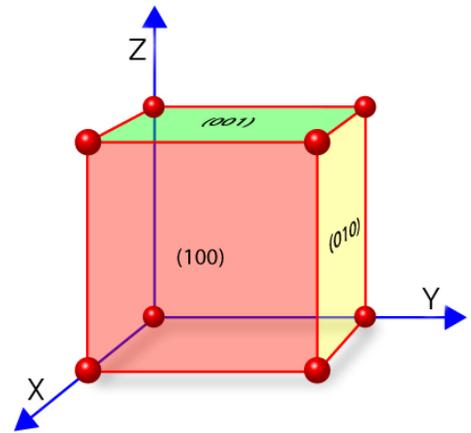
Vectors parallel to the primary vectors are shown as  $\langle 100 \rangle$ ,  $\langle 010 \rangle$ , or  $\langle 001 \rangle$ . Notice in the graphic to the left, the primary vector is  $[010]$  and the vectors parallel to it are denoted  $\langle 010 \rangle$ .

### Plane Notation

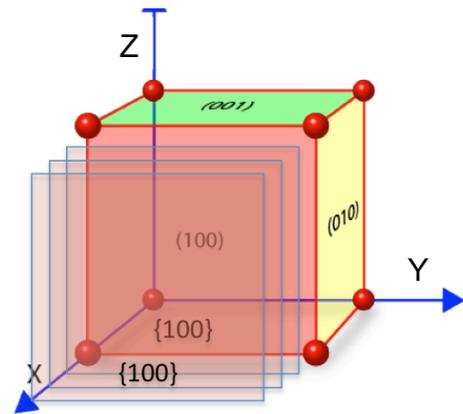
Crystal planes are perpendicular to their corresponding axis or vector. For example, the plane perpendicular to the  $[100]$  vector or x-axis is the  $(100)$  plane (shown in red in the figure to the right).

Each crystal plane has a unique notation.

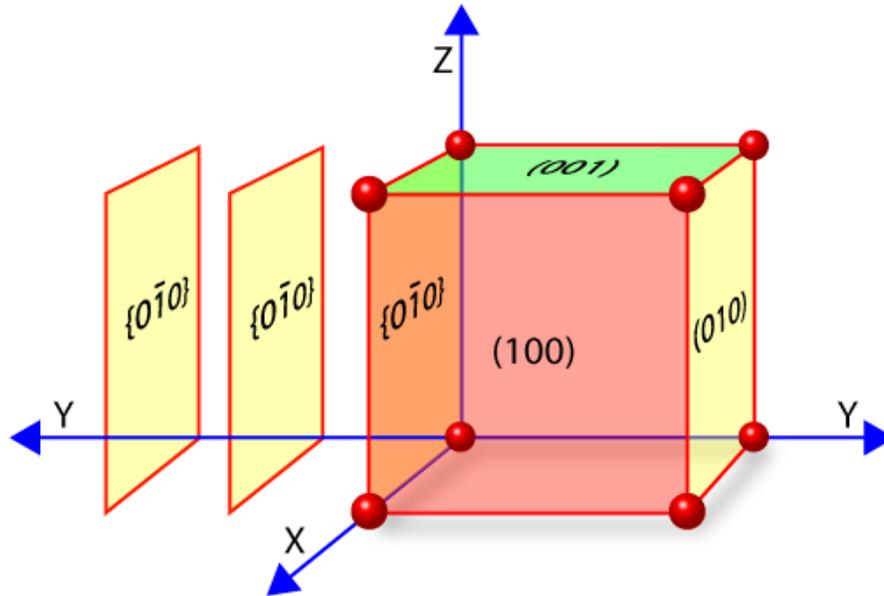
- $(1,0,0)$  or  $(100)$  is perpendicular to the x-axis (Red)
- $(0,1,0)$  or  $(010)$  is perpendicular to the y-axis (Yellow)
- $(0,0,1)$  or  $(001)$  is perpendicular to the z-axis (Green)



Alternate planes or parallel planes are shown in  $\{ \}$ , such as  $\{100\}$ ,  $\{010\}$ , and  $\{001\}$ . The figure to the right shows the  $(100)$  plane and a set of planes  $\{100\}$  parallel to it.



Miller index notation can also refer to a "negative" plane, or a parallel plane on the opposite side of the origin (0,0,0) or the opposite plane of the unit cell. For instance, the  $(0\bar{1}0)$  plane would refer to the plane parallel to the (010) plane on the opposite side of the unit cell or one unit from the origin on the negative y (-y) axis. The graphic below illustrates this. As you can see, the reference plane in the unit cell is one unit from the origin in the positive direction (010). The plane opposite (010) in the unit cell is denoted  $(0\bar{1}0)$  as are the additional planes in the  $-y$  direction.



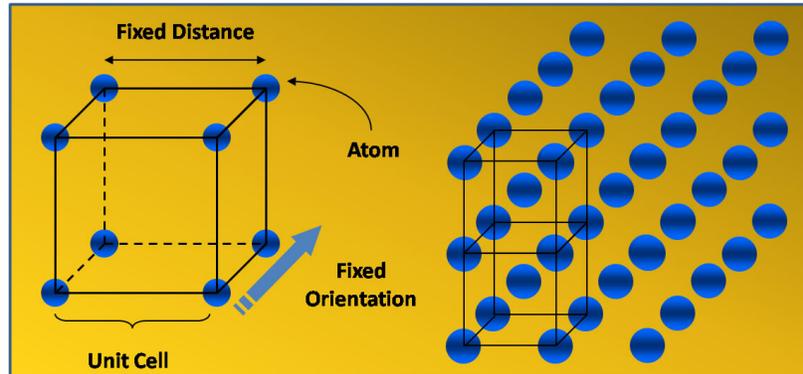
To better understand Miller Index Notation, stop and take a few minutes (7:41 to be exact), to view this video: [An Activity on Miller Index Notation](#). This video illustrates what we have been discussing about vector and plane identification and notation.

[If the above link doesn't work, copy and paste this URL: <https://youtu.be/iFqRUqwAWvo> ]

## The Unit Cell

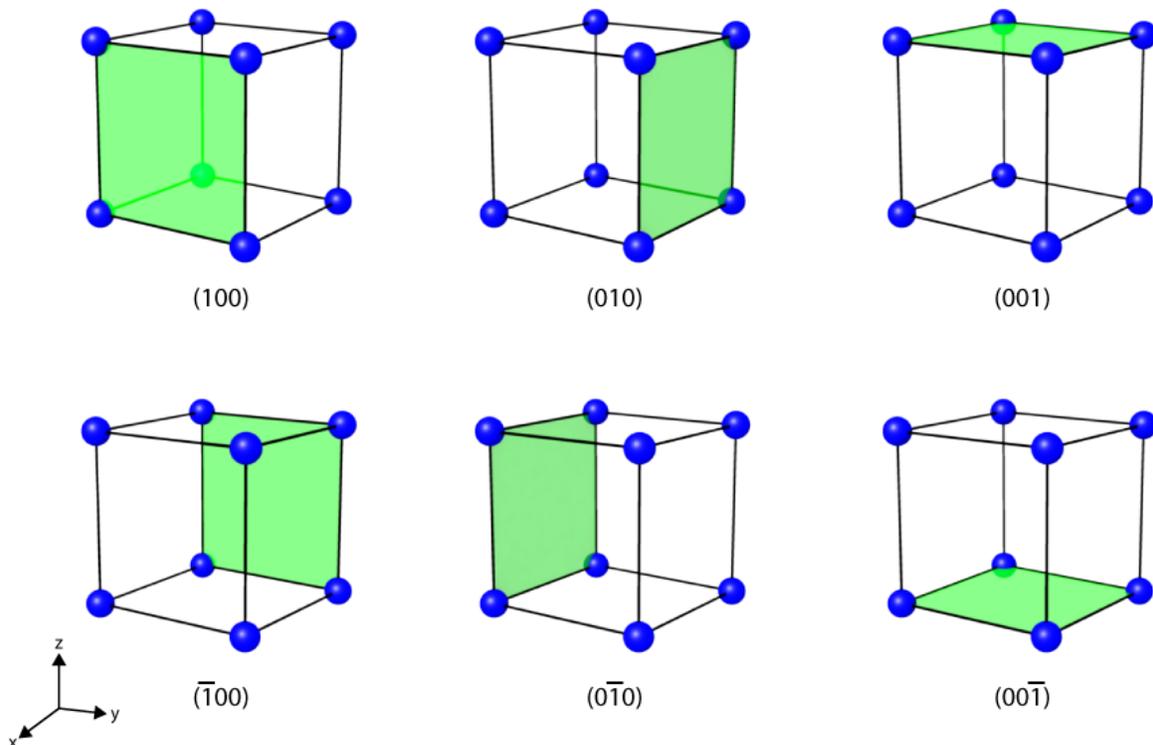
The unit cell is the simplest repeating unit in a crystal. In a single crystal, all unit cells are identical and oriented the same way (fixed distance and fixed orientation). The opposite faces of a unit cell are parallel (*see graphic of unit cell below*). The edge of the unit cell connects equivalent points. The resulting structure is a lattice.

The figure below illustrates a unit cell for a crystalline structure.

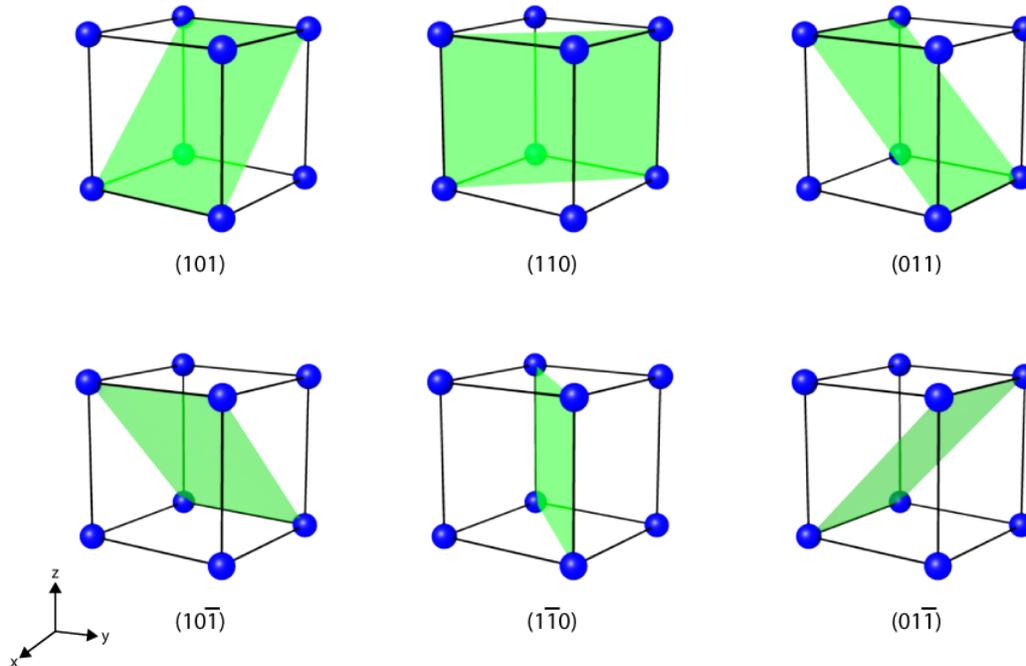


## Miller Indices and the Unit Cell

The  $(100)$ ,  $(010)$ ,  $(001)$ ,  $(\bar{1}00)$ ,  $(0\bar{1}0)$  and  $(00\bar{1})$  planes form the faces of the unit cell.

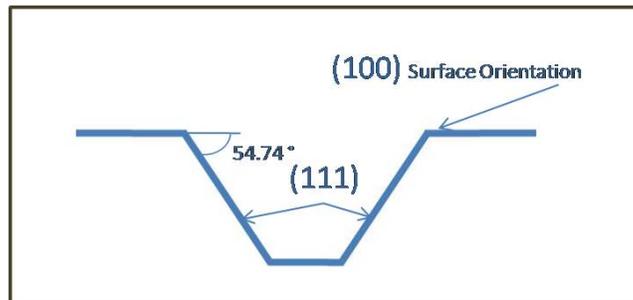
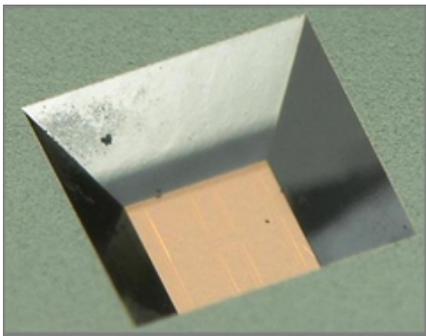


The  $(101)$ ,  $(110)$ ,  $(011)$ ,  $(10\bar{1})$ ,  $(1\bar{1}0)$  and  $(01\bar{1})$  planes form the sections through the diagonals of the unit cell and are denoted below. Study these planes and relative notations and make sure you understand them.



### Why is this important?

Shown below on the left is a microscopic image of the backside of a  $(100)$  silicon wafer. The chemical reaction between a potassium hydroxide (KOH) etchant and the  $(100)$  silicon substrate, results in this desired anisotropic etch along the  $(111)$  crystal plane. Because of the crystalline structure and bonds of the crystal in the  $(100)$  silicon, material (silicon) is selectively removed (or etched) along the  $(100)$  and  $(111)$  planes, leaving the desired cavity. The etch occurs both vertically (down the  $(100)$  planes) and sideways (along the  $(111)$  planes) at an etch rate of 400:1, meaning that the vertical etch of the  $(100)$  plane is 400 times faster than the sideways etch of the  $(111)$  plane. This is because the lattice of the  $(111)$  plane is the denser or has more silicon atoms on its surface than the surface of the  $(100)$  planes. The angle of the  $(111)$  plane is always  $54.74^\circ$  relatively to the  $(100)$  plane in a silicon crystal. The predictability of this chemical reaction on a monocrystalline silicon wafer allows for a micro-cavity that can be used for many purposes.



Backside of etched silicon substrate  
 Courtesy of the MTTC / University of New Mexico

## Activity Objectives and Outcomes

### Activity Objective

- To use the correct Miller index notations for different planes and vectors in crystal structures.

### Activity Outcome

By the end of this activity you should be able to how to determine the Miller Index notation for a variety of planes and vectors within a Cartesian coordinate system and relative to a unit cell at the origin of the system.

### **Resources**

SCME Crystallography Overview for MEMS PK

### **Supplies / Equipment**

#### Supplies for each team (provided by instructor)

- 3 sticks or rulers (representing the x, y, z axes)
- Tape
- 1- piece of cardboard approximately 12"x12" in size (representing a “plane”)
- 1 – 18” piece of string (representing a “vector” or direction)

This activity should be performed in teams of 2 or 3 in order to promote discussion and a better understanding of the concept.



### **Documentation**

- Answers to the Post-Activity Questions

### **An on-line tutorial**

Again, you can refer back to this tutorial while you are doing this activity.

### **[An Activity on Miller Index Notation](#)**

**[\[https://youtu.be/iFqRUqwAWvo\]](https://youtu.be/iFqRUqwAWvo)**

## Activity: Miller Indices Models

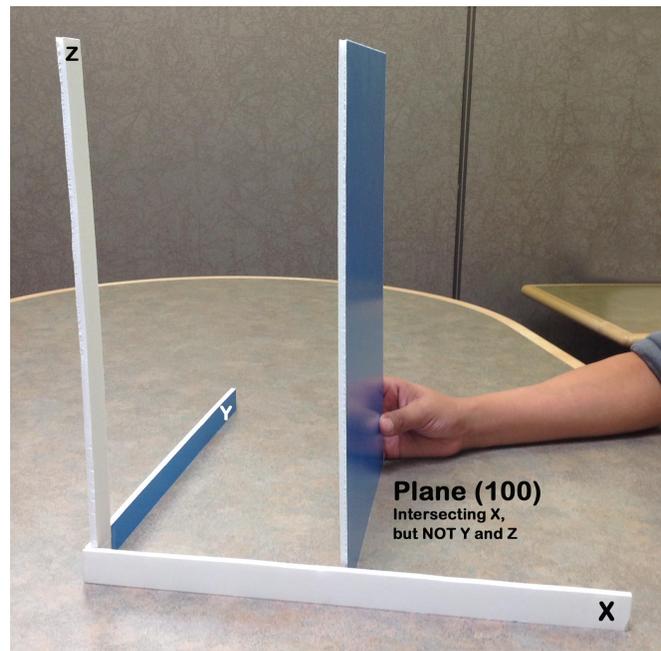
### Procedure

Complete this activity with one or two other students.

1. Create a Cartesian coordinate system using the three rulers or sticks. Designate the x, y, or z-axis. For the purpose of this exercise, use the Cartesian orientation shown in the "Crystal Planes" image shown previously in this activity. Make sure that your team members know which ruler represents which axis (x, y, or z).

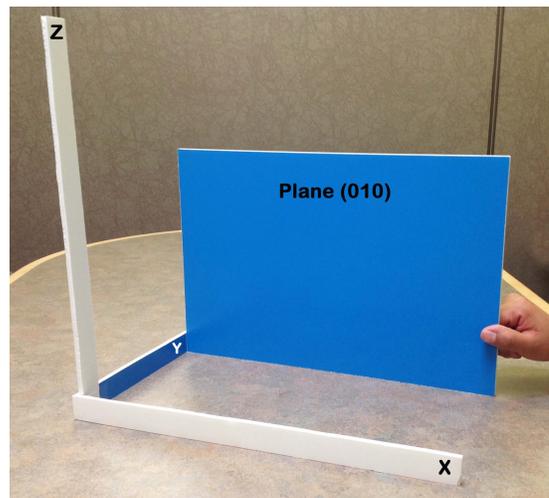


2. Position the piece of cardboard perpendicular to and in the middle of the "x" axis (1 unit length), and parallel to the y-z plane. The cardboard in this orientation represents the (100) crystal plane.



- Using the string, indicate the  $[100]$  vector. Remember that this vector is perpendicular to the  $(100)$  plane.

- Position the piece of cardboard perpendicular to and in the middle of your "y" axis. The distance should represent 1 unit length. The cardboard in this orientation represents the  $(010)$  crystal plane.



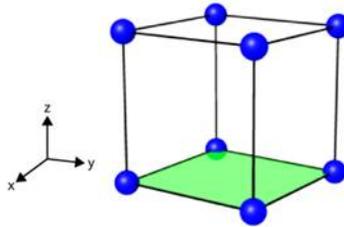
- Using the string, show the  $[010]$  vector, the vector perpendicular to the  $(010)$  plane and one unit from the origin.

6. Position the cardboard to represent the (001) crystal plane.
7. Use the string and show the [001] vector. Make sure that everyone in your team agrees.
  
8. Using the cardboard and the string model the (110) plane and the [110] vector. Make sure that everyone in your team agrees.
  
9. Now position the cardboard in the (111) orientation and the string for the [111] vector.
  
10. Model the ( $\bar{1}00$ ), ( $0\bar{1}0$ ) and ( $00\bar{1}$ ) planes.
  
11. Model the (101), (011), ( $10\bar{1}$ ), ( $1\bar{1}0$ ) and ( $01\bar{1}$ ) planes.
  
12. Using the string, again model the following vectors. Create a drawing below that illustrates these vectors relative to a unit cell.

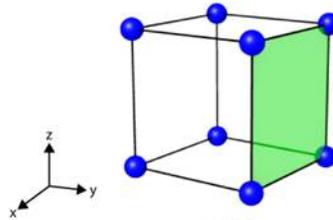
[100], [010], [001], [011], [110], [111]

## Post-Activity Questions

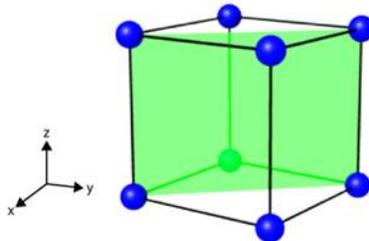
1. What does it mean when a crystal plane is noted like this:  $(\bar{1}00)$ ?
2. Name all of the faces of the "unit cell" using the Miller Index notations.
3. Draw a unit cell and show the (011) plane relative the x-y-z axes.
4. Draw the (101) plane relative the x-y-z axes.
5. Using Miller indices, name the following crystal plane, relative to the unit cell



6. Using Miller indices, name the following crystal plane, relative to the unit cell.



7. Using Miller indices, name the following crystal plane, relative to the unit cell.



## Summary

Crystal orientation is a very important aspect of microsystems fabrication. Knowing the orientation of a crystal is imperative to being able to design and fabricate functional microstructures because the physical, chemical and electrical properties of each plane can be different. The Miller Index allows us to identify and notate specific crystalline planes relative to the Cartesian coordinate system and the unit cell.

## References

1. Gallium arsenide. Wikipedia. 2011. [http://en.wikipedia.org/wiki/Gallium\\_arsenide](http://en.wikipedia.org/wiki/Gallium_arsenide)
2. Lattice Planes and Miller Indices. University of Cambridge. [http://www.doitpoms.ac.uk/tlplib/miller\\_indices/printall.php](http://www.doitpoms.ac.uk/tlplib/miller_indices/printall.php)

## Disclaimer

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