Crystallography Overview

Crystallography Overview PK Activities (3)

Participant Guide

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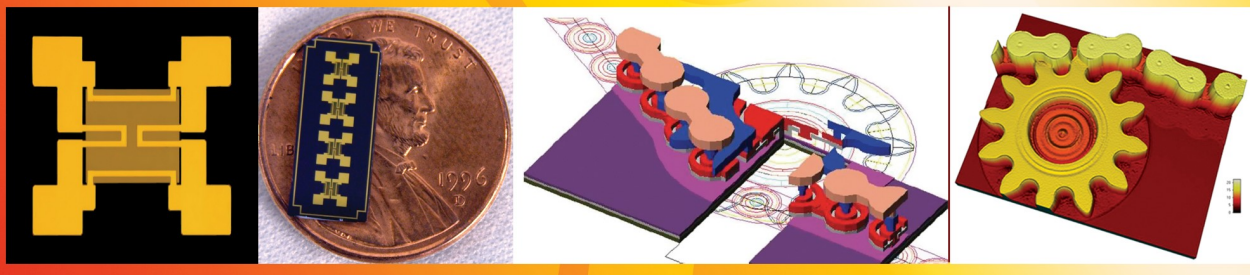

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University of New Mexico

MEMS Fabrication Topic

Crystallography Overview for MEMS

Primary Knowledge (PK)
Shareable Content Object (SCO)

This SCO is part of the Learning Module
Crystallography

Target audiences: High School, Community College.

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Southwest Center for Microsystems Education (SCME)
800 Bradbury Drive SE, Suite 235
Albuquerque, NM 87106-4346
Phone: 505-272-7150
Website: www.scme-nm.org

Crystallography Overview for MEMS

Primary Knowledge
Participant Guide

Description and Estimated Time to Complete

This unit reviews the science of crystallography as it relates to the construction of microsystem (MEMS) components. You will study three types of solids (amorphous, polycrystalline, and crystalline) and will learn how to identify crystal orientation based on Miller indices.

Estimated Time to Complete
Allow 40 minutes maximum.

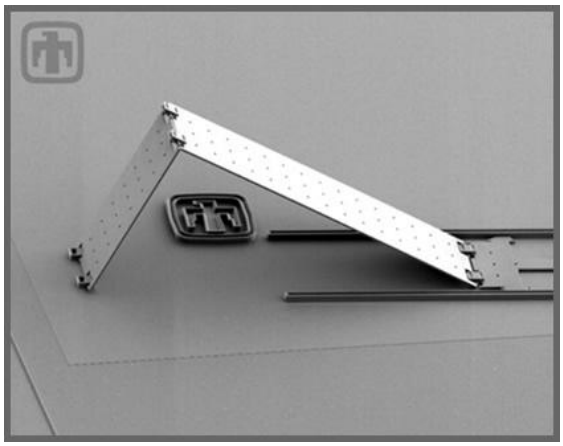
Introduction

Crystallography is the science of determining the arrangement of atoms in solid matter. Solids with an irregular arrangement of atoms are amorphous or noncrystalline structures. Such solids include glass, soot, plastics, and gels. Solids composed of atoms arranged in a definite pattern with a repeating structure are crystalline structures. These structures include diamonds, ice, quartz, and an old favorite, rock candy. All solid matter is either amorphous or crystalline, or a type of crystalline matter called polycrystalline.

One of the objects below is amorphous. The other is crystalline. *Which is which?*

Pretty obvious, isn't it? *Notice the cloudiness of the amorphous glass (bottom left) compared to the clarity of the crystalline diamond (top right).*

Because the molecules of crystalline structures "fit together" so well, a crystal is typically very strong. This characteristic is invaluable for the construction of micro and nanosized devices. The fabrication of microsystems requires a type of crystalline substrate in order to build microsized structures such as cantilevers, diaphragms, gears, comb drives, and electronic circuits. The image to the right is a MEMS popup mirror used to redirect optical data.



MEMS popup mirror
[Courtesy of Sandia National Laboratories, SUMMIT Technologies, www.mems.sandia.gov]

This unit will discusses three topics of crystallography:

- The types of solid matter (amorphous, polycrystalline and crystalline)
- Miller Indices (a method of describing planes and directions within a crystal)
- Growing crystals

Objectives

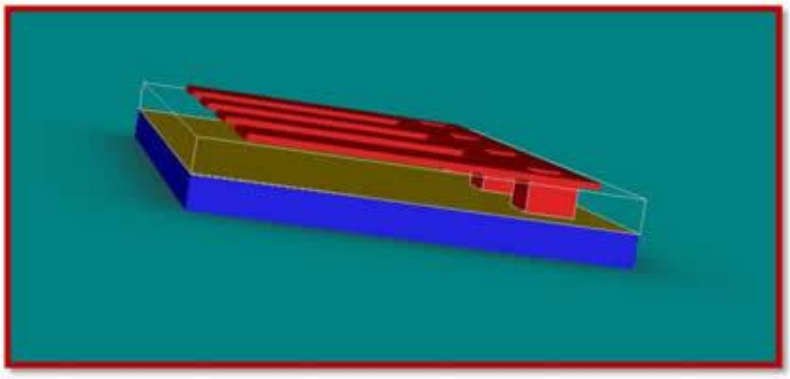
- State at least one example for each type of solid matter (amorphous, polycrystalline and crystalline).
- Discuss the importance of crystal structures in MEMS fabrication.
- Identify the direction of a crystal plane using the Miller index notation.

Key Terms (The key terms are defined in the glossary at this end of this unit.)

Amorphous
Crystalline
Crystallography
Grains
Grain Boundaries
Miller Indices
Polycrystalline
Unit cell

Crystallography

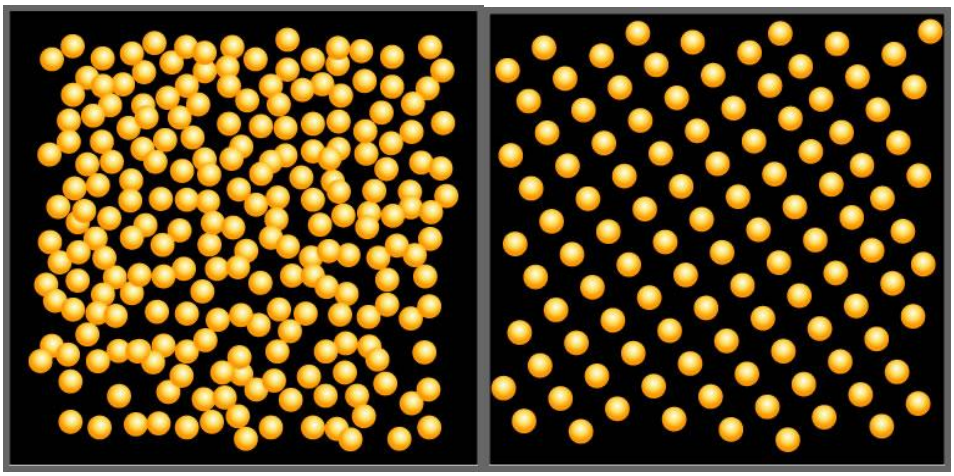
Crystallography is the science of determining the arrangement of atoms in solid matter. This science is important to the advancement of applied sciences and technologies, and material science. It provides information necessary for the development of metal and metal alloy structures, ceramics, glasses, and polymers. For micro and nanotechnologies, it provides information for the design and development of micro and nano-sized components.



Microcantilevers design

The figure above illustrates microcantilevers approximately 100 micrometers long, 30 micrometers wide and 5 micrometers thick. Such cantilevers are etched from a crystalline substrate, usually of silicon. Crystalline structures allow for straight edges as illustrated in the graphic.

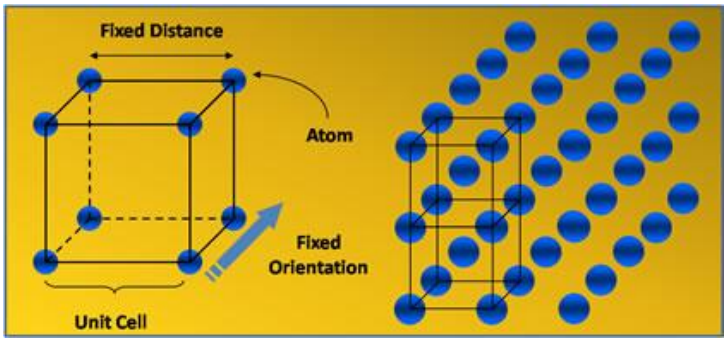
Solid Arrangements



Amorphous vs. Crystalline structures

Matter without a regular arrangement of atoms is called amorphous or non-crystalline. Matter composed of atoms arranged in a definitive pattern with a repeating structure is called a crystal. *(See illustrations above.)* Crystals consist of a repeating structure called a unit cell.

The Unit Cell



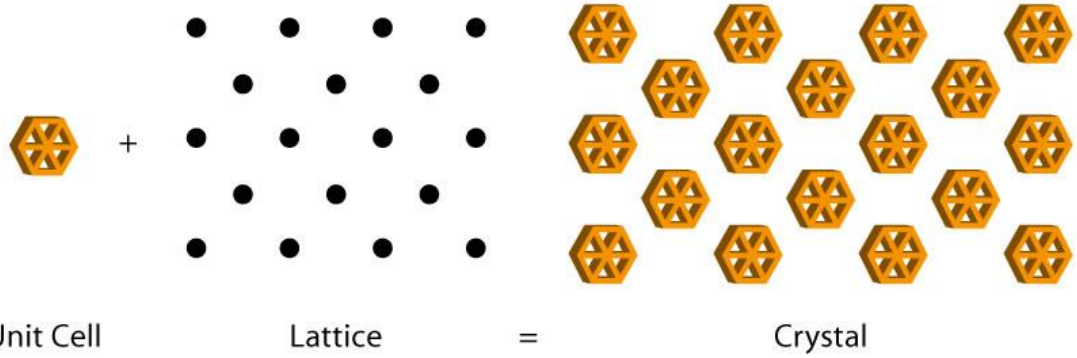
Unit Cell and Unit Cell configuration

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).* The edge of the unit cell connects equivalent points. The resulting structure is a lattice.

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

The Lattice

The pattern of a crystal is like the repeating pattern on wallpaper. The motif is analogous to the unit cell and the arrangement of the motif over the surface is like the lattice.

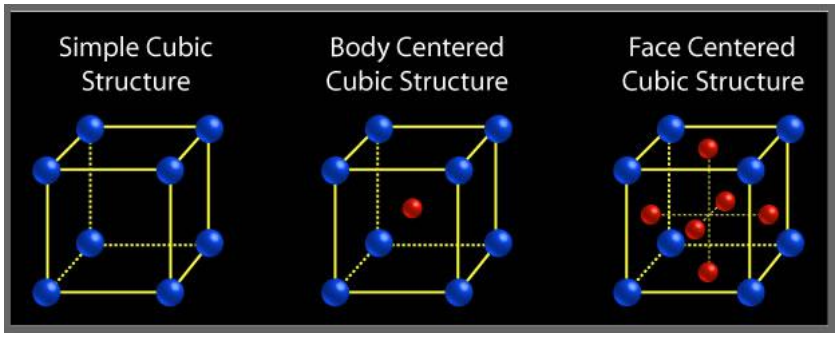


The lattice is a repetition of unit cells and when viewed from different angles or planes one would see different geometries or patterns.

Check out this 3D crystal viewer.[1] This applet allows you to move a crystal around so you can see it from different angles. (Make sure you "Show Bonds" – upper left button. It's easier to see the planes.)

All Unit Cells are Not Alike

There are several different configurations for unit cells. The simplest being the three configurations below.



The *Simple Cubic Structure* is a unit cell consisting of **one atom**. You are probably confused by that because you see eight atoms; however, remember that

- unit cells form a lattice and
- the edge of the unit cell connects to equivalent points.

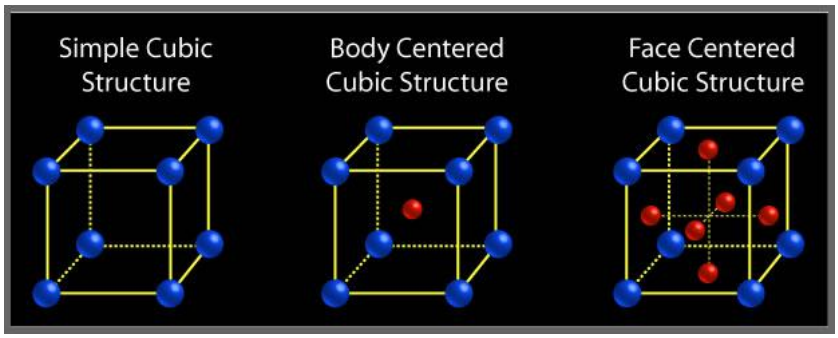
Therefore, each of the atoms you see in the *simple cubic structure* contributes ONLY 1/8 of itself to the unit cell. As the crystal structure forms, seven more unit cells bond with each of the eight atoms. To see this in action, watch an animation of how a body-centered cubic configuration forms a crystal.[2] Pay close attention to how each corner cell bonds to other unit cells.

How many atoms are there

- ***in a "body centered cubic structure"?***
- ***in a "face centered cubic structure"?***

How many atoms are there in a "body centered cubic structure"? ***If you said TWO, you are correct!***

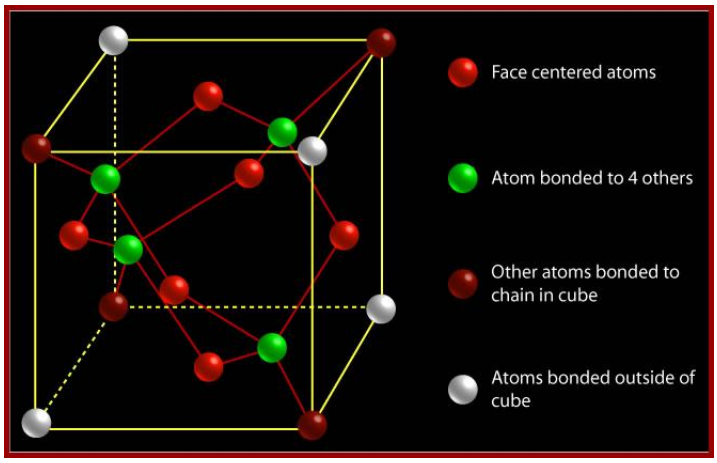
in a "face centered cubic structure"? ***If you said FOUR, you are correct!***



The body centered cubic has ONE atom from the eight corners, then the stand-alone atom on the middle: TWO atoms

The face centered cubic has ONE atom from the eight corners, then ONE-HALF an atom from *each of the face centered atoms:* 1 + ½ * 6 = 4

Carbon Unit Cell



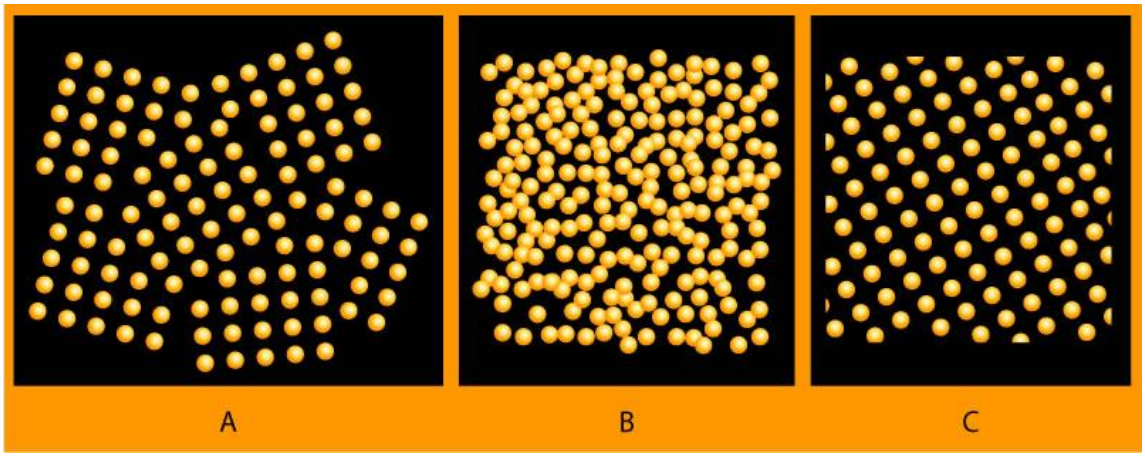
This is the unit cell for Silicon (Si), Germanium (Ge), and carbon (C). Identify the "face-centered atoms".

This unit cell can combine with other unit cells in a variety of ways. To see variety of structures formed by the carbon unit cell, ***Google image Carbon structures***. You should find structures such a carbon sheets, carbon nanotubes, bucky balls (also called fullerenes), and diamonds.

What's What?

Earlier, we talked about solids being crystalline (diamond) or amorphous (glass). However, not all crystals are alike. A true crystal or single crystal is one continuous crystal. Sometimes a crystal is made of many, single crystals. These are polycrystalline structures.

Which of the following graphics (a, b, or c) is crystalline, polycrystalline or amorphous?



Correct answer:

a. polycrystalline
b. amorphous
c. crystalline

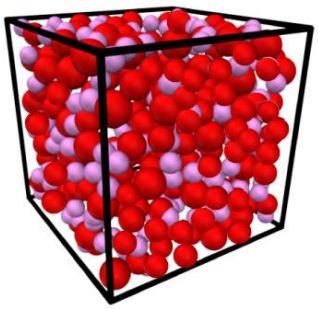
Let's take a closer look at the three arrangements.

Amorphous (Noncrystalline)

Question: What do you think of when you hear the word "amorphous"?

When a solid's atoms are randomly "arranged" in a non-predictable order, the solid is referred to as amorphous. Which of the following are amorphous solids?

- Styrofoam
- Window glass
- Salt
- Wax and paraffin
- A patterned tiled floor
- Peanut brittle



Amorphous solid structure of Silica Glass

If you said all but salt and a tiled floor, you are correct. When you break a piece of peanut brittle, it does not break along a straight edge. Instead it shatters into pieces of different sizes and different shapes. It shatters because it is amorphous, having no definitive edges.

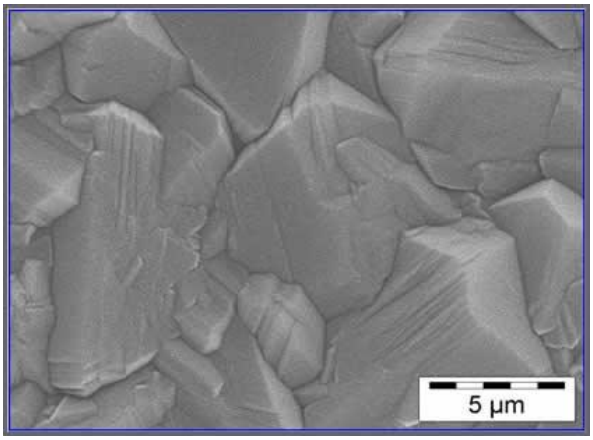
Peanut Brittle

Amorphous solids have the following characteristics:

- No long range order exists at the atomic level. No predictability in the position of atoms, even over a short distance (i.e. a few nanometers).
- An amorphous solid cannot be cut (cleaved) like a crystal. It shatters rather than breaks along a plane.

Amorphous "arrangement"

Polycrystalline



Polycrystalline Diamond
[Courtesy of Prof. Dean Aslam, Michigan State University]

Crystalline matter is either single crystal or polycrystalline (poly being "many").
In both materials the atoms are arranged in a pattern consistent with the unit cell. Diamonds formed in nature are single crystal diamonds. However, polycrystalline diamonds (like the one shown above) are being fabricated for use in high temperature cutting tools, cell phones, and are being explored for use in "MEMS, high-frequency, high temperature and radiation hard device applications".[4] Some metals and metal alloys are polycrystalline. As like diamonds (carbon), silicon can be either polycrystalline or crystalline.

Grains

In polycrystalline materials, the unit cells form small crystals called **grains**. The grains randomly arrange to form the final structure. In the photo, the individual grains of this polycrystalline mineral sample are clearly visible. Each *grain* is a small crystal.

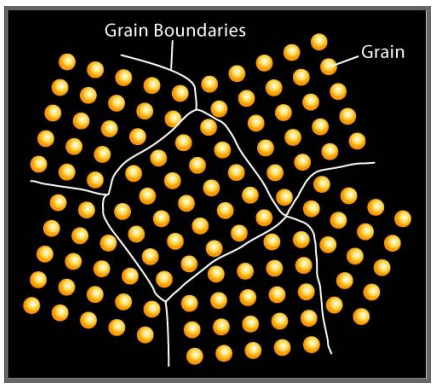
Can you see how the grains connect to each other to form this polycrystalline structure?

In amorphous materials, the unit cells are randomly arranged throughout the material – random distances, random orientations. Grain crystals do not form.

Remember the peanut brittle and how it shattered?

How do you think polycrystalline material would break?

If you said that it would break according to the individual *grains*, you were correct! However, in polycrystalline material the grains are not aligned predictably to each other. In single crystal material, the entire solid is a single gigantic grain. In the figure of the polycrystalline material, note the "grain boundaries".



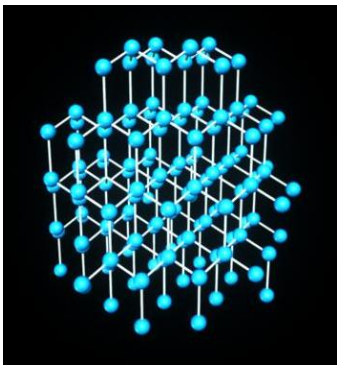
Polycrystalline structure showing grains and grain boundaries

Polycrystalline solids have the following characteristics:

- Long range order exists. Polycrystalline solids consist of crystal grains stuck together; Each crystal grain consists of thousands of atoms with predictable placement.
- Polycrystalline solids do not shatter like amorphous solids. When broken, they tend to break along the grain boundaries (the boundaries form when individual grains are joined).

Based on these characteristics, what are some other examples of polycrystalline solids?

Crystals



Crystals are defined by a regular, well-ordered atomic lattice structure. A lattice consists of stacked planes of atoms. Because the molecules of the crystal fit together and contain strong electrical attractions between the atoms, a crystal is typically very strong.

High quality diamonds consist of tight, dense carbon lattices as illustrated in this image of a diamond structure. The less compact the carbon lattices, the less valuable the diamond. Other crystal solids include gemstones, salt, sugar, some metals, pure silicon, and germanium.

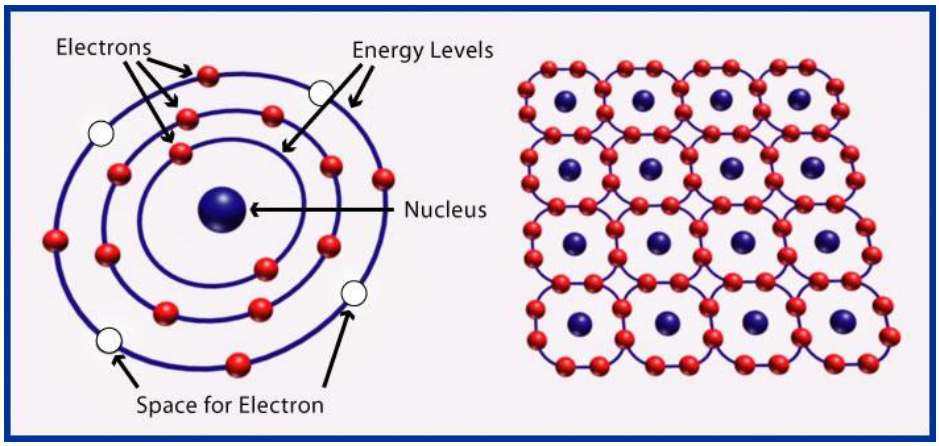
Crystals have the following characteristics:

- Extremely long term order and predictability exists with very few defects. If you could get inside a crystal, you could move from one end to the other and see no difference in the placement of the atoms. The environment is always the same throughout the crystal solid.
- Crystals can be cut along flat planes called cleavage faces. Cutting a crystal is essentially separating one lattice plane from its adjacent plane. This produces a near perfectly flat surface.

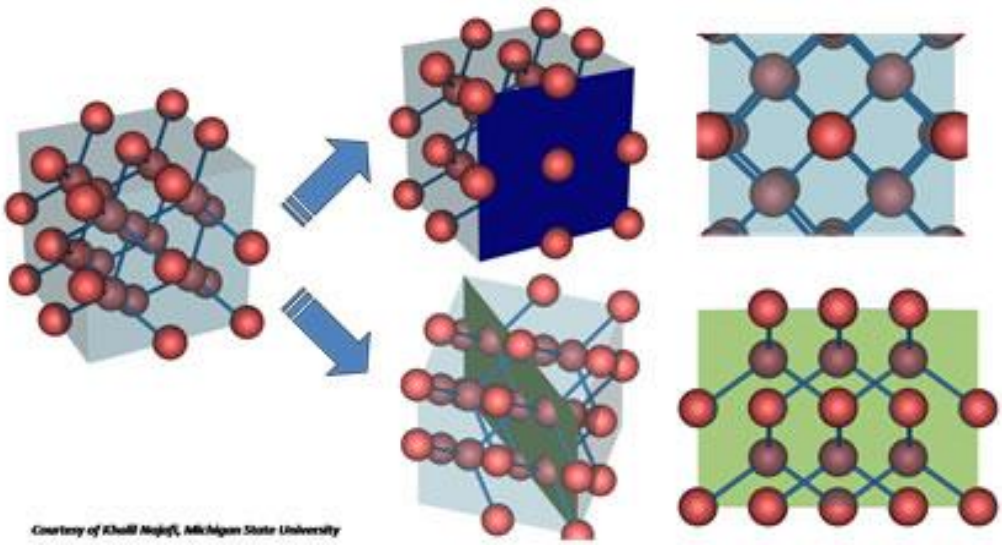
A Closer Look at the Silicon Crystal

Silicon crystal is widely used in micro and nanotechnologies. A silicon (Si) atom has four valence electrons that are *shared* with four other atoms to form four *covalent bonds* when forming a crystal. By sharing electrons this way, each atom's valence shell is complete. This results in solid matter that *is electrically stable* and a *poor conductor of heat.*

In the graphic below, notice that the outer energy level has four electrons and space for four more. On the right, you should see that **each silicon atom** is *bonded to* **four other silicon atoms.** In other words, each "electron space" is filled by one electron from one other silicon atom. The figure on the right is a two-dimensional crystal lattice or sheet.



The orientation of the silicon crystal denotes which crystal plane is exposed on the wafer surface. *(Refer to the graphic below for the following discussion).* The left most image is a silicon crystal. The middle images highlight two different planes within the silicon crystal. Think of looking at the same crystal from two different directions. The images on the right are what you would see looking at the face of each plane. Same crystal, same distance between unit cells, and same orientation of unit cells. However, looking at different planes, presents a different picture.



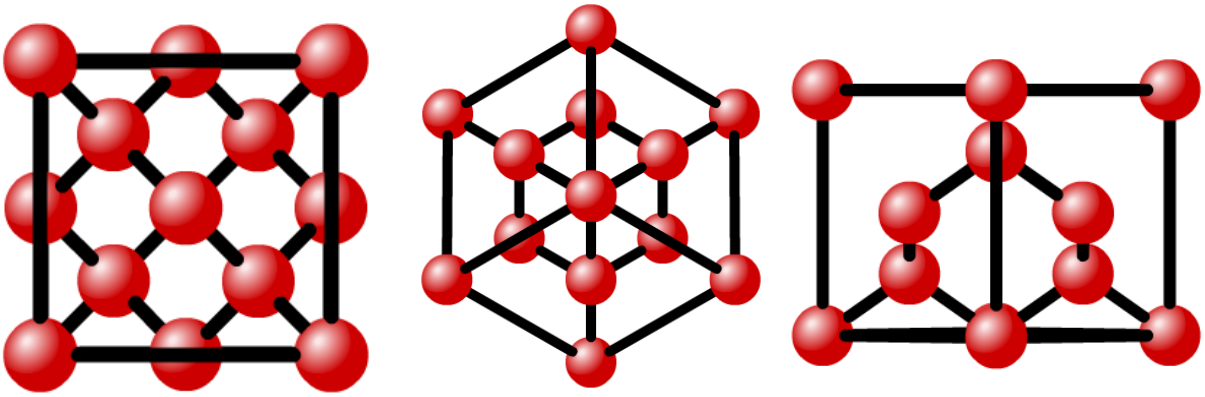
Silicon Crystal Planes
[Graphic courtesy of Khalil Najafi, University of Michigan]

Silicon Properties

The material properties of a silicon wafer change depending on the plane exposed and its arrangement or orientation of atoms. This orientation affects

- the properties of the wafer,
- the number of atoms on the wafer surface, and
- the wafer's conductivity and reaction potential.

Count the number of atoms in the two plane faces shown above right. Revisit 3D crystal viewer[1]. It might help you understand this graphic better. Use the diamond as an example. Rotate the diamond unit cell to find each of the following planes.



Crystal Planes

Planes are the *second level or organization* in crystal structure. They describe the *orientation of the crystal*, which is dependent on the orientation of the individual unit cells within the crystal. Each type of plane is unique, differing in atom count and binding energies and therefore in chemical, electrical and physical properties.

The Miller Index helps us to identify crystal planes.

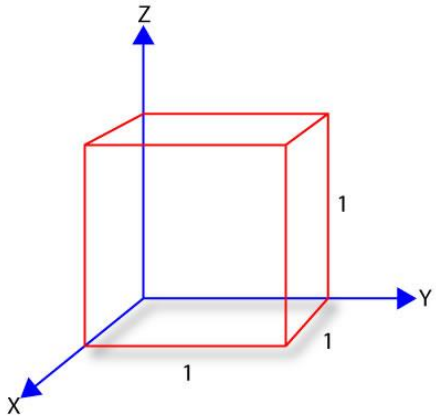
The Miller Index

The Miller index is a roadmap or compass for identifying the crystal planes of crystals. Miller indices are three digit notations that indicate planes and direction 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.

Referring to the graphic "*Cartesian Coordinates",* the

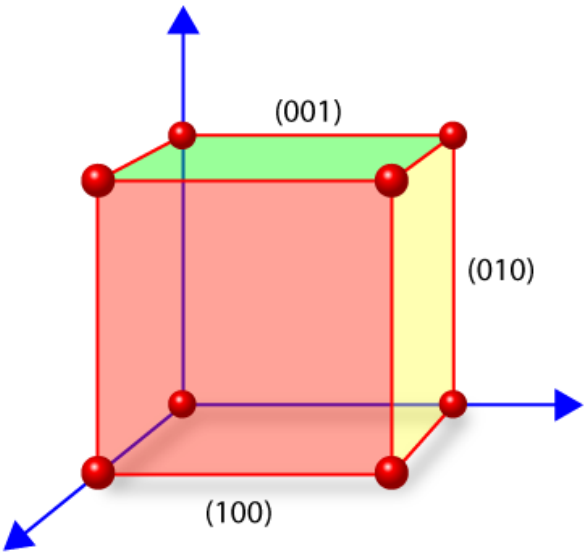
- x-axis vector is denoted [1,0,0]
- y-axis vector is denoted [0,1,0]
- z-axis vector is denoted [0,0,1]

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



Cartesian Coordinates

Identifying the Crystal Plane



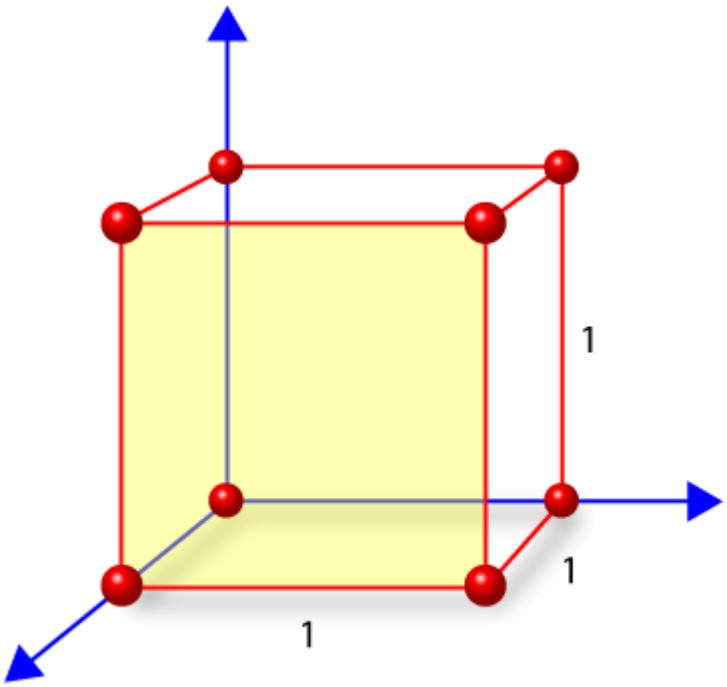
Crystal planes, each perpendicular to its respective vector (or axis)

Crystal planes are perpendicular to their corresponding axis. For example, the plane perpendicular to the [1,0,0] axis or x-axis is the (1,0,0) plane (shown in the figure). Each crystal plane has a unique notation.

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

The above graphic illustrates a unit cell relative to the x-y-z axes.

The (100) Plane



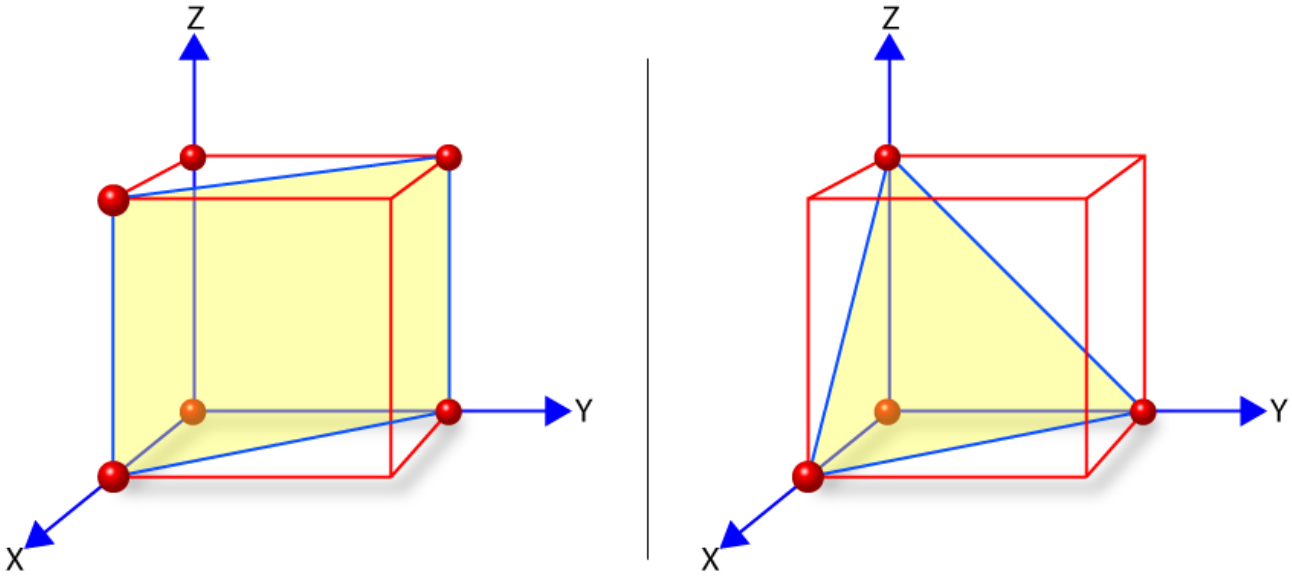
The (100)Plane

The (100) plane is perpendicular to the x-axis, but parallel with the y and z axes. Can you see this in the graphic?

If not, start with the point at which the (100) plane touches the x-axis. Is the plane perpendicular to the x-axis?

Now move along the bottom edge of the plane toward the right. Is this edge parallel to the y-axis? You should now be able to see that the vertical edge of the (100) plane is parallel to the z-axis.

What's What?



What are the Miller indices for each of these planes?

Answers to What's What

What are the Miller indices for each of these planes?
The plane on the left is (110).
The plane on the right is (111).

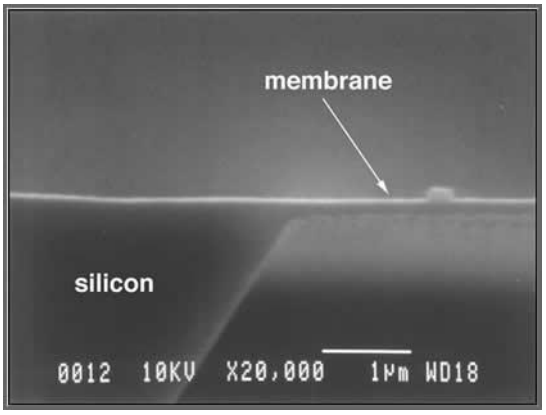
Why is Crystal Orientation Important?

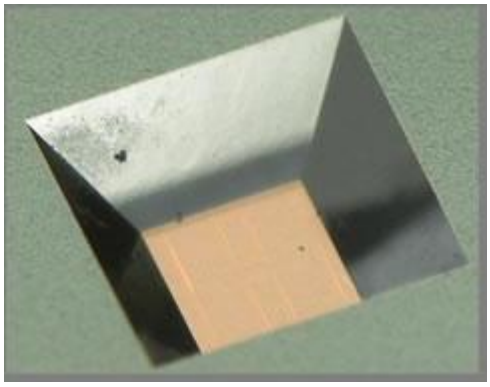
Microsystems consist of structures with defined edges, lengths, widths or thicknesses. They also require certain

- electrical (e.g. resistance),
- mechanical (e.g. bulk modulus), and
- optical (Index of Refraction) properties.

Each of these properties can be different in different orientations.

The structures in the Scanning Electron Microscopy (SEM) images below show a silicon nitride diaphragm (membrane) constructed over a silicon substrate that has been anisotropically etched to provide an opening under the diaphragm. Note the sharp edges of the silicon. This was not accomplished by accident. A (100) silicon substrate and KOH (potassium hydroxide) etchant were used. The chemical reaction between the KOH and the silicon resulted in the anisotropic etch, the selective removal of material in one direction more than in another direction. The silicon atoms were removed at different rates depending on which crystal plane was exposed to the KOH. The picture on the right shows the backside of a wafer.





(Left) Diaphragm (membrane) for MEMS pressure sensor over an etched silicon substrate [SEM courtesy of University of Michigan]
(Right) Backside of etched silicon substrate – blue represents the silicon nitride membrane. [Courtesy of the MTTC / University of New Mexico]

By choosing specific orientation and etchant, one can create a multitude of different shaped structures:

- V-grooves
- Micro fluidic channels
- Cantilevers and bridges
- Mesas or pyramid shaped structures
- Cavities and holes

Determining the orientation

To determine the orientation of a silicon crystal wafer, crystallographers use x-rays aimed at a tiny piece of the wafer containing trillions of identical atoms. The specific periodic arrangement of the atoms within the crystal diffracts the x-rays onto an electronic detector or film. The resulting diffraction pattern on the film or detector gives the crystallographer the information needed to determine the actual orientation of the tiny seed crystal and the spacing of the atoms. A computer reconstructs the orientation from the diffraction pattern. The images below show the resulting patterns of three planes of a silicon crystal. Indicate which image represents each of the following planes. *(Think about the spacing of atoms and the number of atoms in different silicon planes.)*

a. (111)
b. (100)
c. (110)

Crystal orientation of three different planes of a silicon crystal.
X-ray was used to create these images.
[Images printed with permission and from the personal collection of Christopher C. Jones[3]]

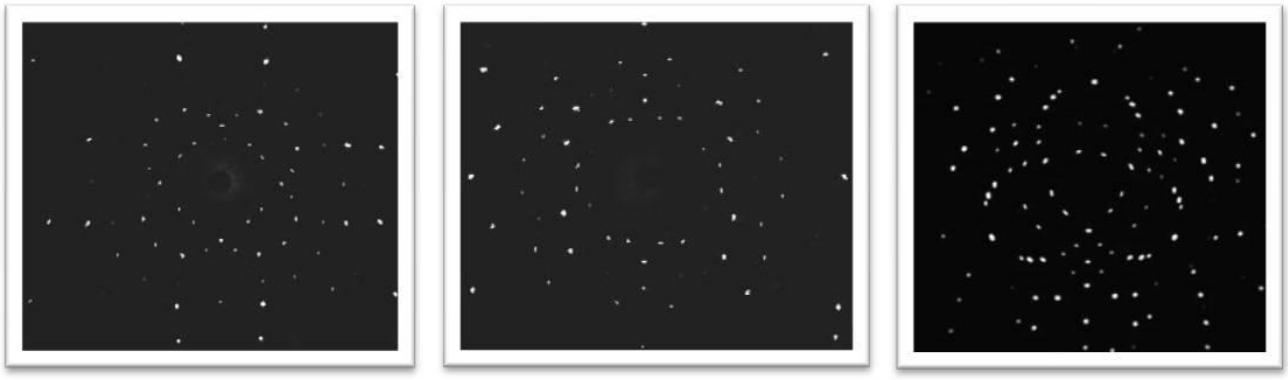
As you can see, there is quite a bit of information in the patterns:

- Spacing between dots
- Relative orientations
- Angle between patterns and different dots

Such a pattern can be reconstructed into a 3-D image for a better view of the crystalline structure.

This same process is used to determine the double helix structure of DNA. Technicians crystallize the DNA, then put an x-ray beam through it. Because they have to use a weak x-ray beam, exposure time is long; however, eventually a diffraction pattern appears.

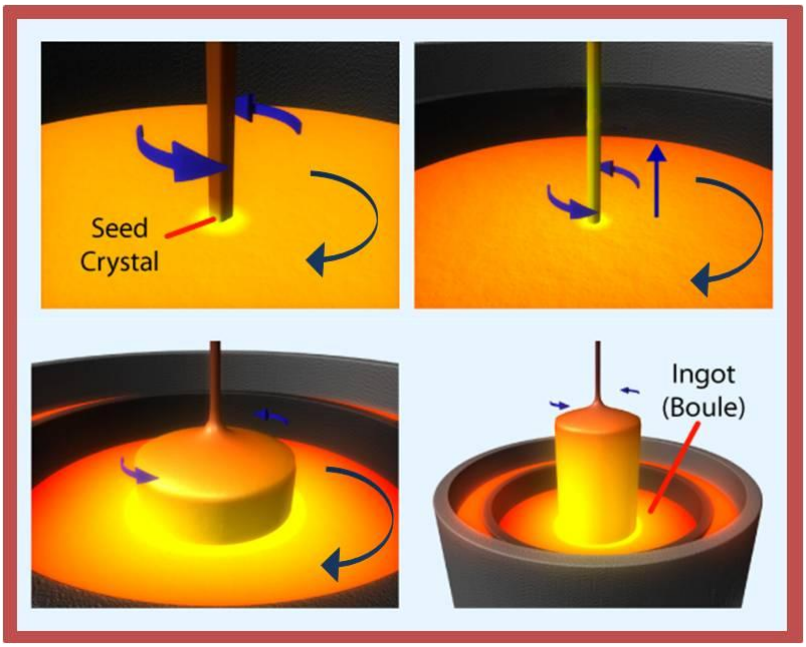
Answer: (100), (110) and (111), respectively (HINTS: The (100) pattern has fewer atoms and right angles are distinct in the pattern. The (111) pattern has the most atoms on the surface.)



Another method to determine the crystal orientation of a silicon wafer is to break it. Remember that a crystal is a lattice structure; therefore, when a silicon wafer breaks it will break along a lattice plane.

To see this for yourself, complete the SCME "Breaking Wafers Activity".

Making a silicon wafer



The CZ (Czochralski) method of growing a silicon ingot

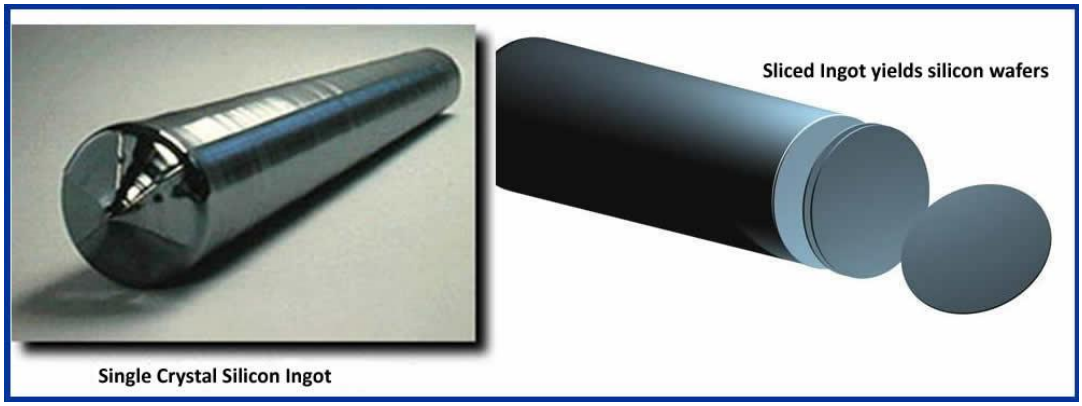
How is a silicon crystal formed and the orientation of a silicon wafer substrate determined?

1. First we start with very pure silicon material (99.999999999% pure!)
2. Melt the pure silicon in a crucible.
3. Lower a seed crystal into the molten silicon *(top left image)*. Silicon atoms in the molten silicon attach to the seed as a crystalline structure.
4. To continue to "grow" the silicon crystal, rotate the seed and the crucible with the molten silicon in opposite directions while slowly pulling the seed crystal upward.
5. The slower the "pull", the larger the diameter of the crystal ingot that forms. (This process is the Czochralski (CZ) Method of growing silicon.)

The seed crystal acts as a starting point for the alignment of the atoms in the molten silicon. The alignment of the seed crystal relative to the molten silicon determines the orientation of the subsequently grown silicon crystal. The wafers cut from this crystal will maintain this orientation.

The Ingot

The resulting ingot is cylindrical in shape, 25.4 mm (~1 inch) to 450 mm (~18 inches) in diameter and several meters long. Once cooled, the ingot is ground to a perfect cylinder. The cylinder is sliced into thin wafers using diamond coated wires or saw blades. Each slice is polished to create silicon wafers, also referred to as substrates. Microsystems are constructed on or within these substrates depending upon the type of process used – surface or bulk, respectively.



Summary

Solid matter is either amorphous, polycrystalline or crystalline. Silicon polycrystalline wafers are widely used as the substrate for microsystems. These wafers provide the electrical and mechanical properties needed to build the components for electromechanical systems. Crystal orientations (100) and (111) are commonly used.

Food For Thought

Explain why the quality of a diamond is determined by its crystalline structure?

Why are only polycrystalline and crystalline materials used as substrates for microsystems components and devices?

Food for Thought / Answers

Explain why the quality of a diamond is determined by its crystalline structure?

Why are only polycrystalline and crystalline materials used as substrates for microsystems components and devices?

Glossary

Amorphous: Without order. Lacking definite form.

Band tailing: A characteristic that helps to define a material as being a conductor, insulator or semiconductor. Band tailing reduces band gap and increases conductivity.

Crystalline: A uniform arrangement of atoms / molecules in all directions.

Crystallography: The science of determining the arrangement of atoms in solid matter.

Grains: Small crystals. Grains are comprised of several unit cells of a crystal.

Grain Boundary: The edge formed by adjourning grains in a polycrystalline structure.

Miller Index: A notation system in crystallography for planes and directions in crystal lattices.

Miller indices: Three integers identifying a type of crystal plane.

Polycrystalline: Solid matter that is made of many smaller crystallites or grains with varying orientation. The variation in direction can be random or directed, possibly due to growth and processing conditions.

Unit cells: A unit of atoms arranged in a definite pattern with a repeating structure. A unit cell is a crystal.

References and Resources

1. "3D Crystal Viewer" Applet. http://www.dawgsdk.org/crystal/index.en
2. Body-centered Cubic". Barbara L. Sauls and Frederick C. Sauls. King's College. Pennsylvania. http://departments.kings.edu/chemlab/chemlab_v2/bcc.html
3. "Crystal Symmetry". Scientific Photographs by Christopher C. Jones. http://minerva.union.edu/jonesc/Scientific.html
4. "Polycrystalline Diamond". Evince Technology. http://www.evincetechnology.com/poly_xtl_dia.html
5. Crystallography Presentation by Matthias Pleil, SCME
6. Crystallography, MATEC

Support for this work was provided by the National Science Foundation's Advanced Technological Education (ATE) Program.

Southwest Center for Microsystems Education (SCME)
University of New Mexico

MEMS Fabrication Topic

The Miller Index Activity

Shareable Content Object (SCO)

This SCO is part of the Learning Module
Crystallography Overview

Target audiences: High School, Community College.

Support for this work was provided by the National Science Foundation's Advanced Technological Education (ATE) Program through Grants #DUE 0902411.

Any opinions, findings and conclusions or recommendations expressed in this material are those of the authors and creators, and do not necessarily reflect the views of the National Science Foundation.

Southwest Center for Microsystems Education (SCME)
800 Bradbury Drive SE, Suite 235
Albuquerque, NM 87106-4346
Phone: 505-272-7150
Website: www.scme-nm.org

The Miller Index Activity

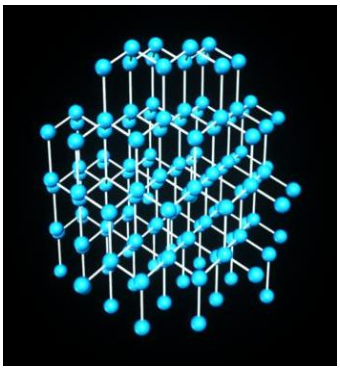
The Crystallography Overview Learning Module
Participant Guide

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.

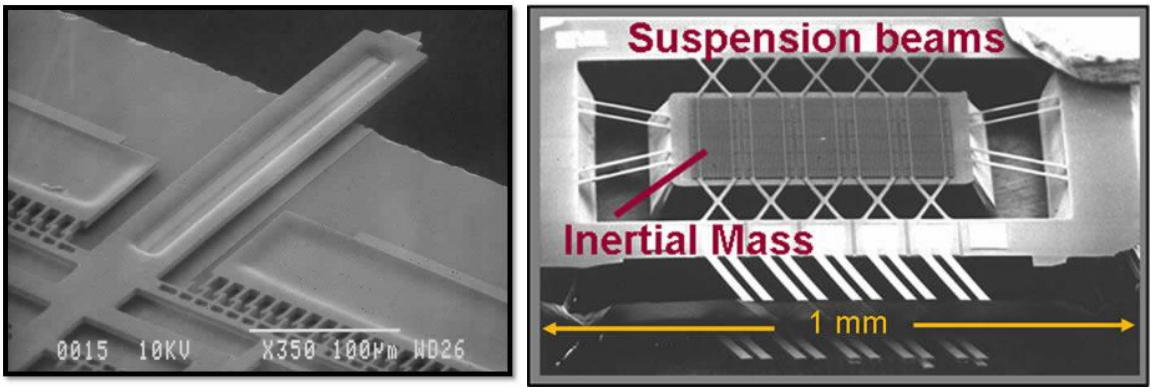
Introduction



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 which 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[1].

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 accelerometer that shows an inertial mass fabricated within a crystal substrate. Components in all three of these images were designed and fabricated using specific planes of silicon crystal.



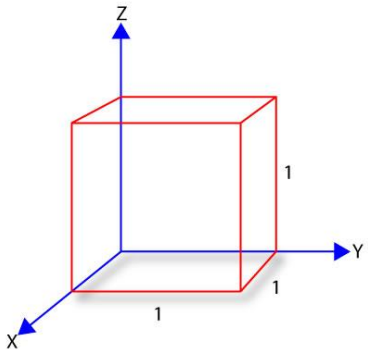
[Cantilever image on the left courtesy of Sandia National Laboratories, Pressure sensor chamber courtesy of the MTTC / University of New Mexico, Accelerometer courtesy of the University of Michigan]

How do we identify the many planes in a crystal structure? Miller index notation is a roadmap or directional compass for identifying the crystal planes and directions within crystals. Miller indices are three digit notations that indicate planes and direction 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.

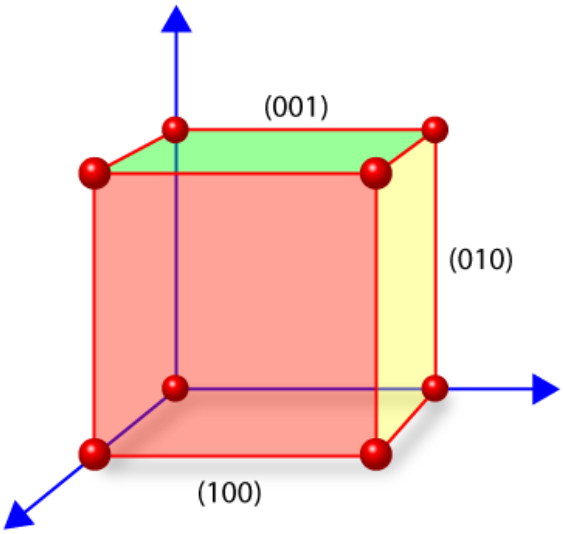
Referring to the graphic "*Cartesian Coordinates",* the

- x-axis vector direction is denoted [1,0,0]
- y-axis vector direction is denoted [0,1,0]
- z-axis vector direction is denoted [0,0,1]

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



Cartesian Coordinates



Crystal planes, each perpendicular to its respective vector (or axis)

Crystal planes are perpendicular to their corresponding axis. For example, the plane perpendicular to the [1,0,0] direction or x-axis is the (1,0,0) plane (shown red in the figure). Each crystal plane has a unique notation.

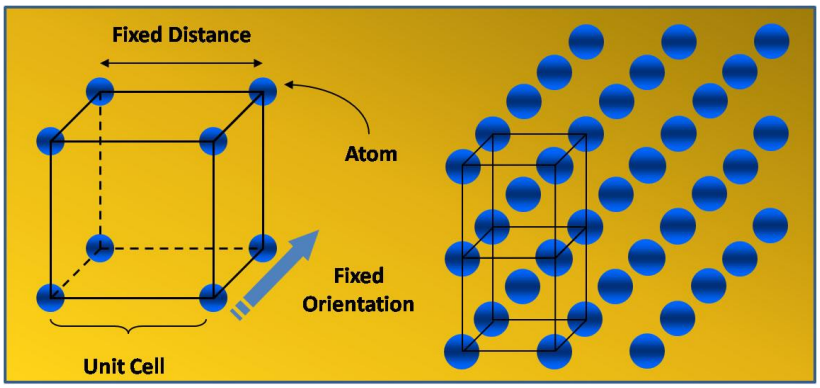
- (1,0,0) or (100) is perpendicular to the x-axis (Red)
- (0,1,0) or (010) is perpendicular to the y-axis (Yellow)
- (0,0,1) or (001) is perpendicular to the z-axis (Green)

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 $(\bar{1}00)$ plane would refer to the plane parallel to the (100) plane, however; it would be one unit from the origin on the negative x (-x) axis or on the opposite side of the unit cell[2].

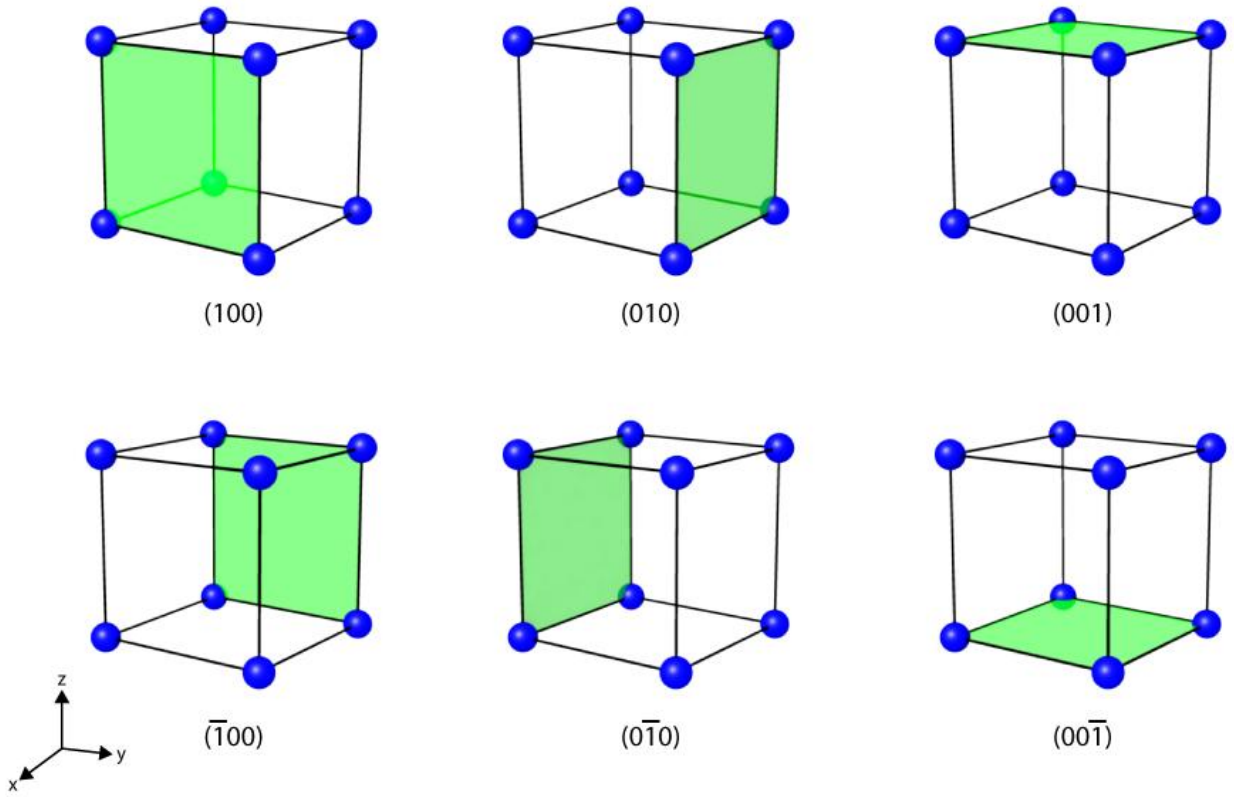
The Unit Cell

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.

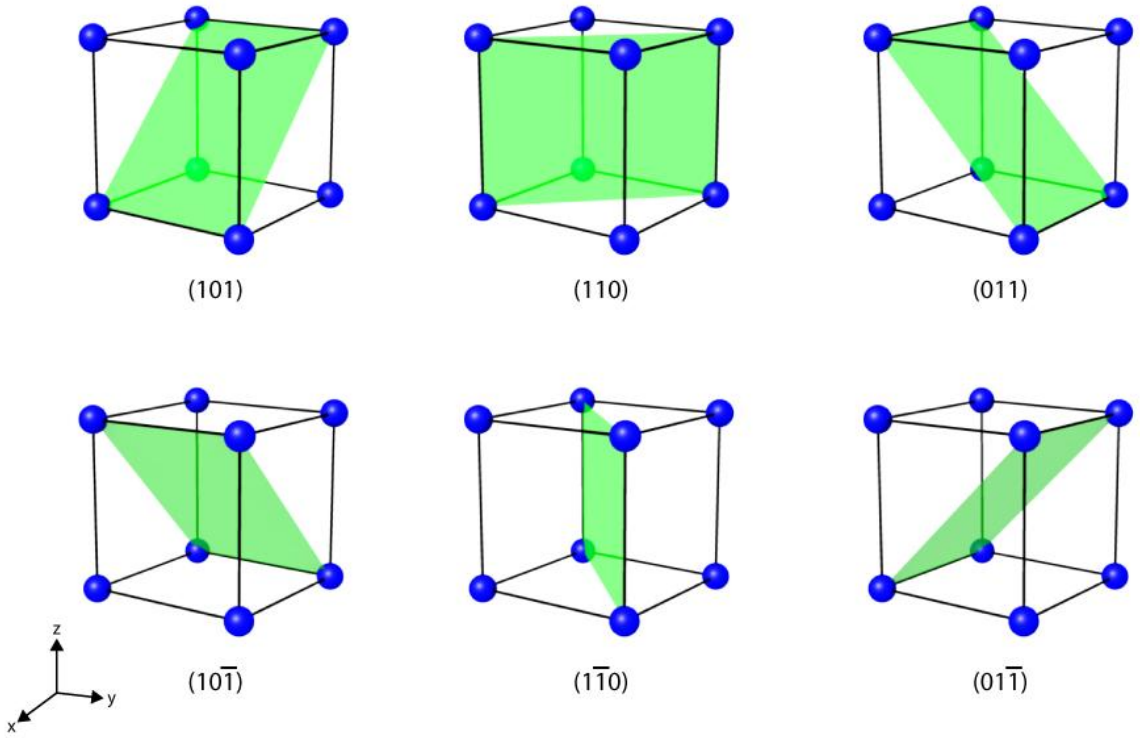
The figure below illustrates a unit cell for a crystalline structure.



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.

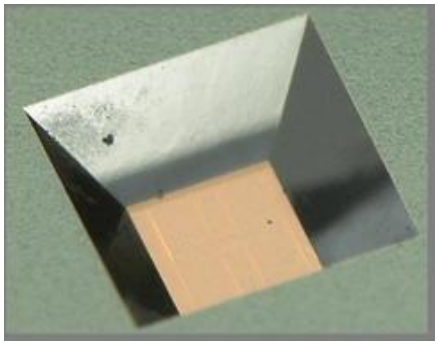


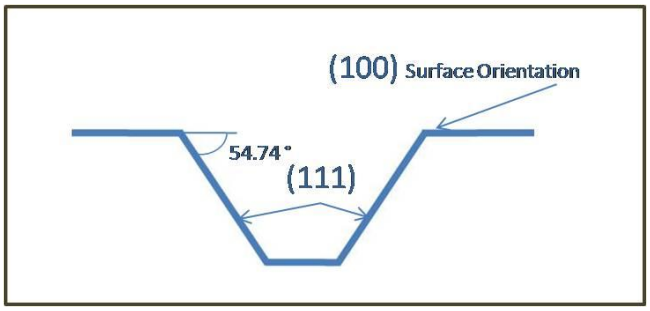
The (101), (110), (011), (10$\bar{1}$), (1$\bar{1}$0) and (01$\bar{1}$) planes form the sections through the diagonals of the unit cell.



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, resulted in a desired anisotropic etch along the (111) crystal plane. Because of the crystalline structure and bonds of the crystal in the (100) silicon, material was selectively removed (or etched) along the (111) plane, leaving the desired cavity. The etch occurs both vertically (down the (100) plane) and sideways (along the (111) plane) at an etch rate of 400:1 meaning that the vertical etch is 400 times faster than the sideways etch. This is because the lattice along the (111) plane is the more dense or more has more silicon atoms on the surface than the (100) plane. The angle of the (111) plane is always 54.74° relatively to the (100) plane in a silicon crystal. The predictability of this chemical reaction allows for a micro-cavity which 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 model the different crystal planes for better visualization of the Miller indices.

Activity Outcome

By the end of this activity you should be able to understand and visualize the basic crystal planes in a crystal structure and match the correct Miller indices to each plane.

Resources

SCME Crystallography Overview for MEMS PK

Supplies / Equipment

Supplies provided by instructor

- 3 yard sticks or rulers (representing the x, y, z axes)
- 1- piece of cardboard approximately 12"x12" in size (representing a "plane")

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

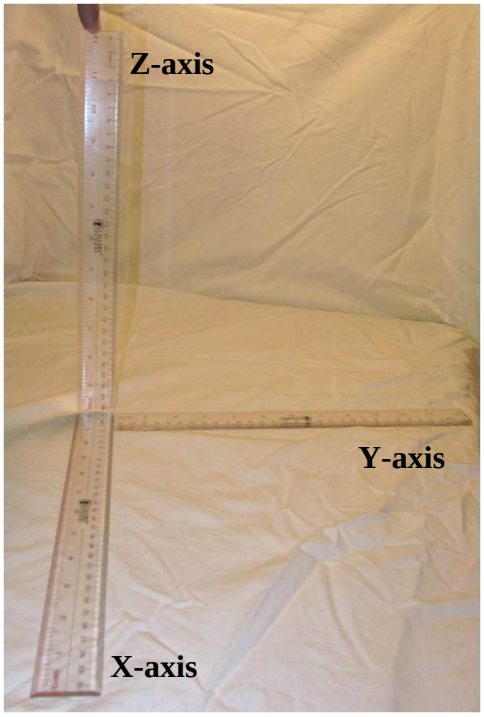
Below is an on-line tutorial that will help you to better understand Miller Indices before starting the activity.

Lattice Planes and Miller Indices
(http://www.doitpoms.ac.uk/tlplib/miller_indices/printall.php), University of Cambridge.

Activity: Miller Indices Models

Procedure

1. Have one or two members of your team create a Cartesian coordinate system using the three rulers. Each ruler represents 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. While one member of your team holds the axes, another should 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.

3. 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.

4. Position the cardboard to represent the (001) crystal plane. Make sure that everyone in your team agrees.

5. Position the cardboard to denote the (110) crystal plane. Make sure that everyone in your team agrees.

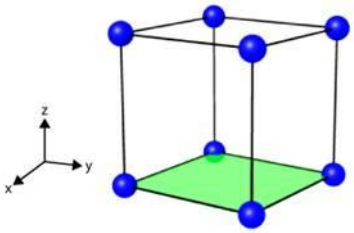
6. Now position the cardboard in the (111) orientation.

7. Model the $(\bar{1}00)$, $(0\bar{1}0)$ and $(00\bar{1})$ planes.

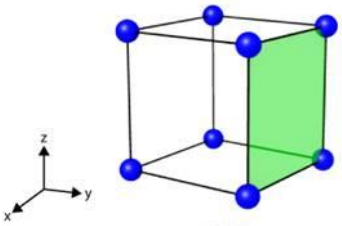
8. Model the (101), (011), $(10\bar{1})$, $(1\bar{1}0)$ and $(01\bar{1})$ planes.

Post-Activity Questions

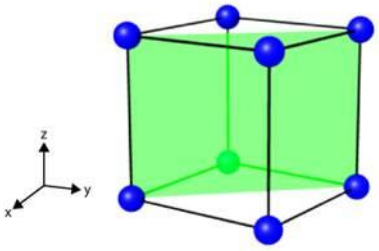
1. What does it mean when a crystal plane is noted like this: $(\bar{1}00)$?
2. Name all of the faces of the "unit cell" using the Miller Index notations.
3. Name all of the planes that form the planes through the diagonals of the unit cell.
4. Draw a unit cell and show the (011) plane relative the x-y-z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



8. 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 micro-structures 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
2. Lattice Planes and Miller Indices. University of Cambridge. http://www.doitpoms.ac.uk/tlplib/miller_indices/printall.php

Support for this work was provided by the National Science Foundation's Advanced Technological Education (ATE) Program through Grants.

Southwest Center for Microsystems Education (SCME)
University of New Mexico

MEMS Fabrication Topic

Breaking Wafers Activity

Shareable Content Object (SCO)

This SCO is part of the Learning Module
Crystallography

Target audiences: High School, Community College.

Support for this work was provided by the National Science Foundation's Advanced Technological Education (ATE) Program through Grants #DUE 0830384 and 0902411.

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Southwest Center for Microsystems Education (SCME)
800 Bradbury Drive SE, Suite 235
Albuquerque, NM 87106-4346
Phone: 505-272-7150
Website: www.scme-nm.org

Breaking Wafers Activity

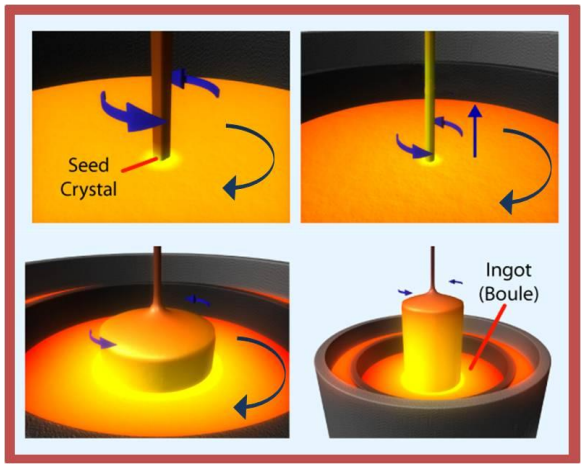
The Crystallography Learning Module
Participant Guide

Description and Estimated Time to Complete

In this activity you will further explore the crystal planes of silicon by breaking two silicon wafers. By the end of this activity, you should be able to tell from a piece of silicon the specific crystal orientation of the silicon crystal.

Estimated Time to Complete
Allow at least 15 minutes to complete this activity.

Introduction



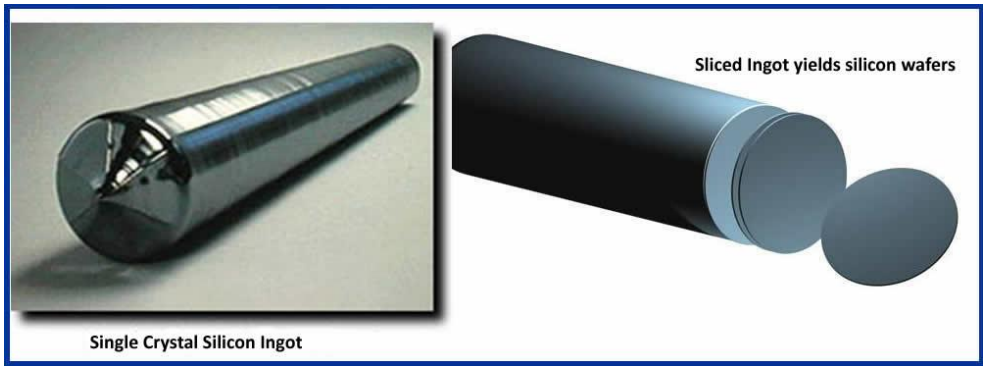
The CZ (Czochralski) method of growing a silicon ingot

How is a silicon crystal formed and the orientation of a silicon wafer substrate determined?

1. First we start with very pure silicon material (99.999999999% pure!)
2. Melt the pure silicon in a crucible.
3. Lower a seed crystal into the molten silicon *(top left image)*. Silicon atoms in the molten silicon attach to the seed as a crystalline structure.
4. To continue to "grow" the silicon crystal, rotate the seed and the crucible with the molten silicon in opposite directions while slowly pulling the seed crystal upward.
5. The slower the "pull", the larger the diameter of the crystal ingot that forms. (This process is the Czochralski (CZ) Method of growing silicon.)

The seed crystal acts as a starting point for the alignment of the atoms in the molten silicon. The alignment of the seed crystal relative to the molten silicon determines the orientation of the subsequently grown silicon crystal. The wafers cut from this crystal will maintain this orientation.

The resulting ingot is cylindrical in shape, 25.4 mm (~1 inch) to 450 mm (~18 inches) in diameter and several meters long. Once cooled, the ingot is ground to a perfect cylinder. The cylinder is sliced into thin wafers using diamond coated wires or saw blades. Each slice is polished to create silicon wafers, also referred to as substrates. Microsystems are constructed on or within these substrates depending upon the type of process used – surface or bulk, respectively.



To determine the orientation of a silicon crystal wafer, crystallographers use x-rays aimed at a tiny piece of the wafer containing trillions of identical atoms. The specific periodic arrangement of the atoms within the crystal diffracts the x-rays onto an electronic detector or film. The resulting diffraction pattern on the film or detector gives the crystallographer the information needed to determine the actual orientation of the tiny seed crystal and the spacing of the atoms. A computer reconstructs the orientation from the diffraction pattern. The images below show the resulting patterns of three planes of a silicon crystal. Indicate which image represents each of the following planes. *(Think about the spacing of atoms and the number of atoms in different silicon planes.)*

a. (111)
b. (100)
c. (110)

_____ _____ _____

[Images printed with permission and from the personal collection of Christopher C. Jones[1]]

What characteristics helped you to identify the correct orientation of these planes?

An easier way to determine the crystal orientation of a silicon wafer is to just break it.
So let's do that in this activity.

Activity Objectives and Outcomes

Activity Objective

- State the crystal orientation of a silicon wafer by breaking the wafer into smaller pieces and observing the resulting shape.

Activity Outcome

By the end of this activity you should be able to look at a piece of a silicon wafer and state its crystal orientation: (100) or (111).

Resource - SCME Crystallography Overview for MEMS PK

Supplies / Equipment

Supplies provided by instructor

- Safety glasses or goggles
- Ice Pick or pointed metal implement (e.g., a Philips screwdriver, a large nail)
- Hammer (For tapping the end of the metal implement)
- Two large sheets of paper or poster paper

Supplies included in kit

- Two silicon wafers of (100) orientation
- Two silicon wafers of (111) orientation
- Wafer holders and packing
- 1 Crystallography Learning Module – Instructor Guide
- 1 Crystallography Learning Module – Participant Guide

Documentation

- Answers to the Post-Activity Questions

Activity: Breaking Wafers

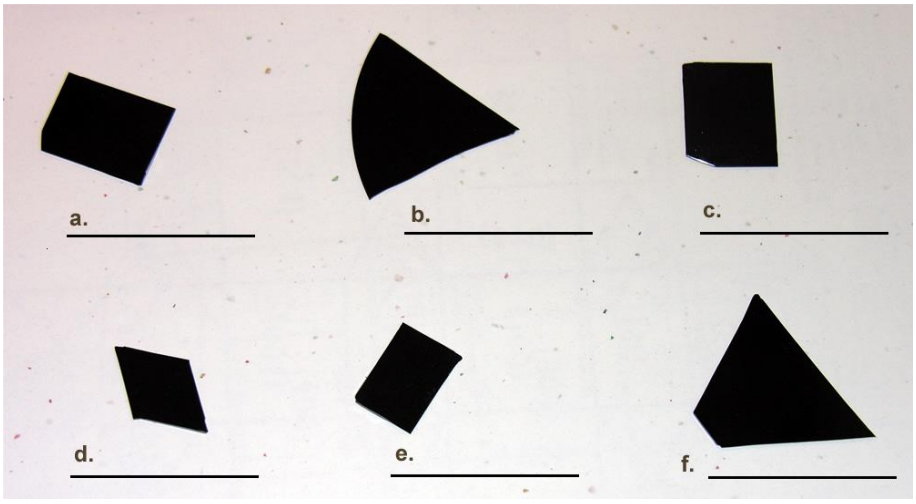
Procedure:

1. Place two pieces of paper or poster paper side-by-side on the table top.
2. Remove one wafer from each of the wafer holders and place them side-by-side on the two pieces of paper.
3. Place another piece of paper over one of the wafers. (This is to minimize wafer shards from flying off the table.)
4. Put on your safety glasses.
5. Place the tip of the ice pick or screw driver close to the center of one of the wafers.

6. With the hammer or your hand, gently, but firmly, tap the handle of the ice pick until you hear the wafer break (snap).
7. Repeat steps 4 and 5 with the second wafer.
8. You will see that that wafers break at either right (90°) angles or at approximately 60° angles.
    a. What is the orientation of the wafer surface plane that breaks at 90° angles: (100) or (111)?
    b. What is the orientation of the wafer that breaks at 60° angles: (100) or (111)?
9. What would be the result of breaking one of the pieces of each wafer?
10. Test out your hypothesis. Break one of the pieces of each wafer.
11. Answer the Post-Activity Questions

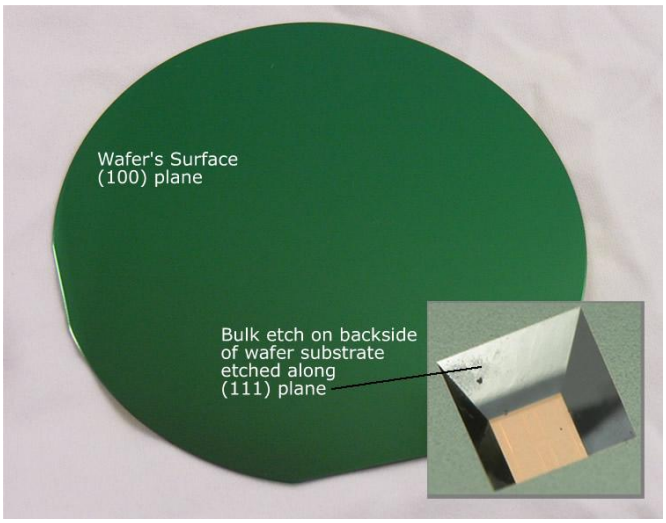
Post-Activity Questions

1. In this activity, you broke two silicon wafers. One wafer had a (100) crystal surface plane orientation and the other a (111) surface plane orientation. In the making of the original silicon ingot, what determined the crystal orientation of the silicon wafer?
2. At what approximate angle did the (111) wafer break?
3. At what approximate angle did the (100) wafer break?
4. Did each wafer continue to break at the same angle when you broke the smaller pieces? Why or why not?
5. Which orientation (100) or (111) has more silicon atoms exposed to the wafer's surface?
6. Why is crystal orientation important in the fabrication of microsystems?
7. Identify the crystal orientation of each of the following pieces of silicon.



Summary

The most commonly used orientation for MEMS fabrication is the (100) and less frequently the (111). These crystal orientation determines the electrical and mechanical properties for components of electromechanical systems. An example of when crystal orientation is very important is in the anisotropic etching of crystalline silicon. For example, KOH (potassium hydroxide) is used to etch crystalline silicon; the (111) plane etches at about 0.0035µm / minute while the (100) plane etches at 1.4µm/minute, about 500 times faster! The picture shows the surface of this wafer as the (100) plane and the results of a KOH backside etch that etched along the (111) plane.



References

1. "Crystal Symmetry". Scientific Photographs by Christopher C. Jones. http://minerva.union.edu/jonesc/Scientific.html
2. Images of wafers, broken wafers and etched wafers courtesy of the Manufacturing Technology Training Center (MTTC) at the University of New Mexico.

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Southwest Center for Microsystems Education (SCME)
University of New Mexico

MEMS Fabrication Topic

An Origami Crystal Activity

Shareable Content Object (SCO)

This SCO is part of the Learning Module
Crystallography

Target audiences: High School, Community College.

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Southwest Center for Microsystems Education (SCME)
800 Bradbury Drive SE, Suite 235
Albuquerque, NM 87106-4346
Phone: 505-272-7150
Website: www.scme-nm.org

An Origami Crystal Activity

Participant Guide

Description and Estimated Time to Complete

In this activity you will use a template to construct a representation of a silicon crystal. The final structure will actually be a rhombicuboctahedron, one of 13 Archimedean solids or a convex polyhedral. Certain faces of the template are marked with specific plane notations from Miller Index. Once the polyhedral is constructed, the markings will illustrate the crystal plane of each face of the polyhedral.

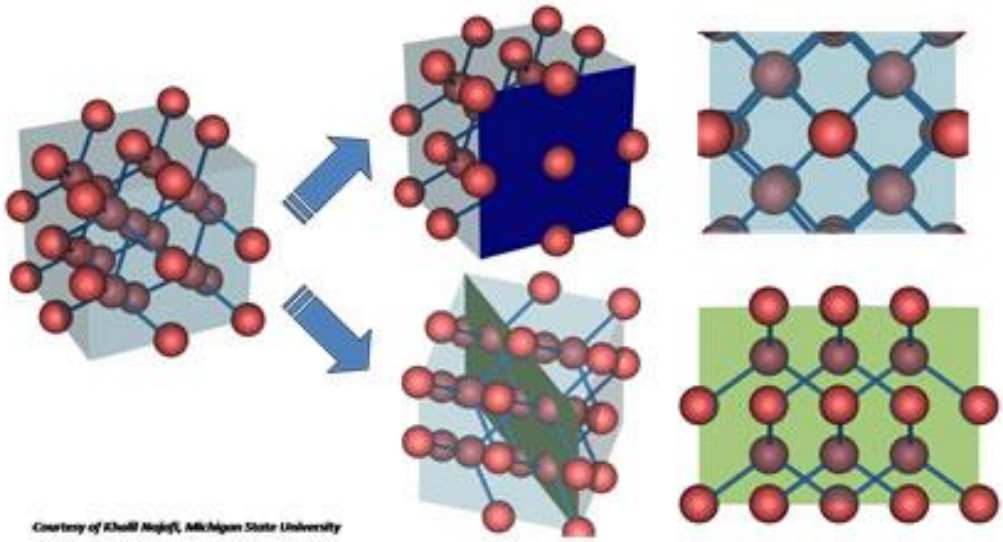
You will use the Japanese art of origami to construct this solid from a template.

Estimated Time to Complete
Allow at least one hour to complete this activity.

Introduction

Crystals are defined by a regular, well-ordered atomic lattice structure. A lattice consists of stacked planes of atoms. The bonds between the atoms are typically very strong.

Silicon crystal is widely used in micro and nanotechnologies. The orientation of the silicon crystal denotes which crystal plane is exposed on the wafer surface. *(Refer to the graphic below in the following discussion).* The left most image shows the silicon crystal structure, also known as face-centered cubic or diamond cubic. It is the same structure carbon forms in a diamond. The middle images highlight two different planes within this structure. Think of looking at the same crystal from two different directions. The images on the right are what you would see looking at the face of each plane. Same crystal, same distance between unit cells, and same orientation of unit cells. However, looking at different planes, presents a different picture.



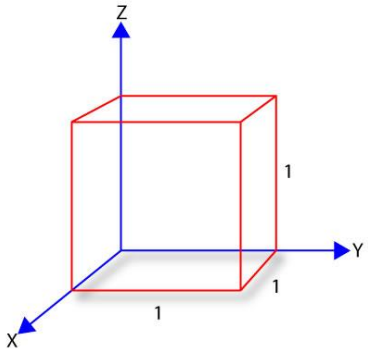
Silicon Crystal Planes
[Graphic courtesy of Khalil Najafi, University of Michigan]

The Miller index is a roadmap or directional compass for identifying the crystal planes and directions within crystals. Miller indices are three digit notations that indicate planes and direction 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.

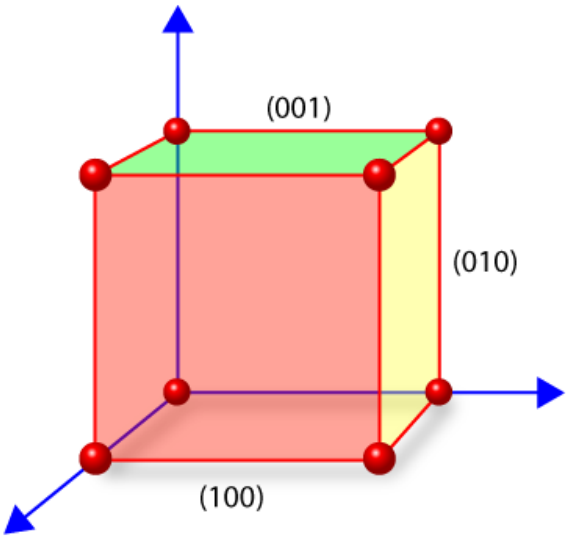
Referring to the graphic "*Cartesian Coordinates",* the

- x-axis vector direction is denoted [1,0,0]
- y-axis vector direction is denoted [0,1,0]
- z-axis vector direction is denoted [0,0,1]

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



Cartesian Coordinates



Crystal planes, each perpendicular to its respective vector (or axis)

Crystal planes are perpendicular to their corresponding axis. For example, the plane perpendicular to the [1,0,0] direction or x-axis is the (1,0,0) plane (shown in the figure). Each crystal plane has a unique notation.

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

Crystal orientations (100) and (111) are commonly used for microsystems fabrication.

Activity Objectives and Outcomes

Activity Objectives

- Using the Japanese art of origami, folding paper into objects, you will construct a rhombicuboctahedron that represents a silicon crystal.

Activity Outcomes

The final product must have clean edges and flat faces. When you work in a small startup company or even a large research lab, many tasks are performed by hand. Attention to detail as well as fine motor skills is a premium! Your outcome should show that you planned your strategy before tackling this task. Take your time and build a quality product! Try not to have excessive tape or glue showing on the finished work.

Resources

Template by Jack Judy, Associate Professor, Electrical Engineering, UCLA

Supplies

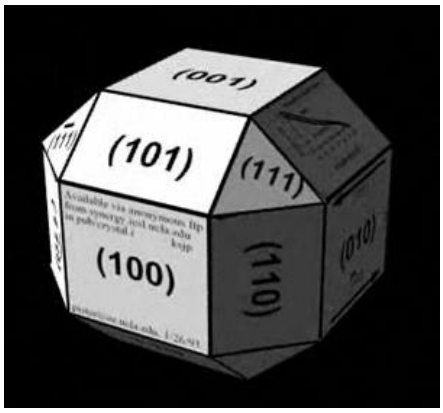
- 12 origami templates printed on cardstock are contained in the SCME Crystallography kit. If you do not have the kit, you can go to http://www-bsac.eecs.berkeley.edu/~pister/crystal.pdf for the template.
- A pair of thin scissors, Exacto knife, or razor blade

Documentation

- The silicon crystal cube
- Post Activity Questions with answers

Activity: An Origami Crystal

NOTE: For simplification purposes, we will refer to the final outcome as a "cube" rather than a rhombicuboctahedron or polyhedral. The image to the right shows the constructed origami crystal.



Procedure:

1. Watch the video "Origami Crystal animation". *(This video can be downloaded from scme-nm.org – Educational Material – MEMS Fabrication Learning Modules – Crystallography – Origami Crystal Animation.)*
2. Carefully cut out the template provided. Be sure to cut along the thin lines.
3. Fold the tabs and carefully construct the cube. You may have to try several times in order to get it to fit together correctly.
4. Use a small amount of glue or double sided tape to hold your cube together.
5. If you make a mistake and need a new template, be sure to print the template on heavy paper or cardstock.
6. Answer the Post-Activity Questions.

Post-Activity Questions

1. How do the faces of this cube relate to a silicon crystal?
2. What do the "folds" represent relative to a silicon crystal?
3. What is the difference between (010) and $(0\overline{1}0)$?
4. Why do you think crystal orientation is important in the fabrication of microdevices?
5. Look carefully at the final cube. What can you say about the importance of crystal orientation related to following:
    a. Etch rates on the exposed planes?
    b. Oxidation growth rates on the exposed planes?

Summary

A silicon crystal consists of different planes. Each plane has a unique set of characteristics that can affect microsystems fabrication, electrical and mechanical function. Miller Indices identify the various planes and directions within a crystalline solid. The construction of a paper model helps one to visualize the different crystal orientations.

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Southwest Center for Microsystems Education (SCME)
Learning Modules available for download @ scme-nm.org

MEMS Introductory Topics

MEMS History

MEMS: Making Micro Machines DVD and LM (Kit available)

Units of Weights and Measures

A Comparison of Scale: Macro, Micro, and Nano

Introduction to Transducers, Sensors and Actuators

Wheatstone Bridge (Pressure Sensor Model Kit available)

MEMS Applications

MEMS Applications Overview

Microcantilevers (Dynamic Cantilever Kit available)

Micropumps Overview

BioMEMS

BioMEMS Overview

BioMEMS Applications Overview

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Cells – The Building Blocks of Life

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Clinical Laboratory Techniques and MEMS

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Regulations of bioMEMS

DNA Microarrays (GeneChip® Model Kit available)

MEMS Fabrication

Crystallography for Microsystems (Breaking Wafers and Origami Crystal Kits available)

Oxidation Overview for Microsystems (Rainbow Wafer Kit available)

Deposition Overview Microsystems

Photolithography Overview for Microsystems

Etch Overview for Microsystems (Rainbow Wafer and Anisotropic Etch Kits available)

MEMS Micromachining Overview

LIGA Micromachining Simulation Activities (LIGA Simulation Kit available)

Manufacturing Technology Training Center Pressure Sensor Process (Three Activity Kits available)

MEMS Innovators Activity (Activity Kit available)

Safety

Hazardous Materials

Material Safety Data Sheets

Interpreting Chemical Labels / NFPA

Chemical Lab Safety

Personal Protective Equipment (PPE)

Check our website regularly for the most recent versions of our Learning Modules.

For more information about SCME and its Learning Modules and kits, visit our website

scme-nm.org or contact

Dr. Matthias Pleil at mpleil@unm.edu