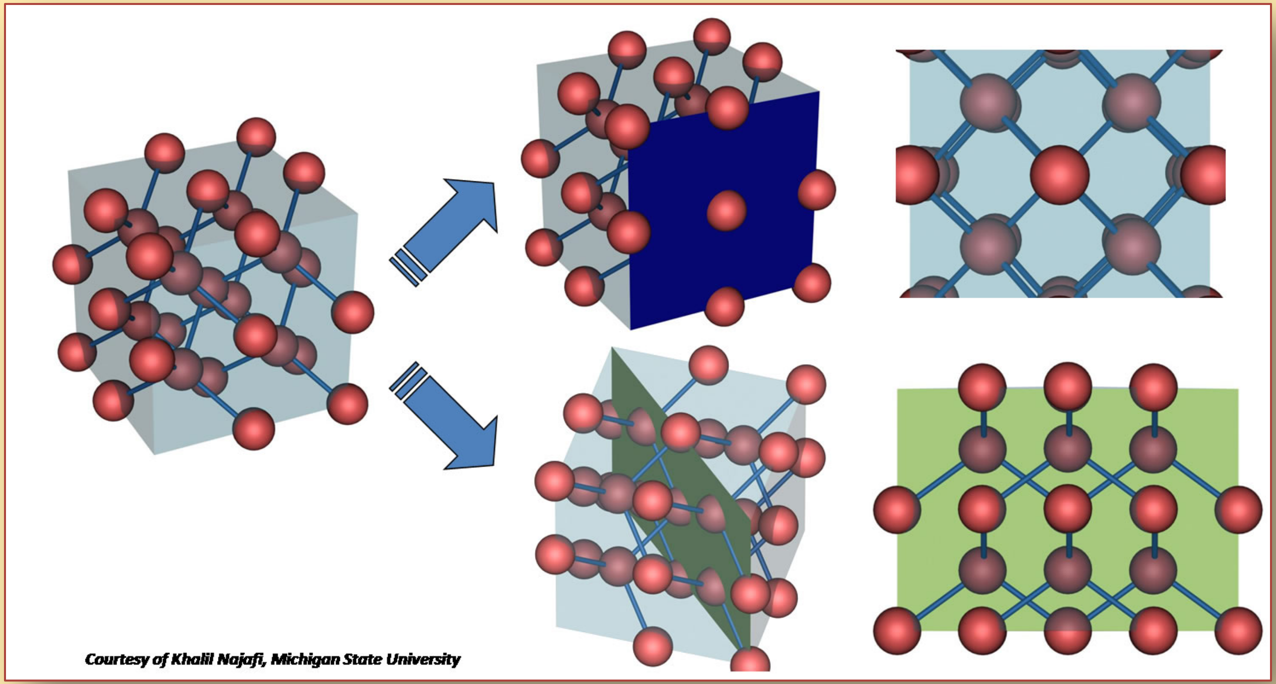
CRYSTALLOGRAPHY OVERVIEW FOR MICROSYSTEMS



Crystal Silicon Planes

Crystallography Learning Module

Unit Overview

This unit reviews the science of crystallography as it relates to the construction of microsystem (MEMS) components.

Three types of solids (amorphous, polycrystalline, and crystalline) are covered as well as how to identify crystal orientation based on Miller indices.

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.

Introduction

- Crystallography is the science of determining the arrangement of atoms in solid matter.
- Irregular arrangements are called amorphous or noncrystalline.
- Definitive patterns with a repeating structure are called crystalline structures.
- All solid matter is either amorphous, crystalline or polycrystalline.

Which of these solids is the crystalline solid?

Introduction

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Which of these solids is the crystalline solid?

Pretty easy to tell, isn't it?
The lower left is cut glass.
The right is a high quality diamond.

What are you familiar with?

- What are some examples of amorphous solid?
- What are some examples of crystalline solids?

What are you familiar with?

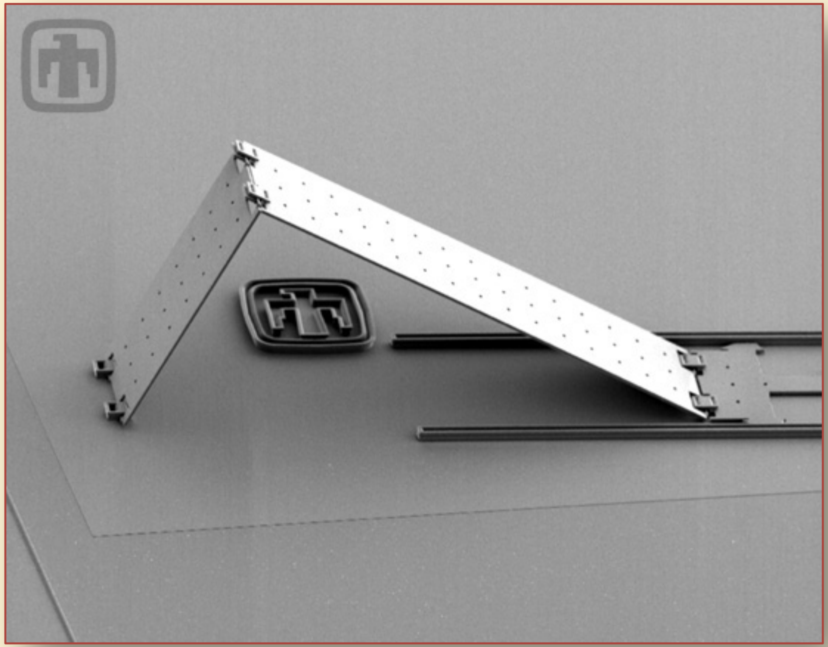
- What are some examples of amorphous solid?
- What are some examples of crystalline solids?

- glass, soot, plastics, gels
- diamonds, ice, quartz, and an old favorite, rock candy

Crystals and MEMS

Because the atoms or molecules of crystalline structures "fit together" so well, a crystal is typically very strong – an important characteristic in the construction of micro and nano-sized devices.

Microsystems require a type of crystalline substrate in order to build micro-sized structures such as cantilevers, diaphragms, gears, comb drives, and electronic circuits.



MEMS popup mirror [Courtesy of Sandia National Laboratories, SUMMIT Technologies, www.mems.sandia.gov]
This device is made of polycrystalline silicon on a monocrystalline silicon substrate.

What we talk about

This unit discusses three topics of crystallography:

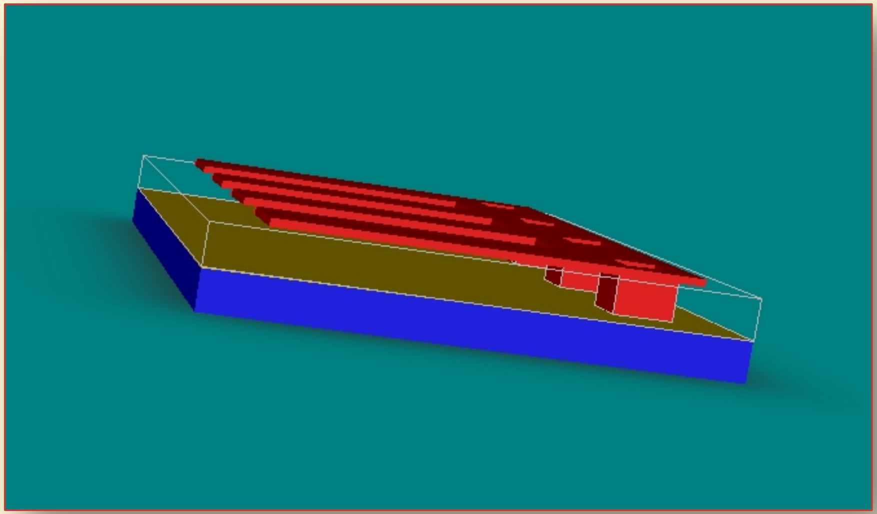
- The types of solid matter (amorphous, polycrystalline and crystalline)
- The Miller Index (a roadmap for identifying planes and directions within a crystal)
- Growing crystals

Crystallography

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

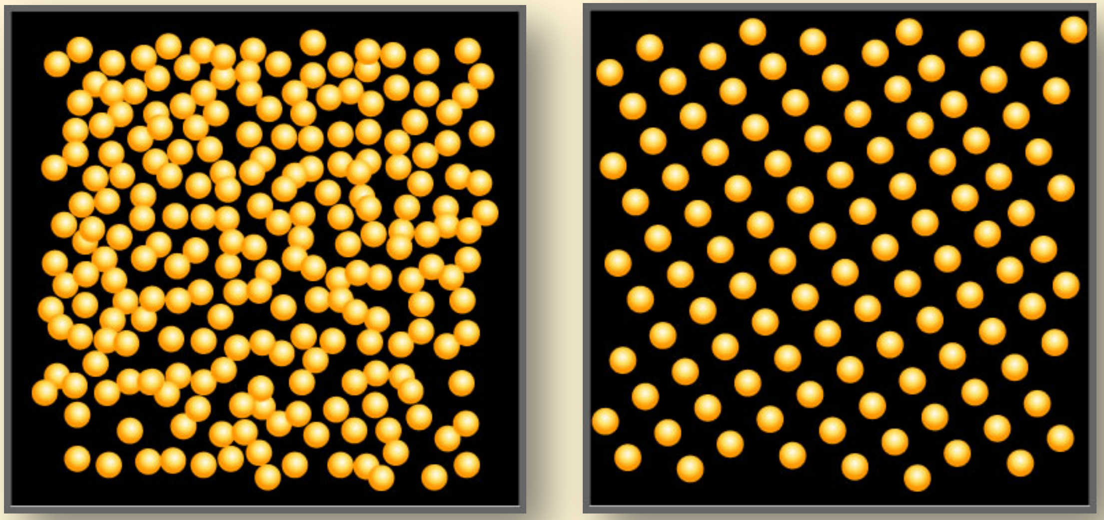
Provides information for the design and development of micro and nano-sized components.

The figure illustrates microcantilevers etched from a crystalline silicon substrate. The microcantilevers are approximately 100 micrometers long, 30 micrometers wide, and 5 micrometers thick.



MEMS cantilevers built by select removal of material underneath and between cantilevers

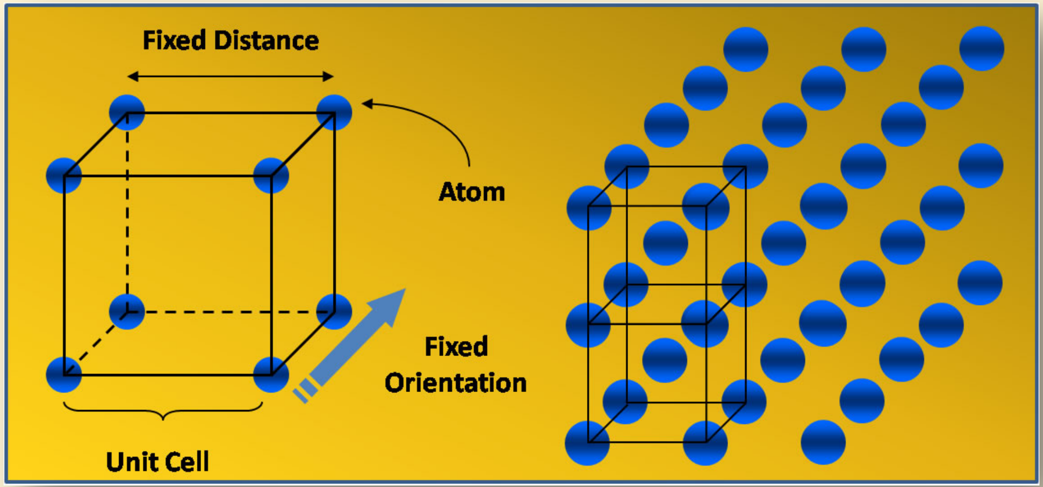
Solid Arrangements



Amorphous (left) and crystalline (right)

- 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.
- The repeating structure is called a unit cell.

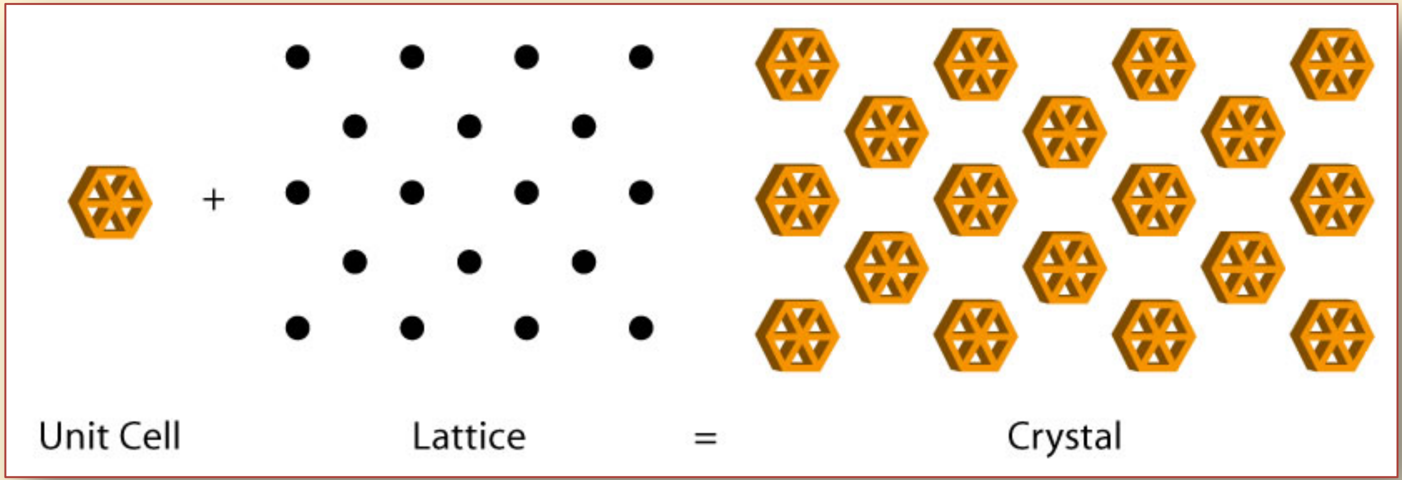
The Unit Cell



Unit cell configuration for a crystal structure

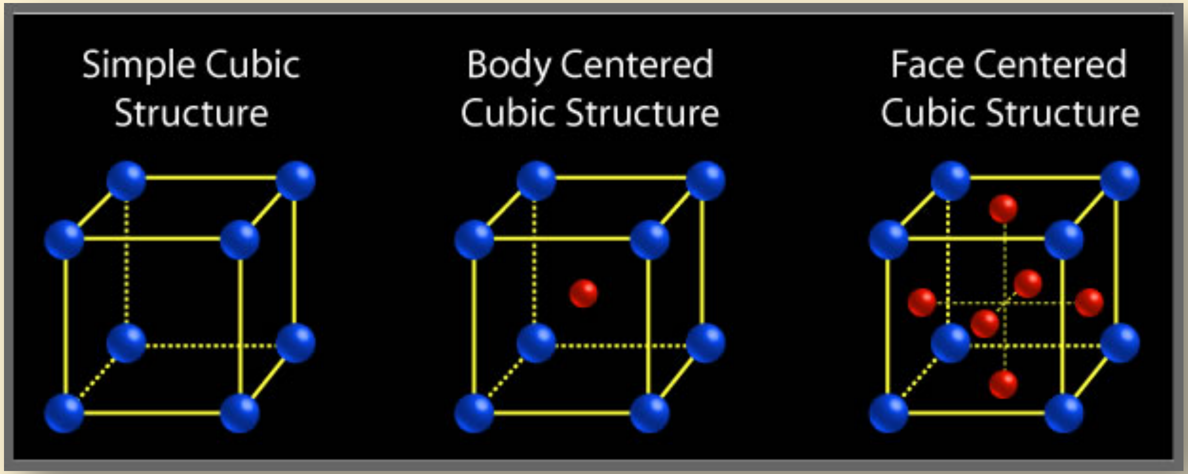
- The simplest repeating unit in a crystal.
- In a single crystal, all unit cells are identical and oriented the same way (fixed distance and fixed orientation).
- The opposite faces of a unit cell are parallel *(see graphic).*
- The edge of the unit cell connects equivalent points. The resulting structure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

The Lattice



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

Unit Cell Configurations

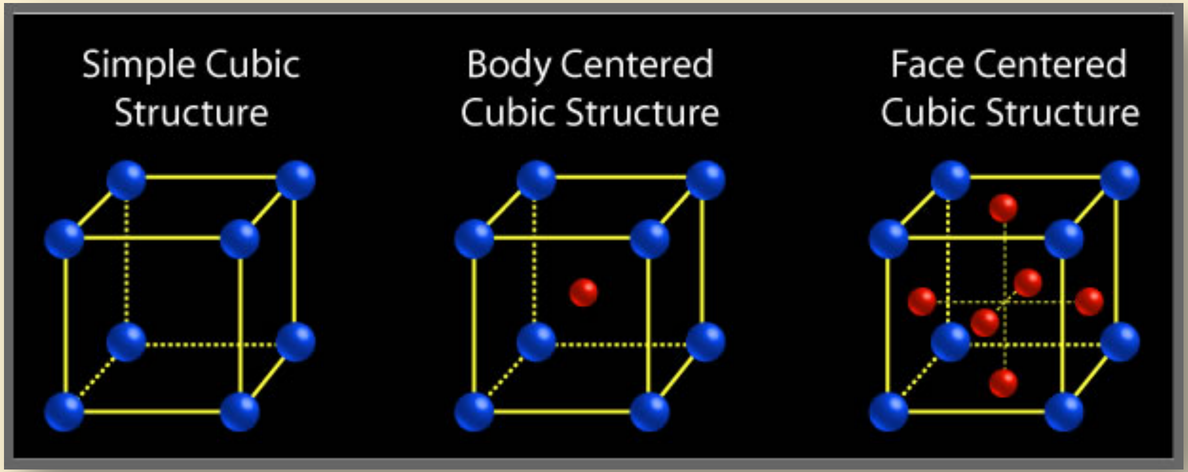


The *Simple Cubic Structure* is a unit cell consisting of **one atom**. Confused? You probably see eight atoms, correct?

- ❖ 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.

All Unit Cells Are Not Alike

There are several different configurations for unit cells.



- To see this in action, watch an animation of how a body-centered cubic configuration forms a crystal. 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"?***

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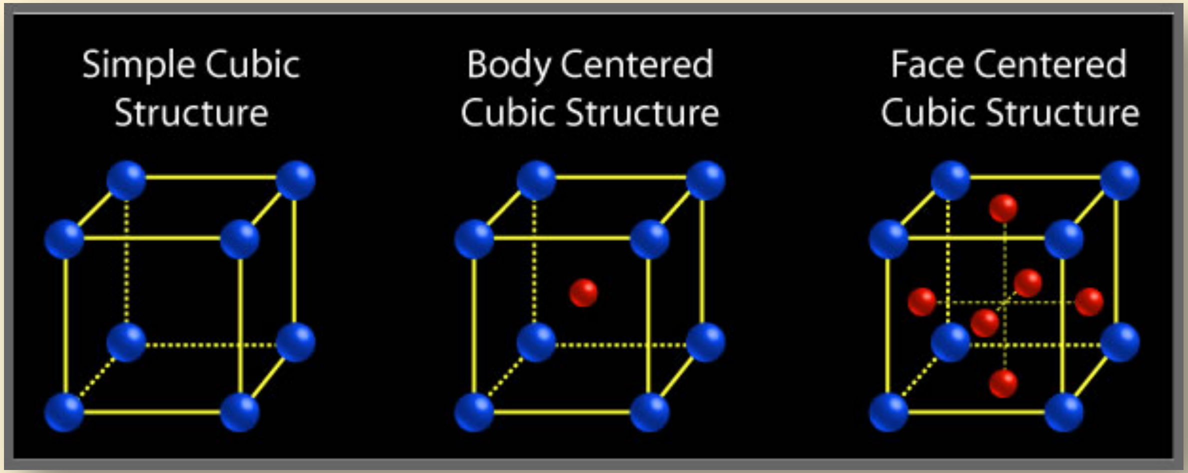


How many atoms are there

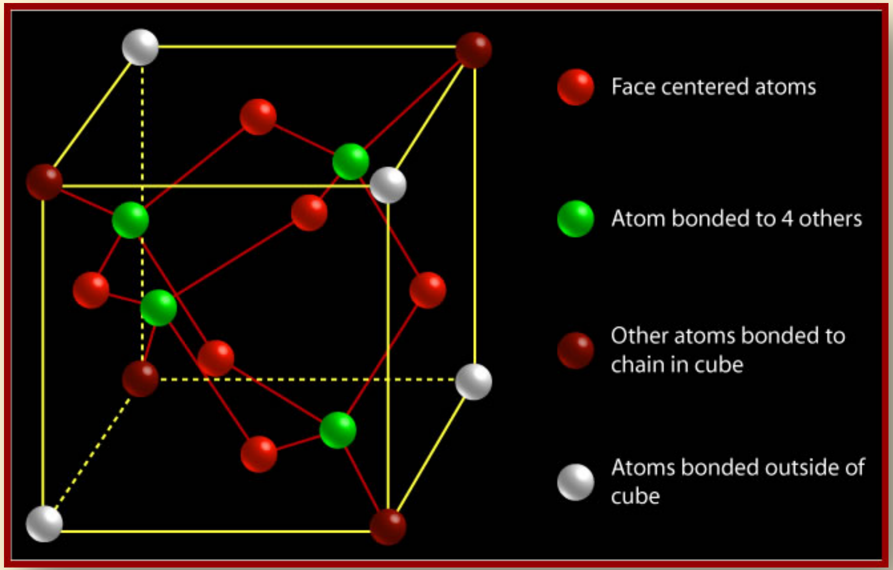
- ***in a "body centered cubic structure"?***

  TWO *(ONE atom from the eight corners, then the stand-alone atom on the middle)*

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

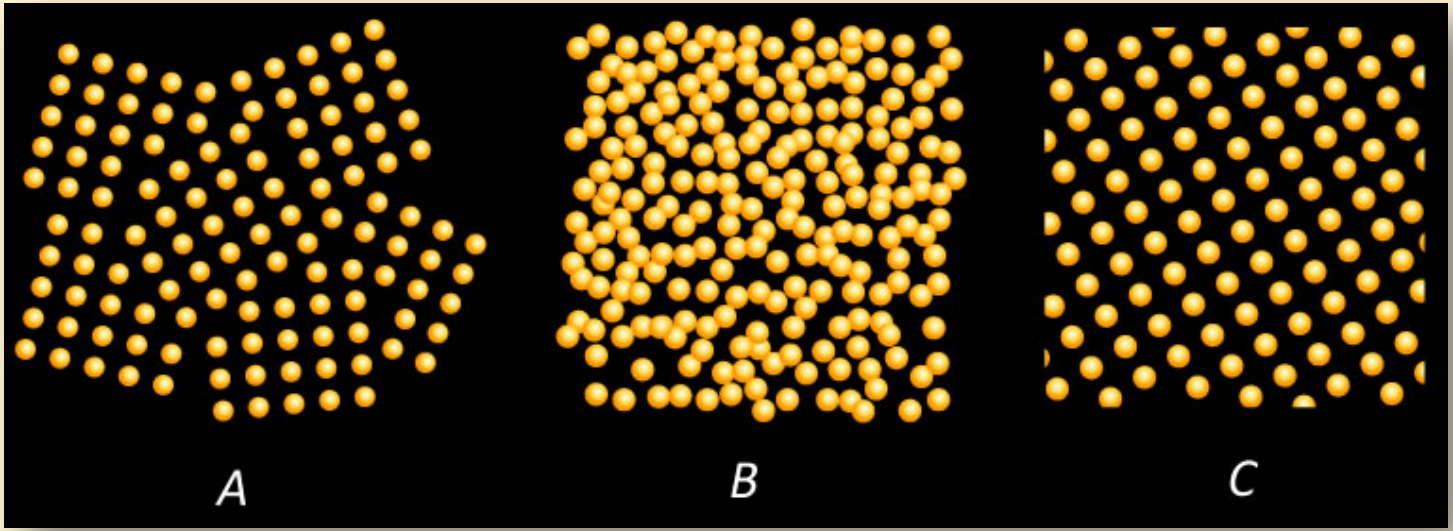
  FOUR *(ONE atom from the eight corners, then ONE-HALF an atom from each of the face) centered atoms: 1 + ½ * 6 = 4)*

Carbon Unit Cell



- Unit cell for Silicon (Si), Germanium (Ge), and carbon (C*). Identify the "face-centered atoms".*
- This unit cell can combines with other unit cells in a variety of ways. To see variety of structures (carbon sheets, nanotubes, bucky balls, diamonds) formed by the carbon unit cell, *Google image Carbon structures*.

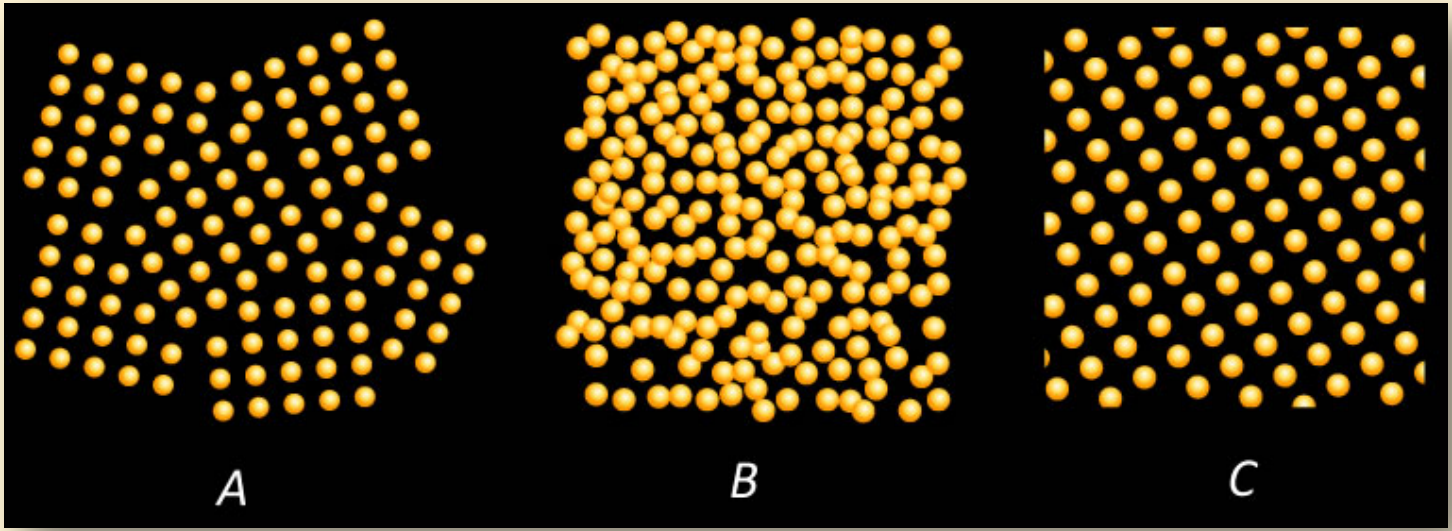
What's What?



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 above graphics (A, B, or C) is crystalline, polycrystalline or amorphous?

What's What?



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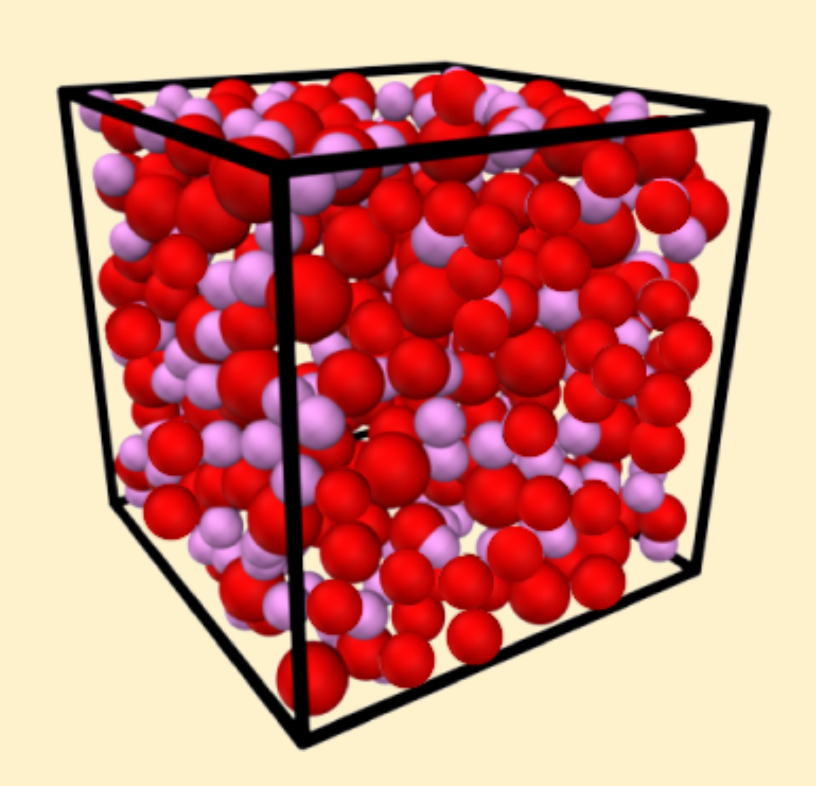
Which of the above graphics (A, B, or C) is crystalline, polycrystalline or amorphous? *A (Polycrystalline), B (Amorphous), C (Crystalline)*

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
- *Amorphous solid structure of Silica Glass*
- Wax and paraffin
- A tiled floor
- Peanut brittle



Amorphous

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.

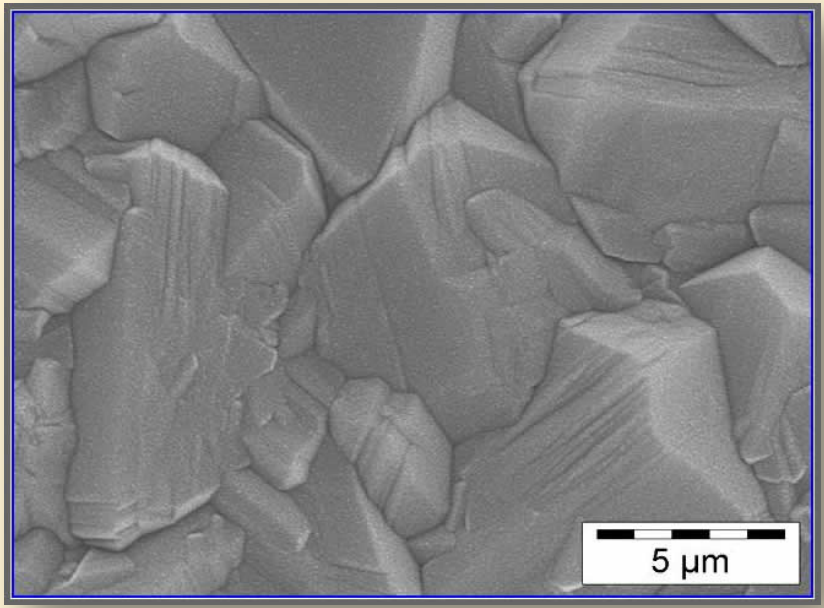
Amorphous Characteristics

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.

Polycrystalline

- Crystalline materials are either made of a single (mono) crystal or many (poly) crystals.
- Jewelry diamonds are usually single crystal carbon structures.
- Silicon used for microtechnology has the same structure of diamonds and can be either polycrystalline or single crystal.
- Some metals and metal alloys that are polycrystalline.



Scanning electron microscope image of a polycrystalline carbon in a diamond structure.

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

Grains

Polycrystalline materials consists of a myriad of small, individual, crystal **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 single crystal.

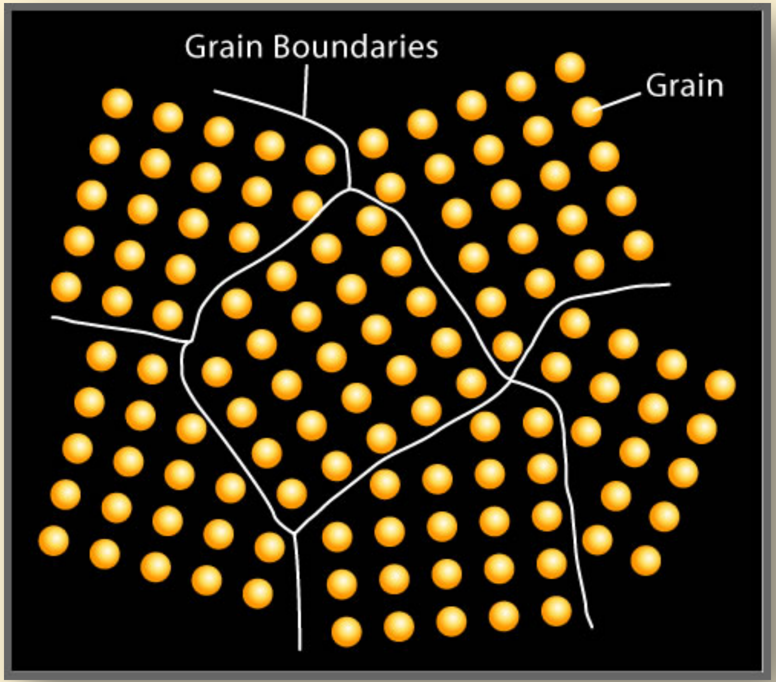
Can you see how the grains connect to each other to form this polycrystalline structure?

Grain Boundaries

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 mono-crystal material, the entire solid is a single gigantic grain.
- In the figure of the polycrystalline material, note the "grain boundaries".



Polycrystalline Characteristics

Polycrystalline solids have the following characteristics:

- Long range order exists. Polycrystalline solids consist of crystal grains stuck together. Each crystal grain consists of billions and billions of atoms in an individual mono-crystal.
- 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).

Crystals

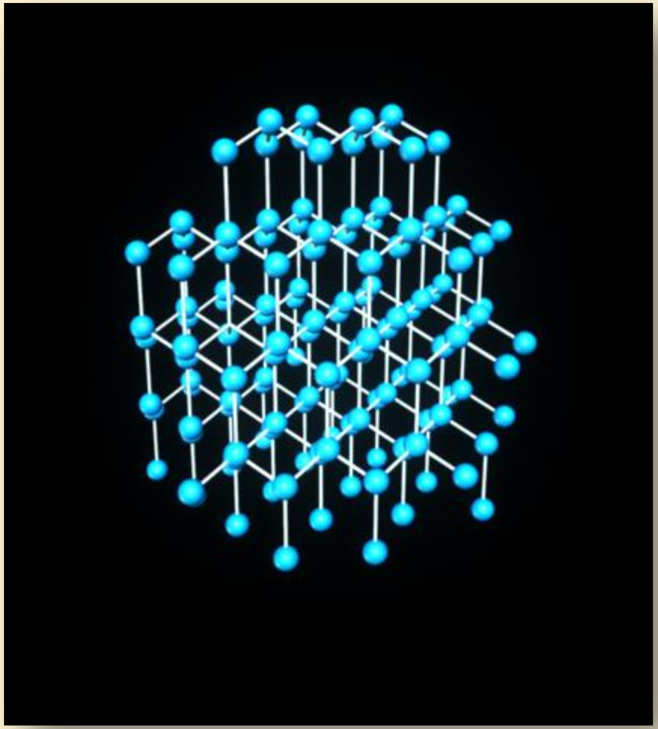
- Defined by a regular, well-ordered atomic lattice structure.
- Lattice consists of stacked planes of atoms.
- Because the atoms of the crystal fit together repeatedly and are held together by strong electrical attractions between each other, a crystal is typically very strong.

Diamond Crystal

High quality diamonds consist of 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.



Crystal Characteristics

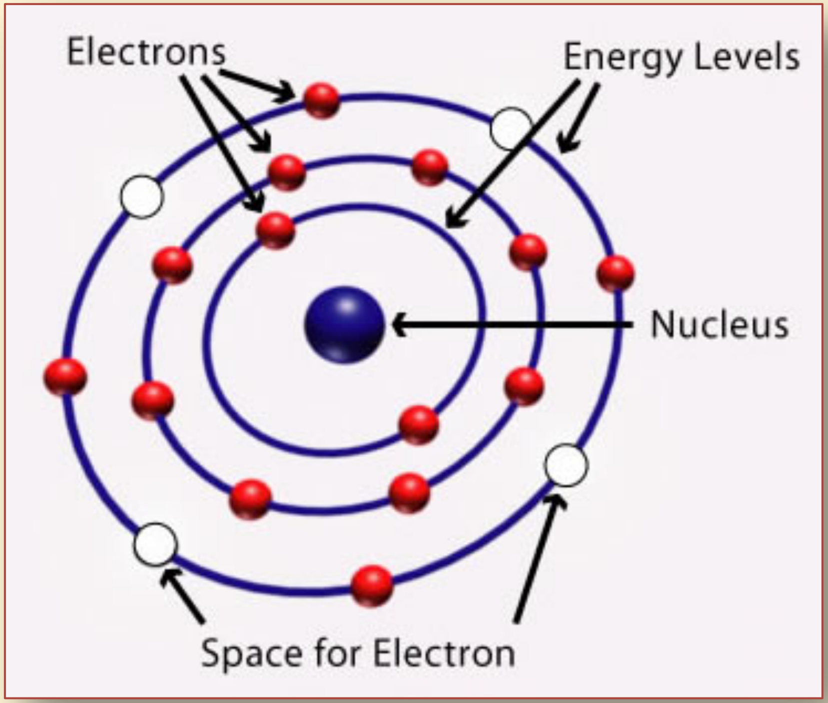
Crystals have the following characteristics:

- Extremely long range 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 Silicon: The Silicon Atom

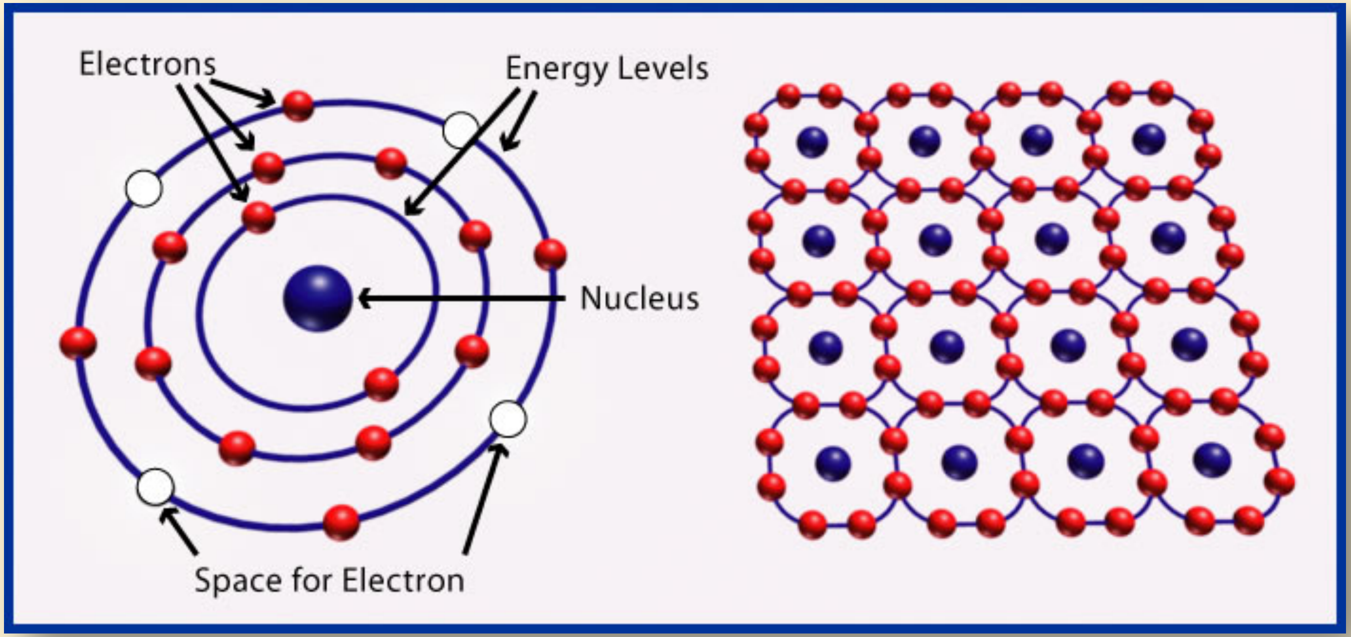
Silicon crystal is widely used in micro and nanotechnologies.

- 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.



The Silicon (Si) Crystal

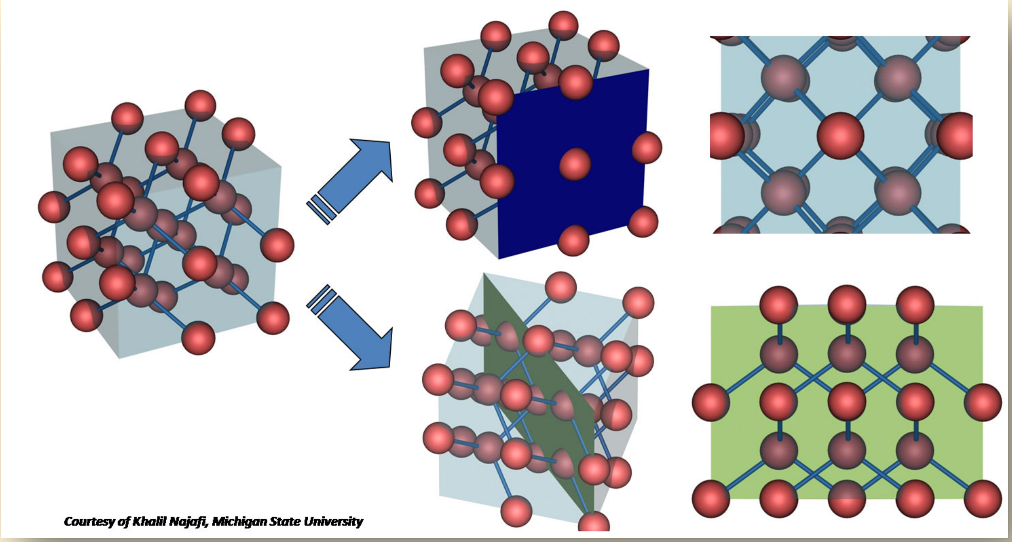
In the graphic below, notice that the outer energy level has four electrons and space for four more. On the right, you can see that **each Si atom** is *bonded to* **four other Si atoms.** In other words, each "electron space" is filled by one electron from one other Si atom. The figure on the right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



Crystal Orientation – Si Planes

Orientation of Si crystal denotes which crystal plane is exposed on the wafer surface *(refer to the graphic below).*

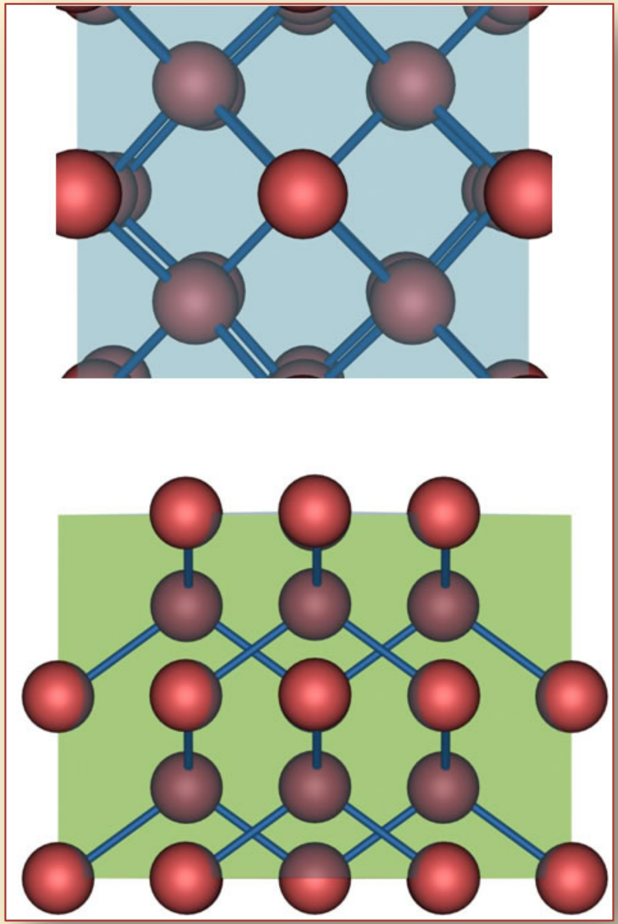
- Left most image is a Si crystal.
- Middle images show two different planes of the Si crystal. *Think of looking at the same crystal from two different directions.*
- Right images are looking at the faces of two different planes in the same crystal, presenting observers with two different looking arrangements of surface atoms.



Same crystal, same distance between unit cells, and same orientation of unit cells. However, looking at different planes, presents a different picture.

Material Properties of Silicon Planes

- Surface properties of a silicon monocrystalline wafer varies based on the orientation of the lattice relative to the wafer surface.
- Etching silicon in potassium hydroxide (KOH) is dependent on this orientation (e.g., What arrangement is presented to the surface?).
- Certain electronic properties depend on the crystal orientation.
- Silicon crystal has different bending (mechanical) properties depending on its orientation to applied stresses.



3D Viewer

Study the different planes of different crystalline structures at

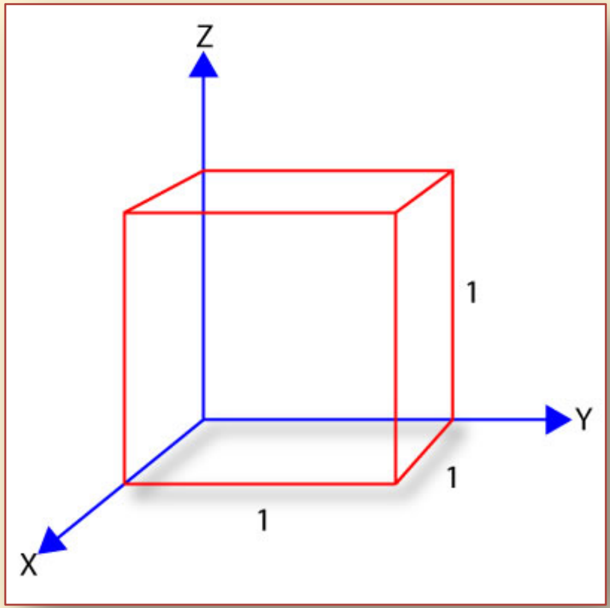
[3D Viewer.]

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 digits notations that indicate planes and direction within a crystal. These notations are based on the Cartesian coordinate system of x, y, and z.



Referring to the graphic

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

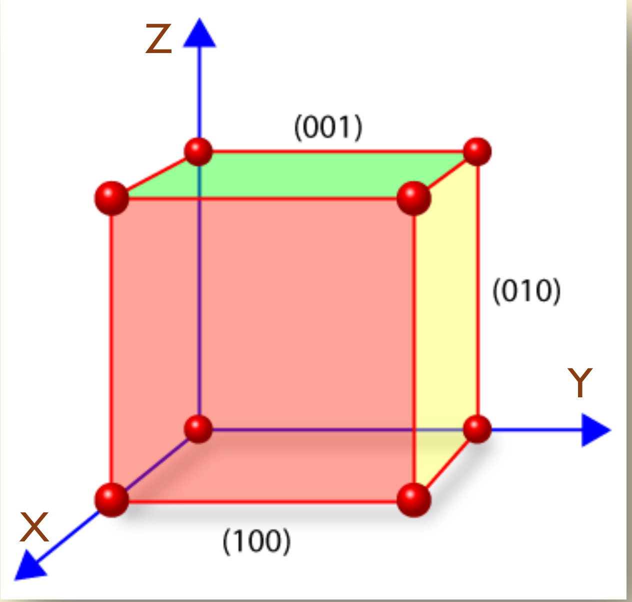
(Think of the "1" as being "1 unit" out from the origin or 0,0,0.

Identifying the Crystal Plane

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



Before going to the next slide, make sure you can see how each plane is perpendicular to its corresponding axis.

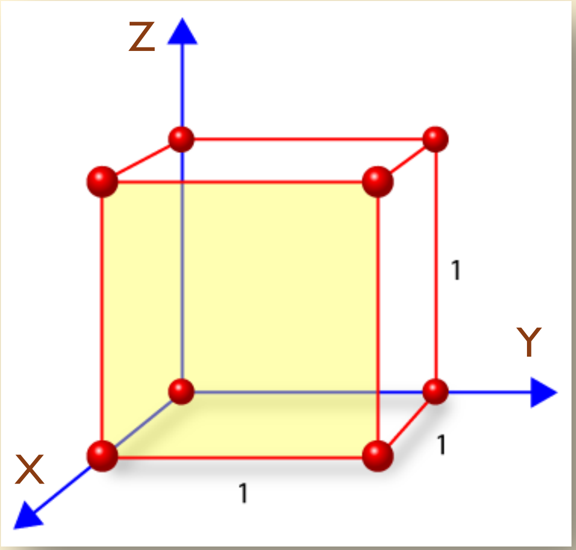
The (100) Plane

A (100) plane is perpendicular to the x-axis (the <100> vector), and is a plane formed by the y and z axes.

Can you see this in the graphic?

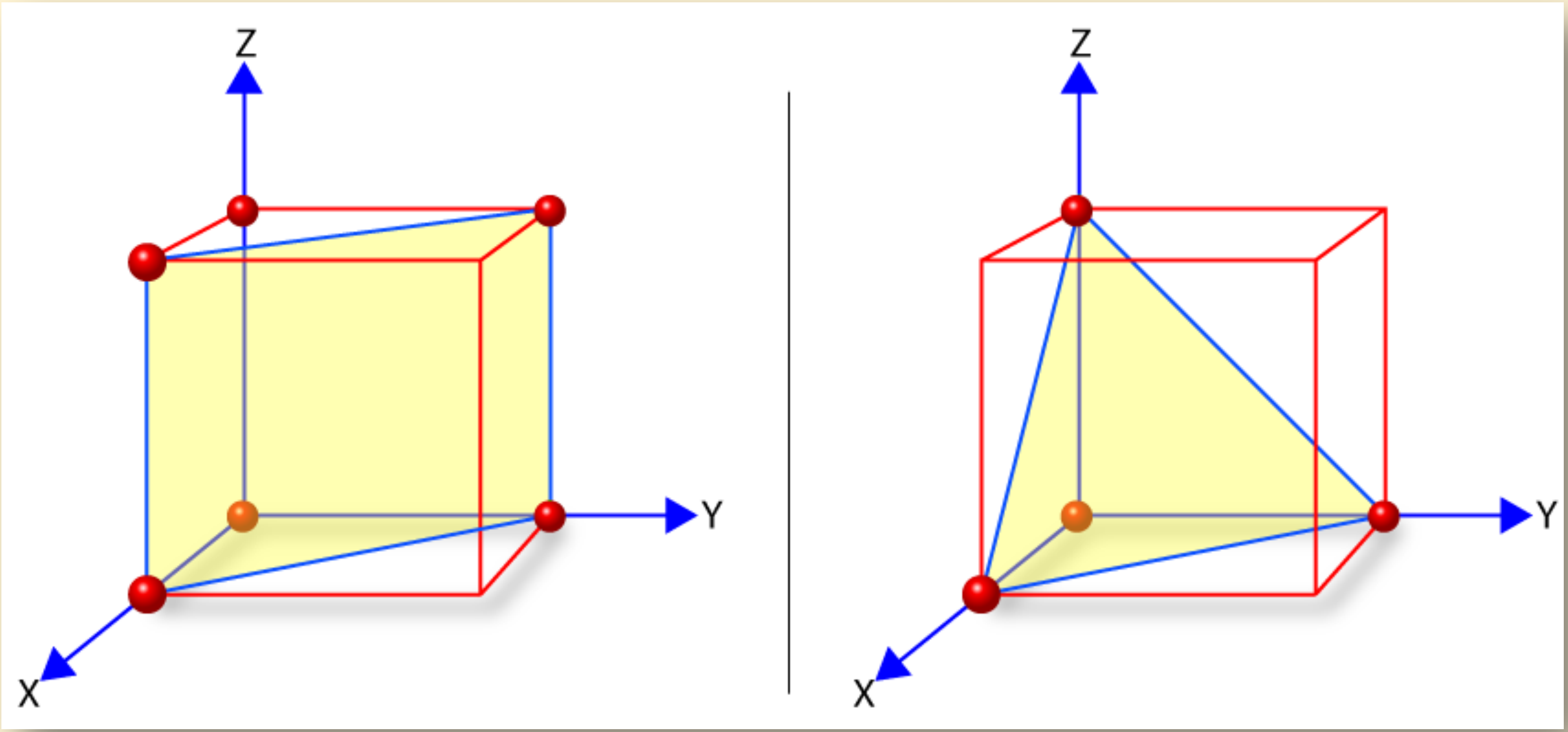
There are an infinite number of parallel planes in a crystal structure.

For example, take a deck of cards and place them on edge, perpendicular to the table top, but parallel to each other. That would denote several (100) planes in a crystal structure.



What's What?

What are the Miller indices for each of these planes?



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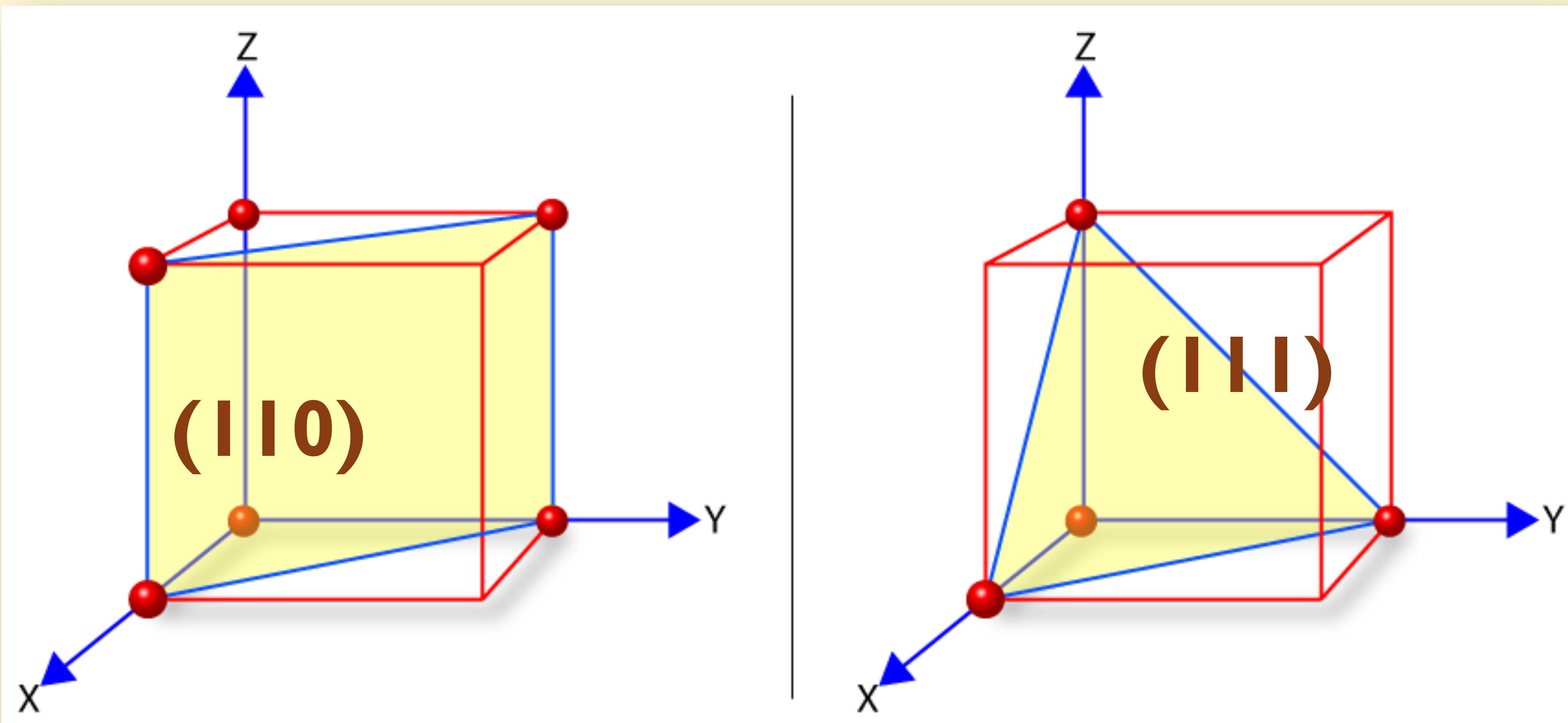


Why is the crystal orientation important?

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

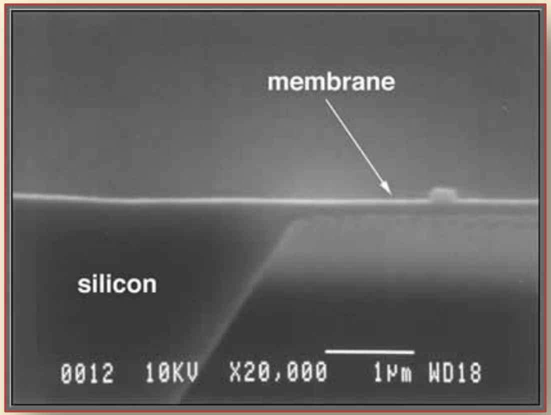
- electrical (e.g., resistance),
- mechanical (e.g., bulk modulus), and
- optical (Index of Refraction) properties.

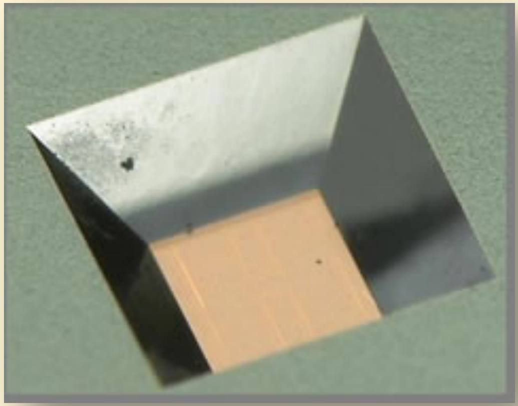
Each of these properties can be different for the different crystal orientations.

Silicon Crystal Etch

These images show a silicon nitride diaphragm constructed over a monocrystalline silicon substrate that has been anisotropically etched to provide an opening under the diaphragm.

To achieve this structure, a (100) silicon substrate and KOH (potassium hydroxide) etchant were used.





(Left) Diaphragm for MEMS pressure sensor over an etched silicon substrate. [SEM courtesy of University of Michigan] (Right) Backside view of etched silicon crystal wafer. The green is a silicon nitride hard mask on the back side of the wafer. The silver edges of the opening are planes of a silicon wafer, and the tan is a silicon nitride membrane on the front of the wafer. [Courtesy of the MTTC / University of New Mexico]

MEMS Structures

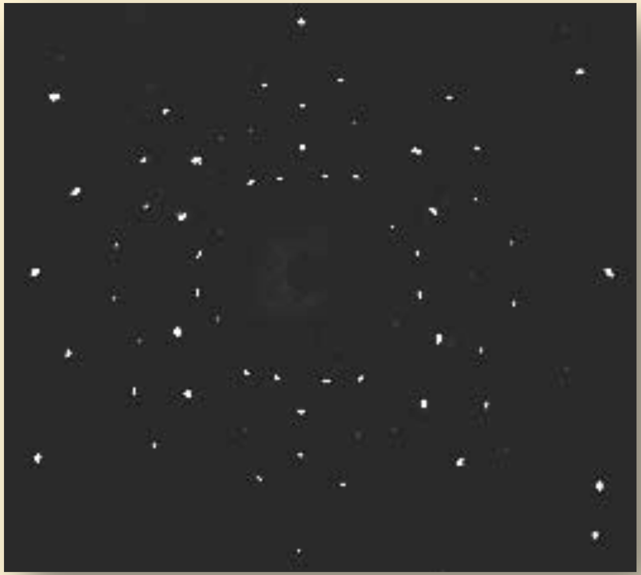
By choosing specific wafer crystal orientation and type of etchant, one can create a multitude of different shaped structures:

- 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 crystalline structure, x-rays are aimed at a tiny crystal containing trillions of identical atoms.

- The crystal scatters the x-rays onto an electronic detector or film.
- The x-rays are said to diffract.
- The resulting diffraction pattern provides information needed to determine the actual orientation of the tiny seed crystal and the spacing of the atoms



X-ray diffraction pattern of a plane of a silicon crystal. [Image printed with permission from and from the personal collection of Christopher C. Jones]

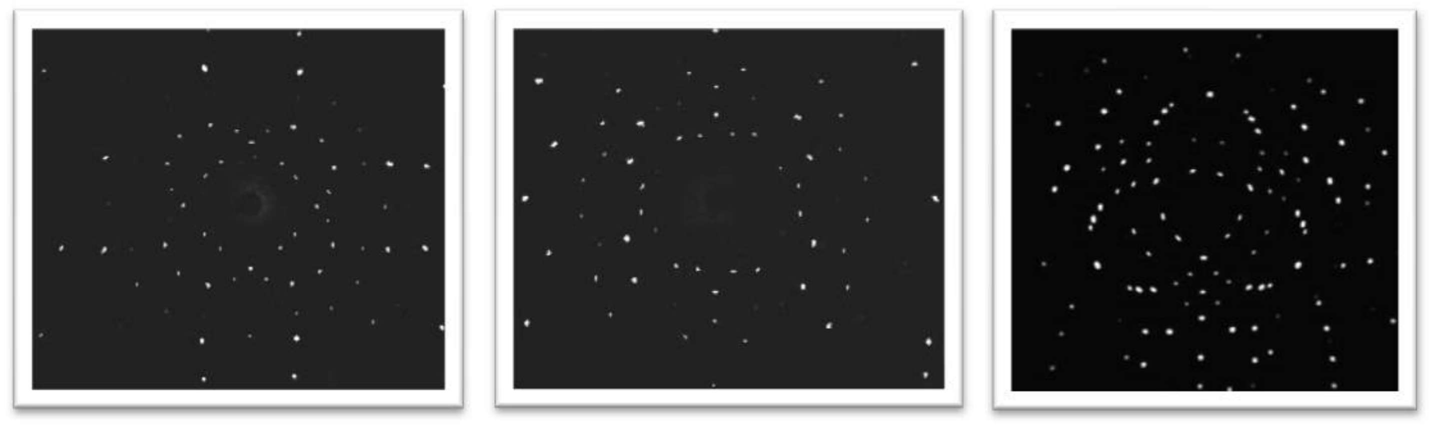
What is its Orientation?

Which image represents which of the following 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 from and from the personal collection of Christopher C. Jones]

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b) (100)

c) (110)

(100) **(110)** **(111)**

Crystal orientation of three different planes of a silicon crystal.
X-ray was used to create these images.
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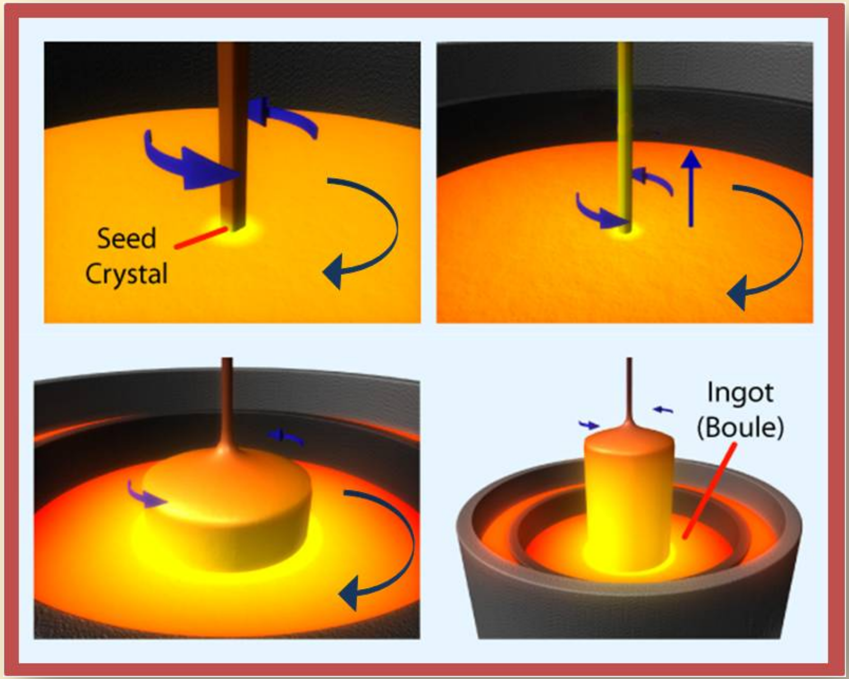
Making a Silicon Crystal

- Pure silicon (99.9999999999% pure!) is melted in a crucible.
- A seed crystal is lowered into the molten silicon *(top left image)*.
- Silicon atoms in the melt align to the seed crystal's orientation. As the seed crystal is slowly pulled from the melt, a large crystal ingot or boule is formed.
- The seed and the crucible with the molten silicon are rotated in opposite directions as the seed is slowly pulled upward.



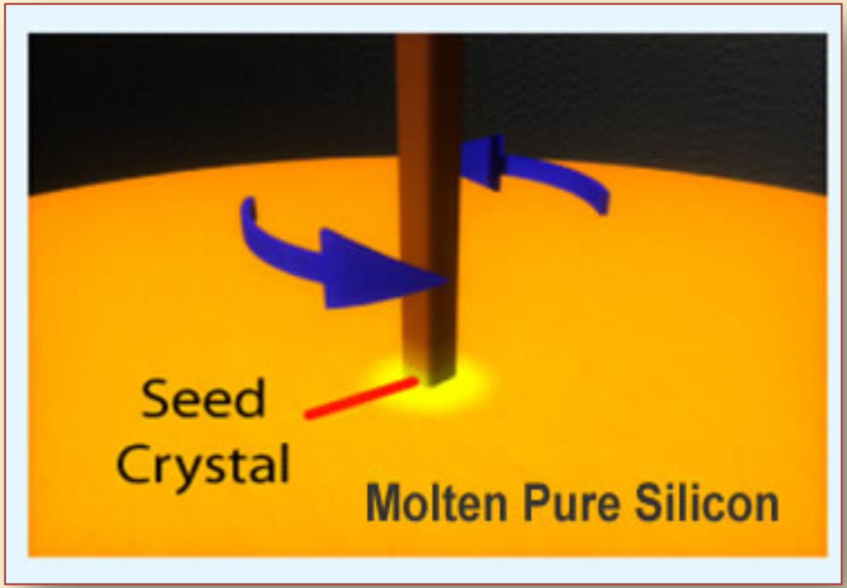
The Czochralski (CZ) Method of Growing an Ingot of Silicon Crystal

The slower the "pull", the larger the diameter of the crystal ingot that forms.

The Seed Crystal

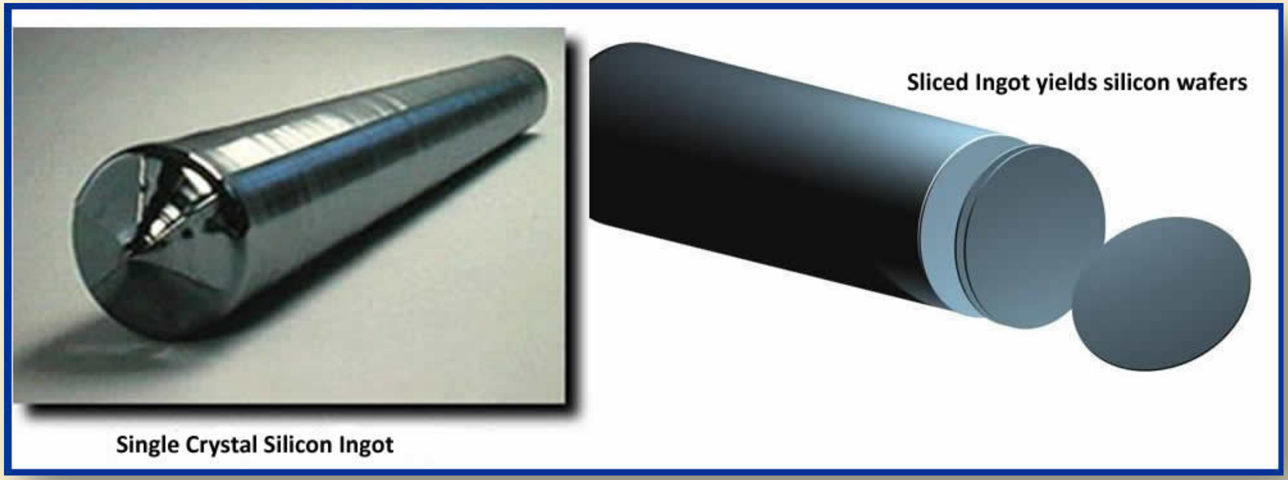
The seed crystal acts as a starting point for the alignment of the atoms in the molten silicon.

The alignment of the seed crystal relative to the molten silicon determines the orientation of the subsequently grown silicon crystal.



The Ingot

- The 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.
- 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.



Summary

- Solid matter is either amorphous, polycrystalline or crystalline.
- Mono-crystalline silicon 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 orientation (100) and (111) are commonly used.

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