Crystallography

An Introduction

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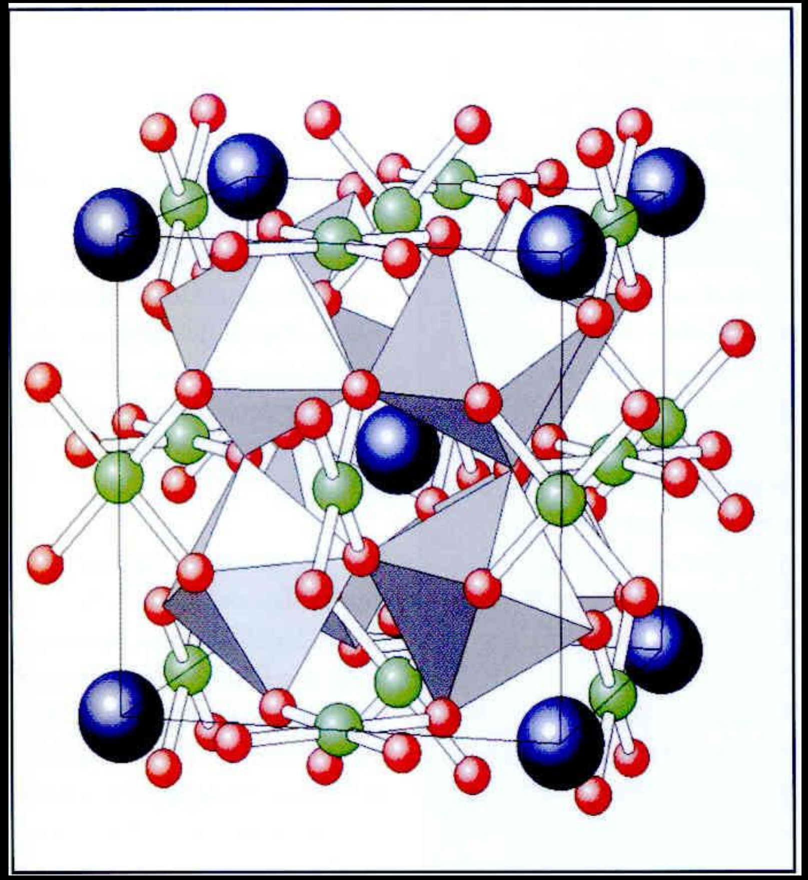
What is Crystallography?

- "The science that examines the arrangement of atoms in solids" (1)

- How are things organized on an atomic level?

- *Why* are they packed that way?

- 2014 is the International Year of Crystallography!



https://www.physik.uni-augsburg.de/en/prof/chemie/bilder/3-Structure_o_a_perovskite-related_material.jpg

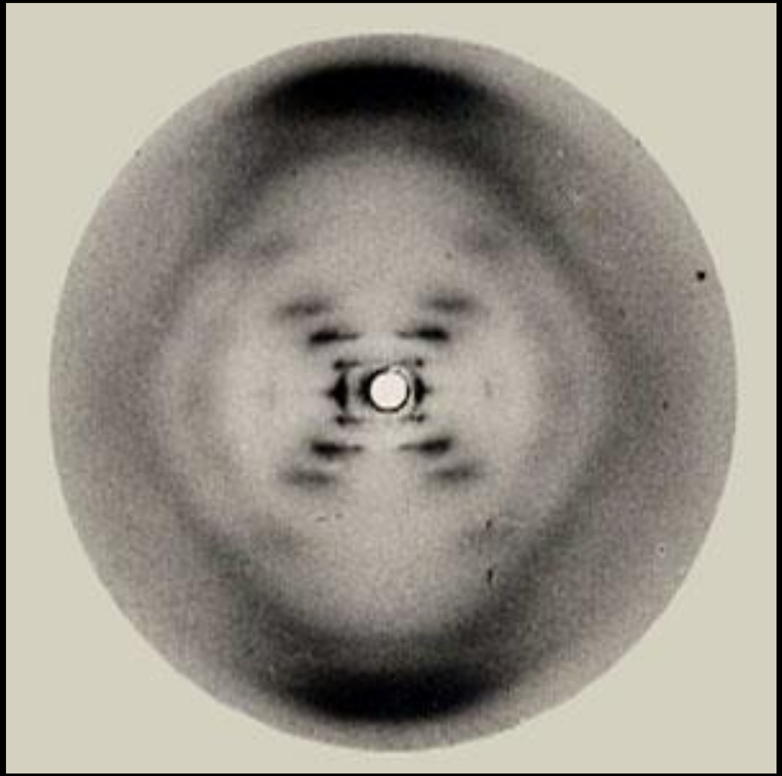
Brief History

- Before X-Rays, Crystallography was largely mathematical, dealing with packing, symmetry in 3D, and lattices (2).
- Kepler wrote of the packing of spheres (like atoms!)
- Many French and German mathematicians formulated these ideas.

- These formed the basis for modern crystallography, made possible by x-rays (x-ray diffraction!).
- Pioneered by William H. and William L. Bragg

Why is it important?

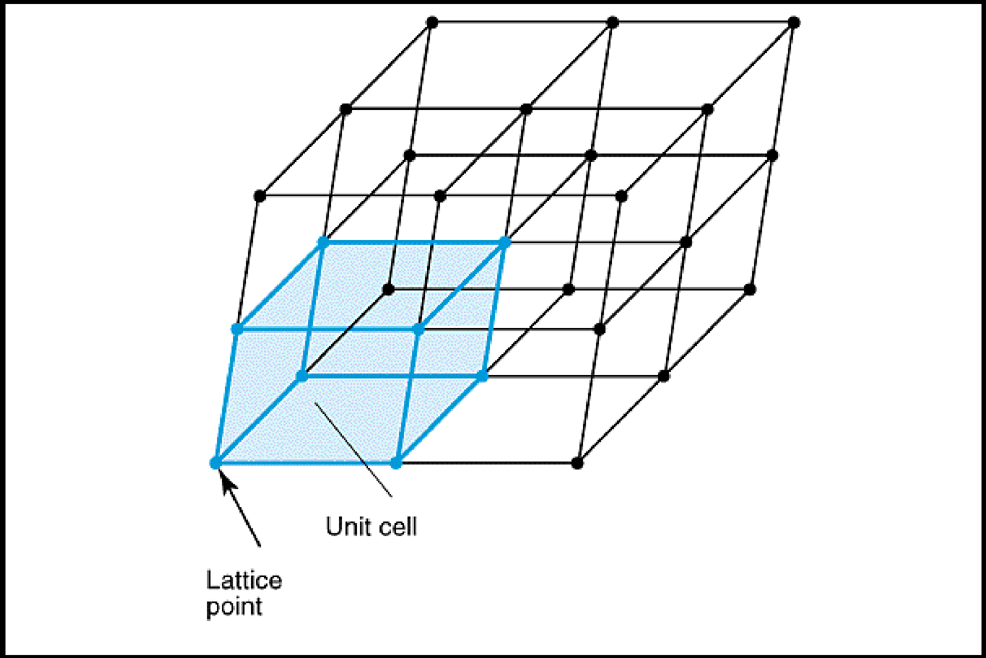
- Many properties of materials are dependent on the crystal structure.
- Examples: Strength, Deformation, Optical and Electrical Properties.
- Understanding how atoms are arranged allows us to begin understanding how it works!
- Example- DNA & Rosalind Franklin



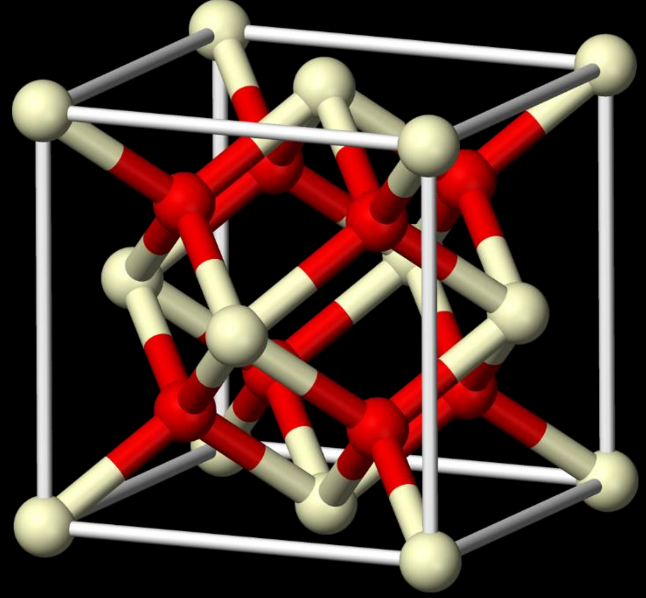
http://learn.crystallography.org.uk/wp-content/uploads/2013/11/DNA_fibre_pattern.jpg

The Unit Cell

- The "Building Block" of a crystal
- Each atom takes a place in a *lattice*- an infinite mathematical collection of repeating points in all directions. Periodic!
- Understanding the properties of the unit cell allows us to know the properties of the crystal as a whole (Example- Volume/atom)

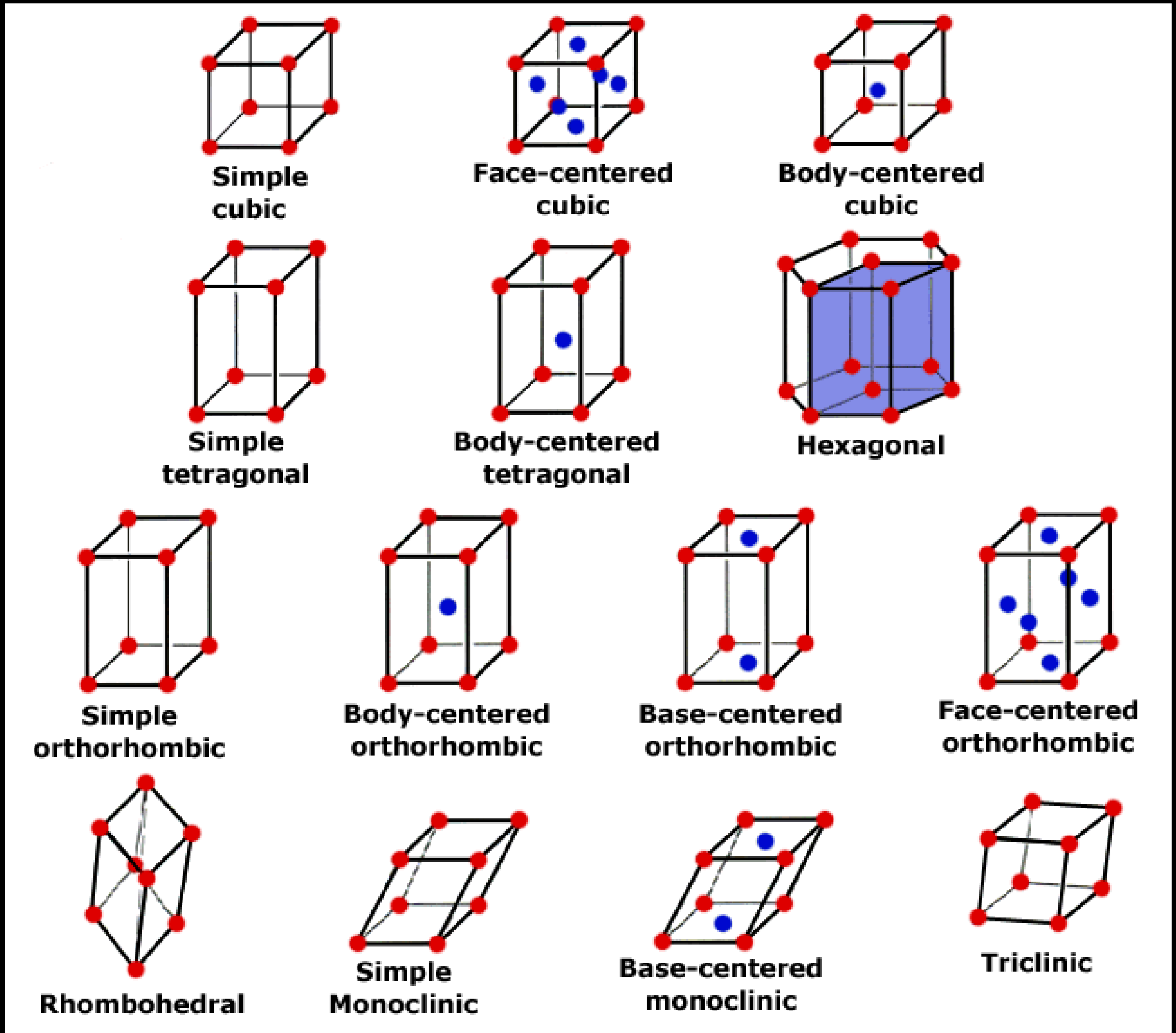


http://www.learneasy.info/MDME/focus/materials/enmat/LECTURES/Lecture-04/webpages/crystals_files/FG11_030.GIF



https://upload.wikimedia.org/wikipedia/commons/1/13/Ceria-unit-cell-3D-balls.png

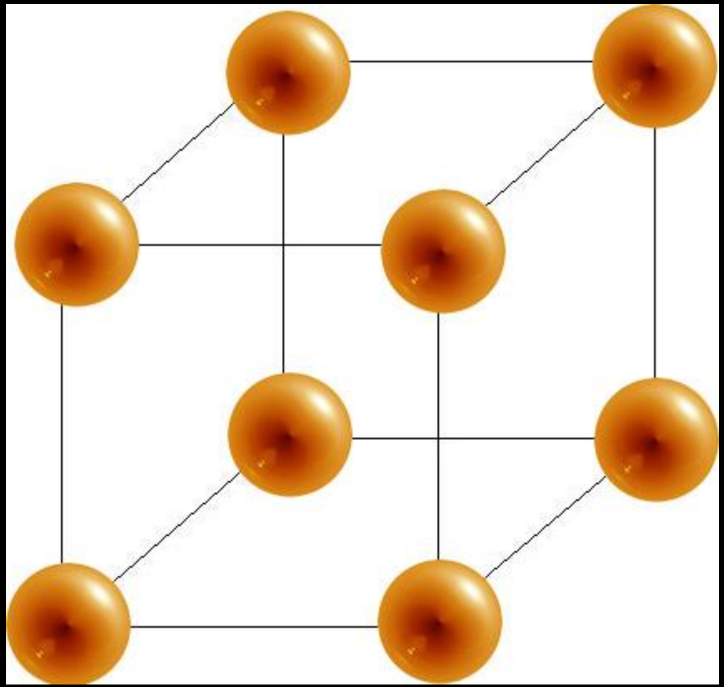
The 14 Bravais Lattices/Crystal Systems



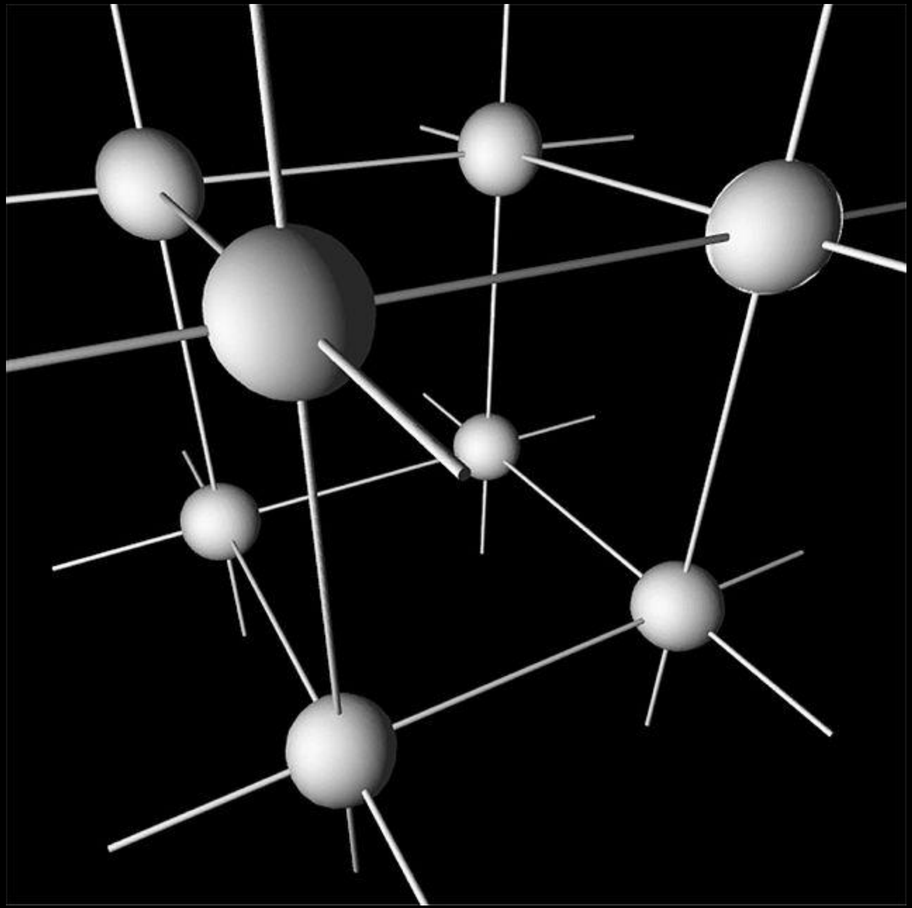
http://www.seas.upenn.edu/~chem101/sschem/bravais.gif

Simple Cubic (SC) (also known as P-Primitive)

- Simplest Crystal Structure!
- Not very common…only Po.
- This structure is not space efficient!



http://chemwiki.ucdavis.edu/@api/deki/files/8736/simple_cubic_jpeg.jpg?revision=1

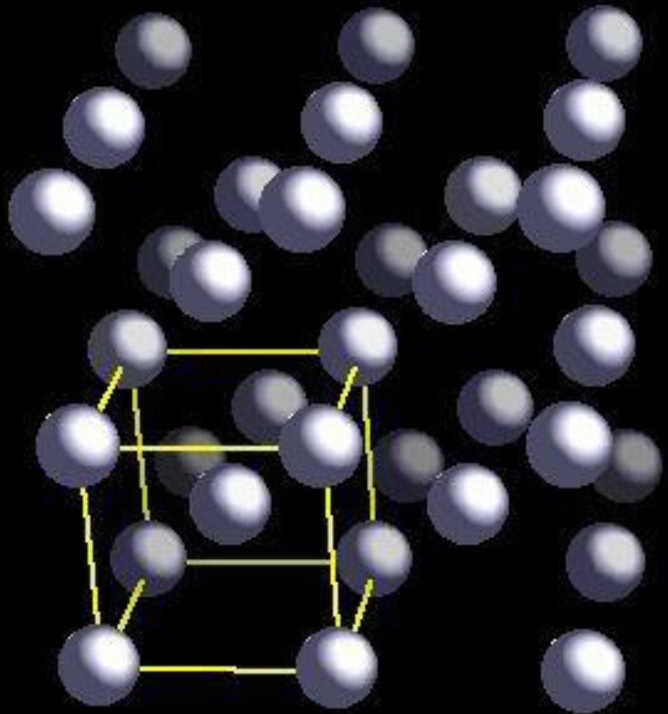


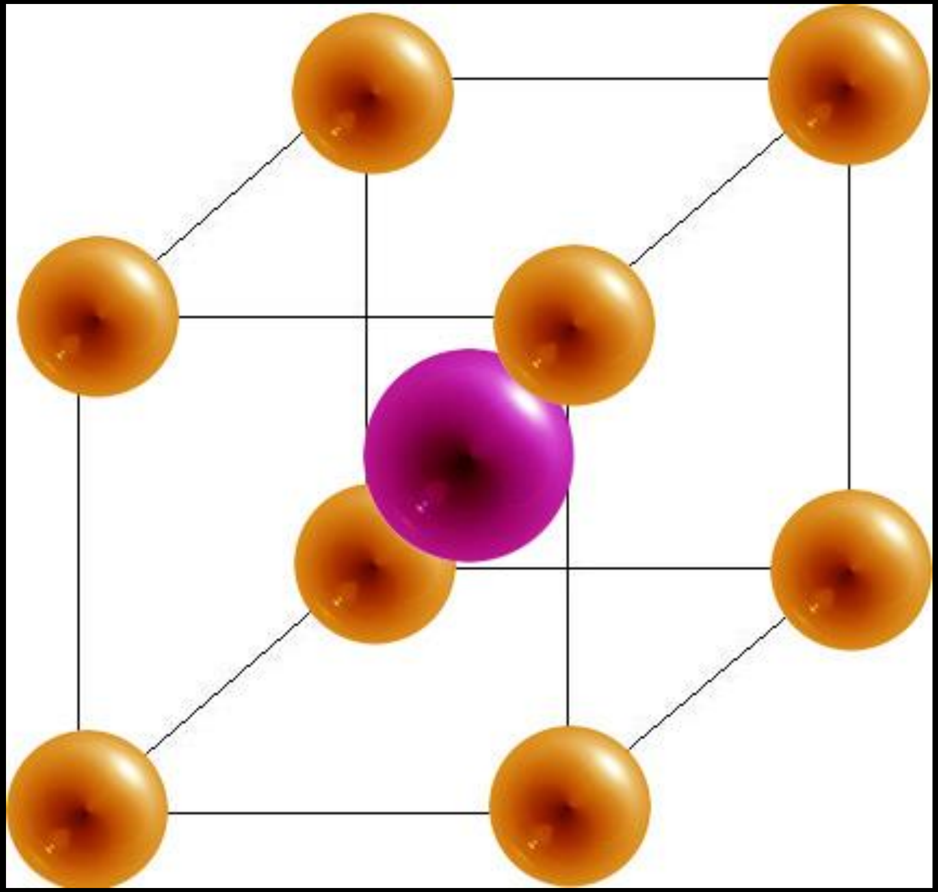
https://en.wikipedia.org/wiki/Cubic_crystal_system#mediaviewer/File:Kubisches_Kristallsystem.jpg

Body-Centered Cubic (BCC)

- Common in nature, especially metals.
- Examples: Cr, Fe, Nb, V, W

http://www.webelements.com/_media/elements/crystal_structure_image/Li-bs.jpg

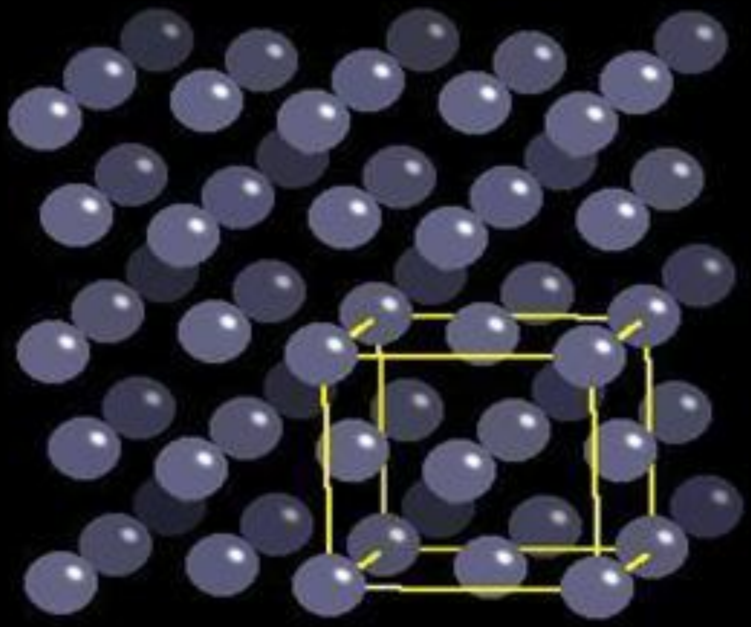




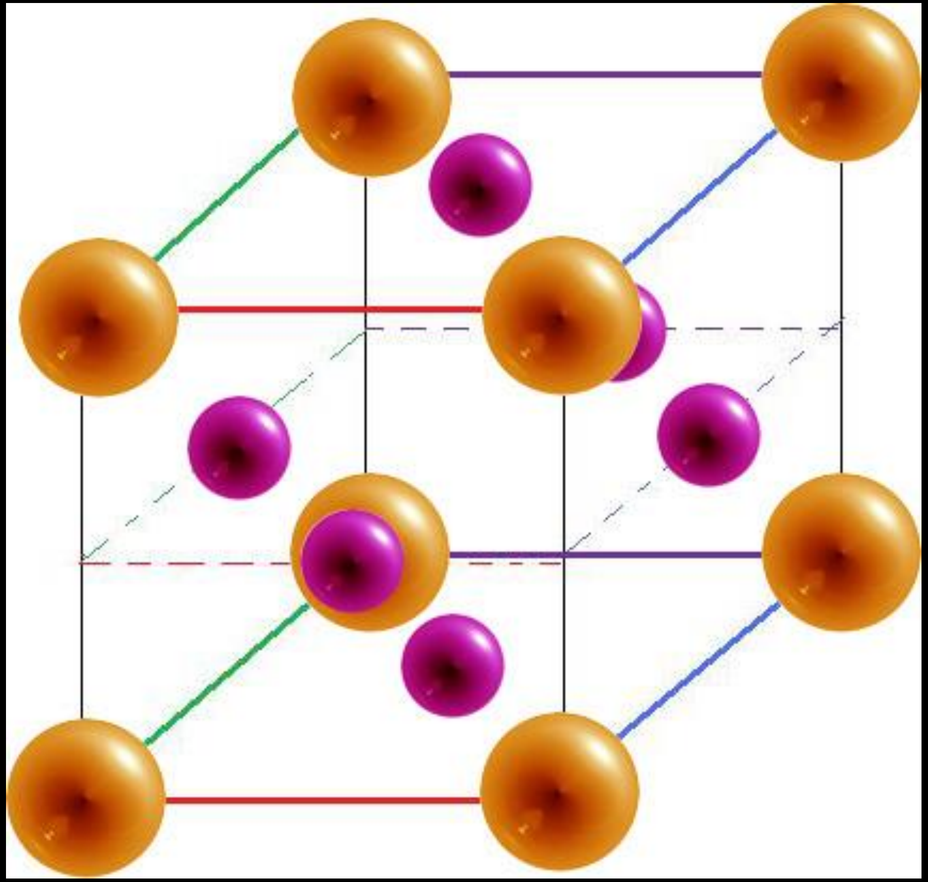
http://chemwiki.ucdavis.edu/@api/deki/files/8729/body_centered_cubic_jpeg.jpg?size=bestfit&width=163&height=156&revision=1

Face-Centered Cubic (FCC)

- Very Common in Metals, good for models.
- Examples: Fe, Al, Cu, Ca, Au, Ag…



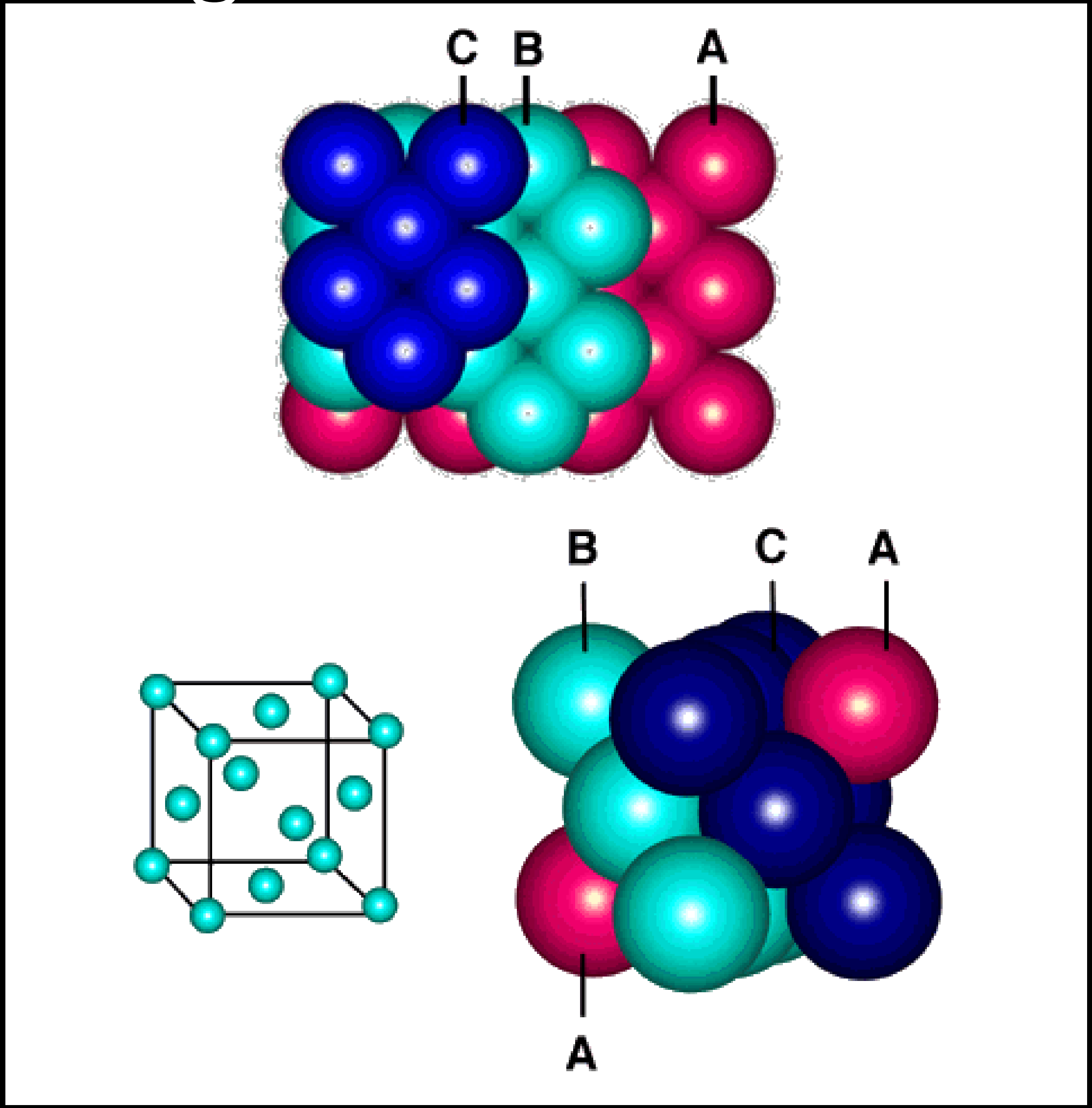
https://courses.physics.illinois.edu/phys466/sp2013/projects/2004/Team1/image015.jpg



http://chemwiki.ucdavis.edu/@api/deki/files/8732/face_centered_cubic_jpeg.jpg?revision=1

From a different angle…

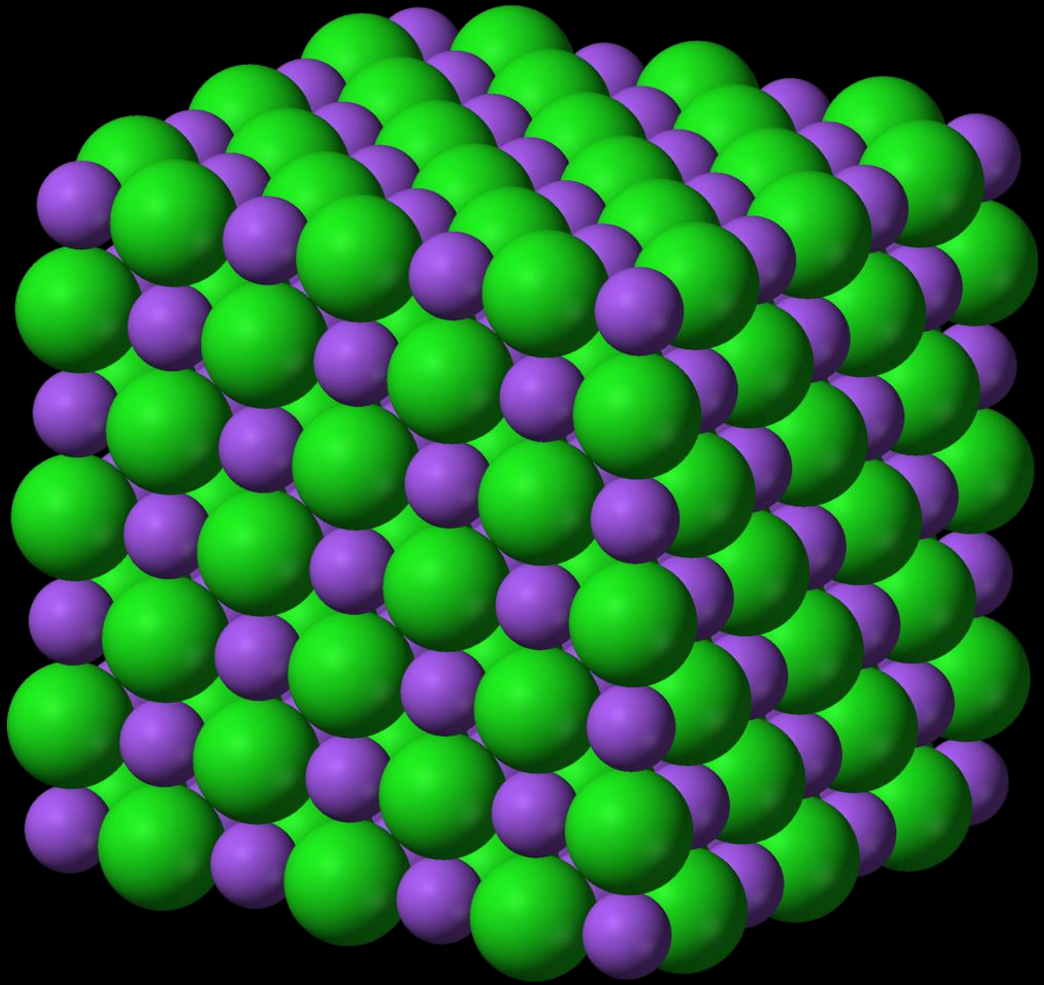
- Alternating packed layers…
- Very efficient at packing atoms close together!



http://www.chemistry.wustl.edu/~edudev/Fullerene/FullereneGraphics/fig6alltf.gif

Describing Directions and Planes in a Crystal

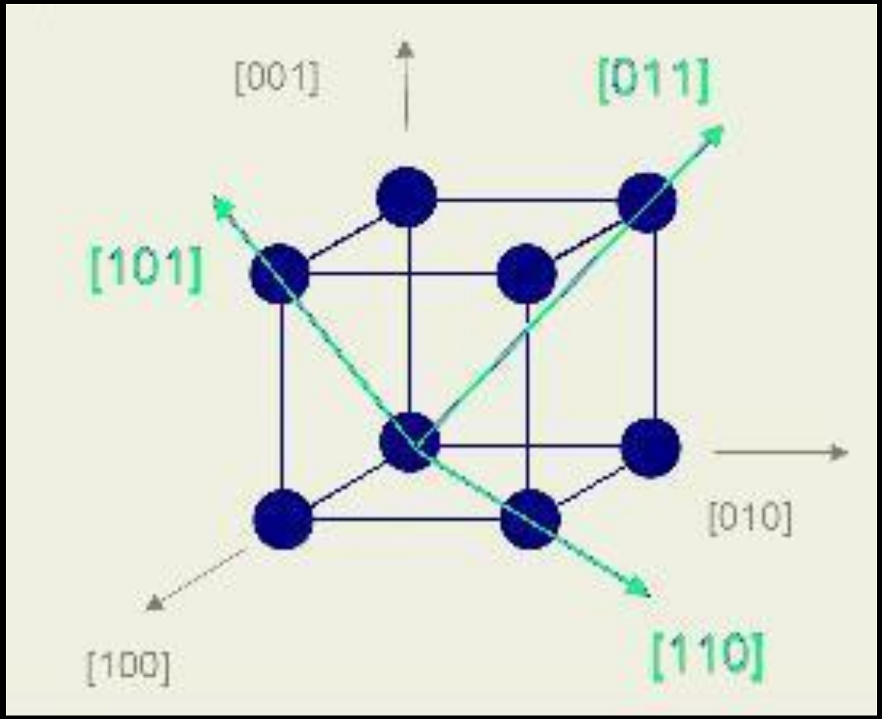
- Different than in mathematics- because crystals are periodic, we want a way to describe families of planes/directions.
- One describes many!
- Deformation, modulus, conductivity can vary along directions and planes (3).



https://upload.wikimedia.org/wikipedia/commons/e/e9/Sodium-chloride-3D-ionic.png

Directions and Miller Indices

- Using a unit cell, we can describe directions throughout the entire crystal!
- Miller Indices- Set of 3 numbers that denote the coordinates of the head of a vector, where tail is at the origin.
- [hkl]. Multiple fractions by common denominator. Negatives denoted by a bar.
- Example- Vector starting at (0,0,0) going to (1/2, 1/3, 1) would have Miller Index [326]
- Going to (-1,-2,1/2) would have Miller Index ? ? ?



http://www.cleanroom.byu.edu/EW_orientation.parts/miller_110.JPG

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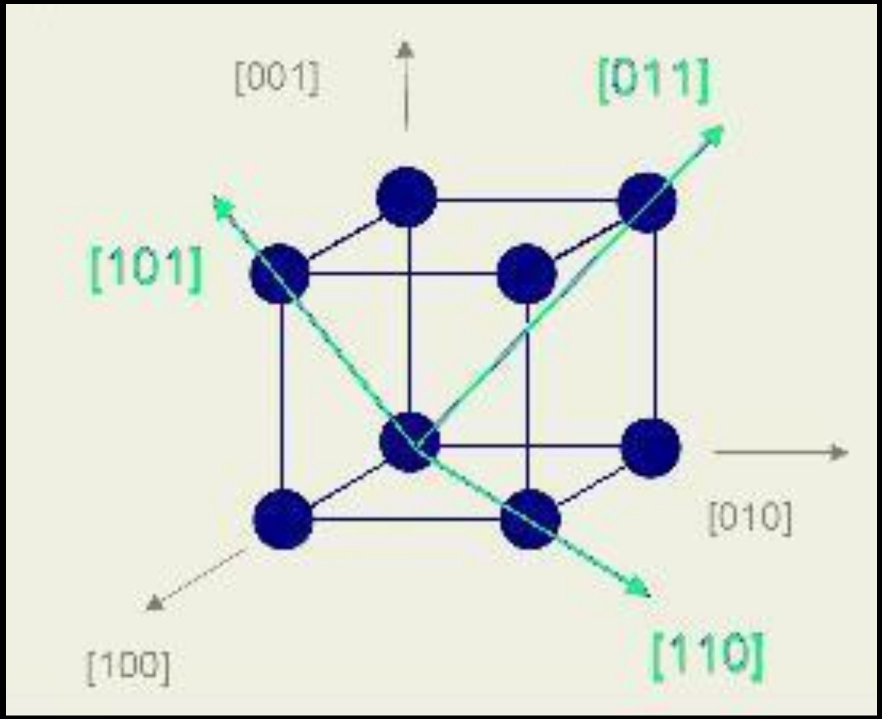

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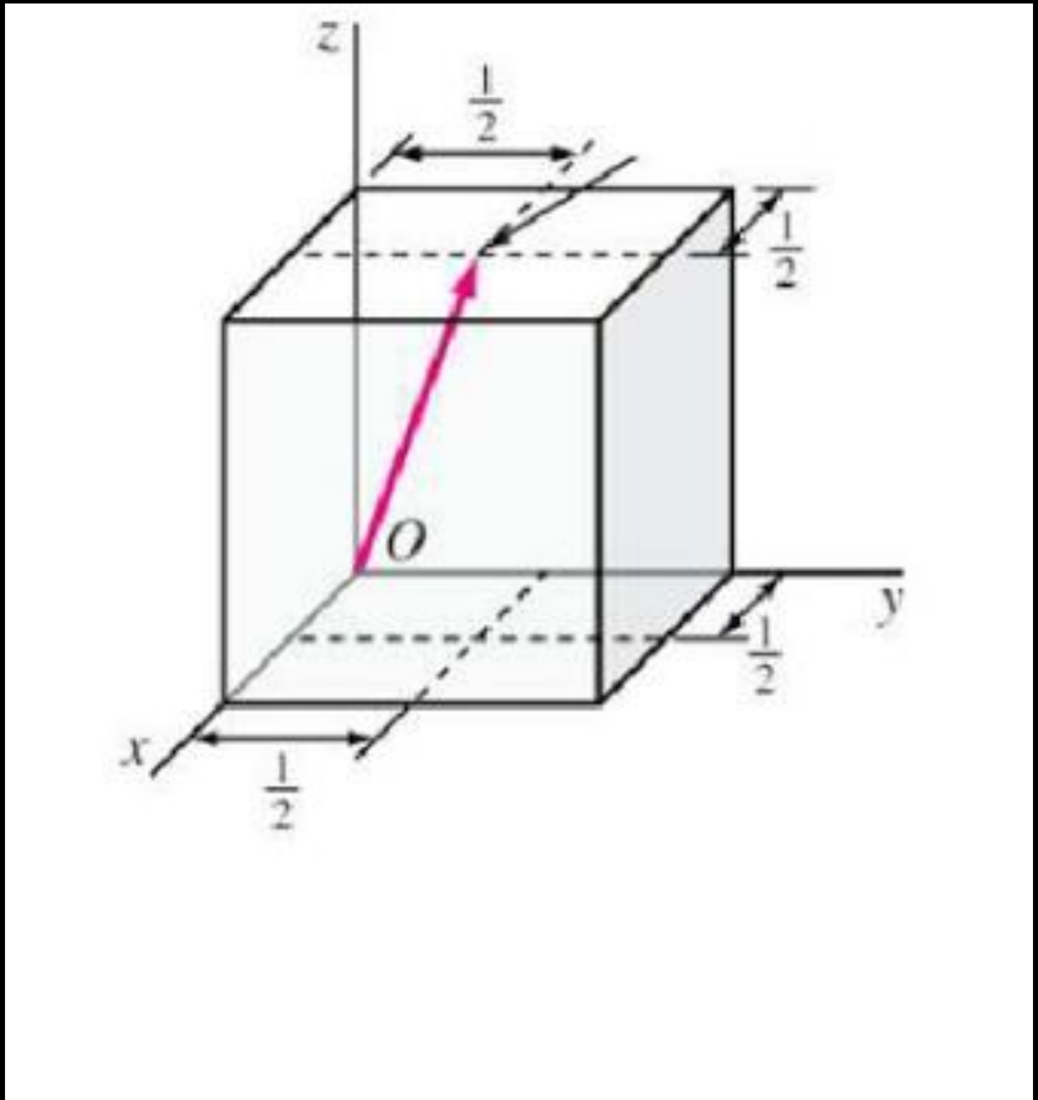
What would be this direction's Miller Index?



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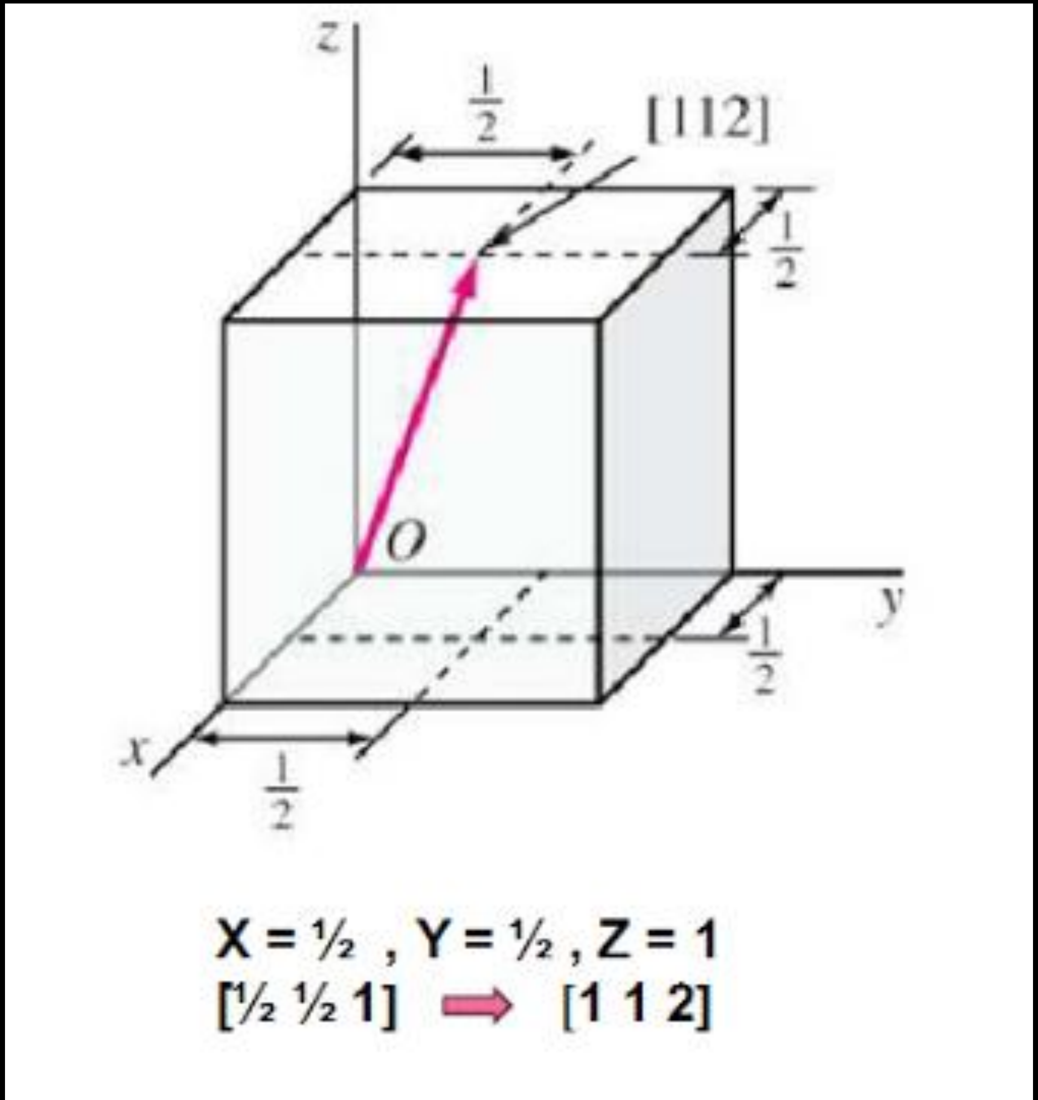

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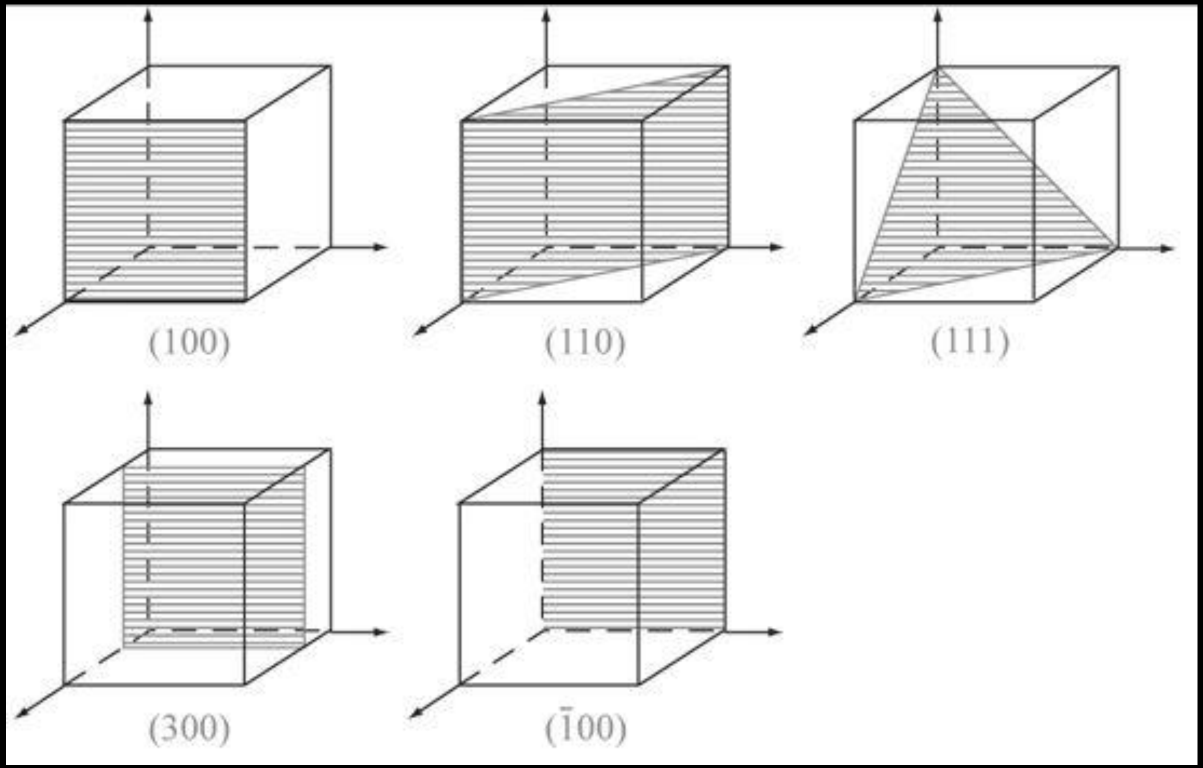
Planes

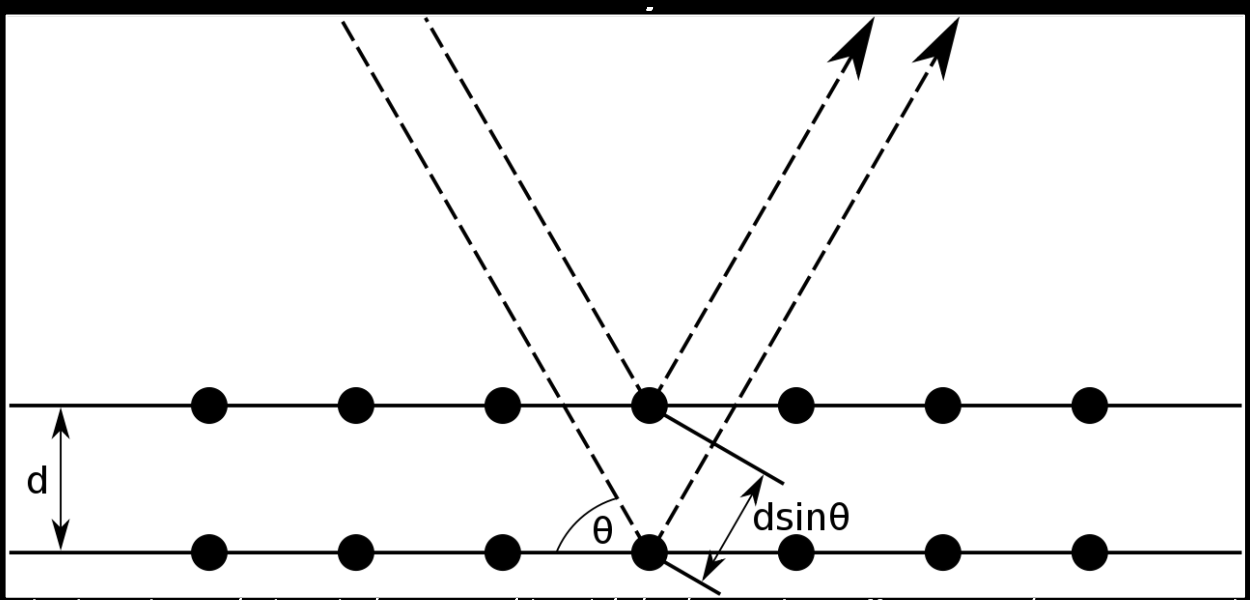
- Like directions, planes can be simplified to 3 numbers. And we can keep it in a unit cell as well!
- Here, each number denotes the reciprocal of the intercept of the plane with each coordinate axis. Still in terms of lowest integers.
- Example: The (123) plane intersects the x-axis at 1, the y axis at 1/2, and the z axis at 1/3.
- For a 0 component, it intersects at infinity- it never intersects the axis.
- Example: (100) is a plane parallel to the yz plane. [100] is normal to (100)



http://eng.thesaurus.rusnano.com/upload/iblock/ca6/index-miller-ok1.jpg

Determining Structure-Diffraction

- Distance between planes in a crystal can be determined by diffraction- scattering of waves reflected by a crystal.
- X-Rays, Electrons, and Neutrons can be used- need to have a wavelength. Two beams of same phase shown at a crystal.
- How much farther does the bottom wave have to travel?



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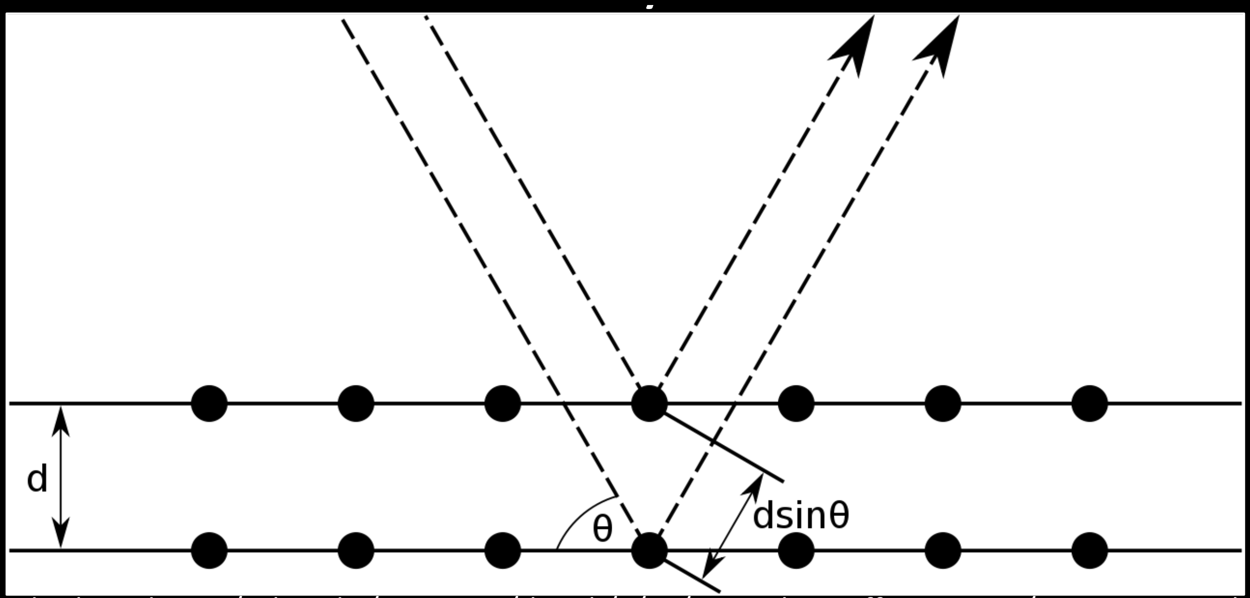
- Bottom wave travels $2dsin\theta$ farther than top wave.



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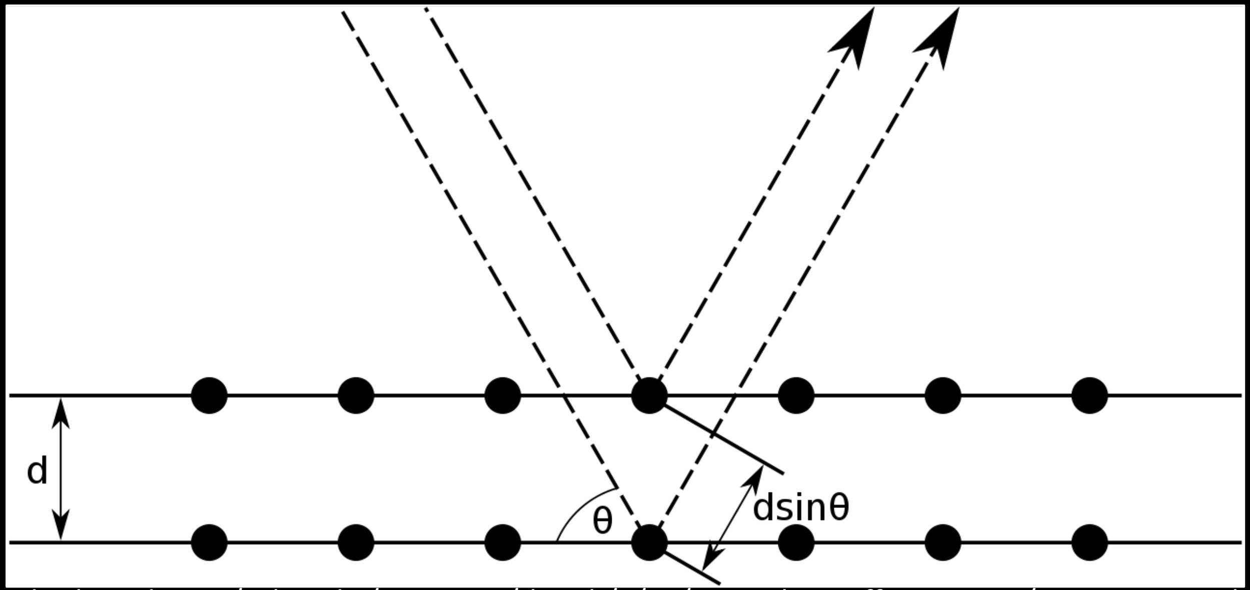
- What do we know if we measure that the two waves constructively interfere?



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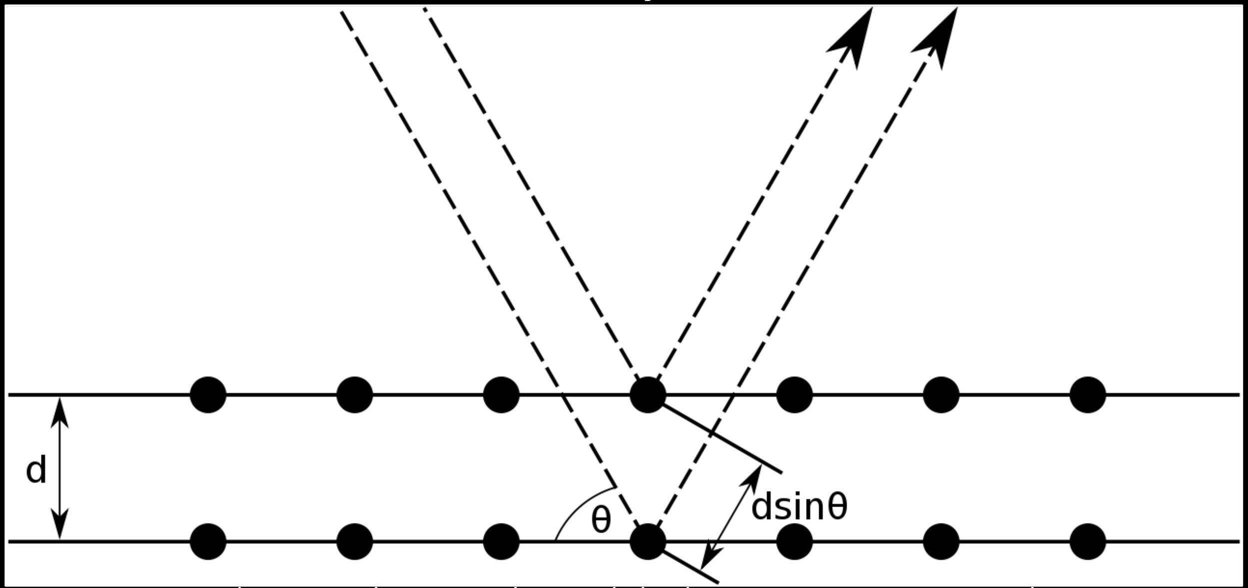
- Bottom wave travels $2dsin\theta$ farther than top wave.
- Waves constructively interfere when both waves are in phase.



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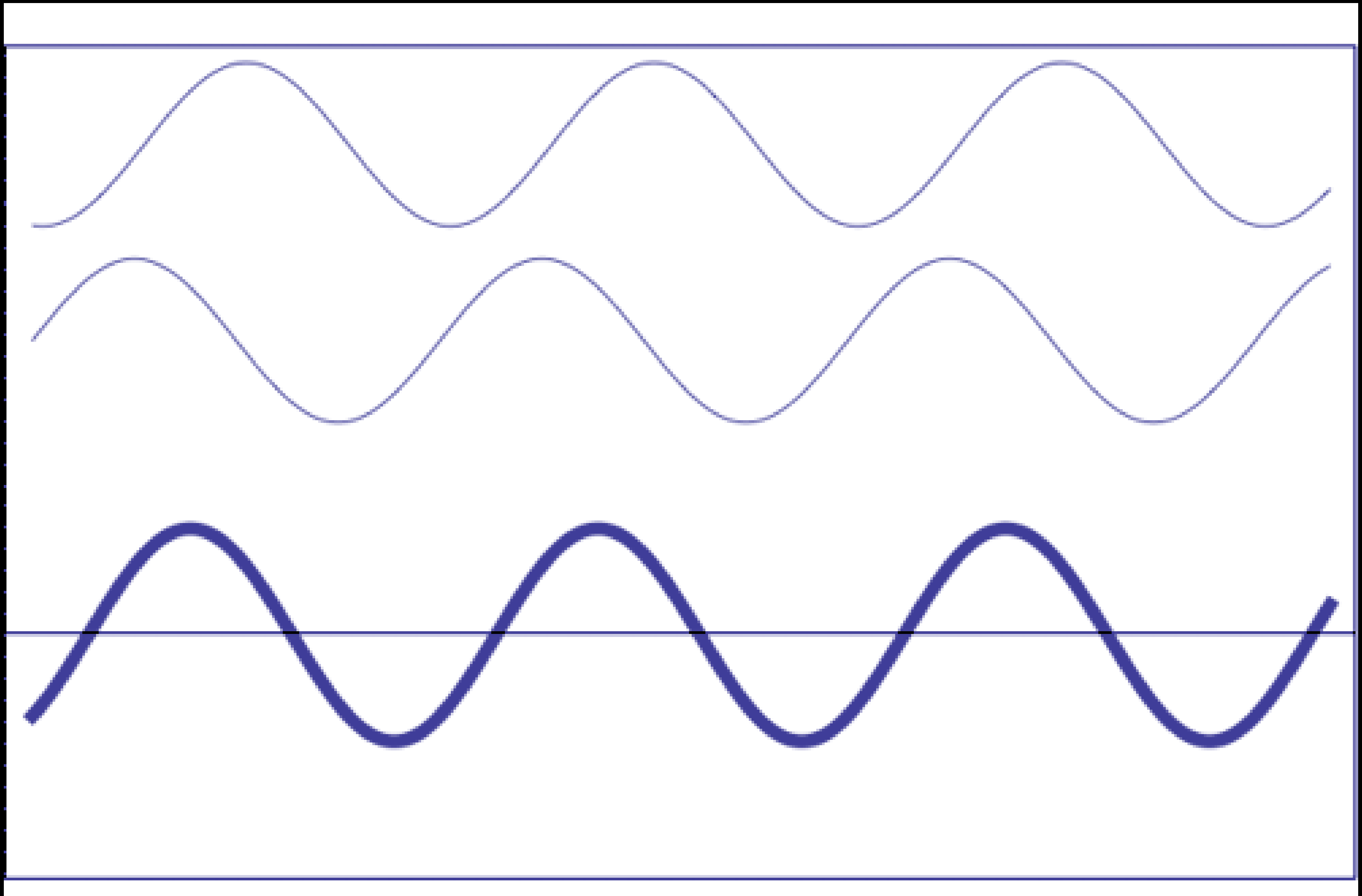

http://www.xtal.iqfr.csic.es/Cristalografia/archivos_05/interferencia-small.gif

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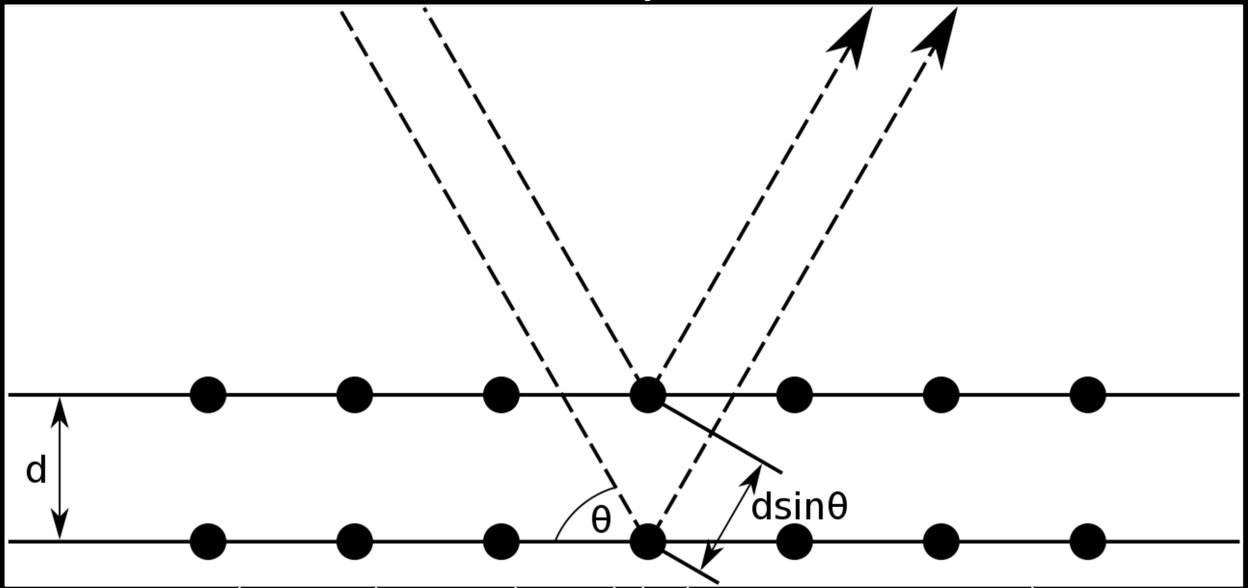

The extra distance traveled by the bottom wave has to be an integer multiple of the wavelength, λ.

https://upload.wikimedia.org/wikipedia/commons/thumb/7/74/BraggPlaneDiffraction.svg/1280px-BraggPlaneDiffraction.svg.png

Determining Structure-Diffraction

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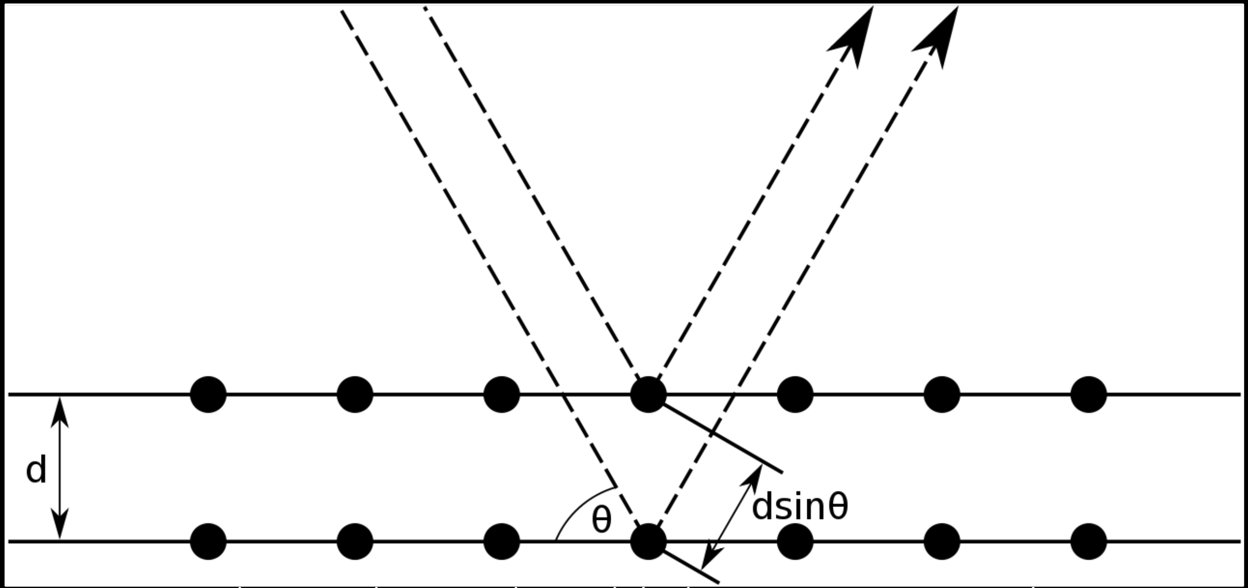
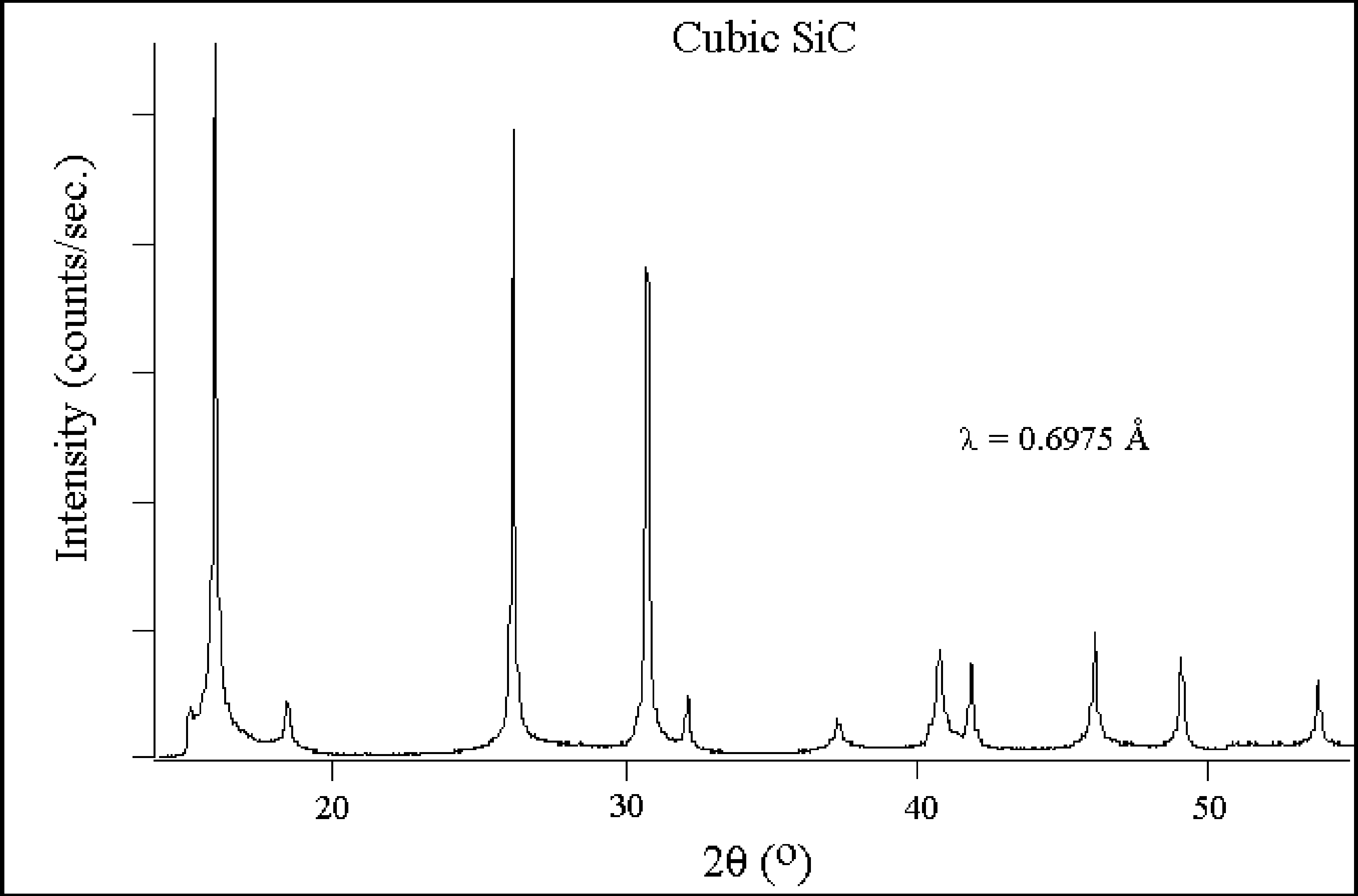
- Bottom wave travels $2dsin\theta$ farther than top wave.
- Waves constructively interfere when both waves are in phase, Bragg's Law:



$$n\lambda = 2dsin\theta$$

https://upload.wikimedia.org/wikipedia/commons/thumb/7/74/BraggPlaneDiffraction.svg/1280px-BraggPlaneDiffraction.svg.png

Rotate crystal to find different planes…



http://www.eserc.stonybrook.edu/ProjectJava/Bragg/SiC1.gif

References

- 1) https://en.wikipedia.org/wiki/Crystallography
- 2) http://www.xtal.iqfr.csic.es/Cristalografia/parte_01_1-en.html
- 3)http://users.encs.concordia.ca/~woodadam/MECH221/Course_Notes/Crystal%20directions%20and%20planes.pdf