Salahaddin University/College of Science
Department of Earth sciences& Petroleum

Theoretical Crystallography course (2022-2023)

A. 1st week — Definition and Concept

B. 2nd week — Crystal systems and Symmetry

C. 3rd week — Miller indices- Wiess parameters- Zone

D. 4th week — Forms of Crystals

E. 5th week — Crystal class (Hermann Mauguin)

F. 6th week — Crystal Projection

G. 7th week — Point groups

*Calculating mark in Crystallography (theory)

1. Exam
2. Homework — Average =15 mark

- Allaby, M., Coenraad, R.R., Hutchinson, S., McGhee, K., O′Byrne, J., Rubin, K. (2008) The Encyclopedia of Earth, A Complete Visual Guide. Weldin Owen Group, Sydney, Australia. 608p.
- Busch, R. M. (2006) Laboratory manual in physical geology. 7th Edition, Pearson Prentice Hall, Upper Saddle River, New Jersey. 302p.
- Coenraad, R.R. (2008) Rocks &Fossils A visual Guide. 2nd Edition, Firefly Book, USA. 304P.
- Hammond, C. (2015) The Basics of Crystallography and Diffraction. 4th Edition. CPI Group (UK) Ltd, Croydon, CR0 4YY. UK. 539p.
- Klein, C. Cornelius, S. Hurlbut, Jr. (1985) Manual of Mineralogy.20th Edition, John wiley & Sons, New York, Chichester, Brisbane, Toronto, Singapore. (After James D. Dana) 596 p.
- Sen, G. (2001) Earth′s Materials Minerals and Rocks. 1st Edition, Prentice Hal, Upper Saddle River, New Jersey.542p.
- Ott, W. B. (2011) Crystallography, An introduction.3rd Edition, Springer Heidelberg Dordrecht London New York, 374p.
- Plummer, C. C. McGeary, D. Carlson, D. H. (2005) Physical Geology. 10th Edition, McGraw-Hill, New York. 580p.
- Tilley, R. J. D. (2006) Crystal and crystal structures. John Wiley & Sons Ltd, The Atrium, Southern Gate, Chichester, England. 270p.

Lecture. 1

Introduction

Aims:

- ❖ Definition
- ❖ Important of crystallography
- ❖ Crystal growth
- ❖ External characteristics of crystal
- ❖ Crystallographic elements

Crystallography: The subject of crystallography includes the description of the characters of crystals in general; of the various forms of crystals and their division into classes and systems; of the methods of studying crystals; including determination of the mathematical relations of their faces, and measurement of the angles between them; finally, a description of compound or twin crystals, of irregularities in crystals, of crystalline aggregates, and of pseudomorphs crystals.

❑ **Crystallography is easily divided into three sections:**

Geometrical, physical, and chemical.

*We will cover the most significant geometric aspects of crystallography.

- During the process of crystallization in the proper environment, crystals assume various geometric shapes dependent on the ordering of their atomic structure and the physical and chemical conditions under which they grow. If there is a predominant direction or plane in which the mineral forms, different habits prevail.
- Example: pyrite often forms equate shapes (cubes), quartz typically is prismatic, and barite tabular.

Why we study Crystallography?

1- It is useful for the identification of minerals. The latter are chemical substances formed under natural conditions and have crystal forms.

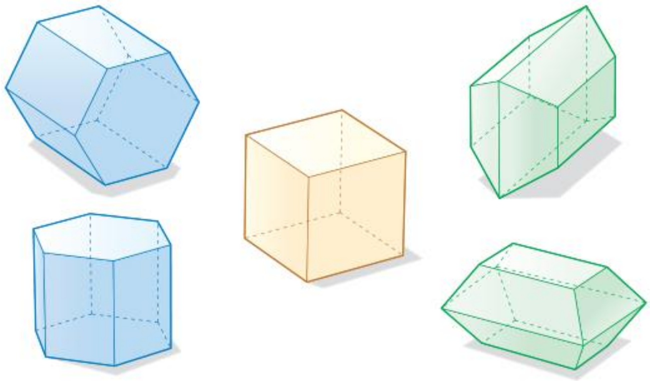
2- Study of crystals can provide new chemical information. In laboratories and industry, we can prepare pure chemical substances by crystallization process.

3- Crystallography is of major importance to a wide range of scientific disciplines including physics, chemistry, molecular biology, materials science and mineralogy.

Crystal

Crystal: Is a regular polyhedral form, bounded by smooth faces, which is assumed by a chemical compound, due to the action of its interatomic forces, when passing, under suitable conditions, from the state of a liquid or gas to that of a solid.

- A polyhedral form simply means a solid bounded by flat planes (we call these flat planes CRYSTAL FACES).
- A chemical compound" tell us that all minerals are chemicals, just formed by and found in nature.
- A crystal normally forms during the change of matter from liquid or gas to the solid state.



Type of crystals

- Classification of crystals depending on the degree of crystallization

Euhedral crystal: All faces of crystal are well-formed.

Subhedral crystal: Crystal has imperfectly developed faces; some of crystal faces are not developed.

Anhedral crystal: A crystal which none of the faces are developed; crystal has not clear faces.

Aggregate crystal: A crystalline substance may occur in such fine grained.

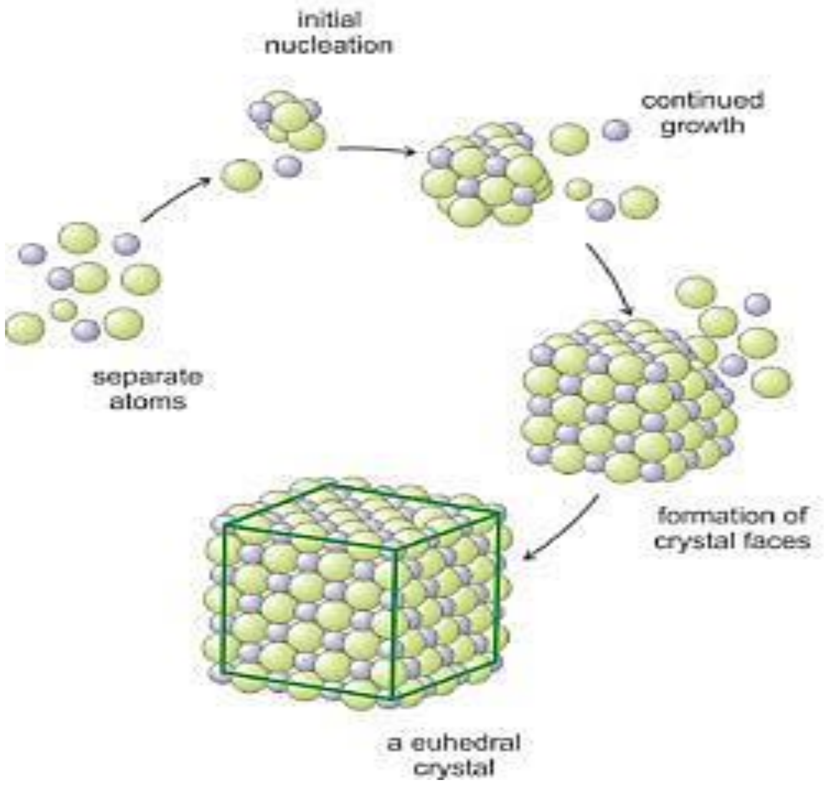
Amorphous: A material that lack of ordered internal atomic arrangement; do not have overall regular internal structure; their constituent particles are arranged randomly; hence, they have no symmetry, and cannot be bounded by faces. Particles are arranged in them in the same way as in liquids, therefore, they are sometimes referred to as super cooled liquids.

Crystal growth

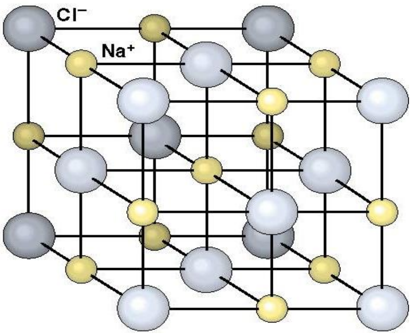
❖ **How are the chemical building blocks (atoms, ions, or ionic clusters) incorporated into a well-ordered crystalline pattern?**

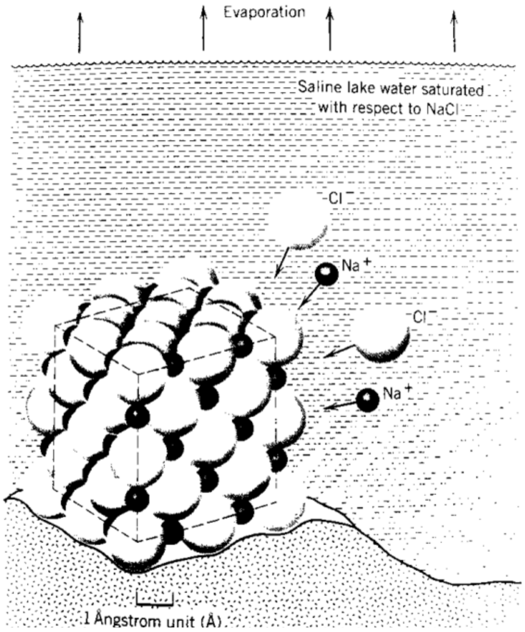
- The first stage in the growth of a crystal is that of nucleation, which implies that growth can commence only after a nucleus has been formed.
- In most cases the nuclei are the initial products of precipitation (in a water environment) or of crystallization (as in melt).
- The nucleus is the result of the coming together of various ions (in the solution or melt) to form the initial regular structural pattern of a crystalline solid.
- The formation of crystals involves the bringing together and ordering of constituent atoms. Crystals grow from a small single molecule to their final visible form. This can happen in many different ways and settings, but the principal mechanisms are three:

  • crystals growing as magma cools
  • crystals precipitating from water
  • crystals forming by chemical reactions



Steps of forming of crystal





- Crystals are formed by repetition in three dimensions of a unit of structure, the limiting surfaces, which are known as the faces of a crystal, depend in part on the shape of the unit cell, also the conditions in which the crystal grows.
- These conditions include all the external influences such as temperature, pressure, nature of solution, direction of movement of the solution, and availability of open space for free growth.

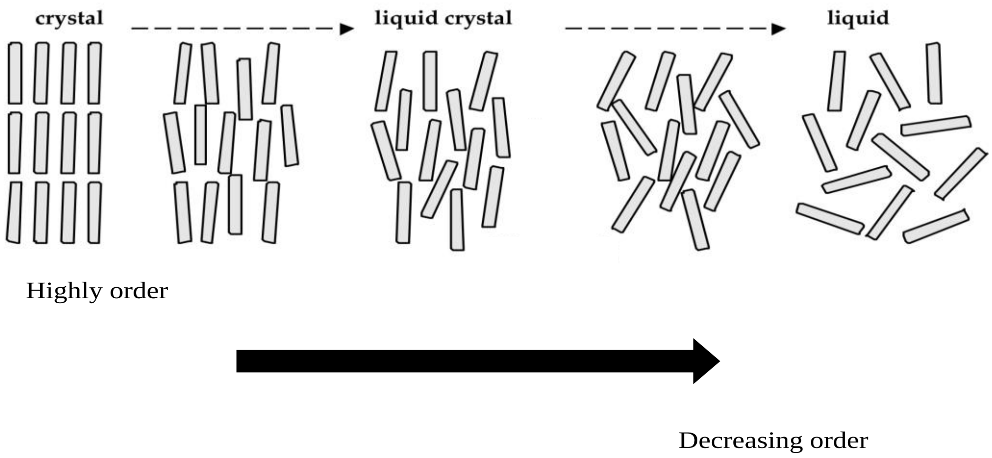
Crystallization: The generation of crystal is known as crystallization.

- Crystals are formed from solutions, melts, and vapors.
- The atoms in disordered states have a random distribution but with changing temperature (T), pressure (P), and concentration they may join in an ordered arrangement characteristic of the crystalline state.
- Examples:

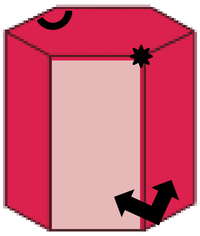
1- Snowflake from H_2O vapor.

2- Igneous rocks from molten magma.

3- Halite from salt water.



Crystal Morphology



Crystal morphology consists of:

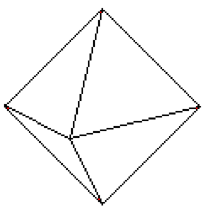
1. Crystal Faces
2. Crystal edge
3. Solid angle
4. Interfacial angle

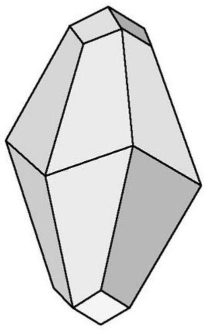
1. Crystal Faces

Crystal faces: The crystal is bounded by flat plane surfaces. These surfaces represent the internal arrangement of atoms and usually parallel to net-planes containing the greatest number of lattice- points or ions.

Faces shape are of two kinds

- ❖ Like faces and unlike faces



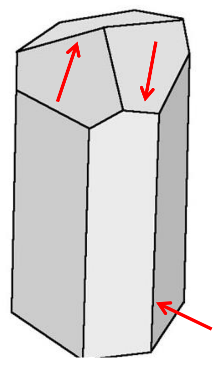


- ❖ Actual crystals deviate, within certain limits, from the ideal forms.
- ❖ First, there may be variation in the size of like faces, thus producing what are defined as distorted forms.

- Second, the faces are rarely absolutely smooth and brilliant; commonly they lack perfect polish, and they may even be rough or more or less covered with fine parallel lines (called striations), or show minute elevations, depressions or other peculiarities.
- Finally; it may note in passing that the characters of natural faces, just alluded to, in general make it easy to distinguish between them and a face artificially ground, on the one hand, like facet of a cut gem; or on the other hand, the splintery uneven surface commonly yielded by cleavage.

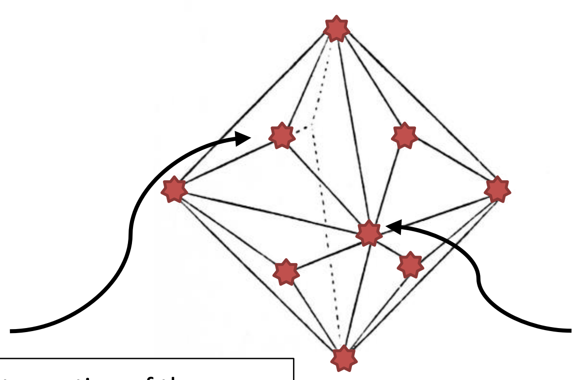
2. Crystal edges

Edge: formed by the intersection of any two adjacent faces. The position in space of an edge depends upon the position of the faces whose intersection gives rise to it.



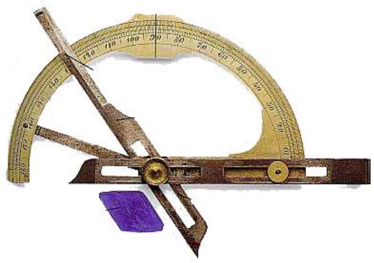
3. Solid angle

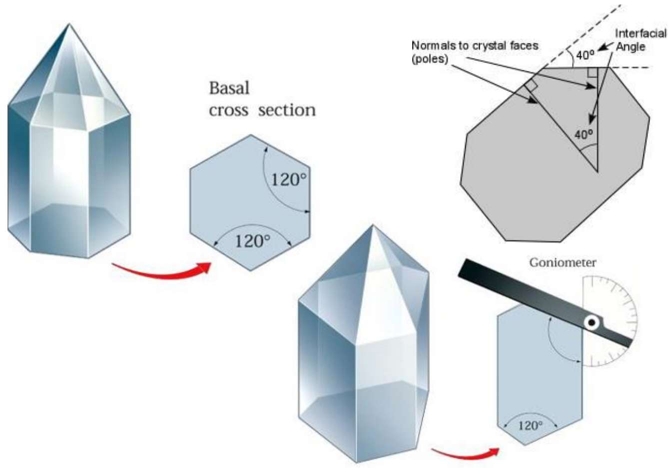
A solid angle is formed by the intersection of three or more faces.



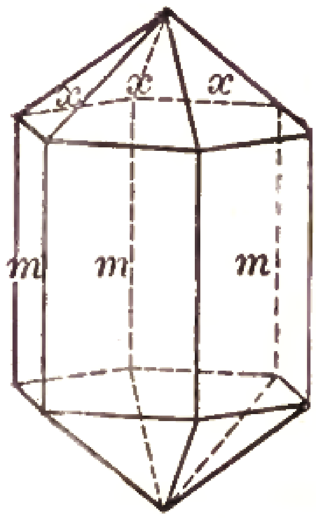
4. Interfacial angle

- Interfacial angle defines such as angle between two crystal faces as the angle between lines that are perpendicular to the faces. Such lines are called the poles to the crystal face.
- The angle can be measured easily with a device called a contact goniometer.





- The angles of inclination between like faces on the crystals of any species are essentially constant, whatever they are found, and whether products of nature or of the laboratory. These angles, therefore, form one of the important distinguishing characters of a species.
- Example: In apatite crystal, the angle between the adjacent faces *x* and *m* (130°) is the same for any two like faces, similarly situated with reference to each other.
- Further, this angle is constant for the species no matter what the size of the crystal may be or from what locality it may come.



Apatite

Diversity of Size: Crystals occur of all sizes, from the merest microscopic point to a yard or more in diameter. It is important to understand, however, that in a minute crystal the development is as complete as with a large one. Indeed, the highest perfection of form and transparency is found only in crystals of small size.

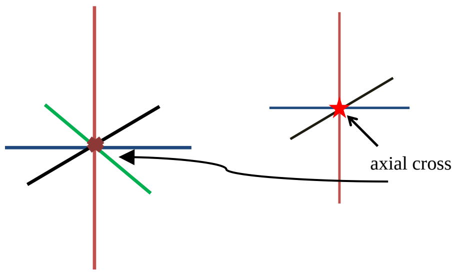
- ❑ Due to a variety of factors, many natural crystals have some degree of distortion to their growth, causing the faces to vary in size and sometimes shape, this problem was resolved by requiring the classroom use of a set of crystal forms, sometimes made of wood or plastic.

Crystallographic elements

Crystallographic axes: Are imaginary straight lines, intersects at the center of the crystal and extending to the mid of the crystal faces, edges or solid angle.

Some characteristic of Crystal axes:

1- They are straight lines.
2- Intersect at a point called axial cross.
3- They are 3 or 4 lines.
4- One of them is vertical others are horizontal.
5- May be equal in length or different.



Axial cross: Is the point of intersection of the three (or four) axes.

Crystallographic axes name:

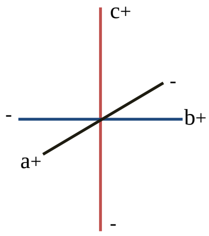
1- **a** axis- horizontal and is oriented front to back.

2- **b** axis- horizontal and is run right to left.

3- The two ends of each of these axes are given the + or – notation by convention.

4- **c** axis is vertical extending from upper to lower in the crystal.

5- The top of **c-axis** is **c+** and the bottom is **c-**; the front portion of the **a-axis** is **a+**, and the back portion is **a-**; the right side of the **b-axis** is **b+** and the left side is **b-**.



Axial angles: They are angles formed as a result of intersection of crystal axes.

1- (α) Alpha angle:

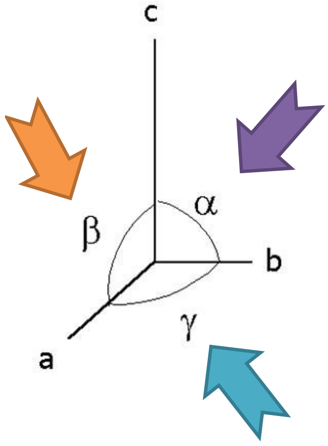
It is located between c-axis and b-axis

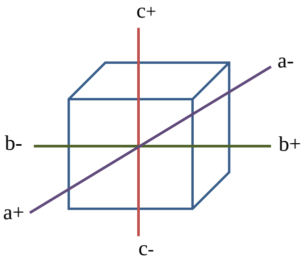
2- (β) Beta angle:

It is located between c-axis and a-axis

3- (γ) Gamma angle:

It is located between a-axis and b-axis





Prepared by
Assistant Lecturer
Baran H. Mustafa