L5: Crystal forms and Miller indices (I)

Tuesday, July 28, 2020 16:33

Time on task: 2 hours (material posted on Sept 7th, Office hours: Monday Sept 21st and Wednesday Sept 23rd)

Goals:

Upon completion of this lecture, you should be able to:

1. Describe the crystal form
2. Determine the Millers indices of each crystal faces

This lecture is complemented with your lab #4 (due on Friday Sept 25)

1. Crystal forms

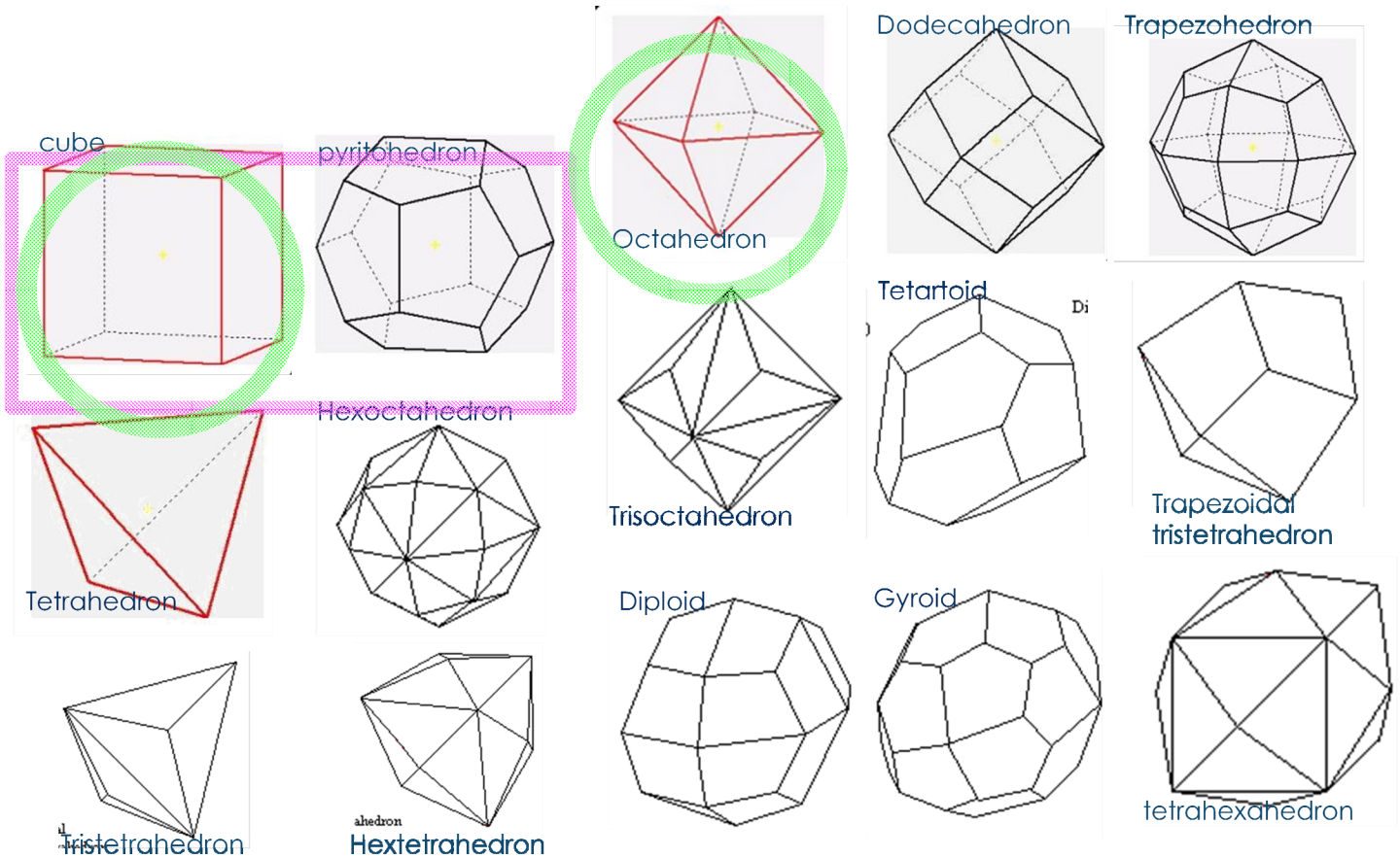
A **crystal form** is a set of crystal faces that are related to each other by symmetry. We distinguish between closed forms and open forms.

A closed form is a set of crystal faces that completely enclose space. Thus, in crystal classes that contain closed forms, a crystal can be made up of a single form. (it can also be made up of several close forms, however, a crystal never mix closed and open forms). All the minerals that belong to the **isometric crystal system** present closed forms.

An open form is one or more crystal faces that do not completely enclose space. Hence, you always need several sets of open forms to describe a crystal morphology.

1.1 Isometric closed forms.

Isometric crystal can present 15 different closed forms or combinations of these closed forms.



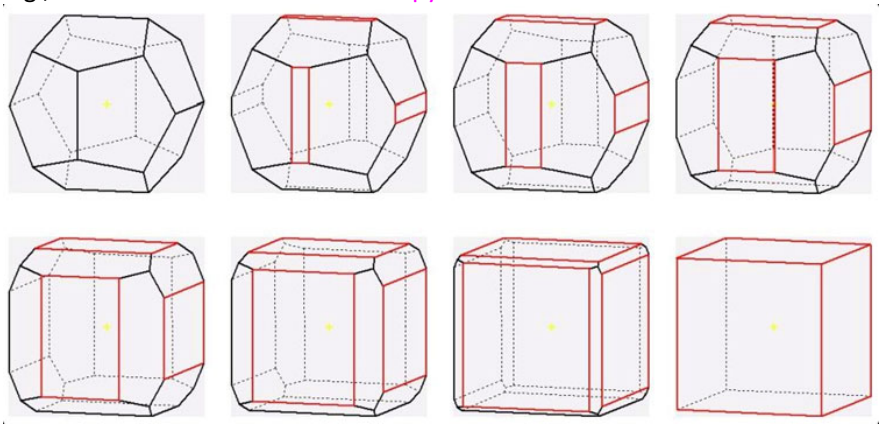
Most of these crystal forms exist in nature. The exception is the Gyroid that has only been observed in experiments. Some minerals can also display various crystal forms.

e.g., Pyrite: cube **pyritohedron** **diploid**

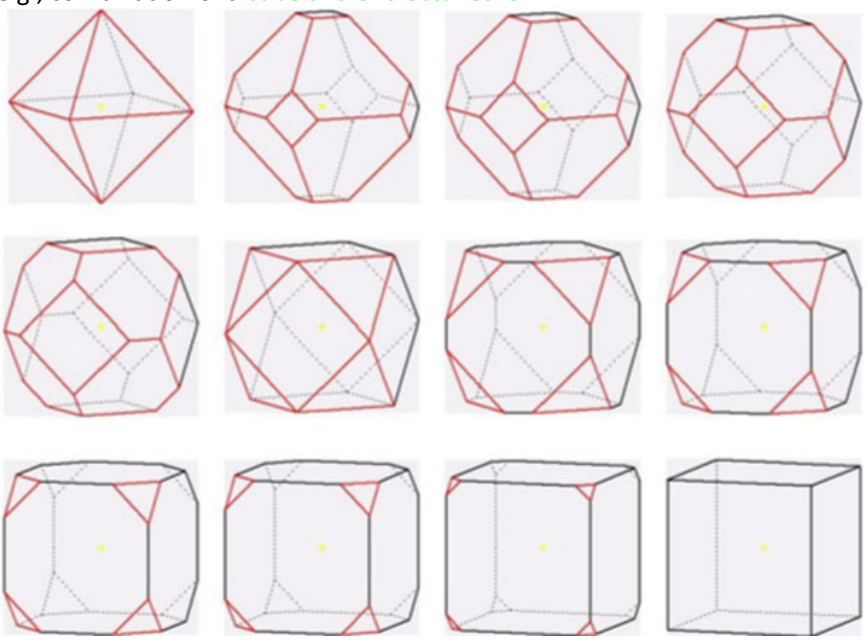


The morphology of a crystal can show several sets of closed forms:

e.g., combination of a cube and of a pyrithohedron



e.g., combination of a cube and of a octahedron



We can usually goes from one crystal form to another by "cutting" the crystals while preserving the symmetry elements. The cut edges are named **truncations** (= edge or angle cut off and replaced by a plane)

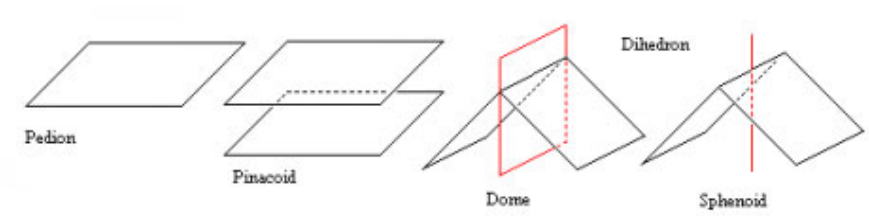
1.2 Non-isometric crystal forms.

They are 4 types of **open forms**:

- **Pedion**: a unique crystal face.

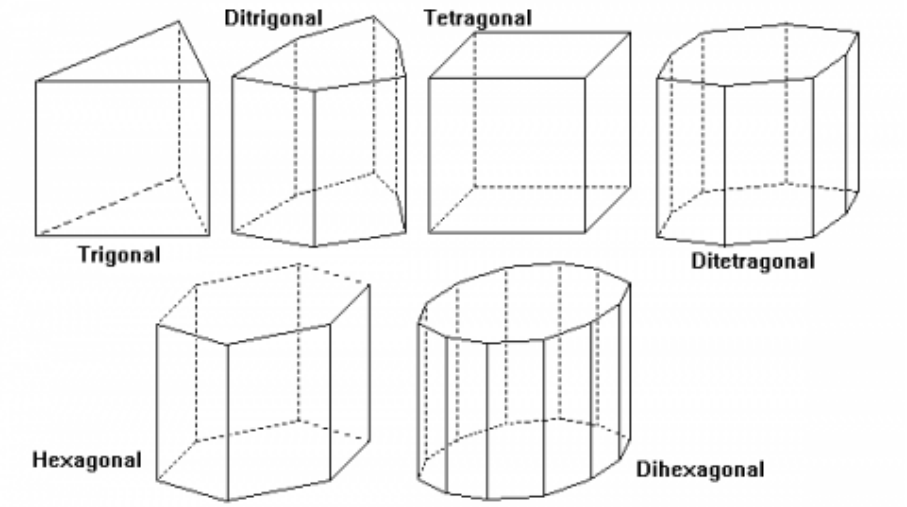
- **Pinacoid/dome/sphenoid**: consists of two parallel faces.

In the pinacoid, the two faces are related by a center of symmetry.
In the dome, the two faces are related by a mirror.
In the sphenoid, the two faces are related by an A2.

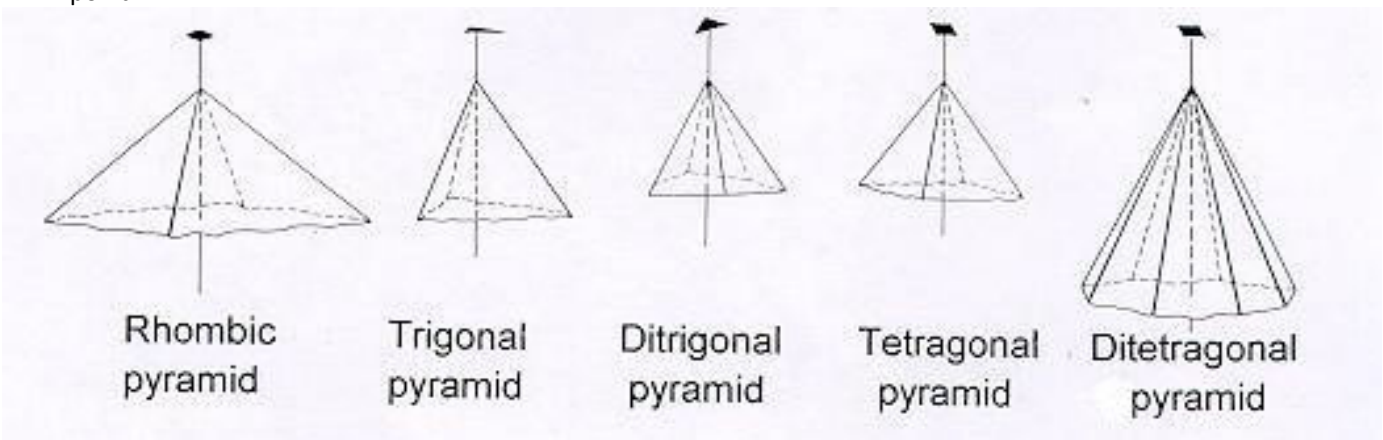


- **Prism**: A "tube" with 3, 4, 6, 8 or 12 mutually parallel faces and consistent angles relating faces.

Prisms are terminated by a dome, a pinacoid or a sphenoid.



- **Pyramid**: A pyramid is a 3, 4, 6, 8 or 12 faced open form where all faces in the form meet, or could meet if extended, at a point.



4-faced form where the faces are related by mirror

3-faced pyramid where faces are related by a A3

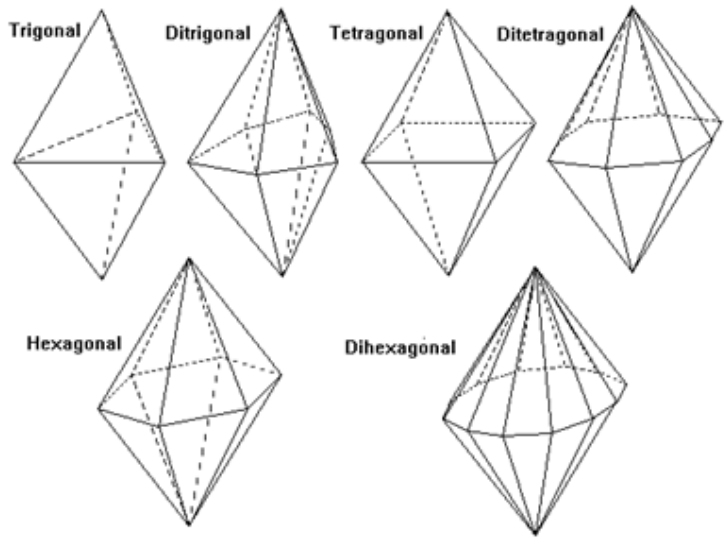
6-faced pyramid where faces are related by a A3

4-faced pyramid where faces are related by a A4

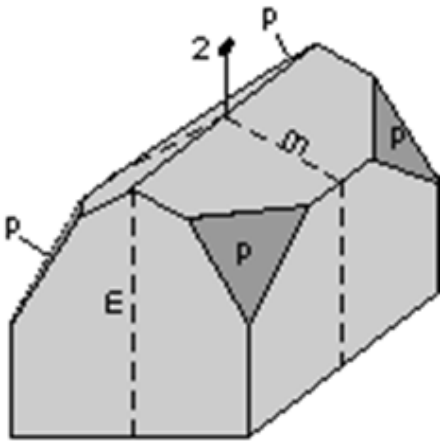
8-faced pyramid where faces are related by a A4

4-faced form where the faces are related by mirror planes or A2.	*3-faced pyramid where faces are related by a A3*	*6-faced pyramid where faces are related by a A3*	*4-faced pyramid where faces are related by a A4*	*8-faced pyramid where faces are related by a A4*

In addition, non-isometric crystals can also display a dipyramid. A **dipyramid** is a closed form consisting of 6, 8, 12, 16, or 24 faces. **Dipyramids are pyramids that are reflected across a mirror plane.**



1.3 examples

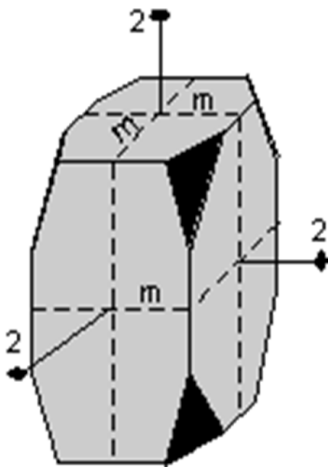


This crystal is composed of:

- 1 rhombic pyramid (the dark gray faces labelled p) (4 faces)
- 2 pinacoids (2*2 faces)
- 1 dome (or sphenoid) (2 faces)
- 1 pedion (1 face)

(total: 11 crystal faces)

Your turn! Describe the forms of this crystal.
(answers are at the end of the personal assessment.)

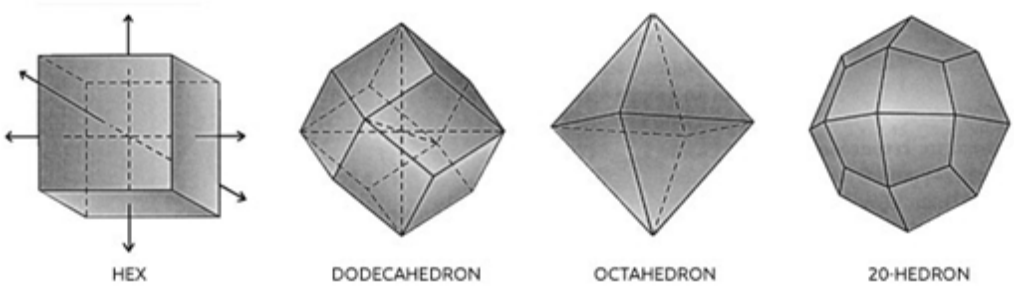


L5: Crystal forms and Miller indices (II)

Thursday, July 30, 2020 9:45

2. Miller indices

Miller indices will allow us to label crystal faces. You already know that the crystal faces are determined by the symmetry elements.



The miller indices allow us to put numbers, i.e, a coordinate system on each of those faces to understand how they are reproduced in three dimensions space.

It's a fairly simple system once we understand how it works.

You can actually identify symmetries of the crystals by looking at the label of each face of the crystal.

2.1. Axial ratios

Modern crystallographers can use x-rays to determine the size of the unit cell, and thus can determine the absolute value of the crystallographic axes.

For example, the mineral forsterite is orthorhombic, the unit cell dimensions are:
a = 4.754 Å, b = 10.1971 Å, c = 5.9806 Å

is hexagonal, with the following unit cell dimensions as determined by x-ray crystallography:

a1 = a2 = a3 = 4.913Å

c = 5.405Å

Axial ratios are defined as the **relative** lengths of the crystallographic axes. They are normally taken as relative to the length of the **b crystallographic axis**. Thus, an axial ratio is defined as follows:

Axial Ratio = a/b : 1 : c/b

- For Triclinic, Monoclinic, and Orthorhombic crystals, where the lengths of the three axes are different, the axial ratio is: a/b : 1 : c/b

e.g., the axial ratio of forsterite (orthorhombic) is 4.754/10.1971 : 1 : 5.9806/10.754
= 0.466 : 1 : 0.587
(new convention: b is the longest: https://www.mindat.org/min-1584.html)

- For Tetragonal crystals where the length of the a and b axes are equal, this reduces to 1 : 1 : c/b

e.g., the axial ratio of zircon is 1 : 1 : 5.982/6.607 = 1:1:0.905 (https://www.mindat.org/min-4421.html)

- For Isometric crystals where the length of the a, b, and c axes are equal this becomes 1 : 1 : 1

e.g., the axial ratio of pyrite is 1 : 1 : 1 (https://www.mindat.org/min-3314.html)

- For Hexagonal crystals where there are three equal length axes (a1, a2, and a3) perpendicular to the c axis this becomes: 1 : 1 : 1: c/a

e.g, the axial ratio of quartz is 1:1:1:5.405/4.913
= 1:1:1:1.1001

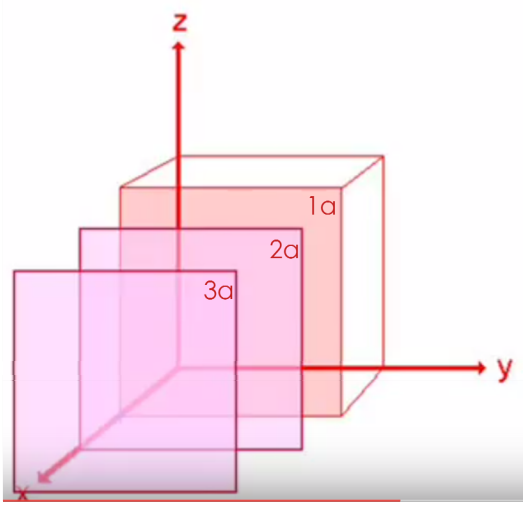
2.2. Intercepts of crystal faces

A crystal face can be defined by how it intercepts the crystallographic axes.

Two very important points about intercepts of faces:

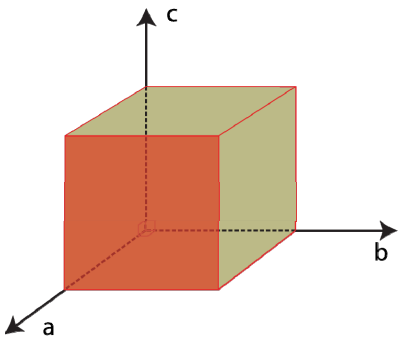
- **The intercepts are relative values, and do not indicate any actual cutting lengths.**
- **Since they are relative, a face can be moved parallel to itself without changing its relative intercepts**.
  (in other words, parallel plans have the same intercept coordinates)

These three plans have the same relative coordinates



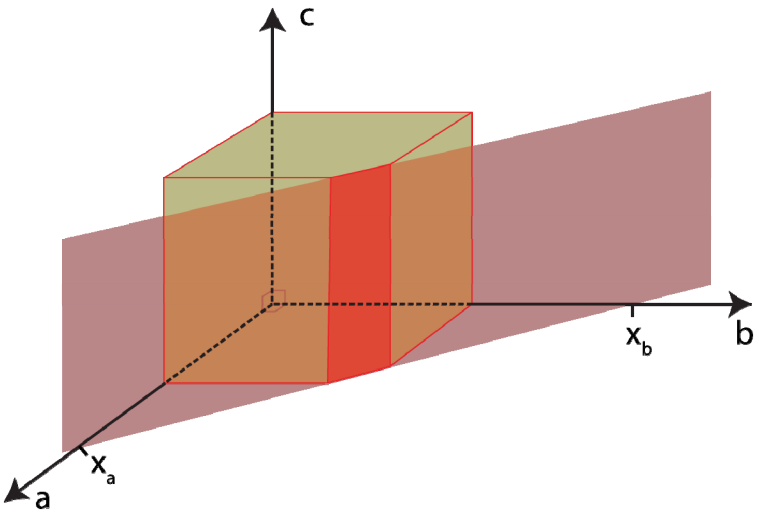
1. A crystal face intersects only one of the crystallographic axes.

e.g., the red face intersects the a-axis but does not intersect the b- and c- axes. The coordinates of the intercept are: xa, ∞b, ∞c. (cut the a-axis in x, never cut b or c)
Because the intercepts are relative values (not actual coordinates), we can normalize the length to 1: 1a, ∞b, ∞c.

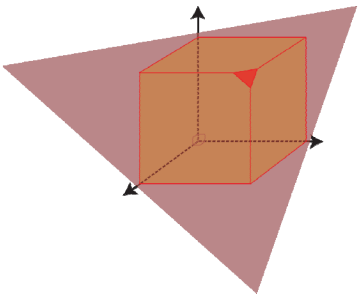


2. A crystal face intersects two of the crystallographic axes.

e.g., the red face intersects the a-axis and the b-axis but never intersects the c-axis, the coordinates of the intercept are: xa, xb, ∞c. (cut the a-axis in x, b-axis in x, never cut or c)
Because the intercepts are relative values (not actual coordinates), we can again normalize the lengths: 1a, 1b, ∞c.



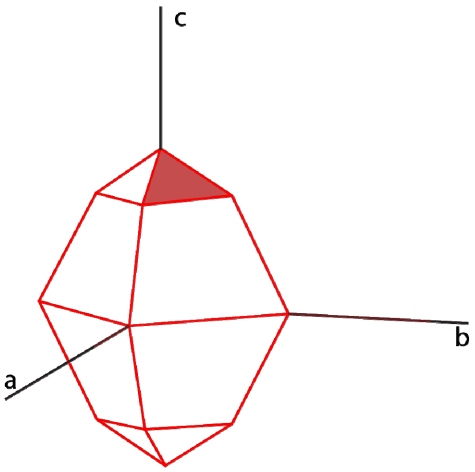
3. A crystal face that intersects all 3 axes.
e.g., In this example the red face is assumed to intersect the a, b, and c crystallographic axes at one unit length on each. The coordinate of the interface are: **1a, 1b, 1c.**

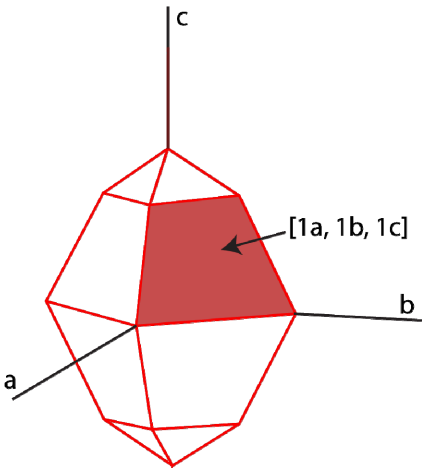


The issue is we usually don't know the size of the unit cell when we examine a crystal. Hence, it is difficult to know what number to give the intercept of a face, unless one face is chosen arbitrarily to have intercepts of 1.

Thus, the first step is to identify the crystallographic axes and the convention is to assign the largest face that intersects all 3 crystallographic axes the coordinates: 1a, 1b, 1c. This face is called the unit face.

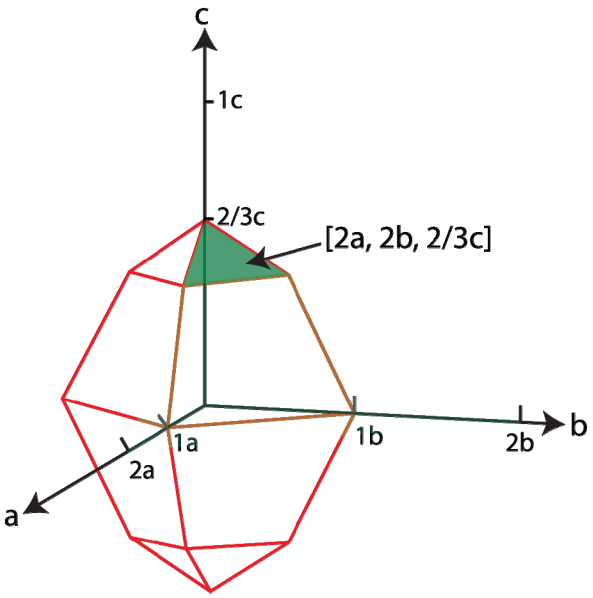
e.g., in this orthorhombic crystal, two types of faces cut the three axes:





We will choose the right one as the unit face as this face is more developed.

All the other face coordinates will be defined relative to this one.



Dealing with "∞" sign and fractions however, is not super convinient to label the faces. So crystallographers have developed another way of identifying or indexing faces. This conventional notation called the **Miller Index**.

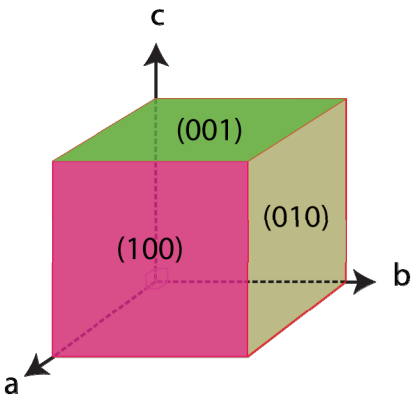
2.3. Miller indices

Miller indices are reciprocal of the coordinates of each crystal face.

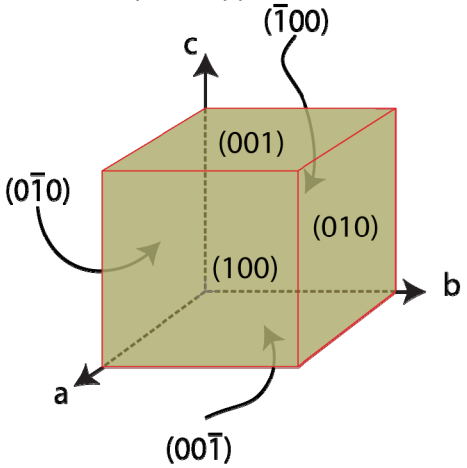
Notation: in parentheses, no comma, no fraction.

Example:

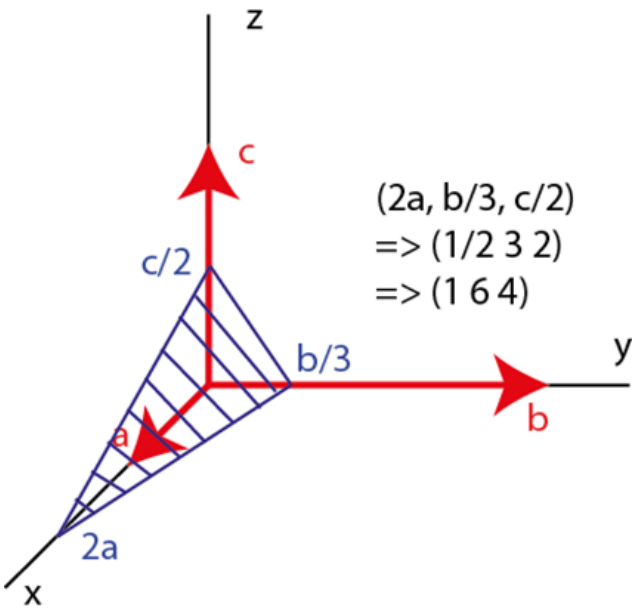
- Pink face: (1/1,1/∞,1/∞)=(1 0 0)
- Yellow face: (1/∞, 1/1,1/∞)=(0 1 0)
- Green face: (1/∞,1/∞,1/1)=(0 0 1)



Additionally, the opposite sides of each face are designed with negative signs.



Example: This plan cut the a-axis in 2, the b-axis in 1/3 and the c-axis in 1/2.
Hence, the coordinates of this plan are (2a, b/3, c/2).

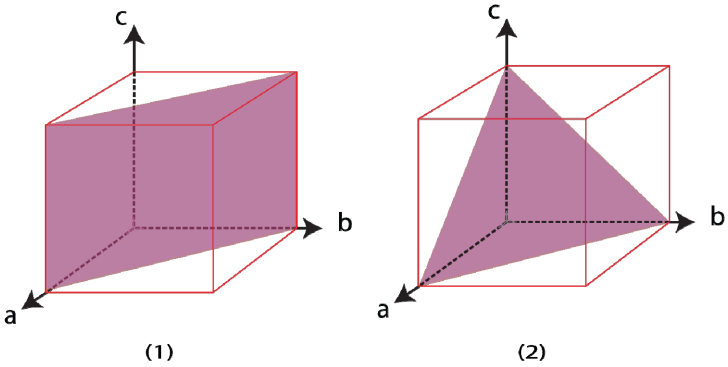


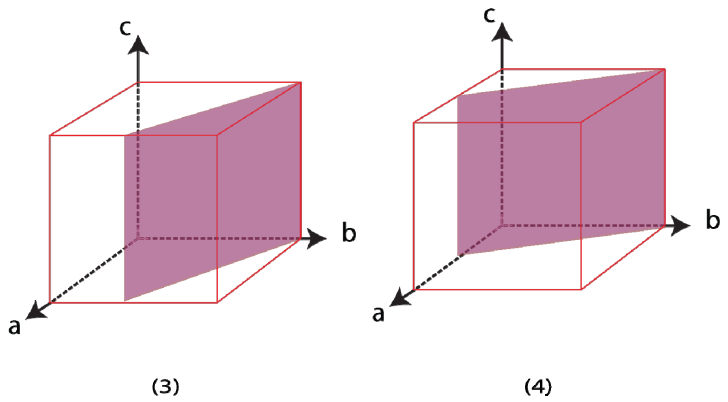
The reciprocal of the coordinates are:
a-axis: 1/2
b-axis: 1/(1/3) = 3
c-axis: 1/(1/2) = 2

We do not use fraction in Miller indices, hence, we multiply everything by a factor 2 (we can do that as the coordinates are relative, not absolute - remember, parallel faces have the same coordinates):

Miller indices: (1 6 4)

Your turn! Give the Miller indices of the pink plan (answers are at the end of your personal assessment).





L5: Personal assessment

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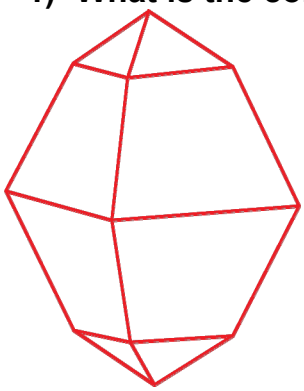
After reviewing the second lecture, you should be able to answer these questions:

1) **What is the correct way to describe this crystal?**



A - four tetragonal pyramids
B - one rhombus dipyramid and two rhombus prisms
C - two rhombus dipyramids
D - one rhombus dipyramid and 4 pinacoids

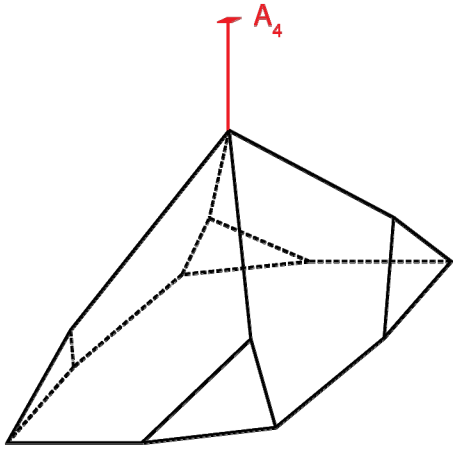
2) **An orthorhombic crystal can present a tetragonal prism.**

A - True
B - False

3) **An hexagonal crystal can present a trigonal pyramid.**

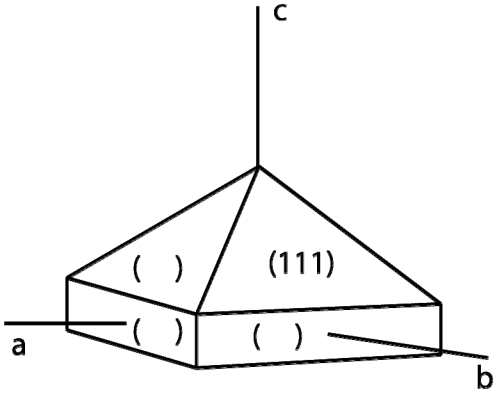
A - True
B - False

4) **What is the correct way to describe this crystal?**

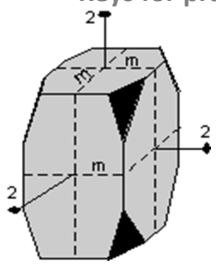


A - two tetragonal pyramids and a pedion
B - one tetragonal pyramid, one tetragonal prism, and a pedion
C - two rhombus pyramids and a pedion
D - one tetragonal pyramids, two sphenoids and a pedion

5) Find the Miller indices of the three other visible faces



Keys for practices:



1 rhombic dipyramid (8 faces)
1 rhombic prism (4 faces)
1 pinacoid (2 faces)
Total 14 faces

Miller indices: 1) (100); 2) (111); 3) (210); 4) (120)