12.108 Structure of Earth Materials

I. Lecture 1: Minerals and Symmetry Operations

Definition of a mineral

A mineral is a naturally occurring homogeneous solid usually formed by inorganic processes. It has a definite chemical composition and a highly ordered atomic arrangement.

In detail—

1. *Naturally occurring*: Minerals are not man-made, but are produced by natural processes. A diamond found in the earth, for example, is a mineral, but a diamond synthesized in a lab is not.

2. *Homogeneous*: A mineral cannot be physically separated into simpler chemical compounds.

3. *Solid*: Liquids and gases are not minerals. Water, for example, is not a mineral, but ice is.

4. *Formed by inorganic processes*: Petroleum and coal are not minerals.

5. *Definite (but generally not fixed) composition*: Minerals can be expressed by chemical formulas, such as SiO_2 for quartz. However, some minerals like feldspars have variable compositions. The composition of plagioclase, for example, ranges from $NaAlSi_3O_8$ to $CaAl_2Si_2O_8$.

6. *Ordered atomic arrangement*: Minerals have long-range 3D atom order. Solids like glass that lack long-range atomic order are called amorphous and are not minerals.

Symmetry

The long-range 3D order of minerals may be defined in terms of molecule-scale building blocks that are arranged in a regular manner. The way these building blocks are arranged is described by symmetry. Symmetry not only describes a mineral's atomic order, but also controls physicals properties such as cleavage and habit (Neumann's Principle).

2D Symmetry Operations

Symmetry operations consist of an element and an operator.

| Operation	Element	Operator
Translation	vector	distance
Rotation	axis	angle
Reflection	mirror	distance

A. Translation

Translations of molecule-scale building blocks lead to long-range atomic order. This symmetry operation will be explored in more detail in Lecture 2; this lecture focuses on symmetry operations that don't require translations.
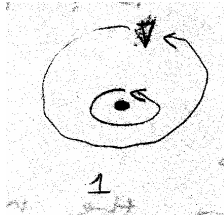

B. Reflection

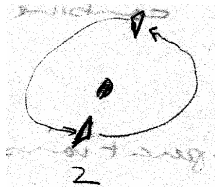Mirror planes are designated by *m*.

6|∂ (m)
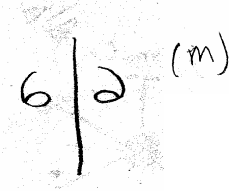
C. Rotation

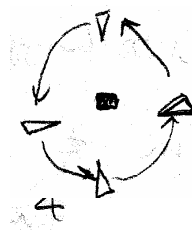The angle of rotation α about an axis must be the quotient of 360° and an integer n.

$$\alpha = 360°/n$$

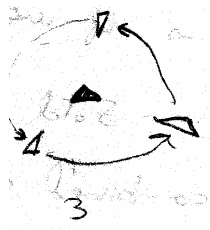When n = 1, an object is completely rotated about the rotation axis and exhibits 1-fold symmetry.

When n = 2, an object is rotated α = 180° around the rotation axis and exhibits 2-fold symmetry.

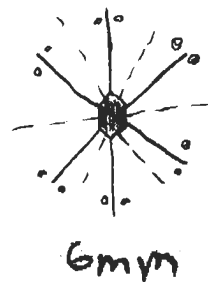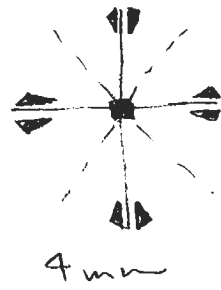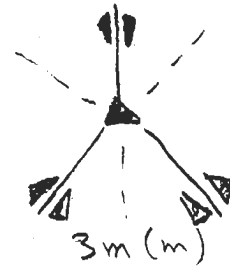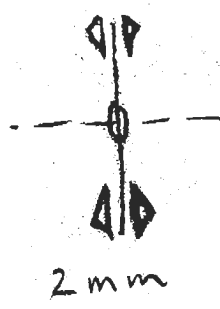| n	α	Symmetry
3	120	3-fold
4	90	4-fold
5		*will be addressed later
6	60	6-fold

D. Combined Operations

Some symmetry operations may be combined to form more complex operations. For example, rotating a mirror plane *m* about an axis combines rotation and reflection.
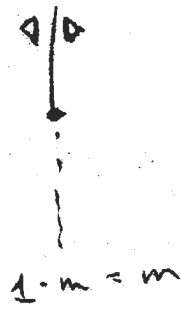
Reflection, rotation, and their combinations produce ten planar point groups. These groups express all the possible symmetries about a point in two dimensions.
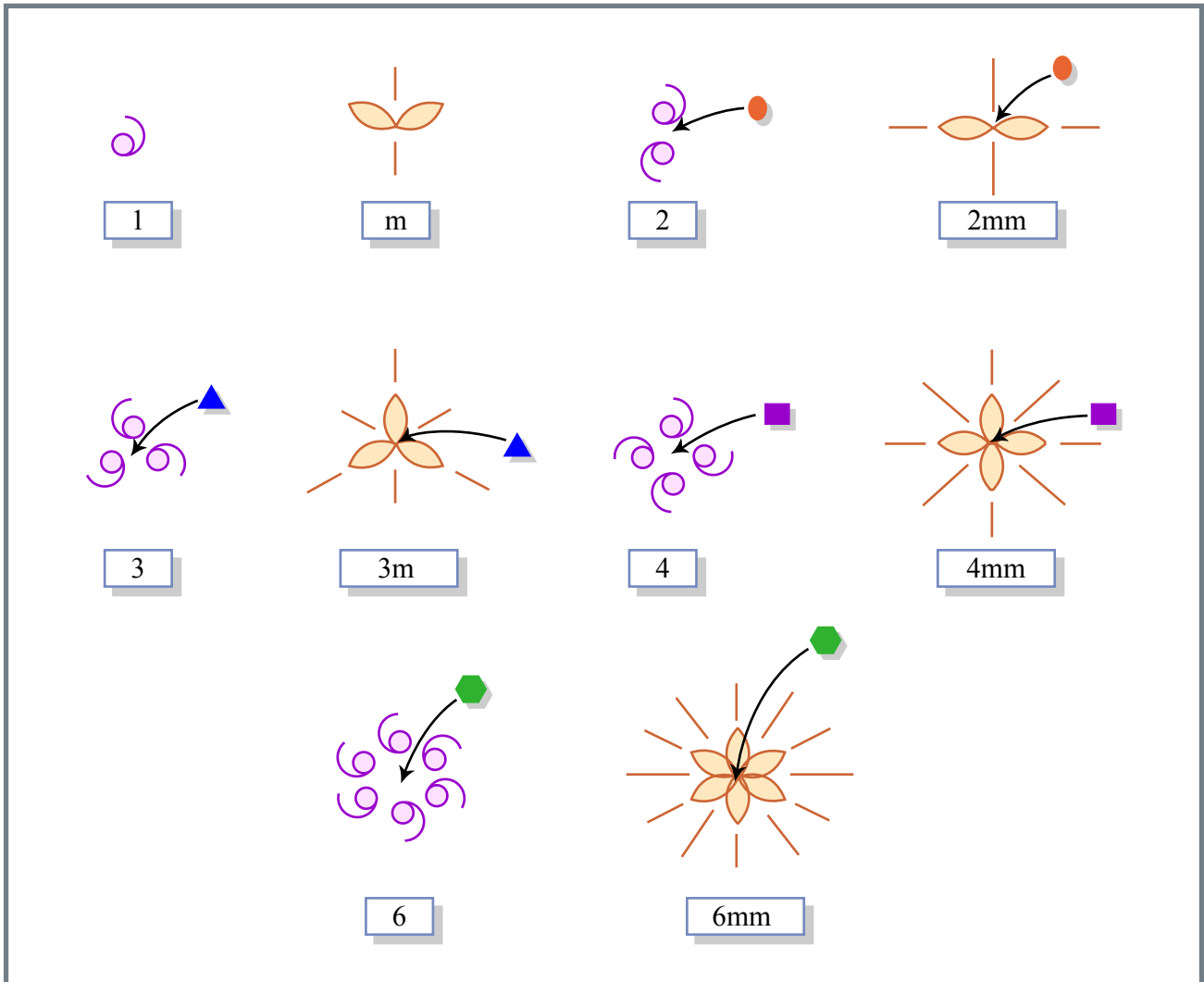
1	m	2	2mm
3	3m	4	4mm
	6	6mm	

(Adapted from Klein and Hurlbut, Jr. Manual of Mineralogy. New York: John Wiley and Sons, Inc., 1993. 117)

D. Inversion

The inversion operation inverts an object through an inversion center i. The inverted object is formed by drawing imaginary lines from the original object through the inversion center and out an equal distance on the other side. In two dimensions, the operation is equivalent to a 2-fold rotation. Symmetry about a point in three dimensions will be covered in a later lecture.

II. Lecture 2: Translation and 2D Plane Groups

Crystals are three-dimensional periodic arrays of a group of atoms. This group of atoms may be $(SiO_4)^{-4}$ or H_2O, for example, and is called a motif. The motif is repeated via vector translations in three dimensions and forms a lattice. In earth materials, the translations are on the order of 0.5 to 2.0 nm.
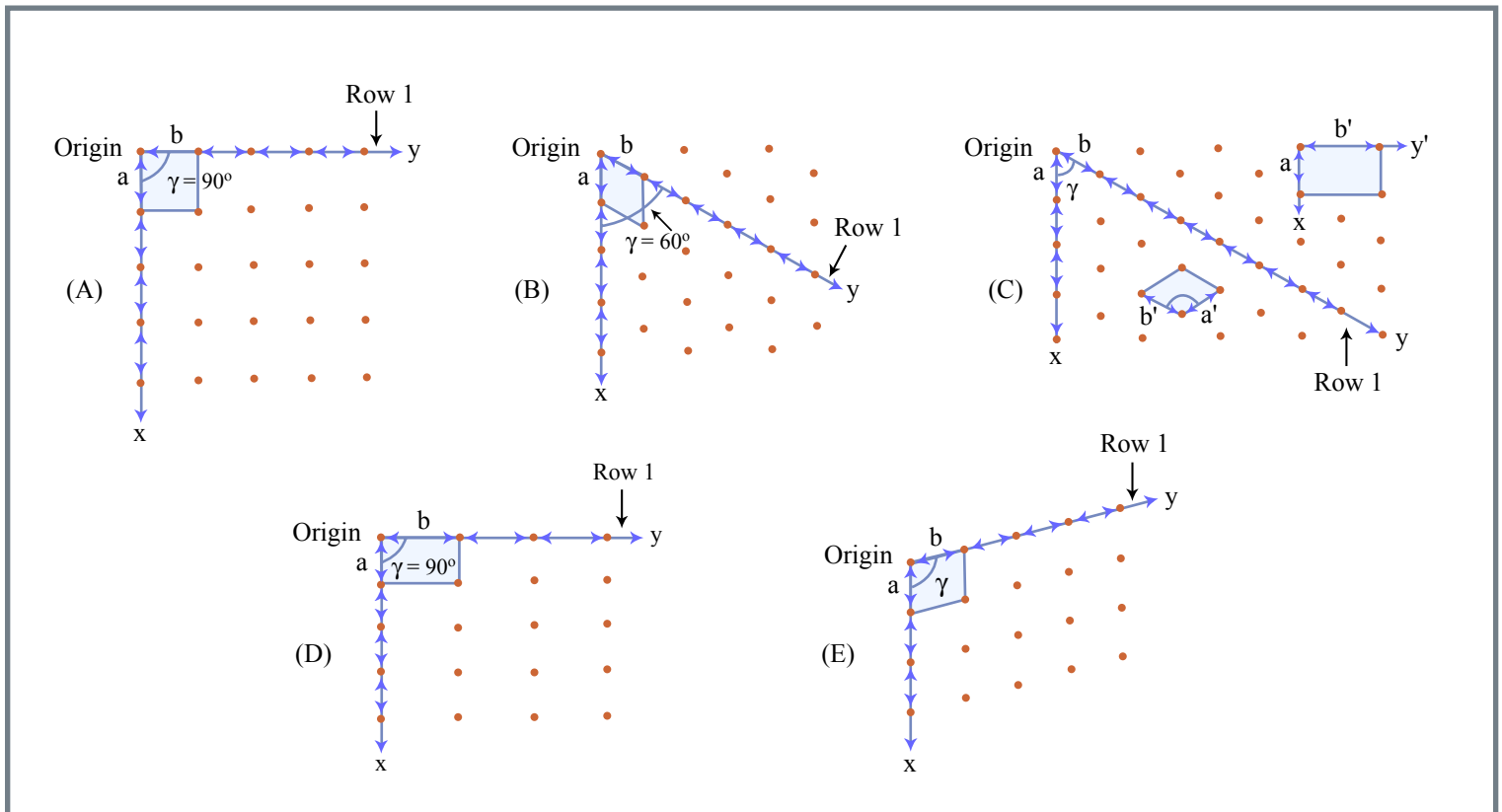
Translations and Lattices in 2D

In diagram below, the motif is represented by points called lattice points. Note that the environment of every point is identical to that of every other point.
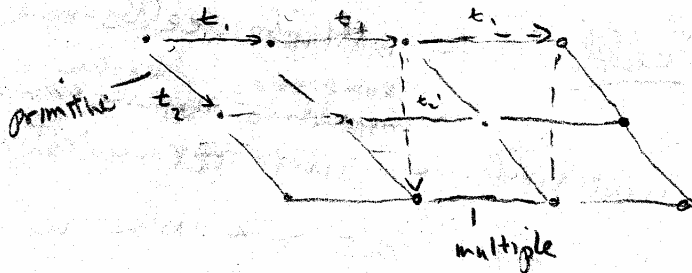
The polygon building blocks that compose a lattice are called unit cells. Primitive unit cells contain only lattice nodes and multiple unit cells contain an extra node within the cell. The smallest unit cell is called the reduced unit cell

In two dimensions, there are only five distinct lattices.

(Adapted from Klein and Hurlbut, Jr. Manual of Mineralogy. New York: John Wiley and Sons, Inc., 1993. 113)

Combining Point Symmetry Operations with 2D Translations

A lattice must be compatible with the point symmetry of the motif it repeats. This restraint limits the motif's possible symmetries. Understanding how requires a mathematical approach to symmetry operations.

Vector and Matrix Digression

Performing inversion or reflection operations requires matrix multiplication.

Example 1. Invert point (x, y, z) through the origin to find (x', y', z').

$$x' = -1x + 0y + 0z$$
$$y' = 0x + -1y + 0z$$
$$z' = 0x + 0y + 1z$$

$$\left.\begin{array}{c} \\ \\ \\ \end{array}\right\} \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$
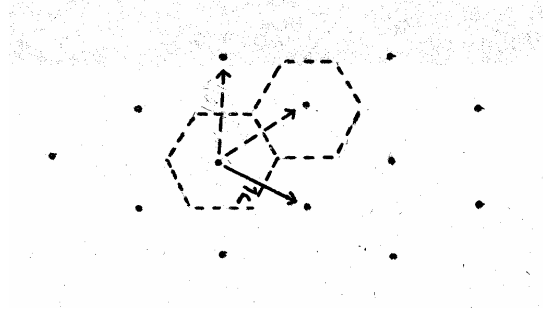
$$I$$

I represents the inversion matrix.

Example 2. Develop the generic formula for the rotation of (x, y, z) about the axis defined by x = 0, y = 0.

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} \cos\frac{2\pi}{n} & -\sin\frac{2\pi}{n} & 0 \\ \sin\frac{2\pi}{n} & \cos\frac{2\pi}{n} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{matrix} x \\ y \\ z \end{matrix}$$

Back to Rotations and Translations

For a lattice point to have rotational symmetry, the points at the end of the rotated unit vector **r** must also be lattice points.
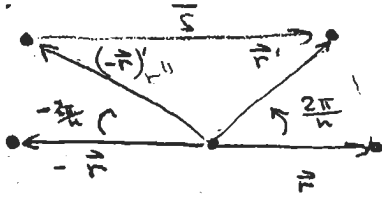

$$\mathbf{r} = \cos{(2\pi/n)}\ \mathbf{i} + \sin{(2\pi/n)}\ \mathbf{j}$$

For a rotation through $2\pi/n$, there must also exist a rotation through $-2\pi/n$. This rotation vector is **r'**.

r' = -cos $(2\pi/n)$ **i** + sin $(2\pi/n)$ **j**

The difference between **r** and **r'** represents a translation vector **s** between lattice points.

s = **r** – **r'** = [cos $(2\pi/n)$ **i** + sin $(2\pi/n)$ **j**] – [-cos $(2\pi/n)$ **i** + sin $(2\pi/n)$ **j**] = 2 cos $(2\pi/n)$ **i**

The magnitude of **s** must be an integral number of lattice translations for a motif with n-fold rotational symmetry to fit into the lattice.
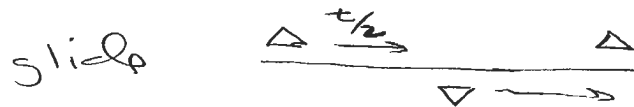
|**s**| = m |**r**|

|**s**| = m [2 cos $(2\pi/n)$]

Evaluate possible rotational symmetries:

n	2 cos $(2\pi/n)$	Ok?
1	2	Yes
2	-2	Yes
3	-1	Yes
4	0	Yes
5	0.6	No
6	1	Yes
7	1.25	No

Glide Reflection

Translation combines with reflection to form the operation depicted below. The element is a glide plane.

Overlaying point operations like rotation, reflection, and glide reflection on the five distinct plane lattices yields 17 plane groups. These plane groups express all the symmetry combinations possible in a plane.

p1

pm

pg

cm

p2

p2mm

p2mg

p2gg

c2mm

p3

p3m1

p31m

p4

p4mm

p4gm

p6

p6mm

(Adapted from Klein and Hurlbut, Jr. <u>Manual of Mineralogy</u>. New York: John Wiley and Sons, Inc., 1993.)