PHYSICS OF CRYSTALS

Chapter 3

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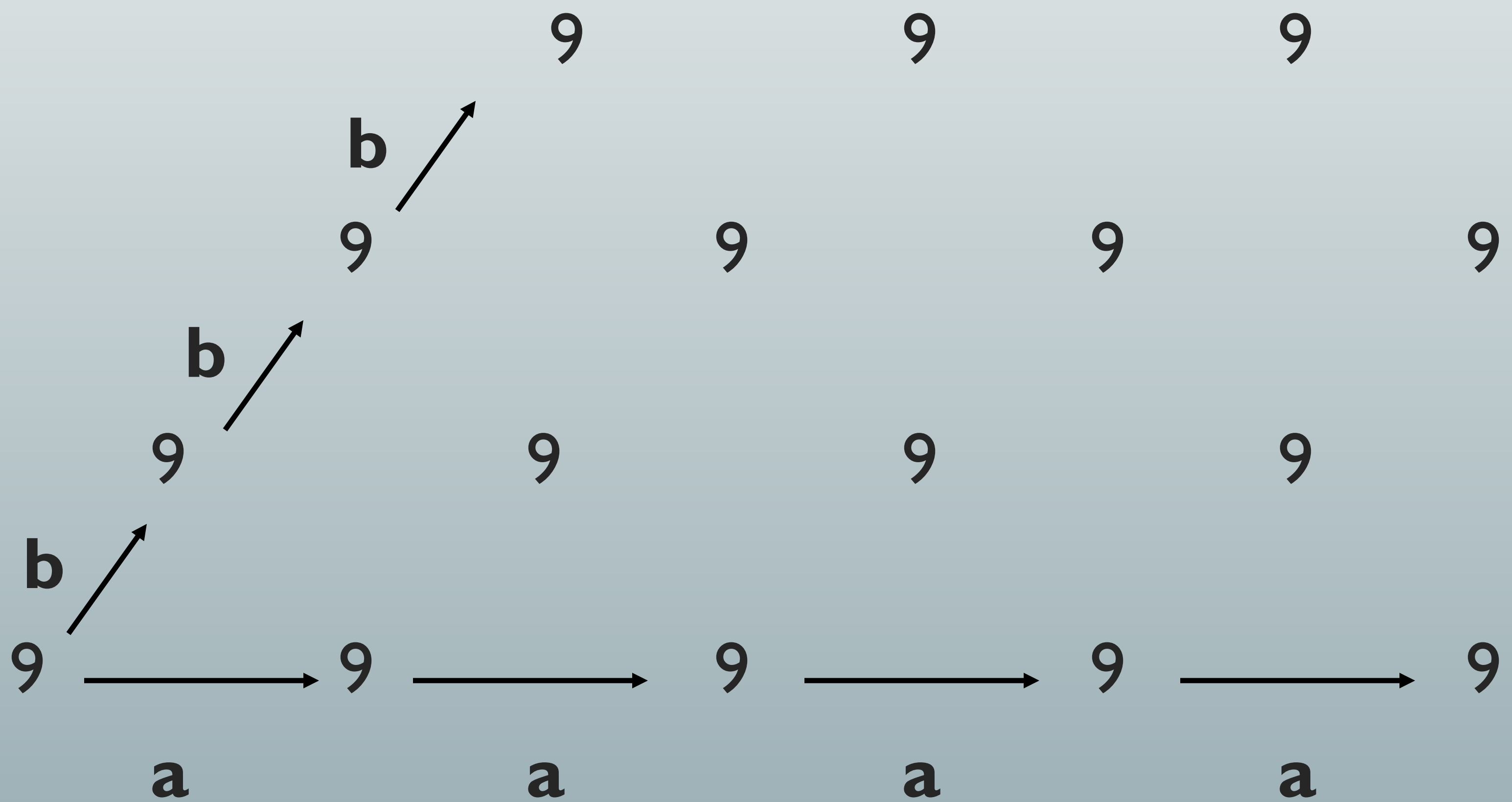
A) TRANSLATION

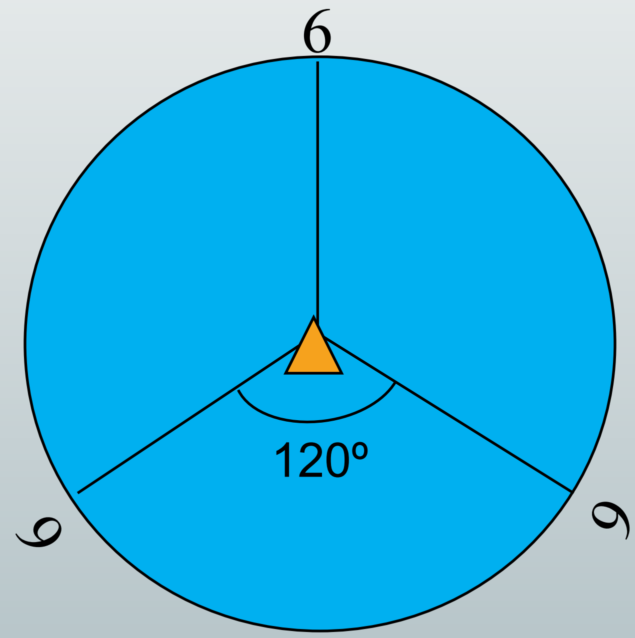
- Öteleme işlemi ile ‘9’ şeklinin düzlemi doldurmasını görüyoruz.

Bu işlem sonucunda katı maddeyi oluşturan moleküllerin biçimleri yani moleküldeki atomları birbirine bağlayan vektör uzunlukları ve bu bağlar arasındaki açı değişmez.



B)ROTATION

- Symmetries of a shape are obtained by rotating a shape around an axis by an angle α. Angle α cannot take every value. If n is an integer, it must obey the relation n.α = 360 °.



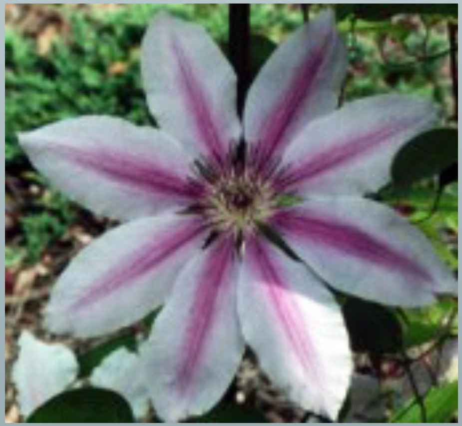
n	1	2	3	4	6
α	360°	180°	120°	90°	60°

In crystals, the symmetry axes (rotation axes) can only be ***two-fold*** (**2**), ***three-fold*** (**3**), ***four-fold*** (**4**) or ***six-fold*** (**6**), depending on the number of times (***order of rotation***) that a motif can be repeated by a rotation operation, being transformed into a new state indistinguishable from its starting state. Thus, a rotation axis of order **3** (3-fold) produces **3** repetitions (copies) of the motif, one every 120 degrees (= 360/**3**) of rotation.
Improper rotations (rotations followed by reflection through a plane perpendicular to the rotational axis) are designated by the order of rotation, with a bar above the number.

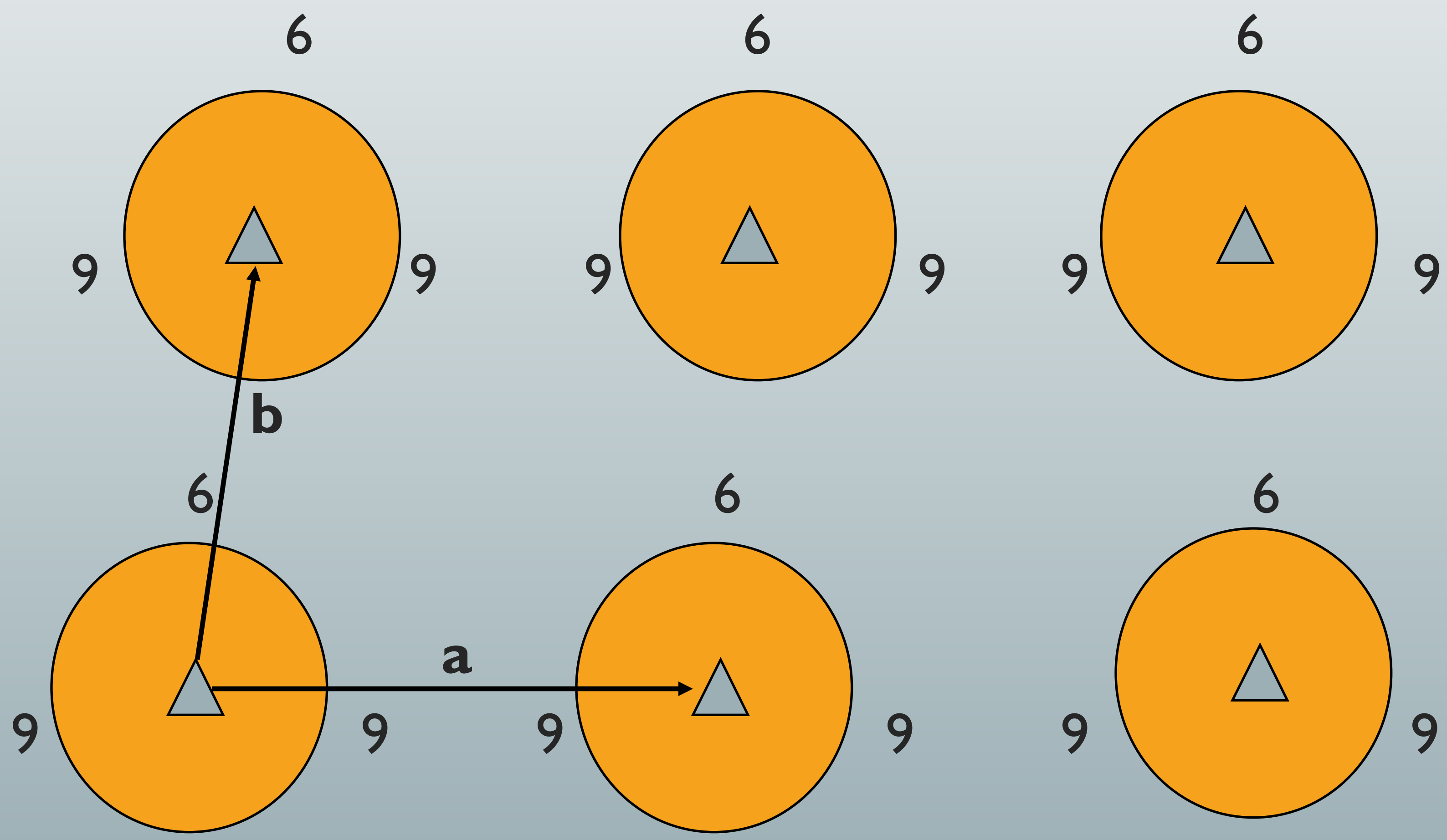
The ***screw axes*** (or helicoidal axes, ie, symmetry axes involving rotation followed by a translation along the axis) are represented by the order of rotation, with an added subindex that quantifies the translation along the axis. Thus, a screw axis of type $\mathbf{6_2}$ means that in each of the 6 rotations an associated translation occurs of **2/6** of the axis of the elementary cell in that direction.

The ***mirror planes*** are represented by the letter **m**.

The ***glide planes*** (mirror planes involving reflexion and a translation parallel to the plane) are represented by the letters **a**, **b**, **c**, **n** or **d**, depending if the translation associated with the reflection is parallel to the reticular translations (***a**, **b**, **c***), parallel to the diagonal of a reticular plane (**n**), or parallel to a diagonal of the unit cell (**d**).

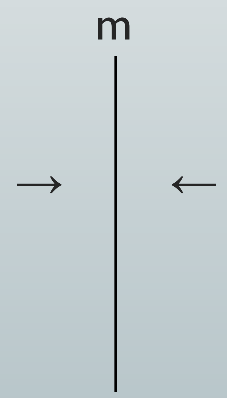


- The figure below shows three molecules connected by triple rotations filling the space by applying t1 and t2 translations to the center of rotation.



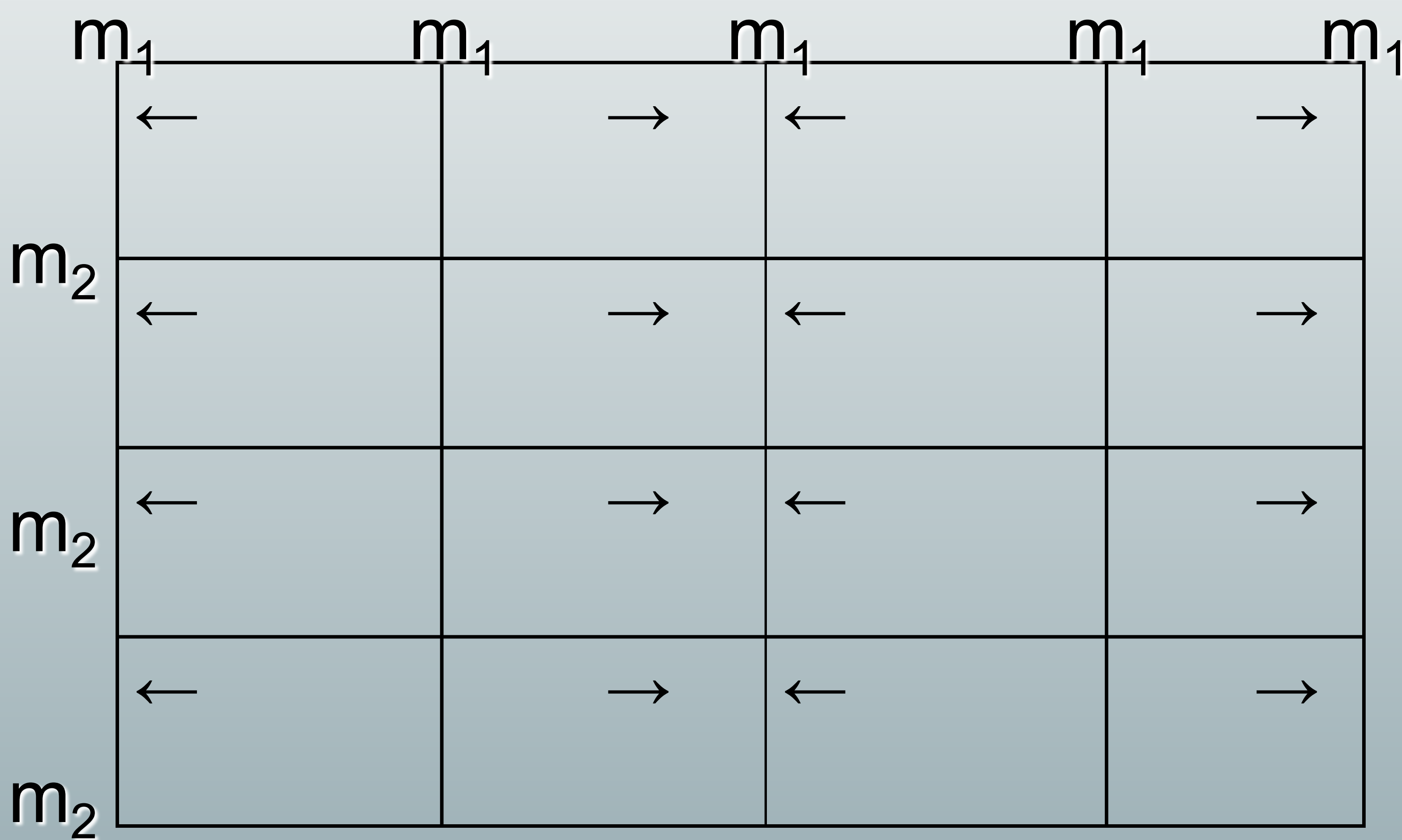
C) REFLECTION

- It is the process of taking symmetry with respect to an m plane. The crystal can have one, two or three planes of symmetry.



refletion from m

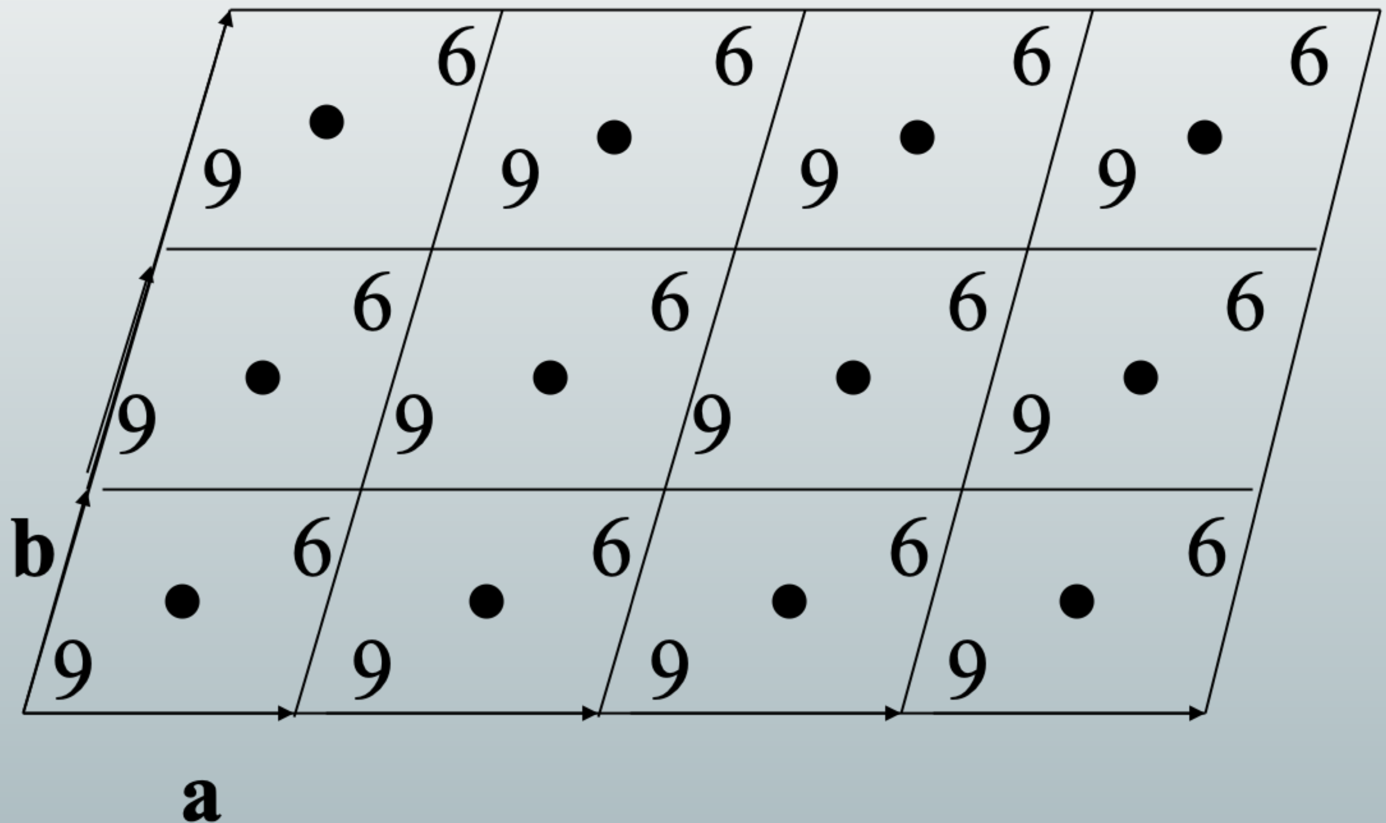
REPEATED REFLECTIONS



D) SYMMETRY CENTER

- The center of symmetry is indicated by i, c or E.
- If molecules are connected to each other by a center of symmetry, the surfaces of a perfectly grown macrocrystal are also connected to each other by a center of symmetry.

9 • 6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b
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9
a

- Translation + rotation compound motion is called Screw axis
- The translation + reflection plane is called the shear plane.
- We will see the compound symmetry elements in space groups later.

BASE AND UNIT CELL

- Crystal is formed by the periodic repetition of structural units in three dimensions. The structural unit consists of four atoms in the copper crystal and four pairs of atoms in the salt crystal (formed by symmetry bonding of Na and Cl atoms). In organic substances, the structural unit can contain hundreds of atoms. This content is called a base.
- The base can be a single atom or molecule, as well as 2, 3, 4, 6, 8, etc. connected by symmetry elements. It can also consist of a large number of molecules.

- The crystal is formed by repeating these bases in large numbers with the help of vectors a, b and c. Vectors a, b and c starting at a point form a parallelepiped. This parallelepiped is called a unit cell.
- Unit cell edges start from 2Å to 100Å and higher values.

SOME CUBICALLY CRYSTALLİZED SUBSTANCES, SİDE LENGTHS A

Demir (Fe)	2.86Å
Lityumoksit (LiO)	4.61Å
Manganez (Mn)	8.89Å
Heksaaminobenzen ($C_6H_{12}N_6$)	15.14Å

- Makroskopik bir kristalde birim hücre sayısı büyüktür.

  Örnek: 0.2 x 0.3 x 0.5 mm boyutlu bir kristalin birim hücre boyutları ortalama 10Å

  ise ;

$$N = \frac{0.02\ cm \times 0.03\ cm \times 0.05\ cm}{(10.10^{-8} cm)^3} = 3.10^{16}$$

  Adet birim hücre vardır. Yani kristalin üç doğrultusunda birim hücre 200.000, 300.000 ve 500.000 kere tekrarlanmıştır.

right and left figures

- Right (congruent) shapes to shapes that can overlap with rotation and translation; Shapes that can overlap with reflection and point symmetry are also called left (enantiomorphic) shapes.
- $\rightarrow$ ile $\leftarrow$ left şekil,

  6 ile 9 right şekillerdir.