CRYSTALLOGRAPHY

UNIT II

SYLLABUS

Cubic System: Symmetry elements - forms and representative mineral of the normal, pyritohedral, tetrahedral and plagiohedral classes. Tetragonal system: Symmetry element and forms of normal, hemimorphic, tripyramidal, pyramidal hemimorphic, sphenoidal and trapezohedral classes.

Cubic sysytem

All those crystals that can be referred to three crystallographic axes, which are- (i) essentially equal in length, (ii) at right angles to each other, and (iii) mutually interchangeable, are said to belong to the isomeric or cubic system.

Axial Diagram:

Since all the three axes are equal and interchangeable, these are represented by the letter a. In the study position, however, the axes may be designated as a1, a2 and a3 the last being vertical. (Fig. 10.16.)

In crystallography, the cubic (or isometric) crystal system is a crystal system where the unit cell is in the shape of a cube. This is one of the most common and simplest shapes found in crystals and minerals.There are three main varieties of these crystals:

Primitive cubic (abbreviated cP and alternatively called simple cubic)

Body-centered cubic (abbreviated cI or bcc)

Face-centered cubic (abbreviated cF or fcc, and alternatively called cubic close-packed or ccp)

Each is subdivided into other variants listed below. Note that although the unit cell in these crystals is conventionally taken to be a cube, the primitive unit cell often is not.

Bravais lattices

The three Bravais lattices in the cubic crystal system are:

The primitive cubic system (cP) consists of one lattice point on each corner of the cube. Each atom at a lattice point is then shared equally between eight adjacent cubes, and the unit cell therefore contains in total one atom (1⁄8 × 8).[1]

The body-centered cubic system (cI) has one lattice point in the center of the unit cell in addition to the eight corner points. It has a net total of 2 lattice points per unit cell (1⁄8 × 8 + 1).[1]

The face-centered cubic system (cF) has lattice points on the faces of the cube, that each gives exactly one half contribution, in addition to the corner lattice points, giving a total of 4 lattice points per unit cell (1⁄8 × 8 from the corners plus 1⁄2 × 6 from the faces). Each sphere in a cF lattice has coordination number 12. Coordination number is the number of nearest neighbours of a central atom in the structure.[1]

The face-centered cubic system is closely related to the hexagonal close packed (hcp) system, where two systems differ only in the relative placements of their hexagonal layers. The [111] plane of a face-centered cubic system is a hexagonal grid.

<u>symmetry elements</u>

(a) Axes of Symmetry:

13 in all.

3 are axes of four-fold symmetry;

4 are axes of three-fold symmetry;

6 are axes of two-fold symmetry.

The three axes of four-fold symmetry are chosen as the crystallographic axes.

(b) Planes of Symmetry:

9 in all.

3 planes of symmetry are at right angles to each other and are termed the principal (axial) planes;

6 planes of symmetry are diagonal in position and bisect the angles between the principal planes.

(c) It has a Centre of symmetry.

Forms

Normal class (galena type)

Following are the forms that commonly develop in the crystals belonging to Isometric System:

i. Cube:

A form bounded by six similar square faces, each of which is parallel to two of three crystallographic axes and meets the third axis. Symbol (100). Fig. 10.17A.

ii. Octahedron:

A form bounded by eight similar faces, each of the shape of an equilateral triangle, each meeting the three crystallographic axes at equal distances. Symbol- (111), Fig. 10.17B.

iii. Dodecahedron:

It is a form with twelve similar faces each of which is parallel to one of the three crystallographic axes and meets the other two at equal distances. (Fig. 10.17 C), Symbol (101)

iv. Trisoctahedron (hhl):

A form of twenty four (24) faces; each face meeting two axes at unit length and to the third at greater than unity. Faces occur in eight groups of three each.

v. Trapezohedron (hll):

A form of twenty four (24) faces each face meeting one axes at unit length and to the other two at greater than unity. Each face is a trapezium.

vi. Tetra-Hexahedron (hol):

Twenty four (24) faces; each face is parallel to one axis and meets other two at unequal distance which are simple multiple of each other; faces occur in six groups of four each.

vii. Hexaocatahedron (hkl):

Forty eight (48) faces; each face meets the three axis at unequal distances.

Pyritohedral class

A. Pyritohedral Class (Pyrite Type):

(a) Symmetry:

7 Axes of symmetry, of which, 3 are axial axes of two-fold symmetry, 4 are diagonal axes of two fold symmetry. 3 Planes of symmetry. A Centre of symmetry.

(b) Forms:

Pyritohedron and Diploid are two typical forms of this symmetry class. Pyritohedron is a hemihedral form having twelve faces and a general symbol (hko) Fig. 10.18 A.

Diploid is a closed form of twenty-four faces that typically occur in pairs (hence the name) and have a symbol (hki)

Tetrahedral Class (Tetrahedrite Type):

(a) Symmetry:

7 axes of symmetry (as in pyrite type), 6 planes of symmetry, diagonal, no center of symmetry.

(b) Forms:

Most typical form of this class is a four sided solid in which each face is an equilateral triangle. It is termed tetrahedron. It has a general symbol of (111). .

C. Plagiohedral Class (Cuprite Type):

(a) Symmetry:

13 axes of symmetry (as in normal class) No planes of symmetry. No Centre of symmetry.

(b) Forms:

Icositedraherons, each of 24 faces, with a symbol (hkl) and commonly enantiomorphous in character are typical forms of this class.

Examples of Isometric Minerals:

A vast number of common minerals crystallize in isometric system.

Following are few mineral examples:

i. Galena

ii. Pyrite

iii. Sphalerite

iv. Spinel

v. Magnetite

vi. Sodalite

vii. Garnet

<u>2. Tetragonal System:</u>

Definition:

The tetragonal system includes all those crystals which can be referred to three crystallographic axes so that:

(i) Two axes are equal, interchangeable and horizontal in position;

(ii) The third axis is either longer or shorter than the other two and is vertical in position; and

(iii) All the three axes are mutually at right angles to each other.

Axial Diagram:

In study position, the crystal is so held that the longer or shorter axis is vertical in position. The one of the horizontal axes is made to run parallel to the observer and the other form front backward. (Fig. 10.20.)

The horizontal axis running away from the observer is designated as a1, that running from right to left is a2, and the vertical axis is designated as c axis.

Axial ratio for the crystal of this system is expressed as a: c.

Classes:

The Tetragonal system includes seven symmetry classes.

Normal Class (Zircon Type):

The symmetry of the normal class (Zircon type) is as follows:

(a) Axis of Symmetry:

5 in all; of these, 2 axes are horizontal and of two fold symmetry, 2 axes are horizontal bisecting the angles made by first set of horizontal axis; they are also of two fold symmetry. 1 axis is vertical and of four folds symmetry (hence tetragonal forms).

(b) Planes of symmetry:

5 in all; of these, 1 plane is horizontal, 2 planes are vertical, 2 planes are vertical diagonal. There is a centre of symmetry.

Forms:

Following forms are met with in the crystals of the Tetragonal System:

a. Basal Pinacoid (001):

An open form with two similar faces. Each face is parallel to the two horizontal crystallographic axes and meets the third, vertical axis at unit length. (Fig. 10.21 A)

b. Prisms:

These are open forms of four or eight faces in which each face is essentially parallel to the vertical crystallographic axes.

Depending on their relation with the other two axes, three types of prisms are recognized in the tetragonal system:

(i) Prism of First Order (110):

Four faces each face meeting the two horizontal axes – at unit lengths and being parallel to the vertical axis (Fig. 10.21B);

(ii) Prism of Second Order (100):

Four faces; each face intercepts only one of the horizontal axes and is parallel to the second axis besides being parallel to the vertical axis (Fig. 10.21 B-100).

(iii) Prism of Third Order or Ditetragonal Prism (hko):

Eight faces each face intercepting the two horizontal axes at different lengths; e.g. 210, 310.

c. Pyramids:

These are closed forms of eight or sixteen faces in which each face essentially meets the vertical crystallographic axis.

Three types of pyramids are recognized on the basis of their relationship with other crystallographic axis:

(i) Pyramid of First Order (hhl):

Eight faces; each face cuts the two horizontal axis at equal length besides intersecting the vertical axis. Example- (221), (223), (111) (Fig. 10.21C)

(ii) Pyramid of Second Order (hol):

Eight faces; each face cuts only one of the two horizontal axes; it is parallel with one horizontal crystallographic axis, Example- (201), (101). (Fig. 10.21D)

(iii) Pyramid of Third Order (hkl):

Also called ditetragonal pyramid is a closed form of 16 faces in which each face cuts all the three crystallographic axes at unequal lengths. Example- (321), (421).

HEMIMORPHIC FORM: It is also derived from a holohedral form and has only half the number of faces as in hemihedral form. In this case, all the faces of the form are developed only on one extremity of the crystal , being absent from the other extremity . In other words , such a crystal will not be symmetrical with reference to centre of symmetry. So, hemimorphism is the property wherein the two ends of a crystallographic axis are not related by symmetry ; thus , the faces that terminate the axis on opposing ends are not symmetrically equivalent . One of the minerals that best exemplifies hemimorphism in its morphology is tourmaline. By virtue of the lack of a centre of symmetry, all hemimorphic crystals also exhibit the property of piezoelectricity. Ultimately , it is the atomic arrangement of the crystals that dictates it is hemimorphic or not. Of the 32 classes, 9 are hemimorphic. In these the two ends of crystallographic axis are not equivalent by symmetry. This requires the absence of the following symmetry elements: a centre of symmetry, a mirror plane oriented perpendicular to the unique crystallographic axis, and a two fold axis of rotation oriented perpendicular to unique crystallographic axis.

<u>TRIPYRAMIDAL CLASS </u>(Scheelite type) Symmetry 1 vertical axis is an axis of 4 fold symmetry One horizontal plane of symmetry Centre of symmetry present Forms The distinctive forms of this class are 1. Tetragonal prism of third order (4faces (hko)) 2. Tetragonal pyramid of third order (8 faces (hkl)) 1. Prism of third order This itself is a square prism identical in appearance to the prism of 1st and 2nd order, represented by 4 faces, each meeting 2 horizontal axis at different length and being parallel to the c axis. Hence general symbol is (hko). The form is considered to be derived from the ditetragonal prism by the development of half of its faces. Hence these are two complimentary forms designated as left and right handed which together account for all the faces of the ditetragonal prism of the normal class. 2. Pyramid of third order It is a square pyramid bounded by 8 similar faces each a triangle. It is similar in appearance to the pyramid of 1st order and 2nd order. Each face meets the 3 crystallographic axes at unequal distances giving the general index (hkl). The form may be considered to be derived from the ditetragonal pyramid by the development of half of its faces. Hence there will be 2 complimentary forms- right and left handed whose faces together will account for the faces of the holohedral form. Other forms of this class- base(001), prism 1st order & 2nd order, p y r a m i

<u>SPHENOIDAL CLASS </u>(Aka chalcopyrite type symmetry) Two vertical diagonal plane of symmetry Three crystallographic axis of two fold symmetry FORMS The typical forms present in this class of the system are sphenoid and tetragonal scalenohedron 1.Sphenoid It is a four faced solid resembling a tetrahedron but each face is isosceles triangle. . It may be considered as derived from the first order pyramid of the normal class by the development of only the alternate faces of the latter. There are therefore possible two complementary forms known as the positive and negative sphenoid .The general symbol of the positive unit sphenoid is (111) and its faces have the indices: 111, 1ത1ത1, 1ത11ത, 11ത1ത. Negative sphenoid has the number (11ത1). Sphenoid 2.Tetragonal scalenohedron It is bounded by eight similar faces, each face is scalene triangle, hence it is called tetragonal scalenohedron The general symbol is (hkl) It may be considered as derived from the ditetragonal pyramid of the normal class by taking the alternate pairs of faces of latter form.

<u>TRAPEZOHEDRAL CLASS SYMMETRY ELEMENTS : </u>AXIS OF SYMMETRY - 4 AXIS OF 2-FOLD SYMMETRY , 1 AXIS OF 4-FOLD SYMMETRY PLANE OF SYMMETRY - ABSENT CENTRE OF SYMMETRY - ABSENT FORMS: The trapezohedral class is analogous to the plagiohedral class of the isometric system, it is characterized by the absence of

any plane or centre of symmetry Vertical axis is an axis of tetragonal symmetry and perpendicular to this there are four axes of binary symmetry GENERAL FORM – (hkl)

28. There are two complementary forms called right and left handed which embraces all the faces of the ditetragonal pyramidof the normal class

Examples of Tetragonal Minerals:

i. Zircon

ii. Vesuvianite

iii. Rutile

iv. Wernerite

v. Cassiterite

vi. Octahedrite

vii. Chalcopyrite

viii. Scheelite

ix. Wulfenite

x. Braunite.

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