MATERIAL SC. (MM1101) ASSIGNMENT

GIVEN BY :-

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BRAVIAS LATTICE , LATTICE DIRECTIONS AND PLANES

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Bravais Lattice refers to the 14 different 3-dimensional configurations into which atoms can be arranged in crystals. The smallest group of symmetrically aligned atoms which can be repeated in an array to make up the entire crystal is called a unit cell. There are several ways to describe a **lattice**.

In geometry and crystallography, a **Bravais lattice**, named after Auguste Bravais (1850),[1] is an infinite array of discrete points generated by a set of discrete translation operations described in three dimensional space by:

$$(1)$$

where the n_i are any integers and $\mathbf{a}_i$ are *primitive vectors* which lie in different directions (not necessarily mutually perpendicular) and span the lattice. The choice of primitive vectors for a given Bravais lattice is not unique. A fundamental aspect of any Bravais lattice is that, for any choice of direction, the lattice will appear exactly the same from each of the discrete lattice points when looking in that chosen direction.

In crystallography, the Bravais lattice concept of an infinite array of discrete points is expanded using the concept of a **unit cell** which includes the space in between the discrete lattice points as well as any atoms in that space. There are two main types of unit cells: primitive unit cells and non-primitive unit cells.

A primitive unit cell for a given Bravais lattice can be chosen in more than one way (each way having a different shape), but each way will have the same volume and each way will have the property that a one-to-one correspondence can be established between the primitive unit cells and the discrete lattice points. The obvious primitive cell to associate with a particular choice of primitive vectors is the parallelepiped formed by them.[2] That is, the set of all points **r** of the form:

$$(2)$$

Using the parallelepiped defined by the primitive vectors as the unit cell has the disadvantage in some cases of not clearly revealing the full symmetry of the lattice. One solution to this is to use the Wigner-Seitz primitive cell (consisting of all points in space that are closer to the given lattice point then to any other lattice point) which does display the full symmetry of the lattice. Another solution is to use a **non-primitive unit cell** which does display the full symmetry of the lattice. The non-primitive unit cell volume will be an integer multiple of the primitive unit cell volume.

The unit cell, whether primitive or not, when replicated once for each discrete lattice point, must exactly fill the entire space with no overlap and no gaps.

The expanded Bravais lattice concept, including the unit cell, is used to formally define a *crystalline arrangement* and its (finite) frontiers. A crystal is made up of a periodic arrangement of one or more atoms (the *basis* or *motif*) occurring exactly once in each primitive unit cell. The *basis* may consist of atoms, molecules, or polymer strings of solid matter. Consequently, the crystal looks the same when viewed in any given direction from any equivalent points in two different unit cells (two points in two different unit cells of the same lattice are equivalent if they have the same relative position with respect to their individual unit cell boundaries).

Two Bravais lattices are often considered equivalent if they have isomorphic symmetry groups. In this sense, there are 14 possible Bravais lattices in three-dimensional space. The 14 possible symmetry groups of Bravais lattices are 14 of the 230 space groups. In the context of the space group classification, the Bravais lattices are also called Bravais classes, Bravais arithmetic classes, or Bravais flocks.[3]

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and 5 – square (tetragonal).

In two-dimensional space, there are 5 Bravais lattices,[4] grouped into four crystal families.

Crystal family	Point group (Schönflies notation)	5 Bravais lattices	
		Primitive	Centered
Monoclinic	C_2	Oblique	
Orthorhombic	D_2	Rectangular	Centered rectangular
Hexagonal	D_6	Hexagonal	
Tetragonal	D_4	Square	

The unit cells are specified according to the relative lengths of the cell edges (a and b) and the angle between them (θ). The area of the unit cell can be calculated by evaluating the norm $\|\mathbf{a} \times \mathbf{b}\|$, where **a** and **b** are the lattice vectors. The properties of the crystal families are given below:

Crystal family	Area	Axial distances (edge lengths)	Axial angle
Monoclinic		$a \neq b$	$\theta \neq 90°$
Orthorhombic		$a \neq b$	$\theta = 90°$
Hexagonal		$a = b$	$\theta = 120°$
Tetragonal		$a = b$	$\theta = 90°$

In 3 dimensions[edit]

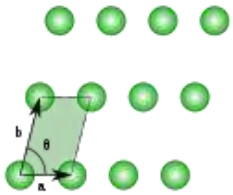
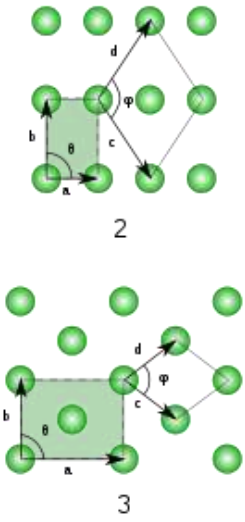
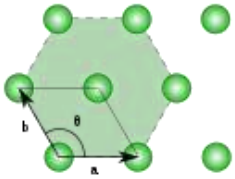
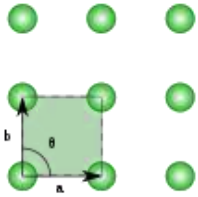
2×2×2 unit cells of a diamond cubic lattice

In three-dimensional space, there are 14 Bravais lattices. These are obtained by combining one of the seven lattice systems with one of the centering types. The centering types identify the locations of the lattice points in the unit cell as follows:

- Primitive (P): lattice points on the cell corners only (sometimes called simple)
- Base-centered (A, B, or C): lattice points on the cell corners with one additional point at the center of each face of one pair of parallel faces of the cell (sometimes called end-centered)
- Body-centered (I): lattice points on the cell corners, with one additional point at the center of the cell
- Face-centered (F): lattice points on the cell corners, with one additional point at the center of each of the faces of the cell

Not all combinations of lattice systems and centering types are needed to describe all of the possible lattices, as it can be shown that several of these are in fact equivalent to each other. For example, the monoclinic I lattice can be described by a monoclinic C lattice by different choice of crystal axes. Similarly, all A- or B-centred lattices can be described either by a C- or P-centering. This reduces the number of combinations to 14 conventional Bravais la

BRAVAIS LATTICES

 1	 2 3	 4	 5
|a| ≠ |b|, θ ≠ 90° m	|a| ≠ |b|, θ = 90° |c| = |d|, φ ≠ 90° o	|a| = |b|, θ = 120° h	|a| = |b|, θ = 90° t

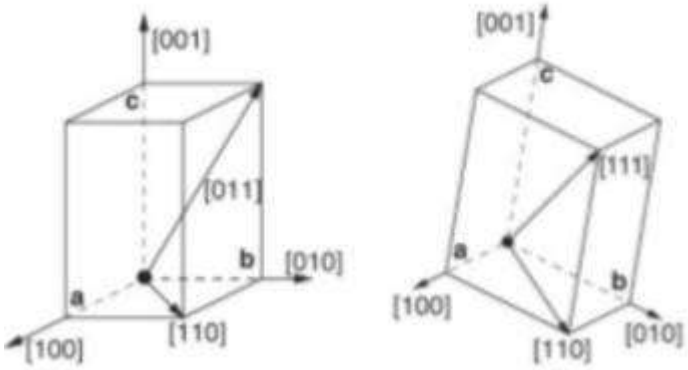
- **Lattice Directions**

Directions in a lattice is denoted by [uvw]

• E.g., [100] denotes the direction parallel to the a-axis in any lattice.

- Negative numbers are denoted with a bar above the number, e.g.,

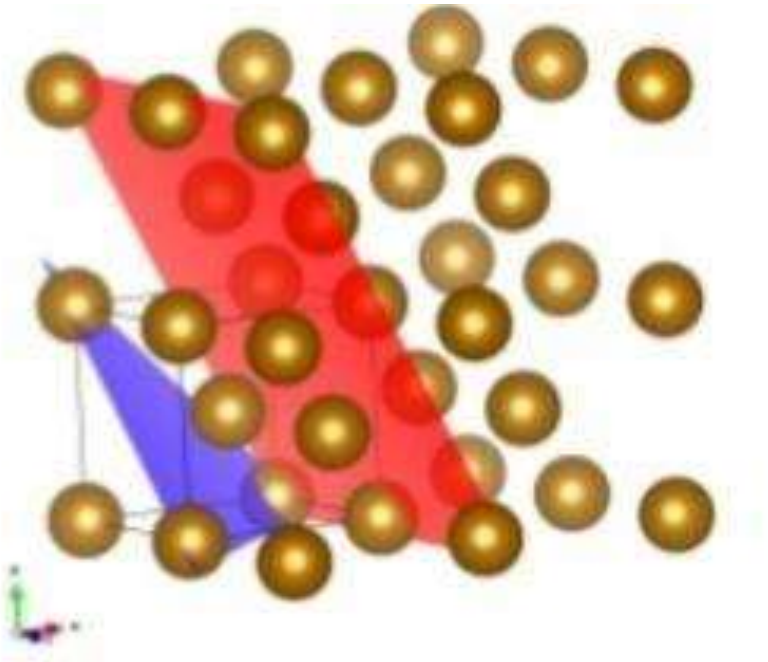
$$[1\,\bar{1}2] \equiv \mathbf{a} - \mathbf{b} + 2\mathbf{c}$$



- **Lattice Planes**

A lattice plane of a given Bravais lattice is a plane (or family of parallel planes) whose intersections with the

lattice are periodic (i.e., are described by 2d Bravais lattices) and intersect the Bravais lattice; equivalently, a lattice plane is any plane containing **at least three noncollinear Bravais lattice points**.



- **Miller indices**

· Lattice planes are represented by Miller indices, denoted as(hkl), where h, k and I are **integers**. Note the use of the **round brackets** instead of the square brackets used for

lattice directions.

• The procedure for determining the Miller indices of a plane

is best illustrated using an example.

Procedure for determining the Miller indicies

Let's say we have a plane in the lattice specified by

a band c.

1. If the plane pass through the origin, displace the

plane by an arbitrary amount so that it does not

pass through the origin (not required for worked

example).

2. Determine the intercepts of plane with three

lattice vectors, in units of the lattice vector

length. If the plane is parallel to one or more of

the axes, this corresponding number is in the

example, these are 1:2:3

3. Invert all three numbers. If the plane is paralel to

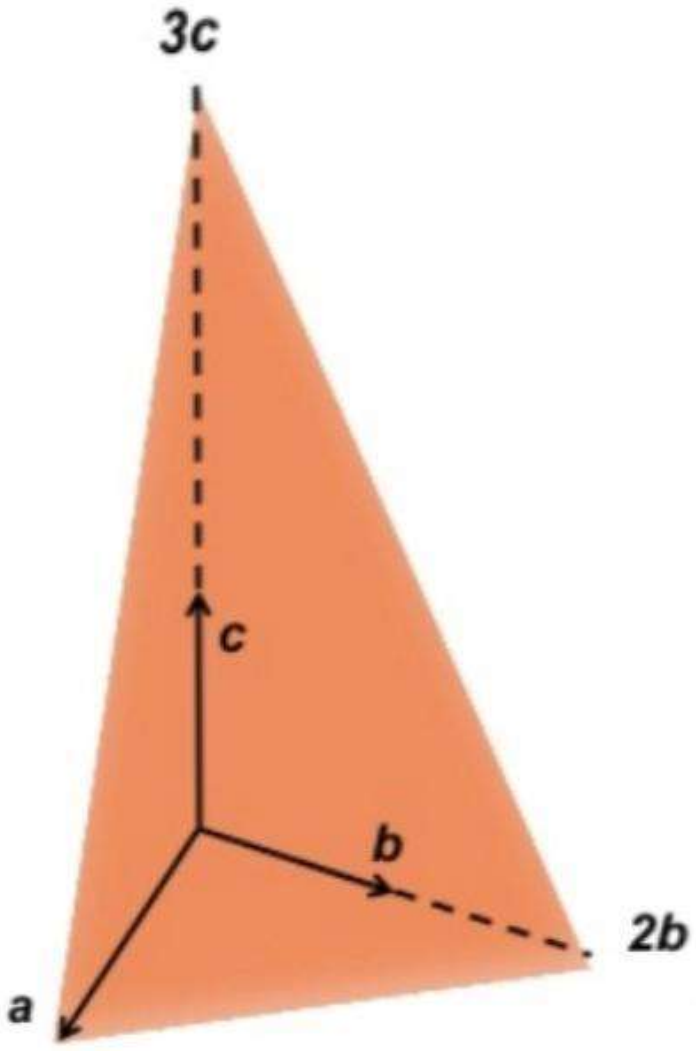
one or more of the axes, this corresponding

number is 1/6 = 0. For the example, we get

1:1/2:1/3

4. Reduce the numbers to the nearest integers

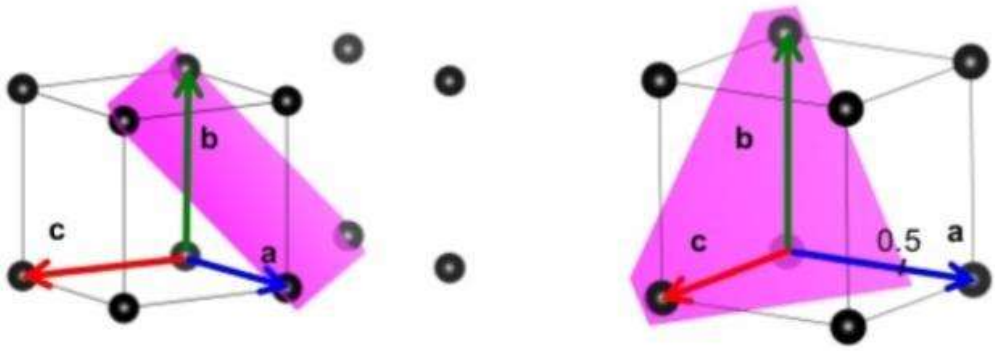
(known as the relative primes). We get (632).



- **Example**

-Determine the Miller indices of the following

Planes

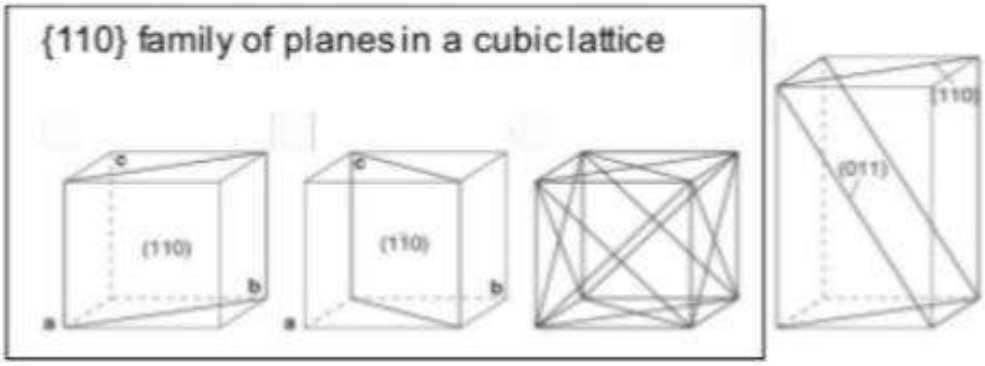


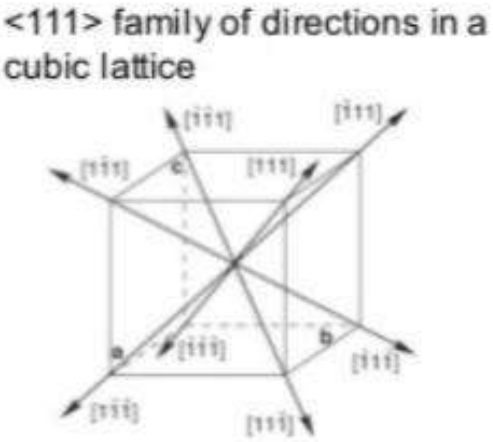
- **Families of planes or directions**

- When the lattice has symmetry (i.e., non-triclinic), certain planes are

equivalent to each other under symmetry. Such families of planes are

represented with a curly brackets, i.e. {**hkl**}.





Similarly, **families of directions** are denoted by <**uvw**>.

- **Permutations of Miller indices**

- From the cubic example, we may observe that all planes in the {110} family is given by permutations of the indices and their negatives:

$$\{110\} = \{(110),(1\bar{1}0),(\bar{1}10),(101),(\bar{1}01),(10\bar{1}),(011),(0\bar{1}1),(01\bar{1})\}$$

. For lower symmetry systems, families are still given by permutations, though not all permutations belong to the same family.

- Rhombohedral: $\{100\} = \{(100), (\bar{1}00), (010), (0\bar{1}0), (001), (00\bar{1})\}$
- Orthorhombic: $\{100\} = \{(100), (\bar{1}00)\}$

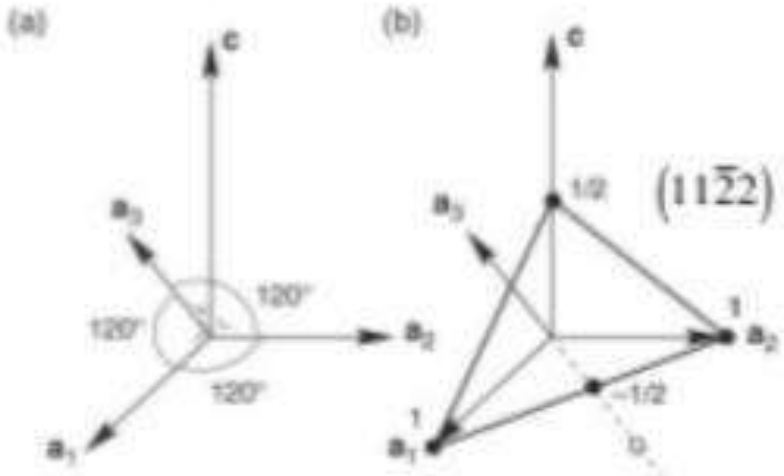
- **Miller-Bravais Indices of Hexagonal Crystal System**

- Hexagonal system is defined by four basis vectors, three of which are

co-planar.

• Miller-Bravais indices are given by intercepts with all four basis

vectors (hkil) i is a redundant index and is given by i = -(h+k)



• The four-index representation allows families of planes for hexagonal

$$\{11\bar{2}0\} = \{(11\bar{2}0),(\bar{1}2\bar{1}0),(\bar{2}110),(\bar{1}\bar{1}20),(1\bar{2}10),(2\bar{1}\bar{1}0)\}$$

systems to be represented as permutations, e.g.,

Miller-Bravais Indices for Directions in

Hexagonal System

• Denoted as ſuvtw).

. By convention, t= -(u+v), similar to indices for planes.

. It can be shown that the relationship between a three-Miller index

[u'v'w] and the corresponding four-Miller index [uvtw] is given by

(please review proof on your own accord):

u, v, t, w ➔u', v', w'

$$u' = 2u + v$$
$$v' = 2v + u$$
$$w' = w$$

u', v', w' ➔u, v, t, w

$$u = \frac{1}{3}(2u' - v')$$
$$v = \frac{1}{3}(2v' - u')$$
$$t = -(u + v)$$
$$w = w'$$

- **Examples**

-Determine the Miller indices of the following

planes.