

Lecture 5: Positions, Directions, and Planes in Crystals

Notation	Meaning	Remarks / Examples
(n_1, n_2, n_3)	Point in the lattice (coordinates)	Commas are mandatory. Example: (1, 0, 2). A bar over an index denotes a negative value, e.g., (1, 0, $\bar{2}$).
$[h\ k\ l]$	Crystallographic direction	Represents a vector direction. No commas are used. Example: $[1\ 0\ 1]$.
$\langle h\ k\ l \rangle$	Family of equivalent directions	All symmetry-equivalent directions. Example: $\langle 100 \rangle$ in cubic crystals.
$(h\ k\ l)$	Crystallographic plane (Miller indices)	Defines a plane via intercepts with the crystal axes. Example: (111).
$\{h\ k\ l\}$	Family of equivalent planes	All symmetry-related planes. Example: $\{110\}$ in cubic crystals.

1. Positions of Atoms

As discussed previously, the position of any point (or atom) inside a unit cell can be specified relative to the **origin** using a position vector:

$$\mathbf{r} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$$

where n_1 , n_2 , and n_3 are integers.

Atomic coordinates are usually expressed in terms of fractional coordinates (x, y, z).

Example-1:

1. The position of an atom at the center of a parallelepiped unit cell corresponds to:

$$\mathbf{r} = \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$$

$$(1/2, 1/2, 1/2)$$

2. The position of an atom at the center of the left face of a parallelepiped unit cell:

$$\mathbf{r} = \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3$$

$$(1/2, 0, 1/2)$$

3. The position of an atom at the center of the right face of a parallelepiped unit cell:

$$\mathbf{r} = \frac{1}{2} \mathbf{a}_1 + \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$$

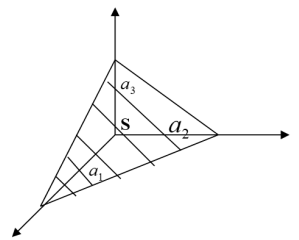
$$(1/2, 1, 1/2)$$

2. Index System of Planes (Miller Indices)

In general, any plane in a crystal can be defined by three points lying in that plane. However, a more practical and widely used method is based on Miller indices.

Procedure for determining Miller indices (hkl):

1. Determine the intercepts of the plane with the crystallographic axes **X**, **Y**, and **Z** in units of the lattice constants **a**, **b**, and **c**. Denote these intercepts by α_1 , α_2 , and α_3 .
2. Take the reciprocals of these intercepts. $1/\alpha_1$, $1/\alpha_2$, and $1/\alpha_3$.
3. Reduce the resulting numbers to the smallest set of integers by multiplying by the least common factor α . $\frac{\alpha}{\alpha_1}, \frac{\alpha}{\alpha_2}, \frac{\alpha}{\alpha_3}$
4. Enclose the integers in parentheses: $(\frac{\alpha}{\alpha_1}, \frac{\alpha}{\alpha_2}, \frac{\alpha}{\alpha_3})$ and are usually written as **(hkl)**.



These integers (hkl) are called the Miller indices of the plane.

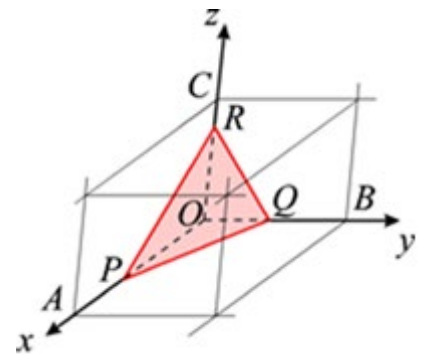
Example-2: Find the Miller indices for the plane shown in the figure.

Where:

$$OP = 3\vec{a}_1$$

$$OQ = 1\vec{a}_2$$

$$OR = \frac{1}{2}\vec{a}_3$$



Solution:

Step 1: Write the intercepts in units of lattice constants

Intercept along a_1 -axis = 3

Intercept along a_2 -axis = 1

Intercept along a_3 -axis = 1/2

Step 2: Take the reciprocals of the intercepts

$$1/3 = 1/3$$

$$1/1 = 1$$

$$1/(1/2) = 2$$

Step 3: Clear fractions to obtain the smallest integers

Multiply all reciprocals by 3:

$$(1/3, 1, 2) \times 3 = (1, 3, 6)$$

Final Answer

The Miller indices of the plane are:

(1 3 6)

Note: Miller indices are written without commas and represent a family of parallel planes.

Special Cases

Zero index:

If a plane is parallel to one of the crystallographic axes, its intercept with that axis is infinite, and the corresponding Miller index is zero.

$$\alpha_1 = 1$$

$$\alpha_2 = \infty$$

$$\alpha_3 = \infty$$

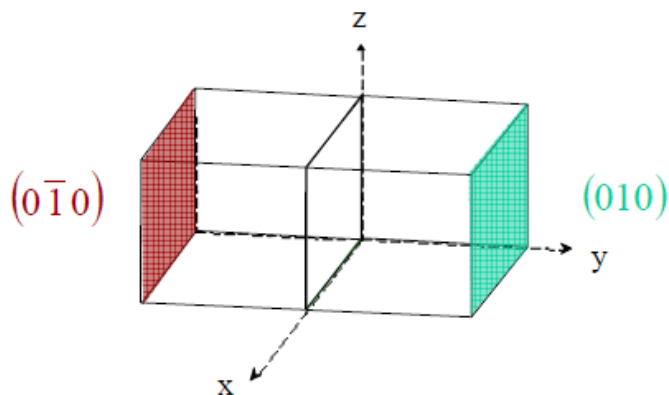
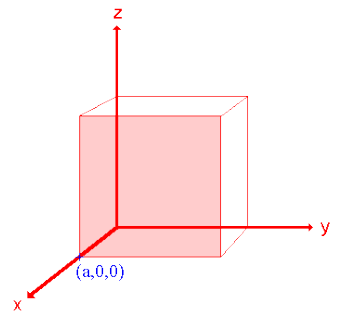
Then, by taking the reciprocal of these numbers, we get:

$$1 \ 0 \ 0$$

That gives us the Miller indices as (1 0 0)

Negative index:

If a plane cuts an axis in the negative direction, the corresponding Miller index is negative and is indicated by a bar over the index.



- ✓ **Question: If the Miller indices are given, is it possible to determine the intercepts of the plane with the crystallographic axes, denoted by a_1 , a_2 , and a_3 ?**

As we learned previously, knowing the intercepts a_1 , a_2 , and a_3 uniquely determines the Miller indices (hkl) of a plane. However, knowing the Miller indices (hkl) does not uniquely determine the intercepts a_1 , a_2 , and a_3 .

Proof:

Since the Miller indices are defined as:

$$h = a / a_1, \quad k = b / a_2, \quad l = c / a_3$$

The intercepts a_1 , a_2 , and a_3 are not uniquely determined because the lattice constants a, b, and c (or an overall scaling factor) may not be known.

Therefore, it is not possible to uniquely determine a_1 , a_2 , and a_3 from the Miller indices (hkl) alone.

A set of symmetry-equivalent planes is denoted, for brevity, by the notation {hkl}. In a cubic crystal, the family {hkl} includes all planes that are equivalent by symmetry.

For example, the family {100} includes all faces of the cube: $(\bar{1}00)$, $(0\bar{1}0)$, $(00\bar{1})$, (100) , (010) , (001) which all have the same Miller indices arranged in different orders.

Exercise-1

For a cubic crystal, consider the plane (210).

- Write the notation for the family of planes equivalent to (210).
- List all the Miller indices of the planes belonging to this family.

3. Directions in Crystals

Directions in crystals are usually specified by two points. We will now explain how to determine the direction of any line in a crystal.

Suppose we want to determine the direction of a given line OA.

$$O\vec{A} = \beta_1 \vec{a}_1 + \beta_2 \vec{a}_2 + \beta_3 \vec{a}_3$$

Multiply by the smallest common factor β so that all components $\beta\beta_1$ $\beta\beta_2$ $\beta\beta_3$ become integers γ_1 γ_2 γ_3 .

We then place these integers inside **square brackets** $[\gamma_1 \ \gamma_2 \ \gamma_3]$. These integers are called the **direction indices**.

Example-3:

In a crystal, suppose a line is given by:

$$O\vec{A} = \vec{a}_1 - \frac{1}{3}\vec{a}_2 + \vec{a}_3$$

Try to determine the direction indices of this line.

Solution

Step 1: Identify the direction ratios

The direction of the line is determined by the coefficients of the lattice vectors:

$$(1, -1/3, 1)$$

Step 2: Clear fractions

To obtain integer direction indices, multiply all components by 3:

$$(3, -1, 3)$$

Step 3: Write the direction indices

Direction indices are written using square brackets. Negative indices are denoted with a bar.

Thus, the direction indices of the line are:

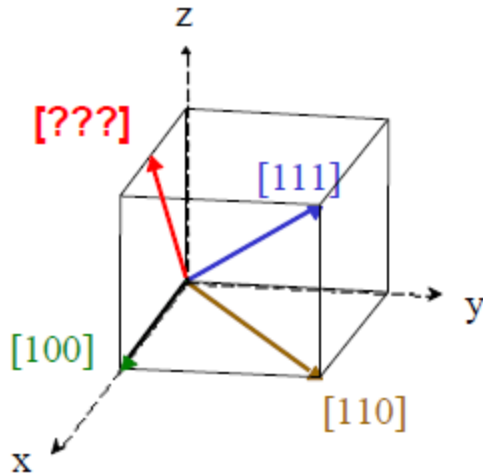
$$[3\bar{1}3]$$

Note: Square brackets denote directions, and a bar over a number indicates a negative value.

Example-4:

The following figure shows the vectors $[111]$, $[110]$, and $[100]$.

However, **what are the direction indices of the vector shown in red?**



✚ A family of symmetry-equivalent directions is denoted by $\langle uvw \rangle$.

For example:

- The family $\langle 100 \rangle$ includes the directions: $[100]$, $[010]$, and $[001]$.
- The family $\langle 110 \rangle$ includes the directions:

$[110]$, $[101]$, $[011]$, $[\bar{1}10]$, $[1\bar{1}0]$, $[\bar{1}\bar{1}0]$, $[\bar{1}01]$, $[0\bar{1}1]$, $[01\bar{1}]$, $[\bar{1}0\bar{1}]$, $[10\bar{1}]$

All these directions have two nonzero components of equal magnitude and one zero component, and they are related to each other by the symmetry operations of the cubic lattice.

The notation $\langle uvw \rangle$ is used to represent a family of crystallographically equivalent directions.

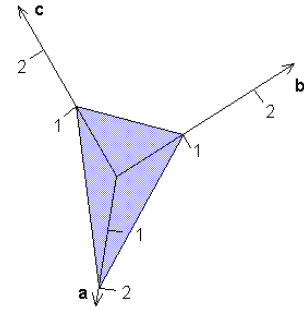
Many physical properties depend on **direction and plane orientation**:

Examples:

- **X-ray diffraction** → diffraction peaks labeled by (hkl)
- **Slip systems** → dislocation motion along $\langle uvw \rangle$ on (hkl)
- **Surface science** → surface energy depends on (hkl)
- **Band structure** → properties differ along $[100]$ vs $[111]$

Exercise 1

Determine the Miller indices of the plane shown in the adjacent figure.



Solution

Step 1: Determine the intercepts

From the figure, the plane intercepts the crystallographic axes at:

a-axis: $2a$

b-axis: $1b$

c-axis: $1c$

Thus, the intercepts in units of the lattice constants are:

$(2, 1, 1)$

Step 2: Take the reciprocals of the intercepts

$(1/2, 1, 1)$

Step 3: Clear fractions

Multiplying all components by 2 gives:

$(1, 2, 2)$

Final Answer

The Miller indices of the plane are:

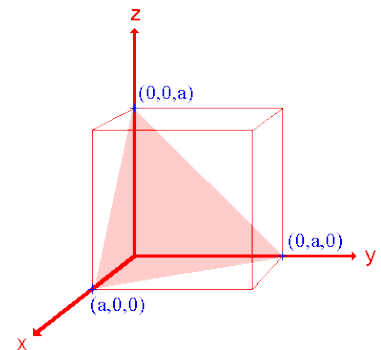
$(1\ 2\ 2)$

More examples:

Intercepts: a, a, a

Fractional intercepts: $1, 1, 1$

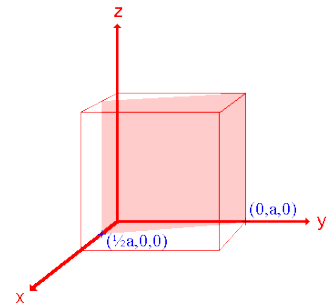
Miller Indices: (111)



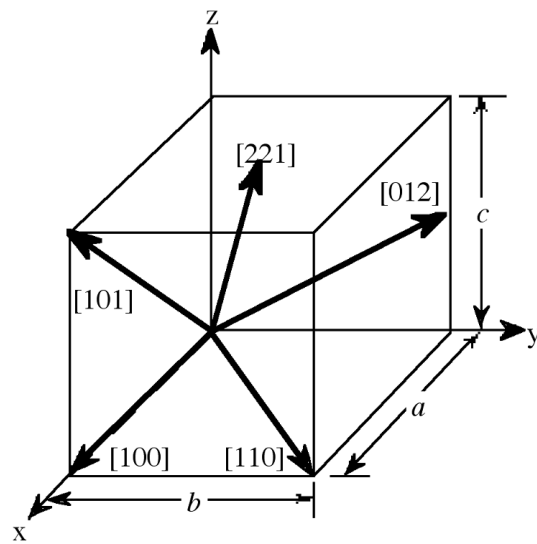
Intercepts: $\frac{1}{2}a, a, \infty$

Fractional intercepts: $\frac{1}{2}, 1, \infty$

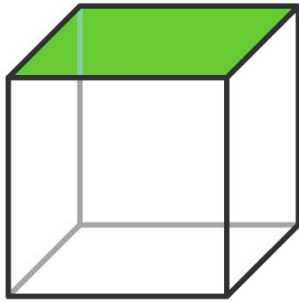
Miller Indices: **(210)**



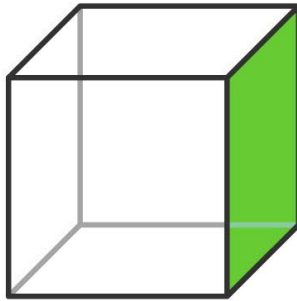
Some directions in a cubic unit cell.



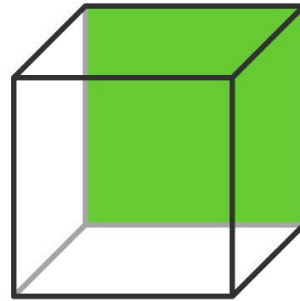
Miller indices of planes in a cubic crystal



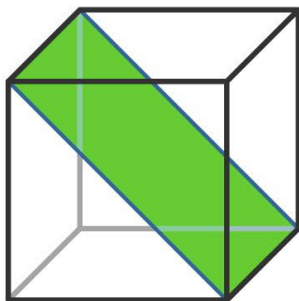
(001)



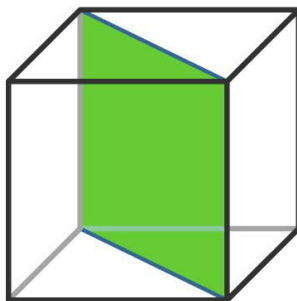
(100)



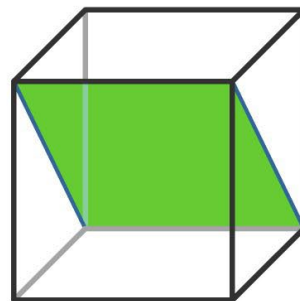
(010)



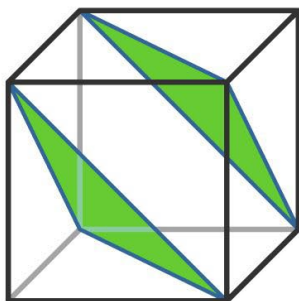
(101)



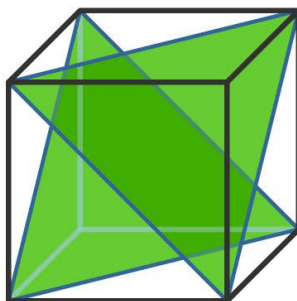
(110)



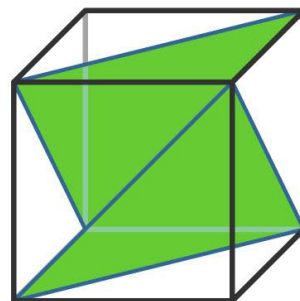
(011)



(111)



(111)



(111)