Families of Lattice Planes

Given any plane in a lattice, there is an infinite set of parallel lattice planes (or family of planes) that are equally spaced from each other.

- One of the planes in any family always passes through the origin.
- The Miller indices (hkl) usually refer to the plane that is nearest to the origin without passing through it.
- You must always shift the origin or move the plane parallel, otherwise a Miller index integer is 1/0!
- Sometimes (hkl) will be used to refer to any other plane in the family, or to the family taken together.
- Importantly, the Miller indices (hkl) is the same vector as the plane normal!

Crystallographic Planes in FCC: (100)

Distance between (100) planes

\[ d_{100} = \frac{a}{2} \]

Crystallographic Planes in FCC: (110)

Distance between (110) planes

\[ d_{110} = \frac{a}{\sqrt{2}} \]

Crystallographic Planes in FCC: (111)

Distance between (111) planes

\[ d_{111} = \frac{a}{\sqrt{3}} \]
Note: similar to crystallographic directions, planes that are parallel to each other, are equivalent.

Comparing Different Crystallographic Planes

For (220) Miller Indexed planes you are getting planes at 1/2, 1/2, 1/2.

The (110) planes are not necessarily (220) planes!

For cubic crystals:

\[ d_{110} = \frac{a}{\sqrt{1^2 + 1^2 + 0^2}} = \frac{a}{\sqrt{2}} \]

Distance between (110) planes

For (220) Miller Indexed planes you are getting planes at 1/2, 1/2, -∞.
The (110) planes are not necessarily (220) planes!

Directions in HCP Crystals

1. To emphasize that they are equal, \( a \) and \( b \) is changed to \( a_1 \) and \( a_2 \).
2. The unit cell is outlined in blue.
3. A fourth axis is introduced \( (a_3) \) to show symmetry.
   - Symmetry about \( c \) axis makes \( a_3 \) equivalent to \( a_1 \) and \( a_2 \).
   - Vector addition gives \( a_3 = -(a_1 + a_2) \).
4. This 4-coordinate system is used: \([a_1, a_2, -(a_1 + a_2), c]\)

Directions in HCP Crystals: 4-index notation

Example

What is 4-index notation for vector \( D \)?

- Projecting the vector onto the basal plane, it lies between \( a_1 \) and \( a_2 \) (vector \( B \) is projection).
  - Vector \( B = (a_1 + a_2) \), so the direction is \([110]\) in coordinates of \([a_1, a_2, c]\), where \( c \)-intercept is 0.
  - In 4-index notation, because \( a_3 = -(a_1 + a_2) \), the vector \( B \) is \([1120]\), since it is 3x farther out.
  - In 4-index notation \( c = [0001] \), which must be added to get \( D \) (reduced to integers) \( D = [1123] \)

Easiest to remember: Find the coordinate axes that straddle the vector of interest, and follow along those axes (but divide the \( a_1, a_2, a_3 \) part of vector by 3 because you are now three times farther out!).

Self-Assessment Test: What is vector \( C \)?

Check w/ Eq. 3.7 or just use Eq. 3.7

1123 -2a_3 without 1/3
Directions in HCP Crystals: 4-index notation

Example

What is 4-index notation for vector D?

- Projection of the vector D in units of [a1 a2 c] gives u' = 1, v' = 1, and w' = 1. Already reduced integers.
- Using Eq. 3.7:

\[ u = \frac{1}{3}(2v' - v), \quad v = \frac{1}{3}(2u' - u), \quad w = w' \]

- In 4-index notation:
  Reduce to smallest integers:

\[ [1123] \]

After some consideration, seems just using Eq. 3.7 most trustworthy.

Miller Indices for HCP Planes

4-index notation is more important for planes in HCP, in order to distinguish similar planes rotated by 120°.

As soon as you see [1100], you will know that it is HCP, and not [110] cubic!

Find Miller Indices for HCP:

1. Find the intercepts, r and s, of the plane with any two of the basal plane axes (a1, a2, or a3), as well as the intercept, t, with the c axes.
2. Get reciprocals 1/r, 1/s, and 1/t.
3. Convert reciprocals to smallest integers in same ratios.
4. Get h, k, i via relation \( i = - (h + k) \), where h is associated with \( a_1 \), k with \( a_2 \), i with \( a_3 \), and l with c.
5. Enclose 4-indices in parenthesis: \( (h \ k \ i \ l) \).

Miller Indices for HCP Planes

What is the Miller Index of the pink plane?

1. The plane’s intercepts \( a_1 \), \( a_2 \), and \( c \) at \( r = 1 \), \( s = 1 \), and \( t = 1 \), respectively.
2. The reciprocals are 1/r = 1, 1/s = 1, and 1/t = 0.
3. They are already smallest integers.
4. We can write \( (h \ k \ i \ l) = (1 \ ? \ ? \ 0) \).
5. Miller Index is \( (1210) \)

Yes, Yes…..we can get it without \( a_1 \)!

1. The plane’s intercepts \( a_1 \), \( a_2 \), and \( c \) at \( r = 1 \), \( s = -1/2 \) and \( t = \infty \), respectively.
2. The reciprocals are 1/r = 1, 1/s = -2, and 1/t = 0.
3. They are already smallest integers.
4. We can write \( (h \ k \ i \ l) = (12?0) \).
5. Using \( i = -(h+k) \) relation, \( k = -2 \).
6. Miller Index is \( (1210) \)

But note that the 4-index notation is unique….Consider all 4 intercepts:
- plane intercept \( a_1 \), \( a_2 \), \( a_3 \), and \( c \) at \( 1, -1/2, 1 \), and \( \infty \), respectively.
- Reciprocals are 1 -2, 1, and 0.
- So, there is only 1 possible Miller Index is \( (1210) \)
Basal Plane in HCP

Name this plane...
- Parallel to $a_1$, $a_2$, and $a_3$
- So, $h + k + l = 0$
- Intersects at $z = 1$

$plane = (0001)$

Another Plane in HCP

$h = 1, k = -1, l = -1, 1 = 0, 1 = 0$

(1 1 0) plane

SUMMARY

- Crystal Structure can be defined by space lattice and basis atoms (lattice decorations or motifs).

- Only 14 Bravais Lattices are possible. We focus only on FCC, HCP, and BCC, i.e., the majority in the periodic table.

- We now can identify and determined: atomic positions, atomic planes (Miller Indices), packing along directions (LD) and in planes (PD).

- We now know how to determine structure mathematically. So how do we do it experimentally? DIFFRACTION.