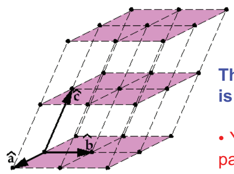
Families of Lattice Planes

Given any plane in a lattice, there is a *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.



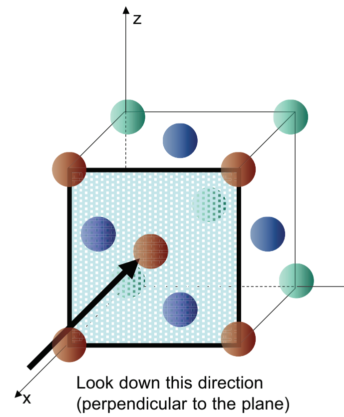
The Miller indices (hkl) usually refer to the plane that is nearest to the origin without passing through it.

• You must always shift the origin or move the plane parallel, otherwise a Miller index integer is 1/0!

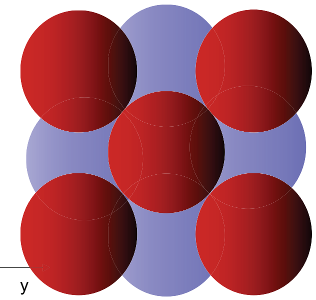
• Sometimes (hkl) will be used to refer to any other plane in the family, or to the family taken together.

• Importantly, the Miller indices (hkl) is the same vector as the plane normal!

Crystallographic Planes in FCC: (100)



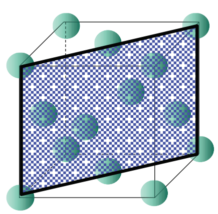
Look down this direction (perpendicular to the plane)

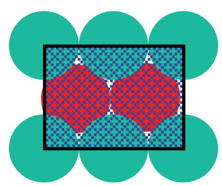


Distance between (100) planes $d_{100} = a$

... between (200) planes $d_{200} = \frac{a}{2}$

Crystallographic Planes in FCC: (110)



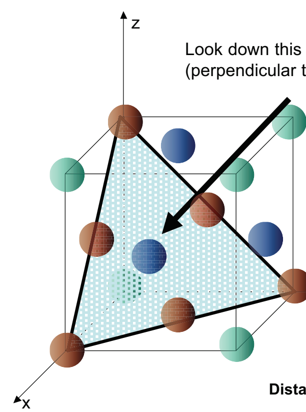


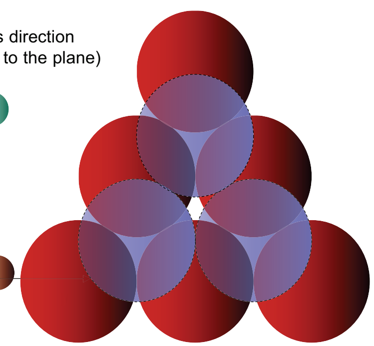
Distance between (110) planes

$$d_{110} = \frac{a\sqrt{2}}{2}$$

Crystallographic Planes in FCC: (111)

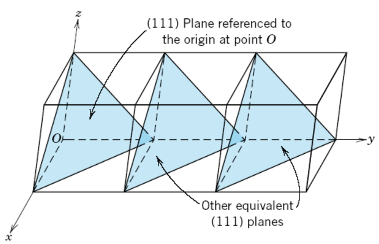
Look down this direction (perpendicular to the plane)





Distance between (111) planes $d_{111} = \frac{a\sqrt{3}}{3}$

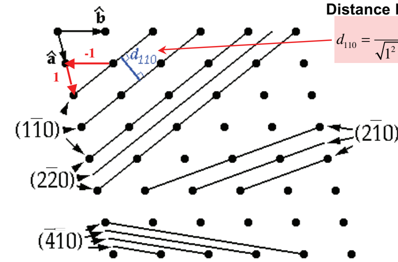
Note: similar to crystallographic directions, planes that are parallel to each other, are equivalent



Comparing Different Crystallographic Planes

Distance between (110) planes

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



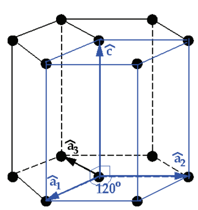
For (220) Miller Indexed planes you are getting planes at 1/2, 1/2, ∞.
The (110) planes are not necessarily (220) planes!

For cubic crystals: $d_{hkl} = \dfrac{a}{\sqrt{h^2+k^2+l^2}}$

Miller Indices provide you easy measure of distance between planes.

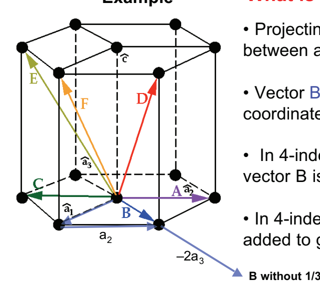
Directions in HCP Crystals

1. To emphasize that they are equal, **a** and **b** is changed to $\mathbf{a}_1$ and $\mathbf{a}_2$.
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: $[\mathbf{a}_1\ \mathbf{a}_2\ -(a_1 + a_2)\ c]$



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 $\frac{1}{3}[11\bar{2}0]$ since it is 3x farther out.

• In 4-index notation **c** = [0001], which must be added to get D (*reduced to integers*) D = $[11\bar{2}3]$

B without 1/3

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

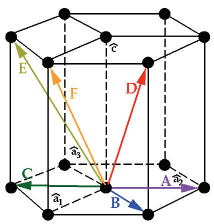
Easiest to remember: Find the coordinate axes that straddle the vector of interest, and follow along those axes *(but divide the a_1, a_2, a_3 part of vector by 3 because you are now three times farther out!)*.

Self-Assessment Test: What is vector C?

Directions in HCP Crystals: 4-index notation

Example

Check w/ Eq. 3.7: a dot-product projection in hex coords.



What is 4-index notation for vector D?

- Projection of the vector D in units of $[\mathbf{a_1}\ \mathbf{a_2}\ \mathbf{c}]$ gives **u'=1, v'=1, and w'=1**. Already reduced integers.

- Using Eq. 3.7:

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

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

- In 4-index notation: $[\frac{1}{3}\frac{1}{3}\frac{\bar{2}}{3}1]$

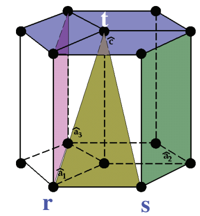
- Reduce to smallest integers: $[11\bar{2}3]$

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!

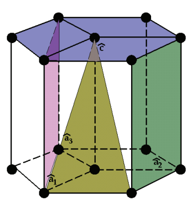


Find Miller Indices for HCP:

1. Find the intercepts, *r and s*, of the plane with any **two** of the basal plane axes ($\mathbf{a_1}$, $\mathbf{a_2}$, or $\mathbf{a_3}$), 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 , l*** via relation ***i = - (h+k),*** *where h is associated with* $\mathbf{a_1}$, *k* with $\mathbf{a_2}$, *i* with $\mathbf{a_3}$, and *l* with **c**.
5. Enclose 4-indices in parenthesis: ***(h k i l)*** .

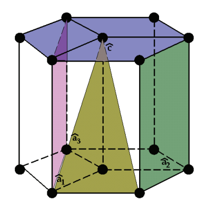
Miller Indices for HCP Planes

What is the Miller Index of the pink plane?



1. The plane's intercept $\mathbf{a_1}$, $\mathbf{a_3}$ and **c** at r=1, s=1 and t= ∞, respectively.
1. The reciprocals are 1/r = 1, 1/s = 1, and 1/t = 0.
2. They are already smallest integers.
3. We can write ***(h k i l) = (1 ? 1 0).***
4. Using ***i = - (h+k) relation, k=–2***.
5. Miller Index is $(1\bar{2}10)$

Yes, Yes….we can get it without a_3!

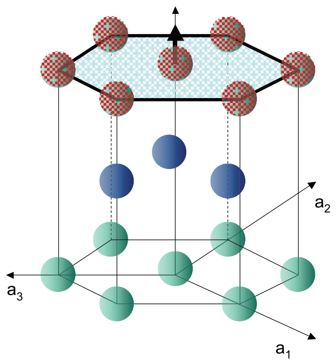


1. The plane's intercept $\mathbf{a_1}$, $\mathbf{a_2}$ and **c** at r=1, s=–1/2 and t= ∞, respectively.
1. The reciprocals are 1/r = 1, 1/s = –2, and 1/t = 0.
2. They are already smallest integers.
3. We can write ***(h k i l) =*** $(1\bar{2}?0)$
4. Using ***i = - (h+k) relation, i=1***.
5. Miller Index is $(1\bar{2}10)$

But note that the 4-index notation is unique….Consider all 4 intercepts:

- plane intercept $\mathbf{a_1}$, $\mathbf{a_2}$, $\mathbf{a_3}$ and **c** at 1, –1/2, 1, and ∞, respectively.
- Reciprocals are 1, –2, 1, and 0.
- So, there is only 1 possible Miller Index is $(1\bar{2}10)$

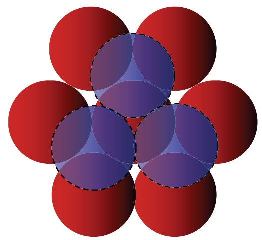
Basal Plane in HCP



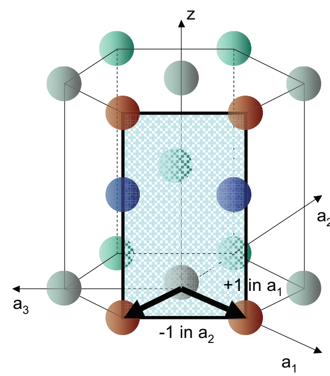
Name this plane…

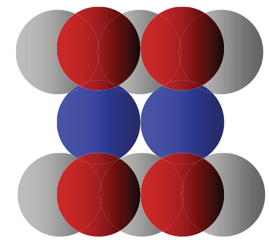
- Parallel to a_1, a_2 and a_3
  - So, h = k = i = 0
- Intersects at z = 1

$$\textit{plane} = (0001)$$



Another Plane in HCP

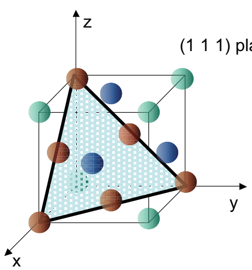


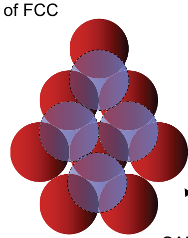


$(1\,\bar{1}\,0\,0)$ plane

h = 1, k = -1, i = -(1+-1) = 0, l = 0

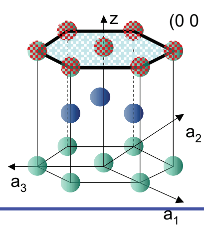
(1 1 1) plane of FCC

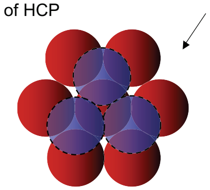




SAME THING!*

(0 0 0 1) plane of HCP





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 to we do it experimentally? DIFFRACTION.*