

## 1 Miller indices

In crystallography, we use Miller indices to specify locations, directions, and planes in a crystal. Standard x-y-z Cartesian coordinates use a basis consisting of three orthogonal axes in three dimensions with unit length. In Miller index notation, we will rely on the lattice vectors of the unit cell as our basis. In 3.091, since we are working with cubic Bravais lattices, the crystallographic lattice vectors are all orthogonal and the same length (with the length specific to a particular solid). With this framework, we can specify an arbitrary point in terms of its projections onto the lattice vectors, much as you would with standard Cartesian coordinates:

$$\text{location} = h\vec{a}_1 + k\vec{a}_2 + l\vec{a}_3$$

where  $\vec{a}_i$  are the unit vectors with some magnitude and direction, and the values of  $h$ ,  $k$ , and  $l$  specify how far to go along each lattice vector. We can express this in shorthand as  $(h, k, l)$ , just like you would write an ordered pair of Cartesian coordinates! A quick note on notation: in Miller indices, the brackets and commas matter a lot! Here's a quick list of the options and what each signifies:

Notation	Representation
$(h, k, l)$	point
$[hkl]$	direction
$\langle hkl \rangle$	family of directions
$(hkl)$	plane
$\{hkl\}$	family of planes

Note that only points use commas! Finally, negative weights can be represented with a bar over the relevant number: travel in the negative  $\vec{a}_1$  direction would be indicated by  $[\bar{h}kl]$ , for example.

Directions and planes can be specified algorithmically:

### Directions

A crystalline direction is defined in the context of a unit cell, and the vector defining the direction always passes through the origin of the unit cell. The vector stretches from the origin to the location specified in terms of the lattice vectors

$$h\vec{a}_1 + k\vec{a}_2 + l\vec{a}_3$$

where it is our job to determine the values of  $[hkl]$ . To determine the crystallographic direction given a picture of a vector in a unit cell:

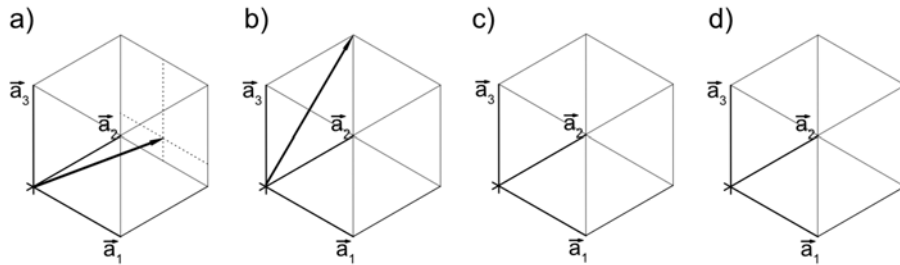
1. Shift the vector such that it intersects the origin of the unit cell (if it doesn't already)
2. Make a mark on the edge of the unit cell where the vector intersects the unit cell frame
3. Determine the fraction of each lattice vector traversed
4. Multiply the fractions by a common multiple to yield integer hkl values which define the direction

Of course you can go the other way as well, from a direction  $[hkl]$  to a drawing. To represent a direction  $[hkl]$  in a unit cell:

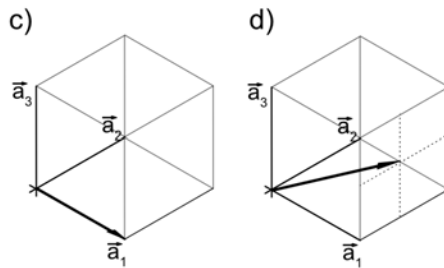
1. Divide through the vector  $[hkl]$  by whichever of  $h$ ,  $k$ , and  $l$  is the largest to yield fractional values

- Place the tip of the vector at the point on the edge of the unit cell defined by the fraction found previously
- Connect the origin to the vector tip

**Example:** For a) and b), determine the crystallographic direction indicated on the unit cell. Then, for c) and d), sketch the direction on the axes provided. For c), sketch [100], and for d), sketch [211].



For a), we can see that the end of the vector is located at  $\frac{1}{2}\vec{a}_1 + 1\vec{a}_2 + \frac{1}{4}\vec{a}_3$ . We can convert this to a crystallographic direction by multiplying through by 4 to get rid of the fractions while preserving the ratios. The direction shown in a) is therefore [241]. For b), the end of the vector is located at  $1\vec{a}_2 + 1\vec{a}_3$ , which is represented as [011]. Finally, the [100] and [211] planes are shown below:



## Planes

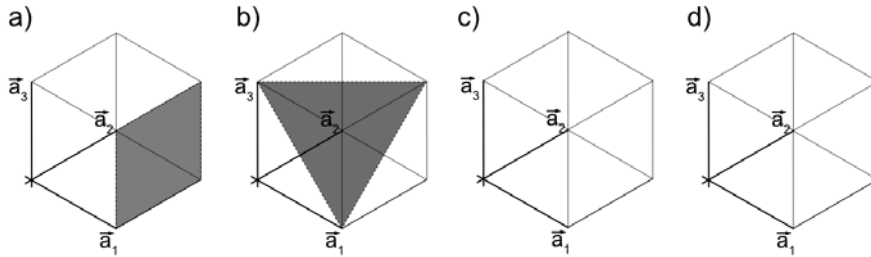
Similar to a crystalline direction a crystalline plane is usually represented in a unit cell, and determined in terms of the lattice vectors  $\vec{a}_1$ ,  $\vec{a}_2$ , and  $\vec{a}_3$ . When given a picture of a plane to identify:

- Make a mark on each edge of the unit cell where the plane intersects the unit cell frame
- Determine the fraction of each lattice vector traversed. If the plane never intercepts a lattice vector, you can note it as intercepting at  $\infty$
- Take the reciprocal of each fractional intercept ( $\frac{1}{\infty} = 0$ ) to yield integer  $hkl$  values which define the plane

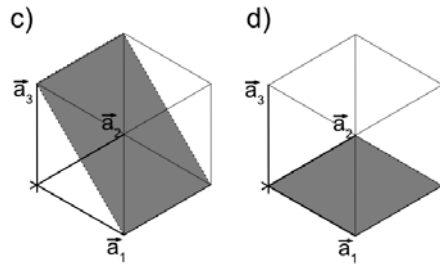
Finally, to sketch a plane given  $(hkl)$ :

- Find the reciprocal value of  $h$ ,  $k$ , and  $l$  ( $\frac{1}{0} = \infty$ )
- Mark the fractional values associated with  $h$ ,  $k$ , and  $l$  on the  $\vec{a}_1$ ,  $\vec{a}_2$ , and  $\vec{a}_3$  axes
- Connect the marks on the edge of the unit cell to form the plane

**Example:** For a) and b), determine the plane shown in the unit cell. Then, for c) and d), sketch the given plane on the axes provided. For c), sketch the (101) plane. For d), sketch the (001) plane.



For a), the plane intersects  $\vec{a}_1$  at the edge of the unit cell, which is 1. It is entirely parallel to  $\vec{a}_2$  and  $\vec{a}_3$ , so we say it intercepts at  $\infty$ . Taking the reciprocals of these intercepts yields  $(\frac{1}{1} \frac{1}{\infty} \frac{1}{\infty})$ , so this must be the (100) plane. For b), the plane intersects  $\vec{a}_1$  at 1 and  $\vec{a}_3$  at 1. If we extend the plane along the positive  $\vec{a}_2$  direction, it doesn't intercept the axis. But we have to remember to consider the other half of the crystal too: if we were to extend the plane backwards, it would intercept  $\vec{a}_2$  at -1. Taking reciprocals,  $(\frac{1}{1} \frac{1}{1} \frac{1}{-1})$  yields the  $(\bar{1}\bar{1}1)$  plane. Finally, the (101) and (001) planes are shown below:



You might notice that some directions and planes in the crystal look the same: the atoms are spaced the same amount. This is due to symmetry in a crystal: for example, if you look down any of the diagonals in a cubic lattice, the atoms you “see” look the same! These equivalent directions and planes are called families. For example, the  $\langle 100 \rangle$  family of directions includes  $[100]$ ,  $[010]$ ,  $[001]$ ,  $[00\bar{1}]$ ,  $[0\bar{1}0]$ , and  $[00\bar{1}]$  in a cubic crystal.

## 2 Interplanar spacing

To find the distance between neighboring parallel planes, we calculate the interplanar spacing,  $d_{hkl}$ .

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

Here,  $a$  is the lattice parameter, usually expressed in [nm].

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