

Miller Indices

Academic Resource Center

Definition

- Miller indices are used to specify **directions** and **planes**.
- These directions and planes could be in **lattices** or in **crystals**.
- The number of indices will match with the dimension of the lattice or the crystal.
- E.g. in 1D there will be 1 index and 2D there will be two indices etc.

Notation Summary

- (h,k,l) represents a point – note the exclusive use of commas
- Negative numbers/directions are denoted with a bar on top of the number
- $[hkl]$ represents a direction
- $\langle hkl \rangle$ represents a family of directions
- (hkl) represents a plane
- $\{hkl\}$ represents a family of planes

Miller Indices for Directions

- A vector \mathbf{r} passing from the origin to a lattice point can be written as:

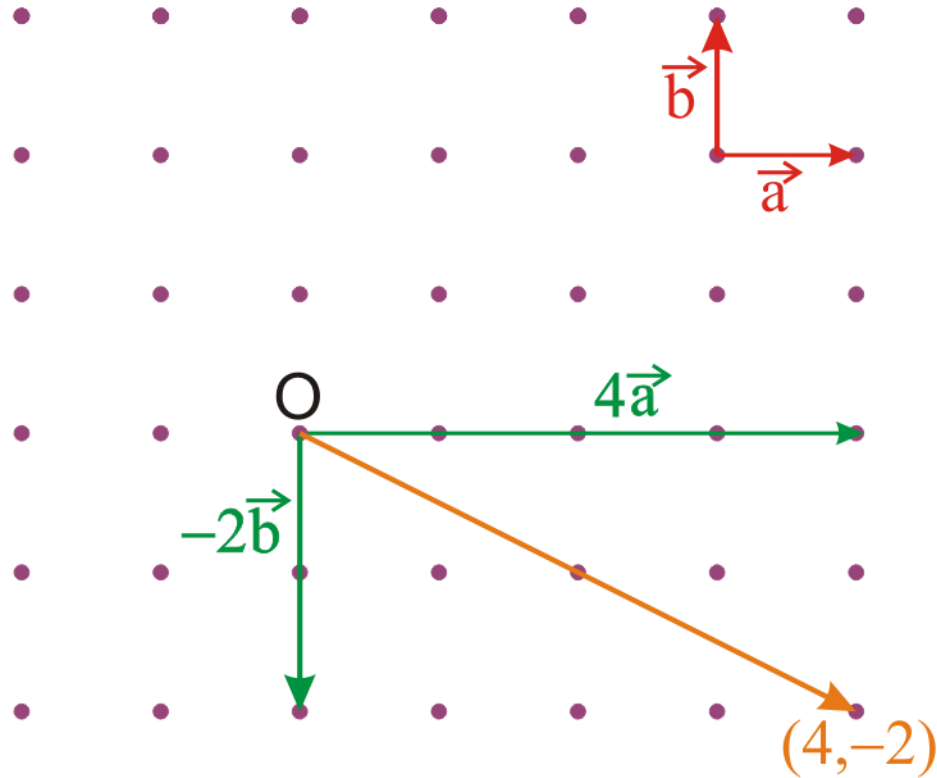
$$\mathbf{r} = r_1 \mathbf{a} + r_2 \mathbf{b} + r_3 \mathbf{c}$$

where, \mathbf{a} , \mathbf{b} , $\mathbf{c} \rightarrow$ basic vectors and

Miller indices $\rightarrow (r_1 r_2 r_3)$

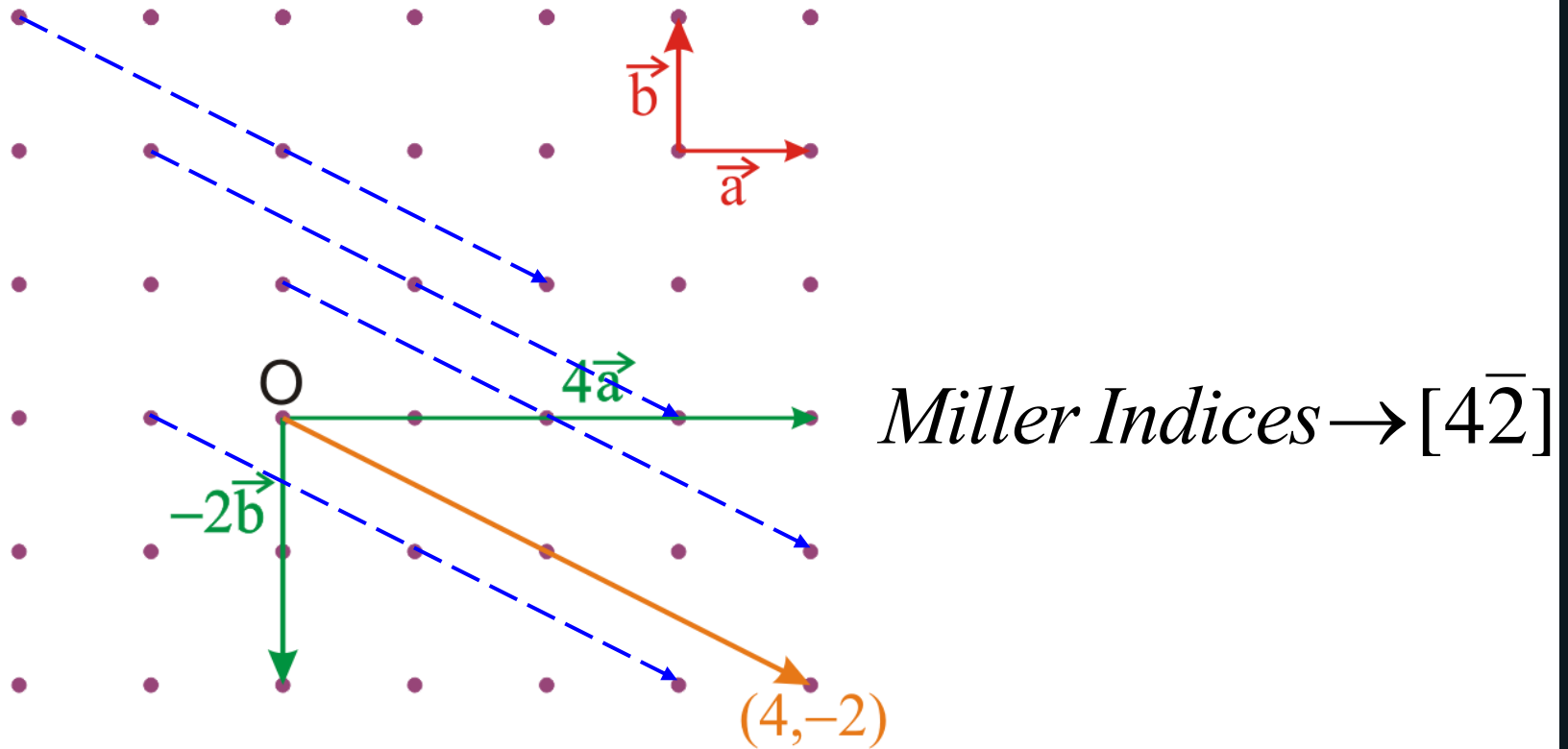
- Fractions in $(r_1 r_2 r_3)$ are eliminated by multiplying all components by their common denominator.
- [e.g. $(1, \frac{3}{4}, \frac{1}{2})$ will be expressed as (432)]

Example



Miller Indices $\rightarrow [4\bar{2}]$

Example (cont'd)



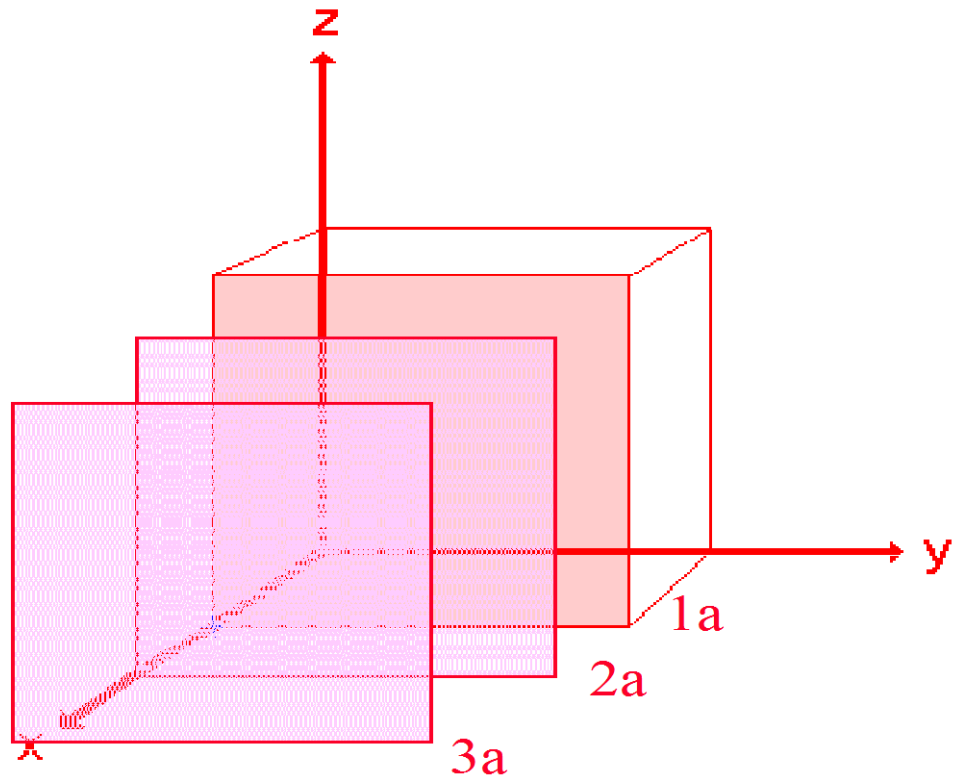
The index represents a set of all such parallel vectors

Miller Indices for Planes: Procedure

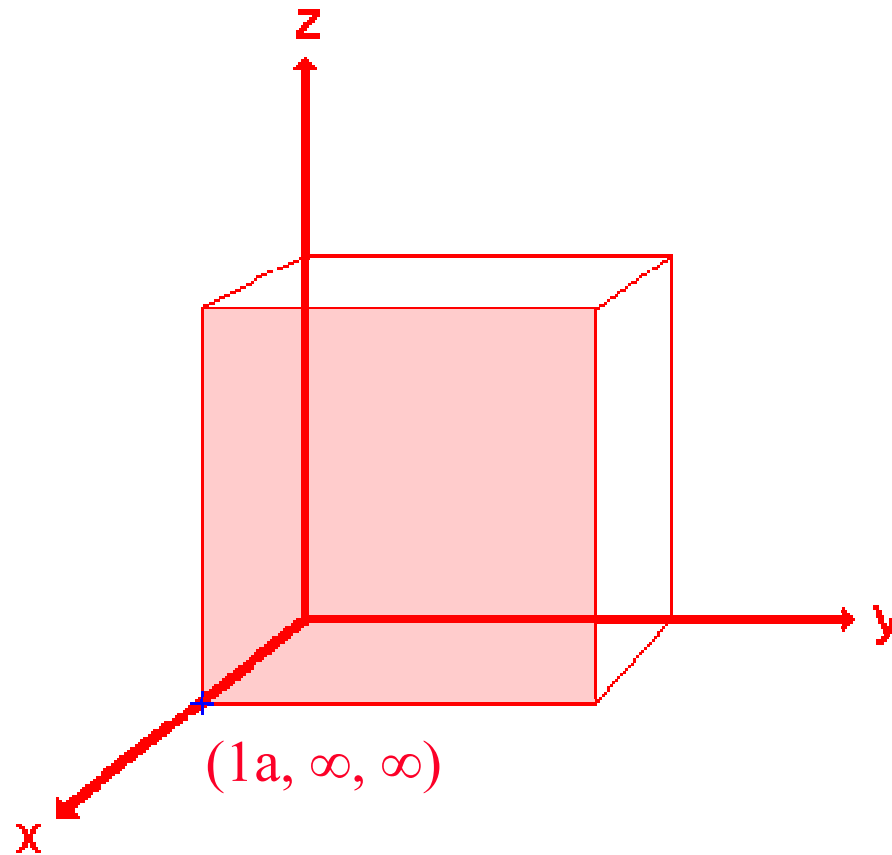
1. Identify the plane intercepts on the x, y and z-axes.
2. Specify intercepts in fractional coordinates.
3. Take the reciprocals of the fractional intercepts.

Miller Indices for Planes: Illustration

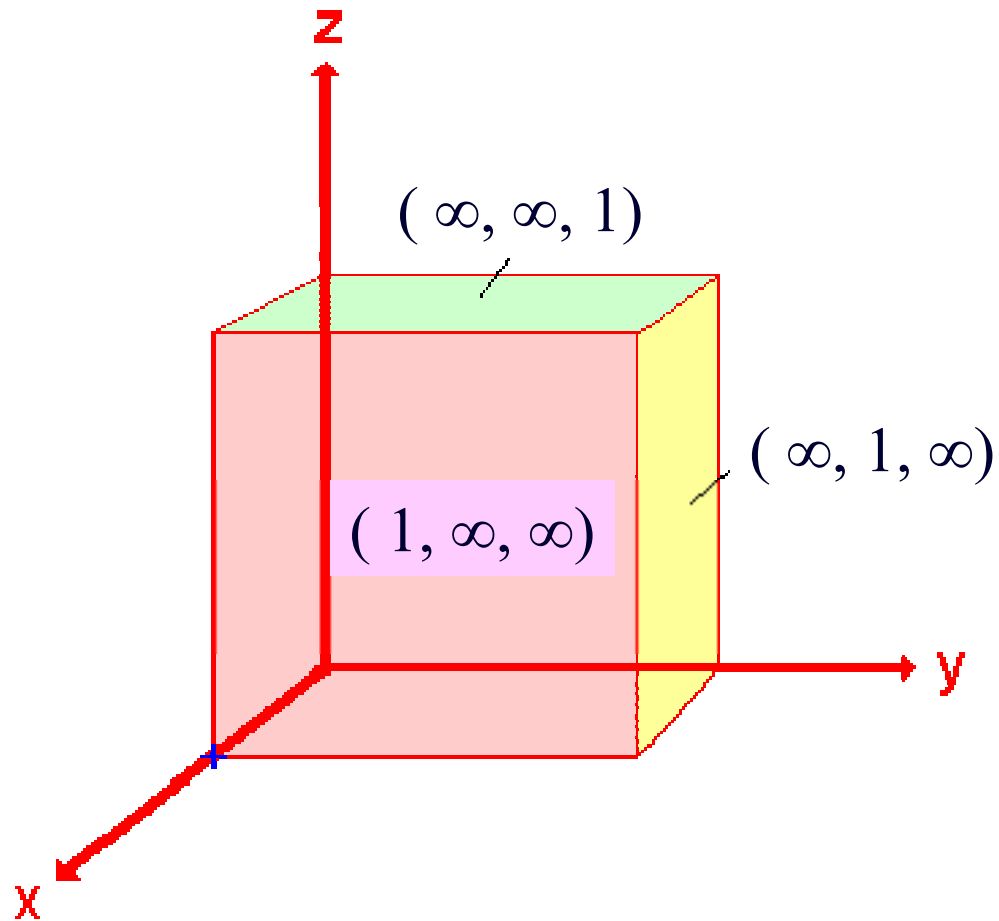
- Consider the plane in pink, which is one of an infinite number of parallel plane each a consistent distance (“ a ”) away from the origin (purple planes)



- The plane intersects the x-axis at point a. It runs parallel along y and z axes.
- Thus, this plane can be designated as $(1, \infty, \infty)$



- Likewise, the yellow plane can be designated as $(\infty, 1, \infty)$
- And the green plane can be written as $(\infty, \infty, 1)$



- Miller Indices are the reciprocals of the parameters of each crystal face. Thus:

- Pink Face

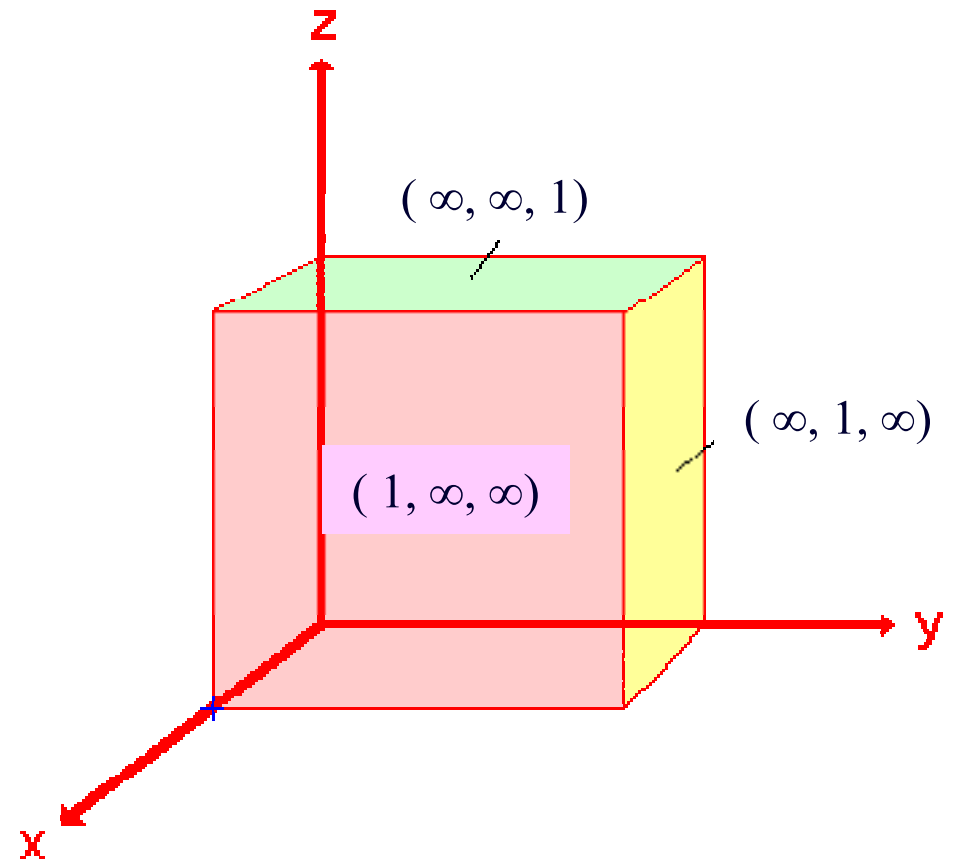
$$= (1/1, 1/\infty, 1/\infty) = (100)$$

- Green Face

$$= (1/\infty, 1/\infty, 1/1) = (001)$$

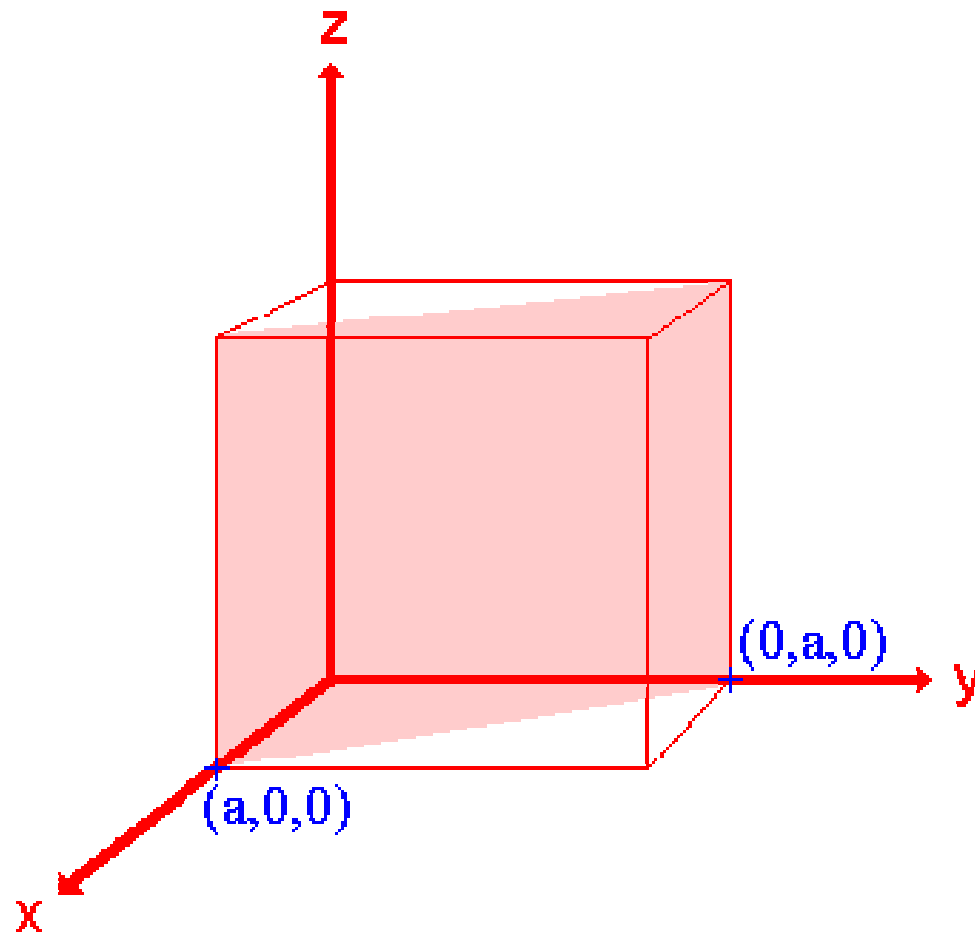
- Yellow Face

$$= (1/\infty, 1/1, 1/\infty) = (010)$$



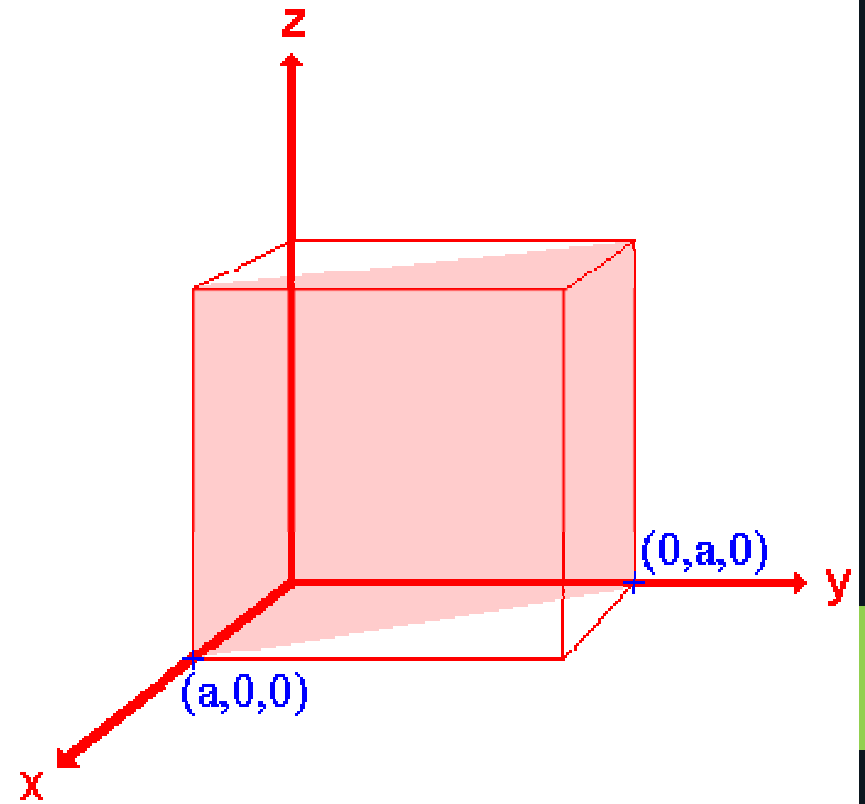
Examples

What's the Miller Index of this plane?



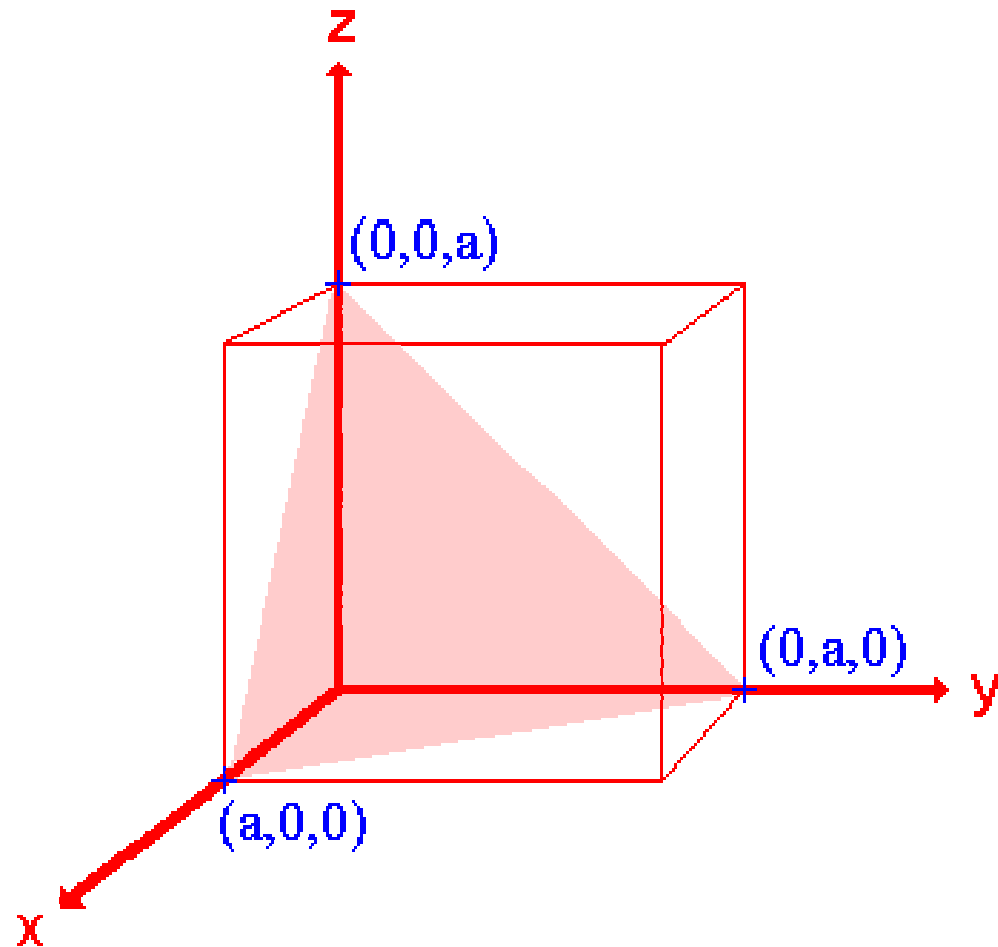
Examples (cont'd)

- The plane of interest cuts two of the crystallographic axes.
- Intercepts: $(1,1, \infty) \rightarrow (110)$



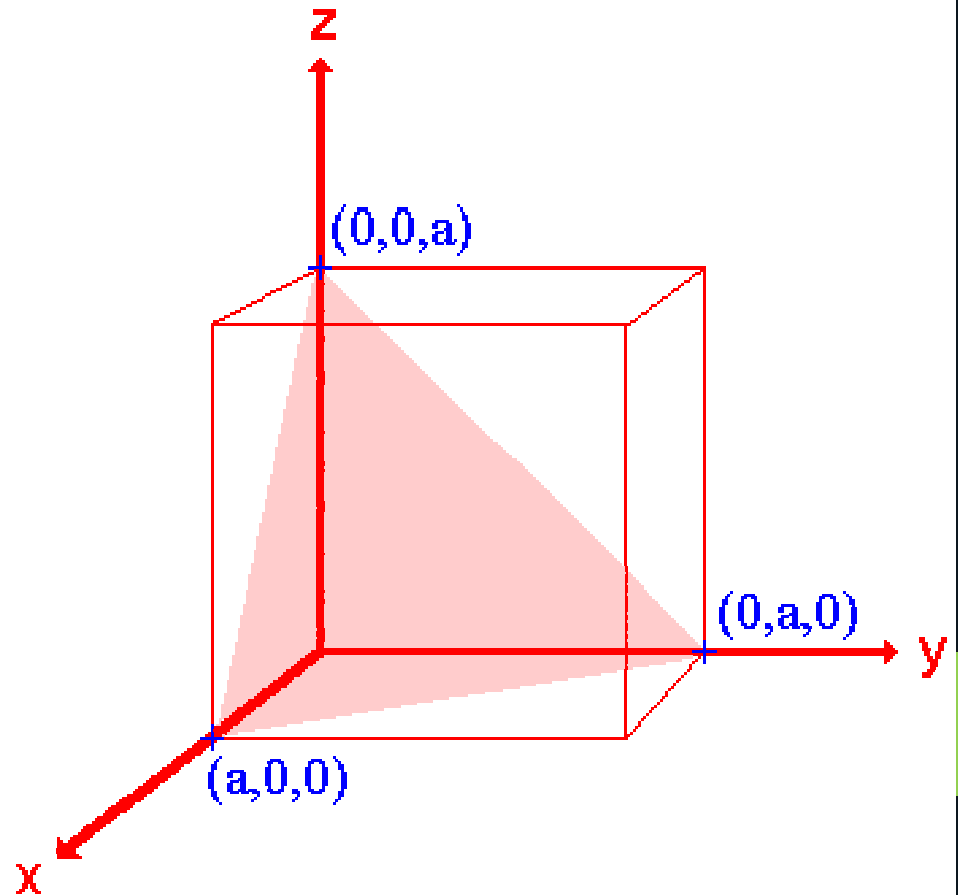
Examples (cont'd)

- Miller Index?



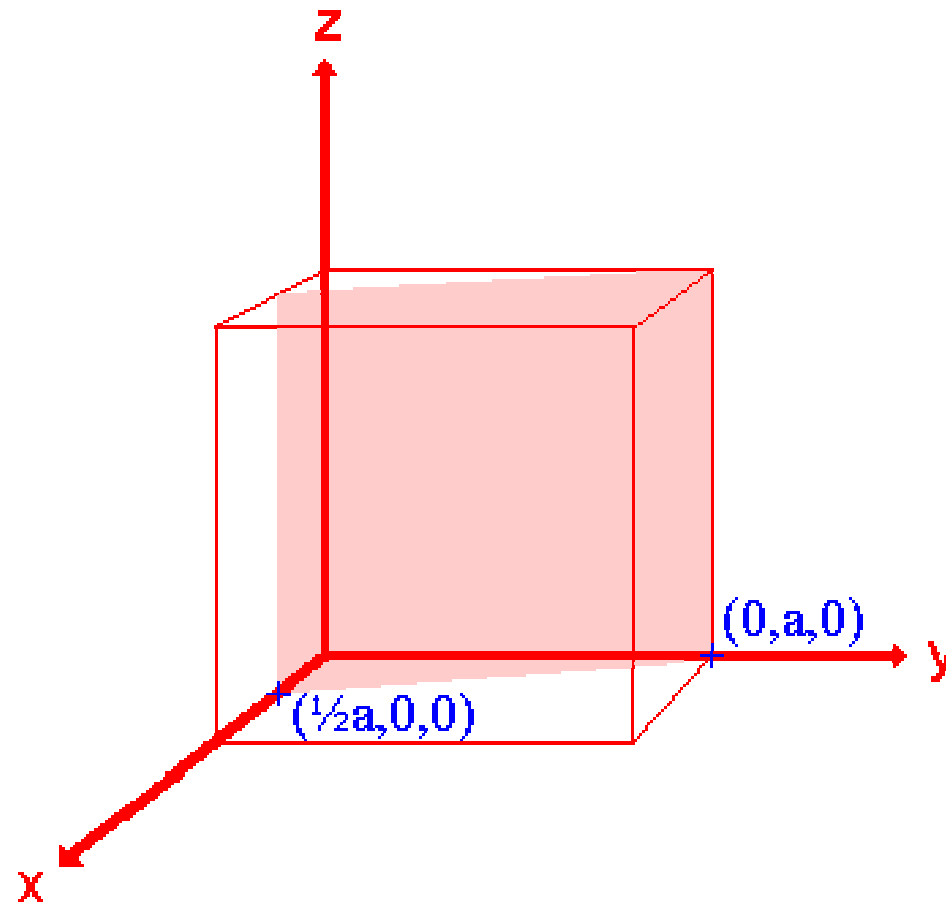
Examples (cont'd)

- This plane cuts all three crystallographic axes.
- Intercepts = $(1,1,1) \rightarrow (111)$



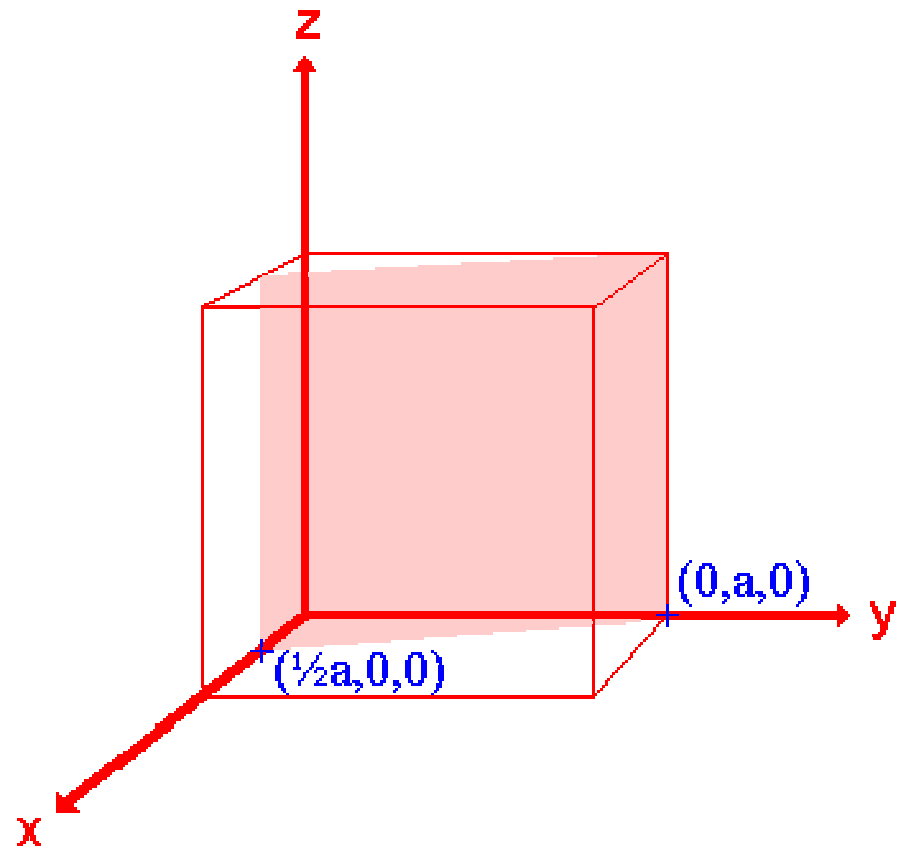
Examples (cont'd)

- Miller Index? (Difficult one)



Examples (cont'd)

- This plane cuts two of the reference axes, but not equidimensionally.
- Intercepts: $(\frac{1}{2}, 1, 0) \rightarrow (210)$



Family of Directions

It's a set of directions related by symmetry operations of the lattice.

Index	Members in family for cubic lattice
$\langle 100 \rangle$	$[100], [\bar{1}00], [010], [0\bar{1}0], [001], [00\bar{1}]$
$\langle 110 \rangle$	$[110], [\bar{1}10], [1\bar{1}0], [\bar{1}\bar{1}0], [101], [\bar{1}01], [10\bar{1}], [\bar{1}0\bar{1}], [011], [0\bar{1}1], [01\bar{1}], [0\bar{1}\bar{1}]$
$\langle 111 \rangle$	$[111], [\bar{1}11], [1\bar{1}1], [11\bar{1}], [\bar{1}\bar{1}1], [\bar{1}1\bar{1}], [1\bar{1}\bar{1}], [\bar{1}\bar{1}\bar{1}]$

Importance of Miller Indices

- In Materials Science it is important to have a notation system for atomic planes since these planes influence
 - Optical properties
 - Reactivity
 - Surface tension
 - Dislocations