Miller Indices

Academic Resource Center

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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.

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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
- <hkl> represents a family of directions
- (hkl) represents a plane
- {hkl} represents a family of planes

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Miller Indices for Directions

- A vector **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, **a**, **b**, **c** → basic vectors and

miller indices → $(r_1 r_2 r_3)$

- Fractions in $(r_1 r_2 r_3)$ are eliminated by multiplying all components by their common denominator.
- [e.g. (1, ¾ ,½) will be expressed as (432)]

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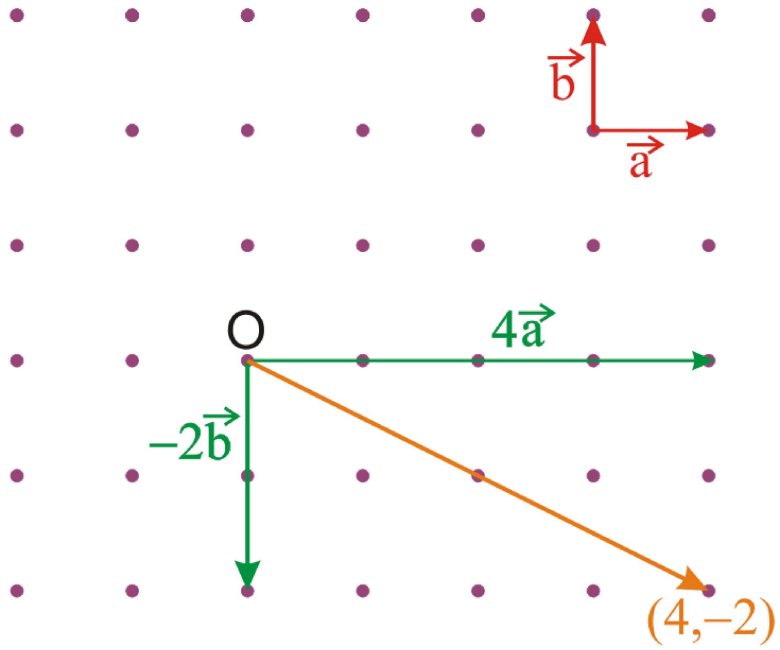
Example



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

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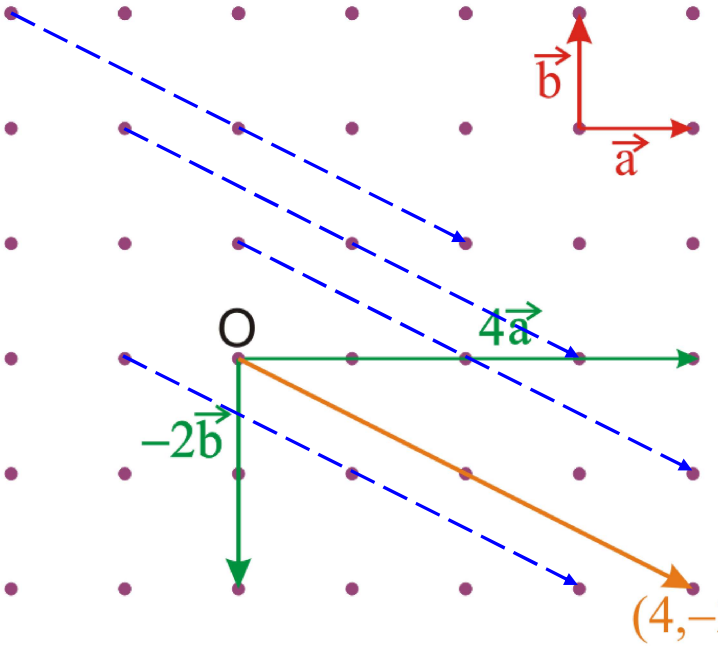
Example (cont'd)



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

The index represents a set of all such parallel vectors

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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.

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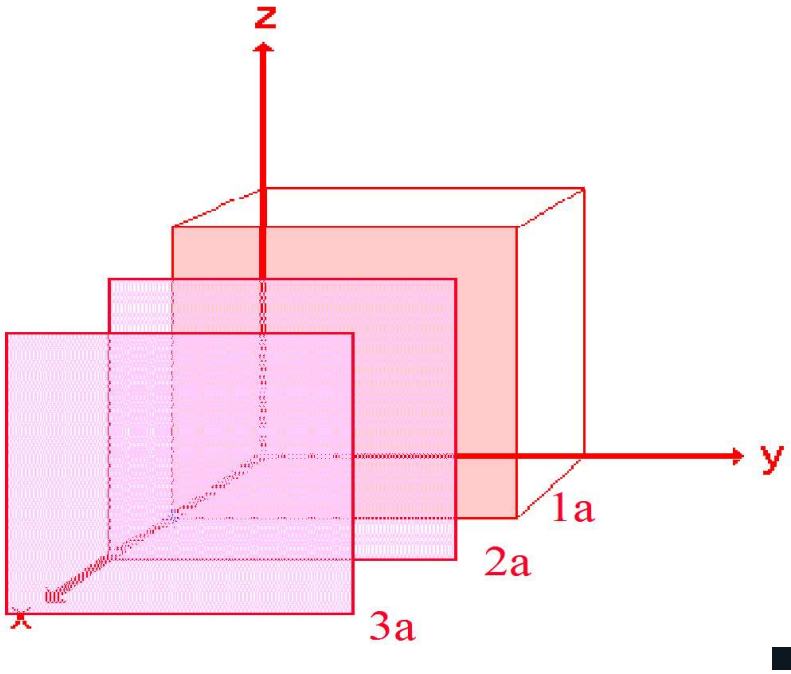
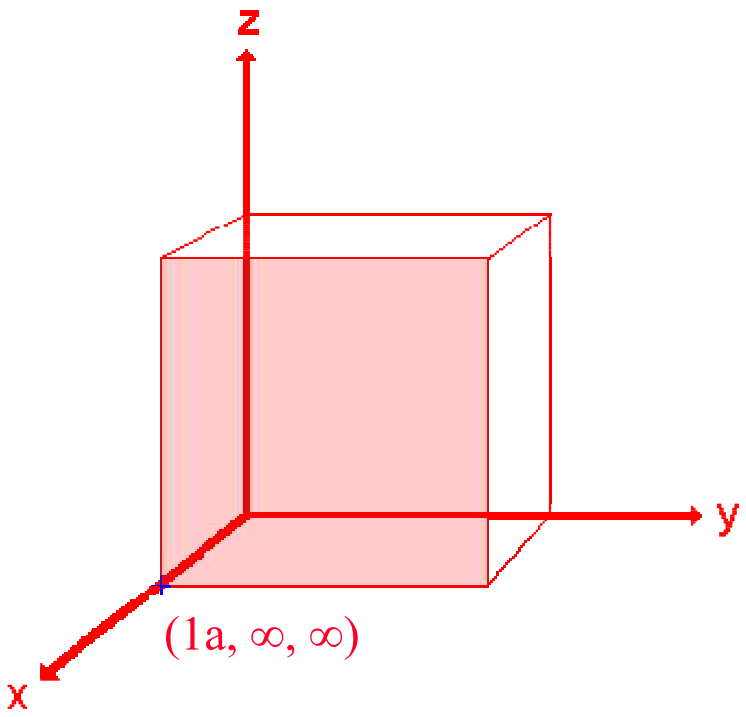
Miller Indices for Planes: Illustration

- 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,∞,∞)



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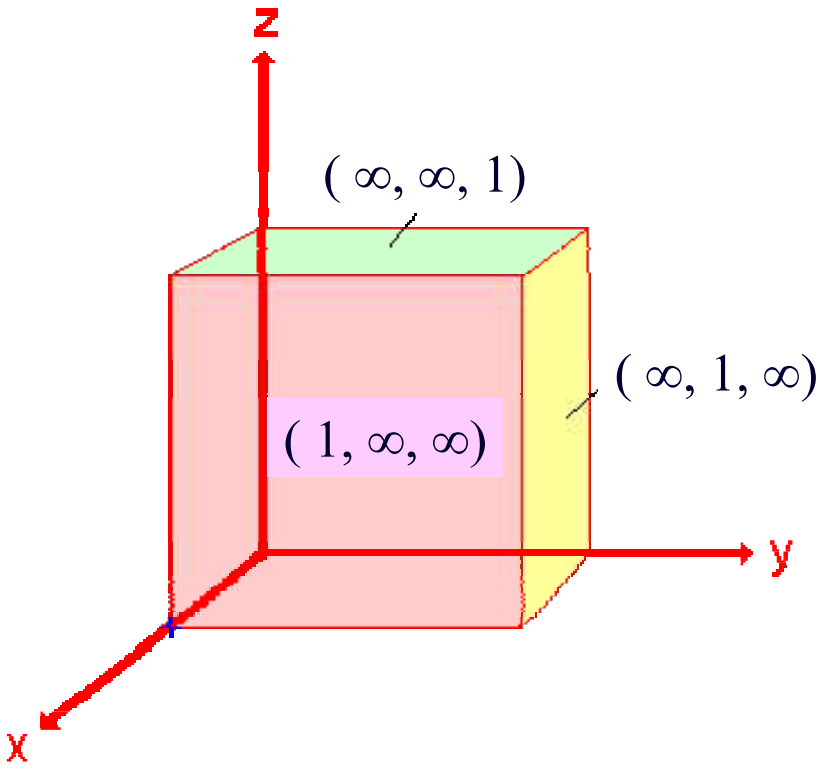
- Likewise, the yellow plane can be designated as (∞,1,∞)
- And the green plane can be written as (∞,∞,1)

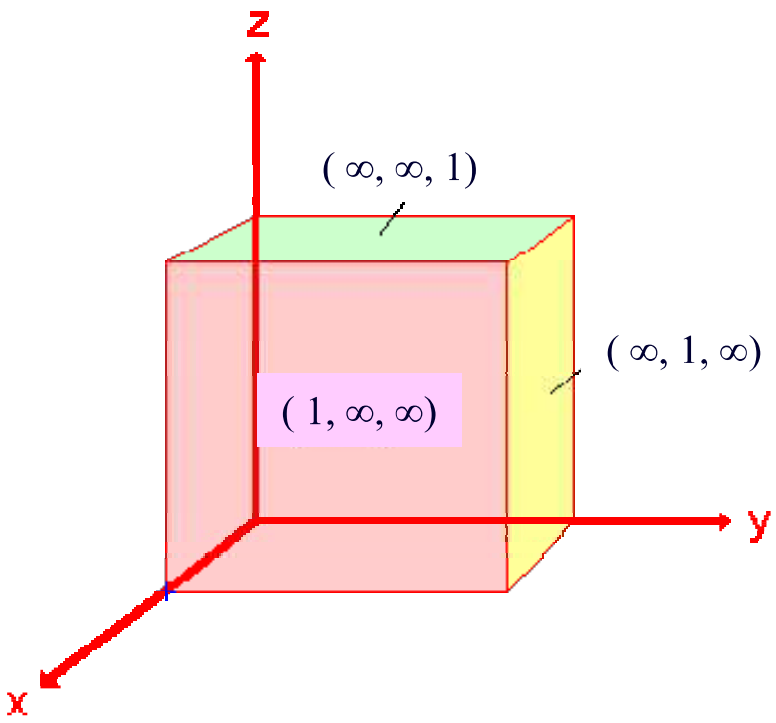


- Miller Indices are the reciprocals of the parameters of each crystal face. Thus:
- Pink Face

  = (1/1, 1/∞, 1/∞) = (100)
- Green Face

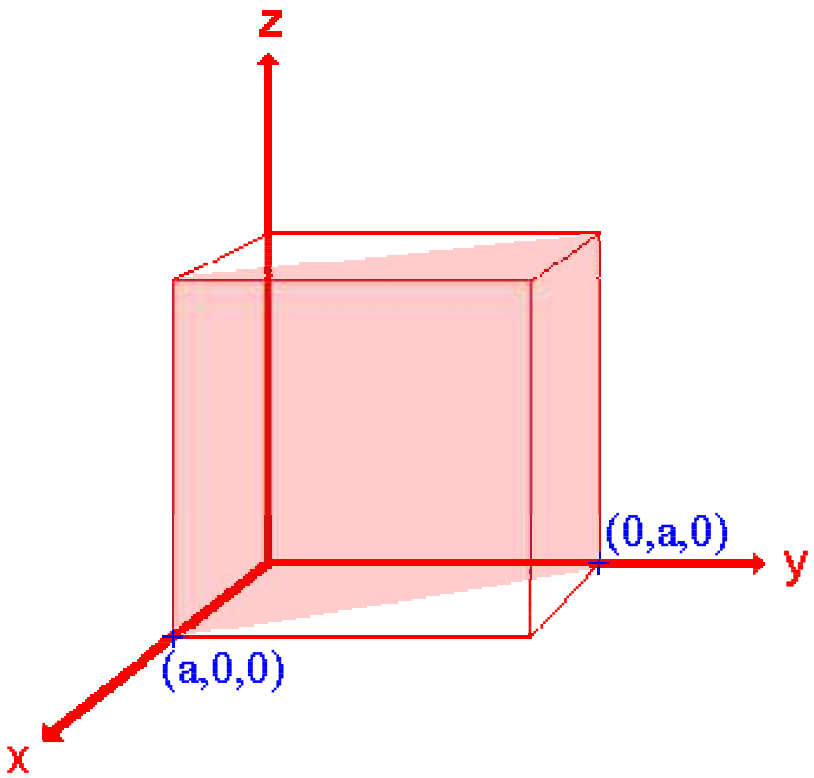
  = (1/∞, 1/∞, 1/1) = (001)
- Yellow Face

  = (1/∞, 1/1, 1/∞) = (010)



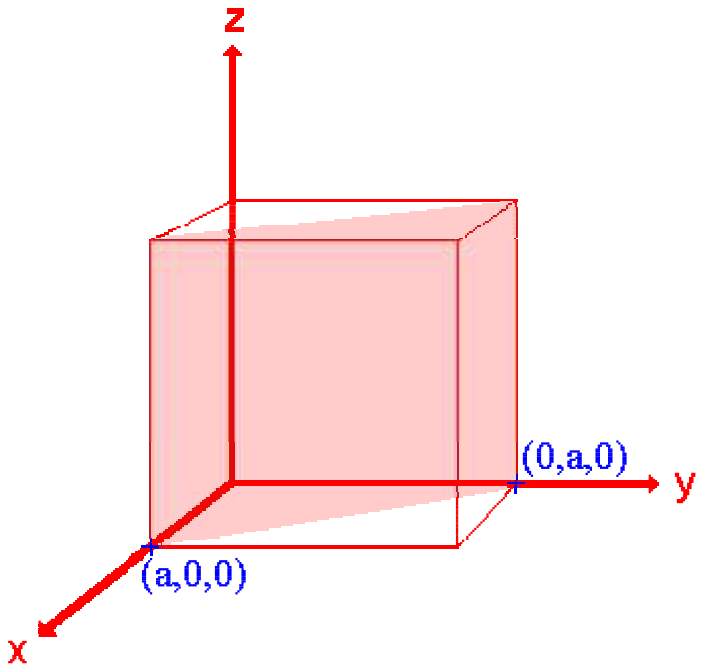
Examples

What's the Miller Index of this plane?



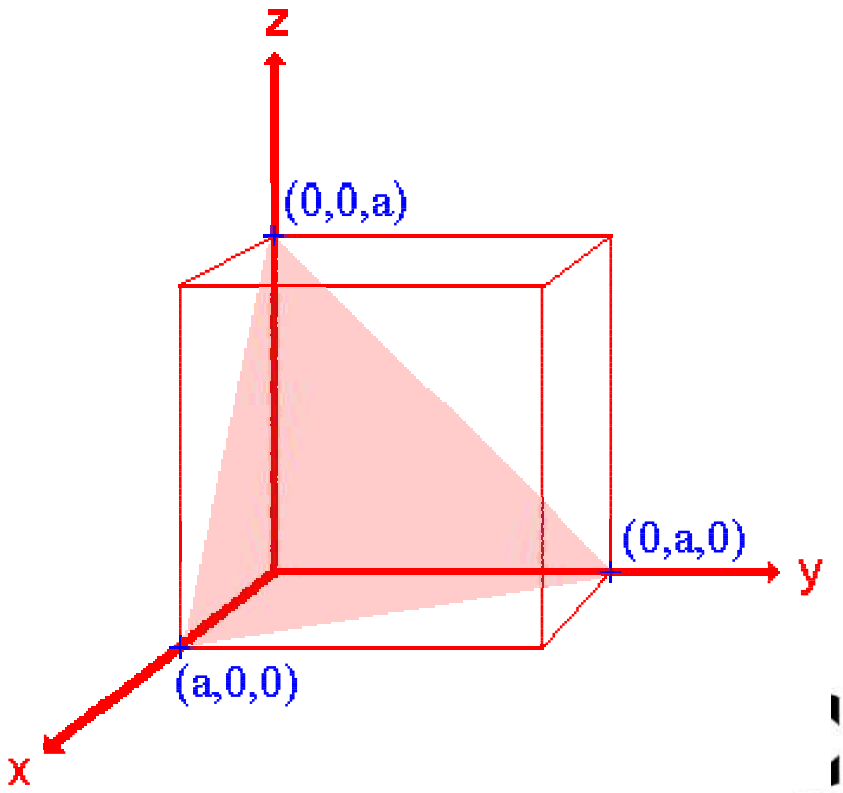
Examples (cont'd)

- The plane of interest cuts two of the crystallographic axes.
- Intercepts: (1,1, ∞) → (110)



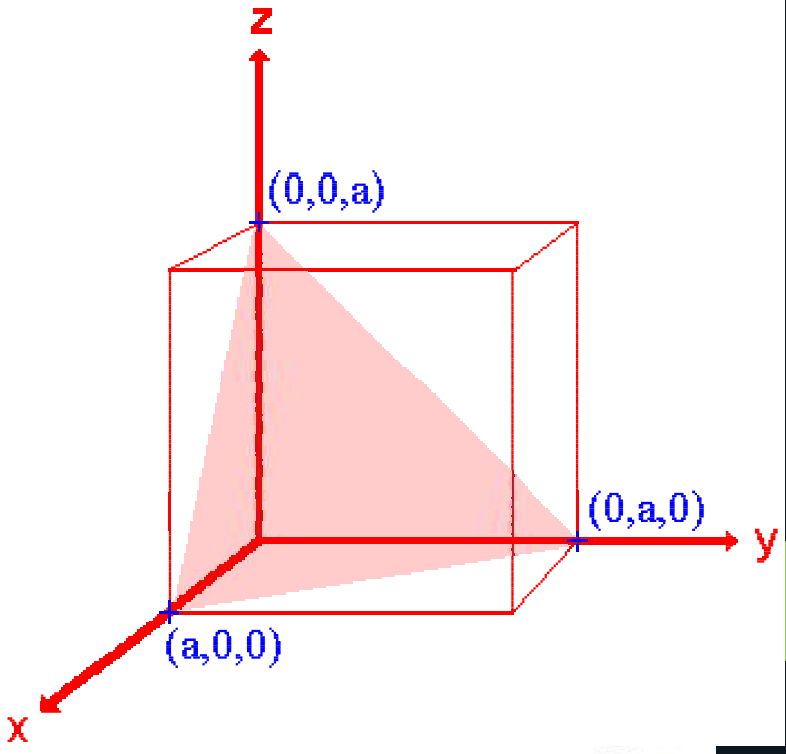
Examples (cont'd)

- Miller Index?



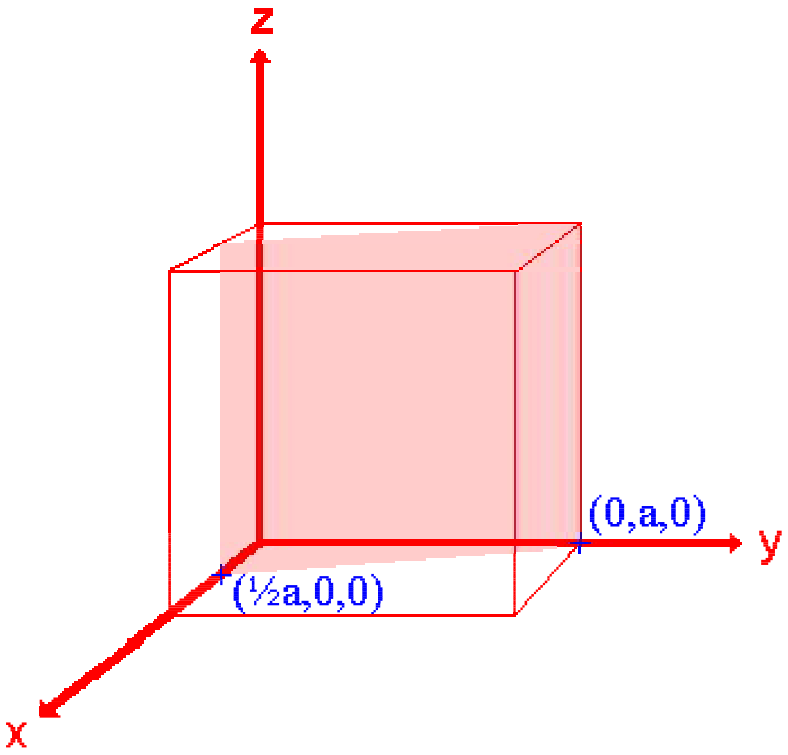
Examples (cont'd)

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



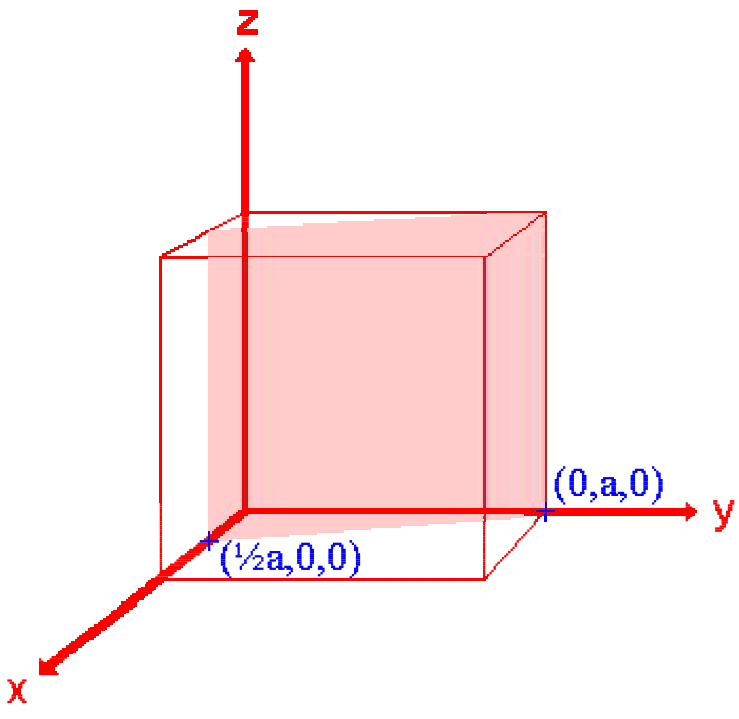
Examples (cont'd)

- Miller Index? (Difficult one)



Examples (cont'd)

- This plane cuts two of the reference axes, but not equidimensionally.
- Intercepts: (½, 1, 0) → (210)



Family of Directions

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

Index	Members in family for **cubic lattice**
<100>	[100],[$\bar{1}$00],[010],[0$\bar{1}$0],[001],[00$\bar{1}$]
<110>	[110],[$\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}$]
<111>	[111],[$\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}$]

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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

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