Miller Indices

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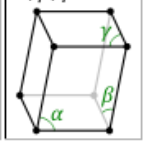
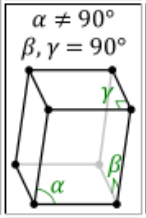
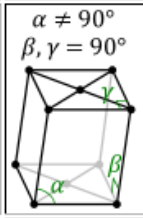
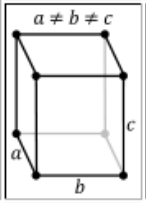
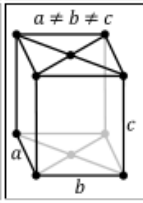
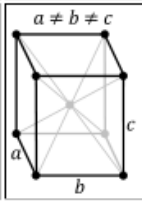
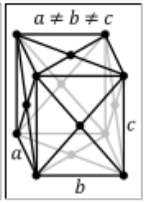
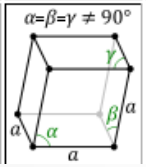
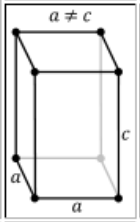
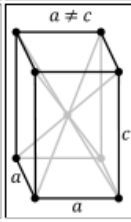
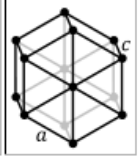
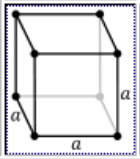
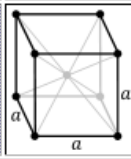
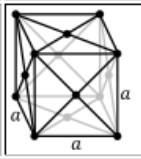
Introduction

- Developed by William Miller – 1839
- Primarily to describe crystalline structures
- Indices used to reference orientation of planes
- Consist of positive & negative integers
- Help determine material properties

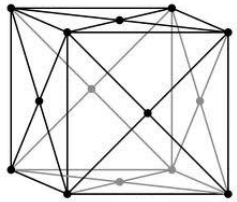
Examples of Crystal Structures

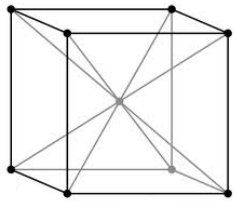
The 7 lattice systems (From least to most symmetric)	The 14 Bravais Lattices			
1. triclinic (none)	$\alpha, \beta, \gamma \neq 90°$ 			
2. monoclinic (1 diad)	simple	base-centered		
	$\alpha \neq 90°$ $\beta, \gamma = 90°$ 	$\alpha \neq 90°$ $\beta, \gamma = 90°$ 		
3. orthorhombic (3 perpendicular diads)	simple	base-centered	body-centered	face-centered
	$a \neq b \neq c$ 	$a \neq b \neq c$ 	$a \neq b \neq c$ 	$a \neq b \neq c$ 
4. rhombohedral (1 triad)	$\alpha=\beta=\gamma \neq 90°$ 			

5. tetragonal (1 tetrad)	simple	body-centered	
	$a \neq c$ 	$a \neq c$ 	
6. hexagonal (1 hexad)			
7. cubic (4 triads)	simple (SC)	body-centered (bcc)	face-centered (fcc)
			

Definitions

- Lattice Parameters
  - Lengths of the edges of a lattice, defined by distance
- Isotropic
  - Uniform in all orientations, regardless of reference point
- Anisotropic
  - Interactive properties are dependent on incident orientation
- Face-Centered Cubic
  - Cubic lattice with atoms on each face
- Body-Centered Cubic
  - Cubic lattice with atom in center





Nomenclature

- Indices expressed as integers
- x, y, z axis correspond to lengths a, b, c
- a, b, c, are inverted to find h, k, l
- Negatives expressed with 'bar': $\bar{1}$, $\bar{2}$, $\bar{3}$, etc.
- ( ) Brackets represent single planes
- { } Brackets represent family of planes

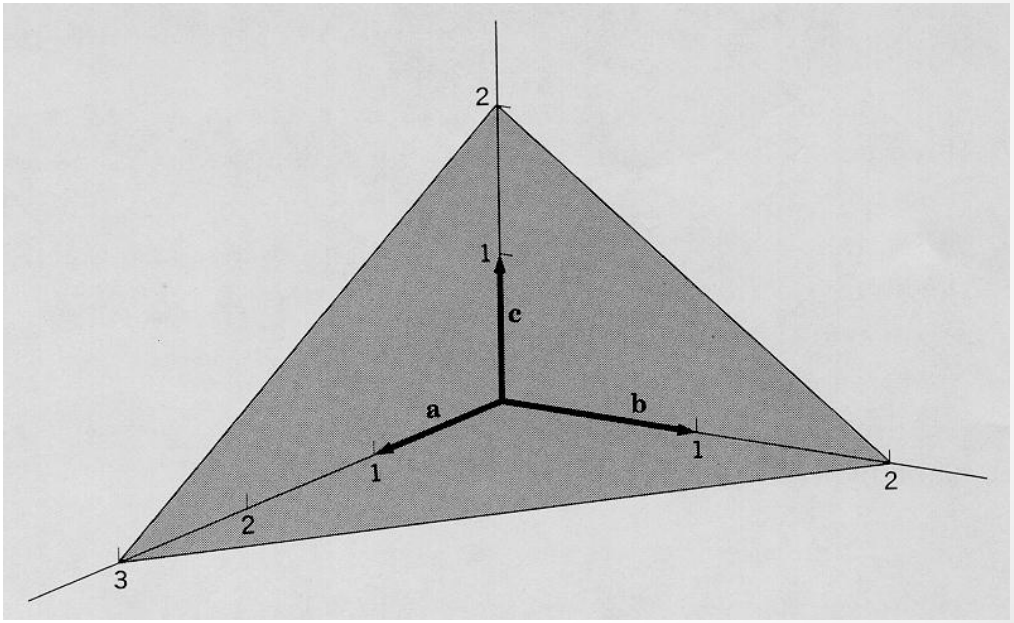
Determine Ratios

- Evaluate axis intercepts
  - Equal to 1/h, 1/k, 1/l
- Invert to find:
  - h, k, l

h = 1/3

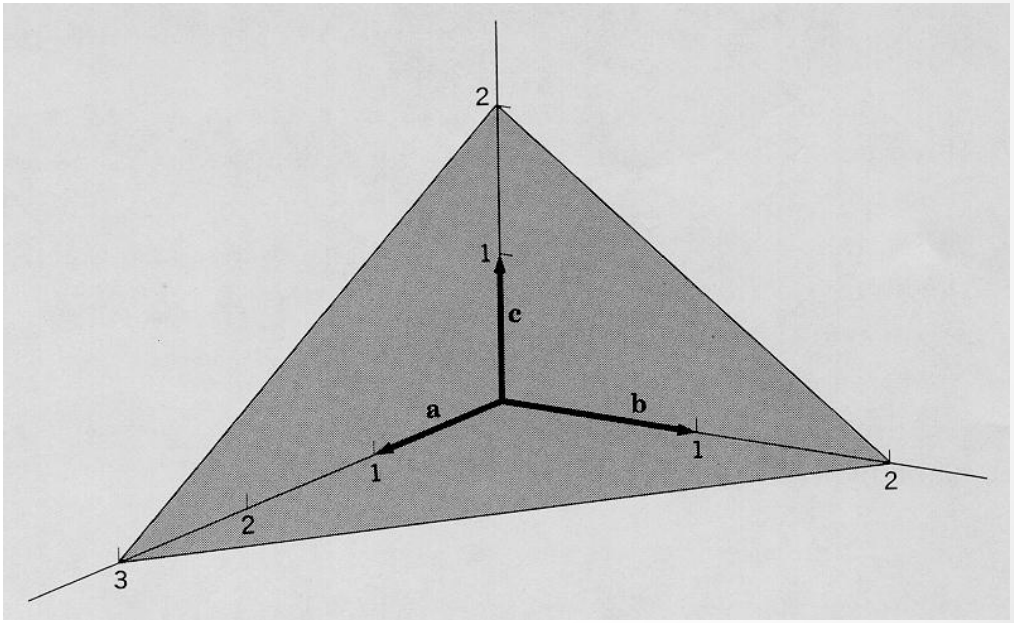
k = 1/2

l = 1/2



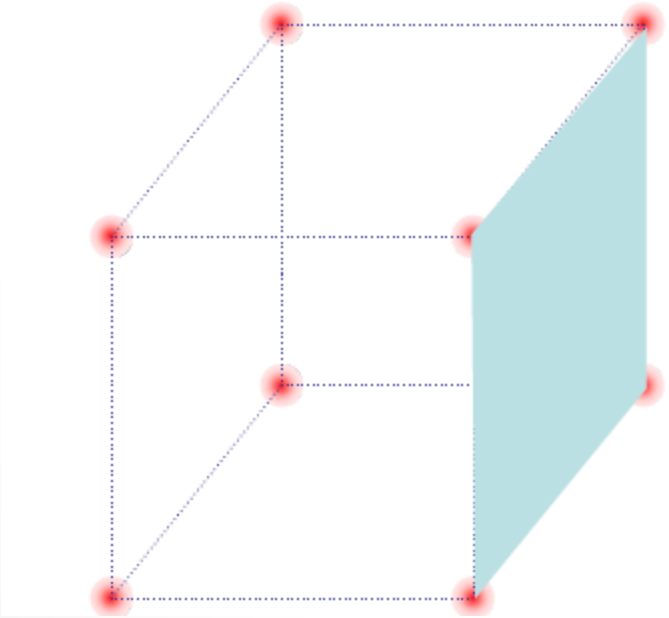
Realization of Indices

- Find smallest integers with same ratio
  - h = 1/3, k = 1/2, l = 1/2
  - h → 2, k → 3, l → 3
- Record index
  - (hkl) = (233)



Planes by Symmetry

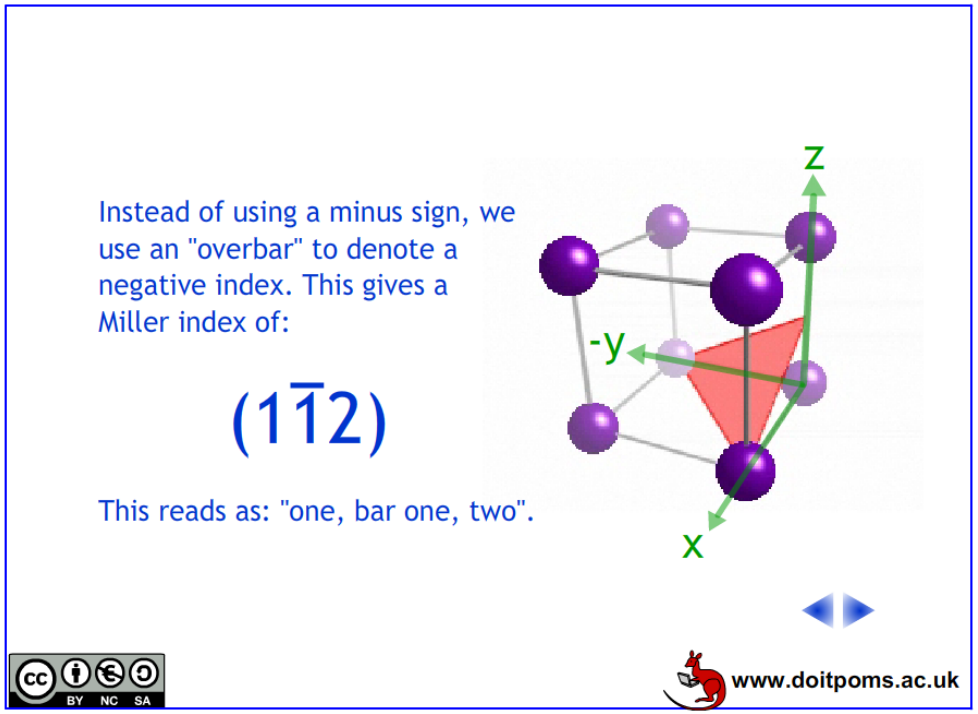
- Planes by symmetry are a ‘family’
- Therefore, {100} consists of (100), (010), (001)



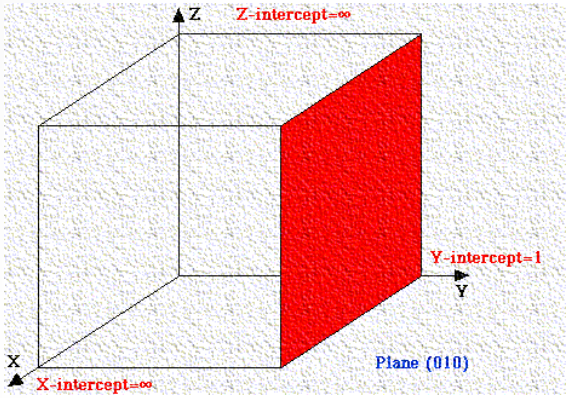
For an isotropic material, (100) is only defined by reference axis

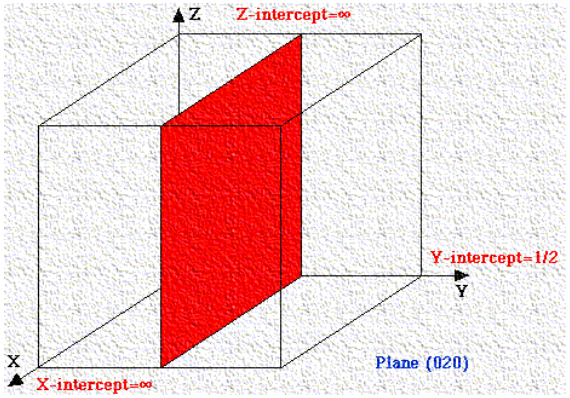
Negative Indices

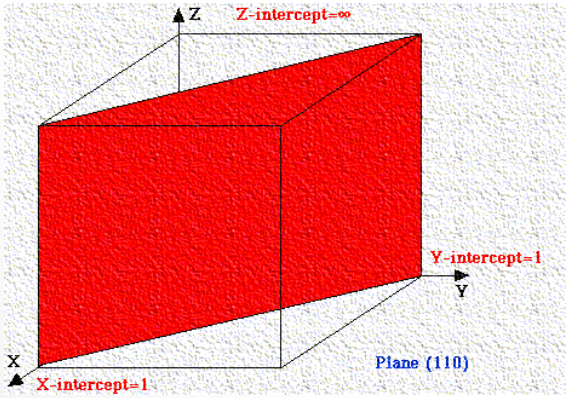
- Leave sign of negative intercept
- Find ratio as normal
- Denote negative with ‘bar’

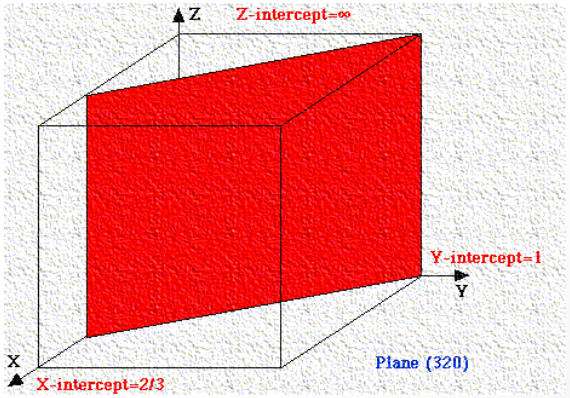


Example of Indices









Applications

- Determine material properties
- Semi-conductor properties depend on structure
- Structure affects energy band-gap
- Band-gap determines wavelengths absorbed/emitted
- Manipulate lattice structure (doping)

References

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