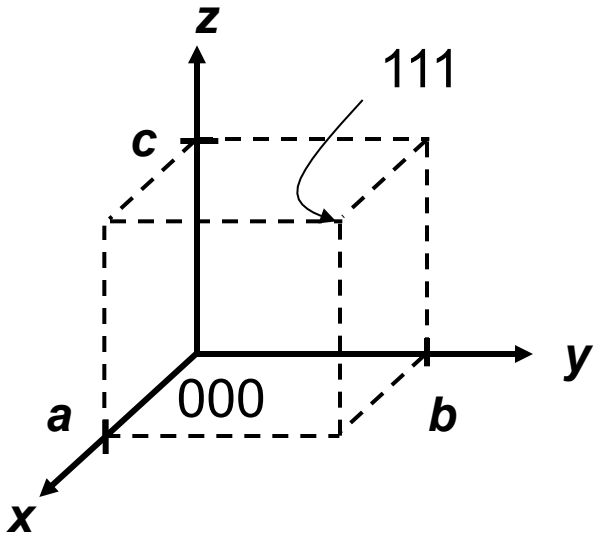
Crystallography revisited

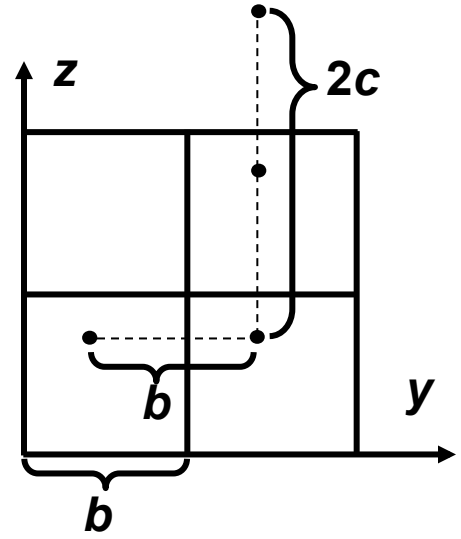
Point coordinates



Point coordinates for unit cell center are: *(a*/2, *b*/2, *c*/2)

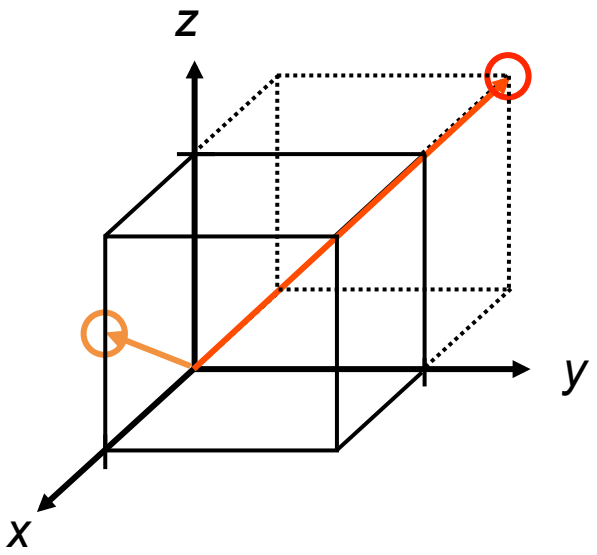
For cubic cells and unit vectors: (½, ½, ½)

and the coordinates for unit cell corner are: (1,1,1)



Translation: integer multiple of lattice constants → identical position in another unit cell

Crystallographic directions



Algorithm

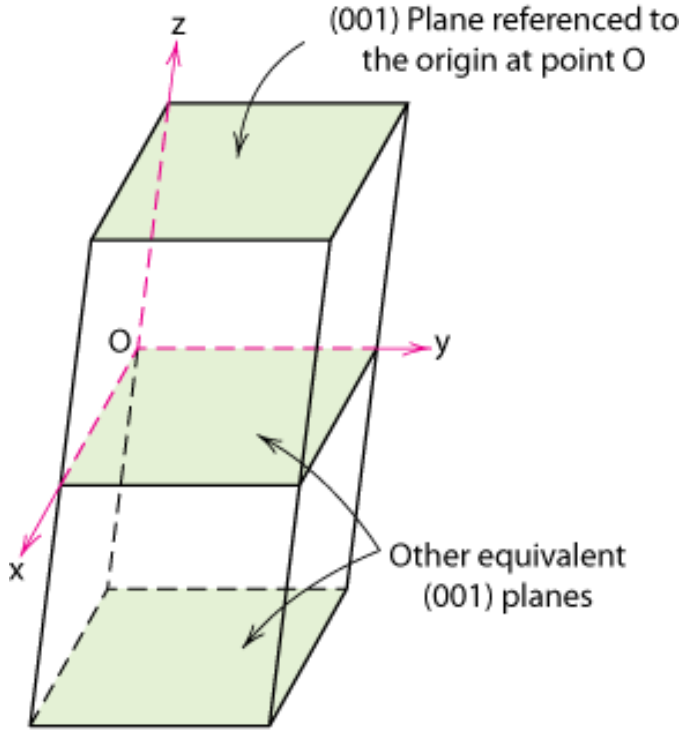
1. Vector repositioned (if necessary) to pass through origin.
2. Read off projections in terms of unit cell dimensions *a*, *b*, and *c*.
3. Adjust to smallest integer values.
4. Enclose in square brackets, no commas: [*uvw*]

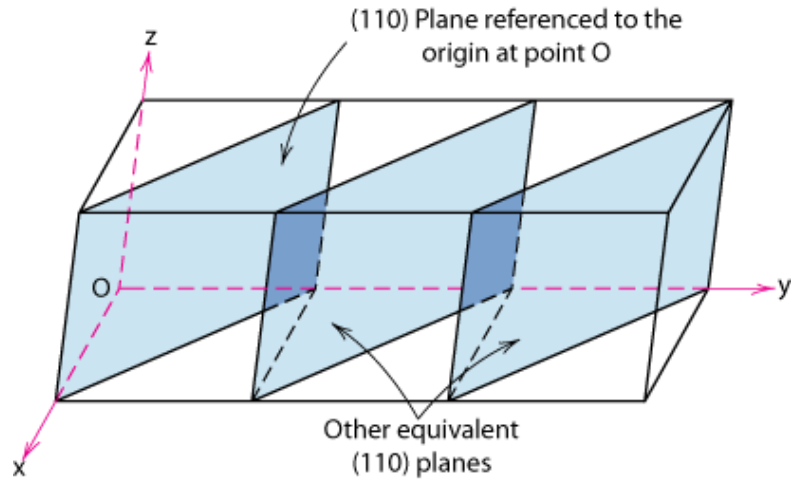
ex: 1, 0, ½ => 2, 0, 1 => [201]

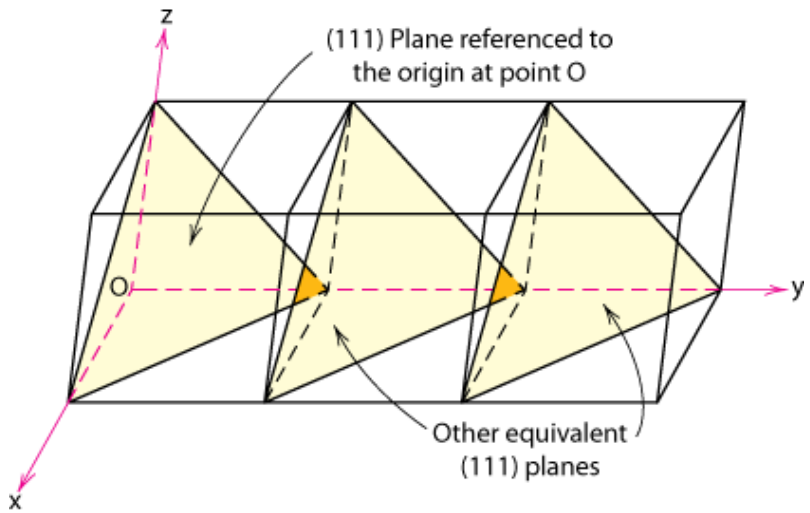
-1, 1, 1 => [$\bar{1}$11] where overbar represents a negative index

Directions of a form: <*uvw*>

Crystallographic planes







Crystallographic planes

Miller indices:

Reciprocals of the (three) axial intercepts for a plane, cleared of fractions & common multiples.

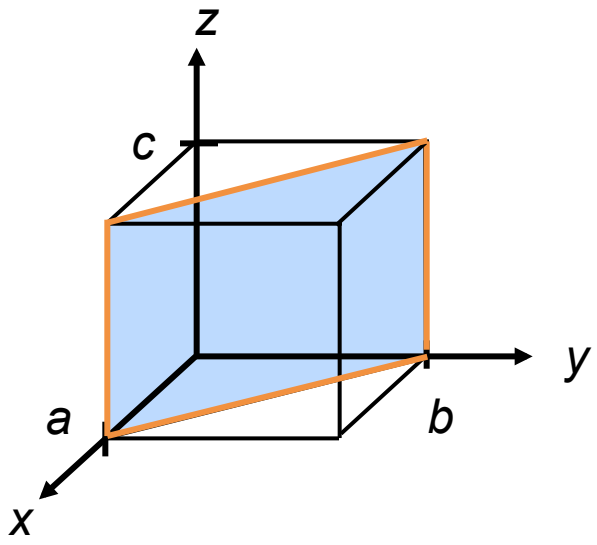
All parallel planes have same Miller indices.

Algorithm

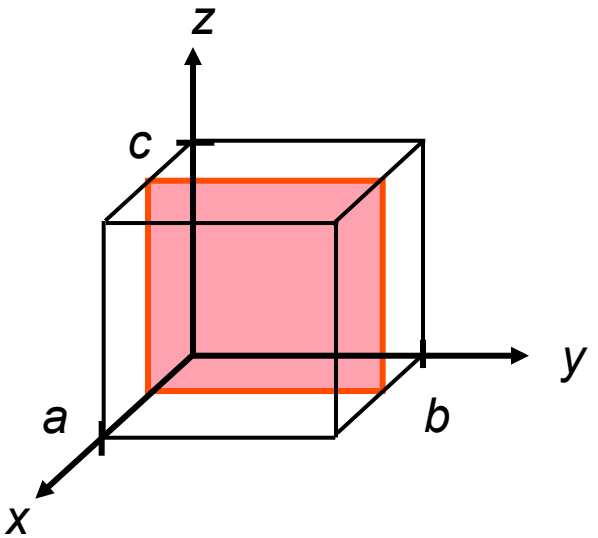
1. Read off intercepts of plane with axes in terms of *a*, *b*, *c.*
2. Take reciprocals of intercepts.
3. Reduce to smallest integer values.
4. Enclose in parentheses, no commas: (*hkl*)

Crystallographic planes

example		*a*	*b*	*c*
1.	Intercepts	1	1	∞
2.	Reciprocals	1/1	1/1	1/∞
		1	1	0
3.	Reduction	1	1	0
4.	Miller Indices	(110)		

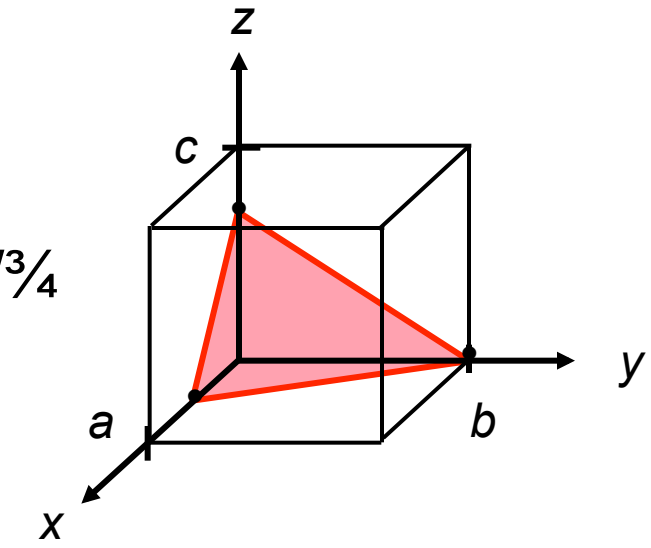


example		*a*	*b*	*c*
1.	Intercepts	1/2	∞	∞
2.	Reciprocals	1/½	1/∞	1/∞
		2	0	0
3.	Reduction	2	0	0
4.	Miller Indices	(100)		



Crystallographic planes

	example	*a*	*b*	*c*
1.	Intercepts	1/2	1	3/4
2.	Reciprocals	1/½	1/1	1/¾
		2	1	4/3
3.	Reduction	6	3	4
4.	Miller Indices	(634)		

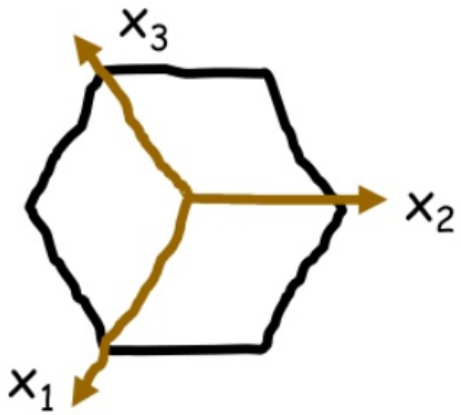


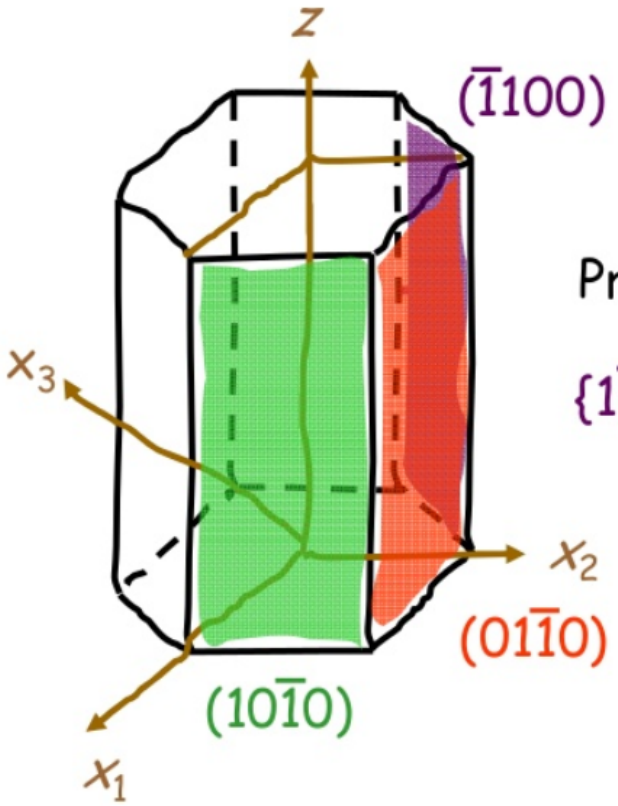
Planes of a form: {*hkl*}

Ex: in cubic systems:
{100} = (100), (010), (001), $(\bar{1}00)$, $(0\bar{1}0)$, $(00\bar{1})$

Crystallographic planes in hexagonal crystals

Introduce a fourth axis in the basal plane





Prismatic planes:

$\{1\bar{1}00\}$ = $(10\bar{1}0)$ $(01\bar{1}0)$ $(\bar{1}100)$

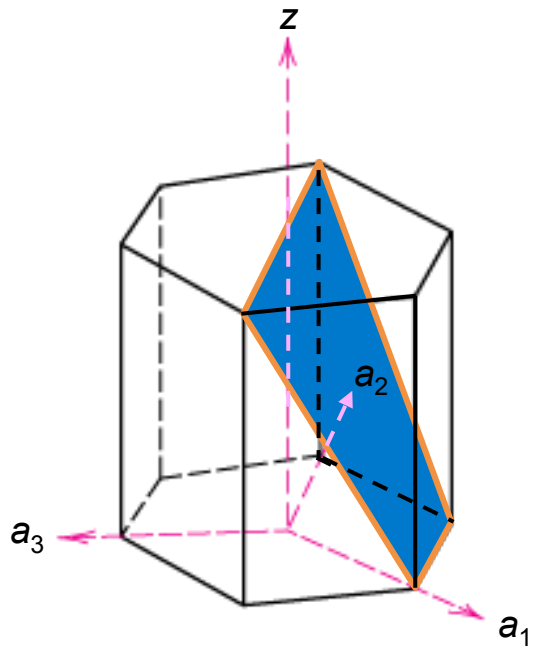
(hkl)=>(hkil) with i=-(h+k)

And with directions? Not so simple see problem 6.

Crystallographic planes in hexagonal crystals

example

		a_1	a_2	a_3	c
1.	Intercepts	1	∞	-1	1
2.	Reciprocals	1	1/∞	-1	1
		1	0	-1	1
3.	Reduction	1	0	-1	1
4.	Miller-Bravais Indices	$(10\bar{1}1)$			



And with directions? Not so simple see problem 6.

Summary of Notation convention for Indices

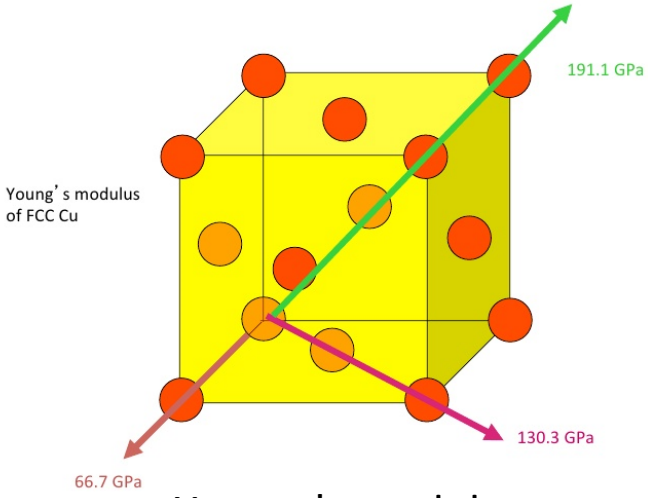
[uvw]	Miller indices of a direction (i.e. a set of parallel directions)
<uvw>	Miller indices of a family of symmetry related directions
(hkl)	Miller Indices of a plane (i.e. a set of parallel planes)
{hkl}	Miller indices of a family of symmetry related planes
[uvtw]	Miller-Bravais indices of a direction,
(hkil)	plane in a hexagonal system

1. Are there grain boundaries in amorphous materials?

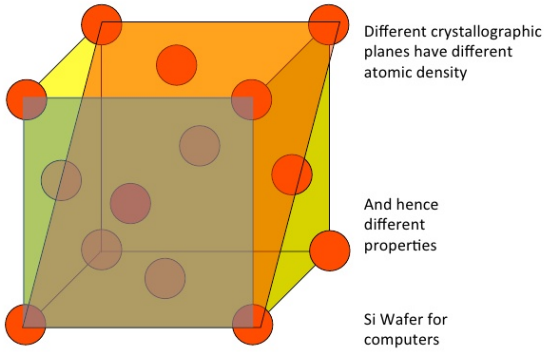
A grain is by definition a monocrystal of reduced dimensions. A grain boundary is the surface between two grains with different crystallographic orientations. Non-crystalline materials (amorphous materials) are not constituted by grains and therefore cannot present grain boundaries.

2. Can crystalline solids be isotropic?

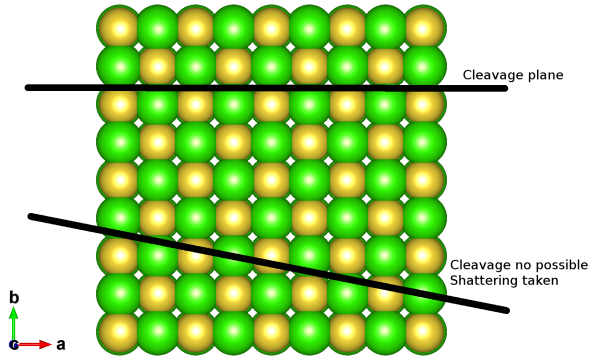
Crystallographic anisotropy is the dependence of property values with the crystallographic orientation taken. This dependence results from composition and interatomic distance differences. Therefore **crystalline solids exhibit intrinsic anisotropic** in many of their properties.



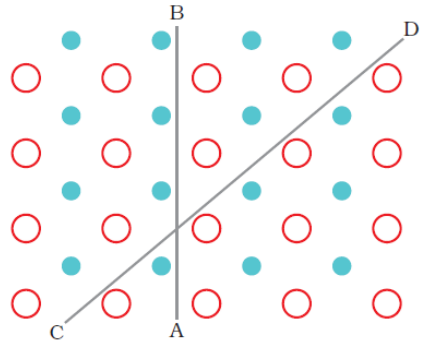
Youngs's modulus



Conductivity



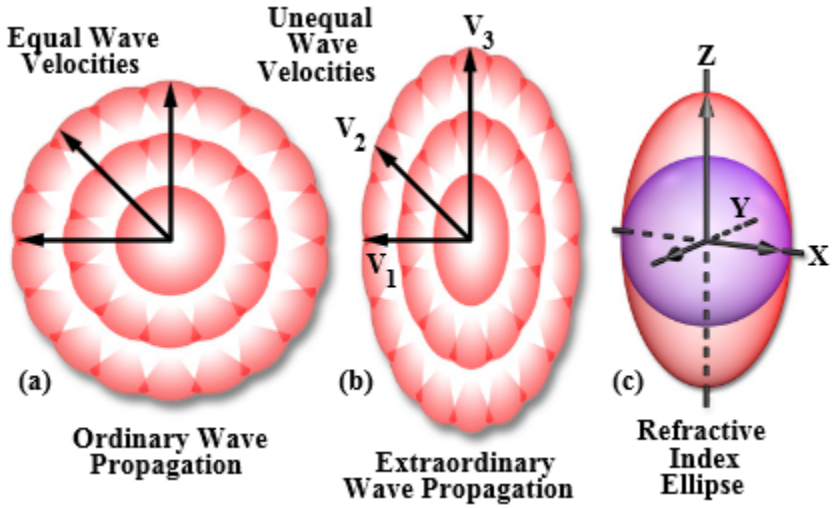
Fracture behavior



Different compositions…

2. Can crystalline solids be isotropic?

Optical properties are isotropic in cubic materials.



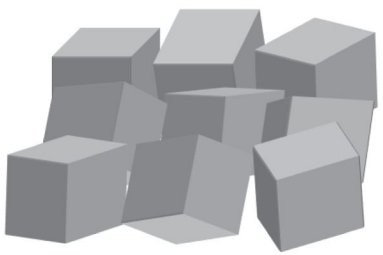
The propagation of waves through an isotropic crystal occurs at constant velocity because the refractive index experienced by the waves is uniform in all directions (a). In contrast, the expanding wavefront may encounter refractive index variations as a function of direction (b) that can be described by the surface of an ellipsoid of revolution.

Non-cubic crystals exhibit often (b),(c) behavior

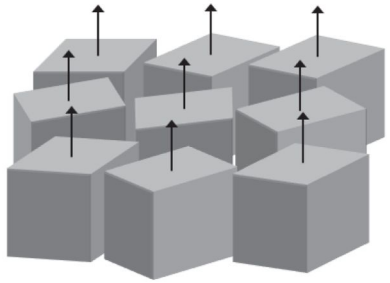
2. Can crystalline solids be isotropic?

Random crystallographic orientation in polycrystals results in isotropy.

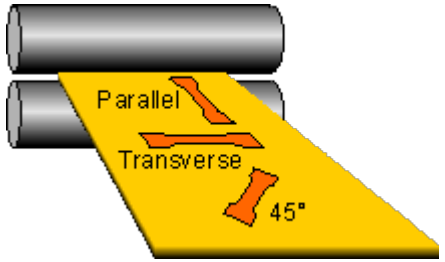
Preferred crystallographic orientation (texture) results in anisotropy.

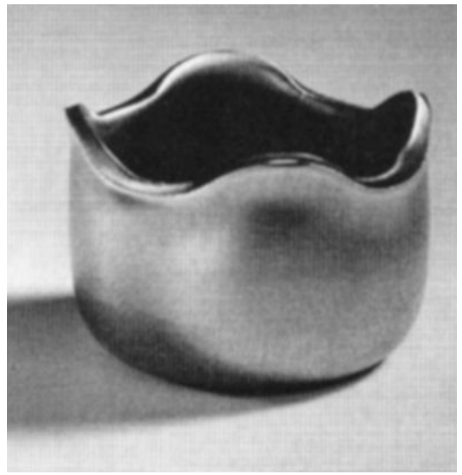


Random



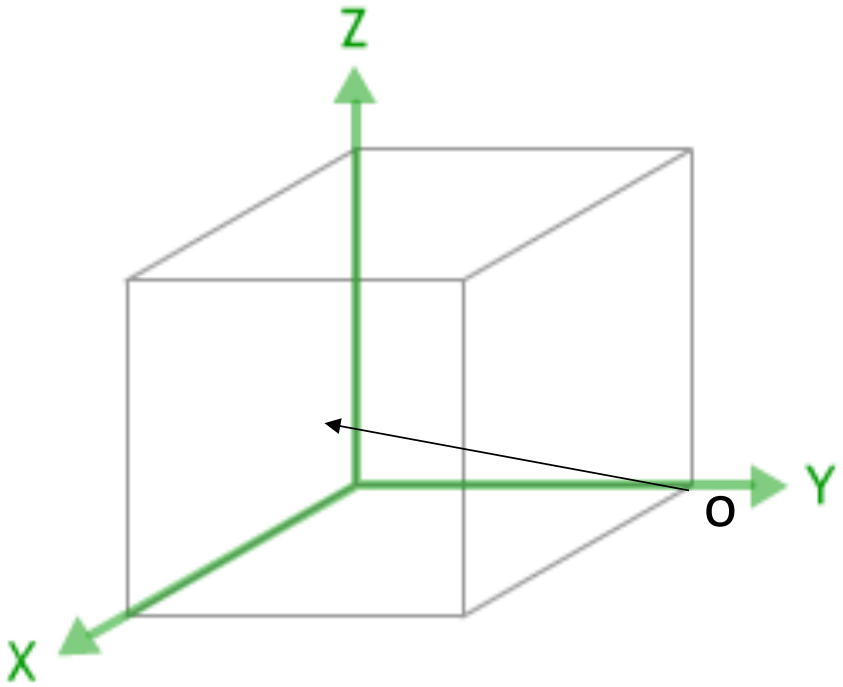
Fiber texture

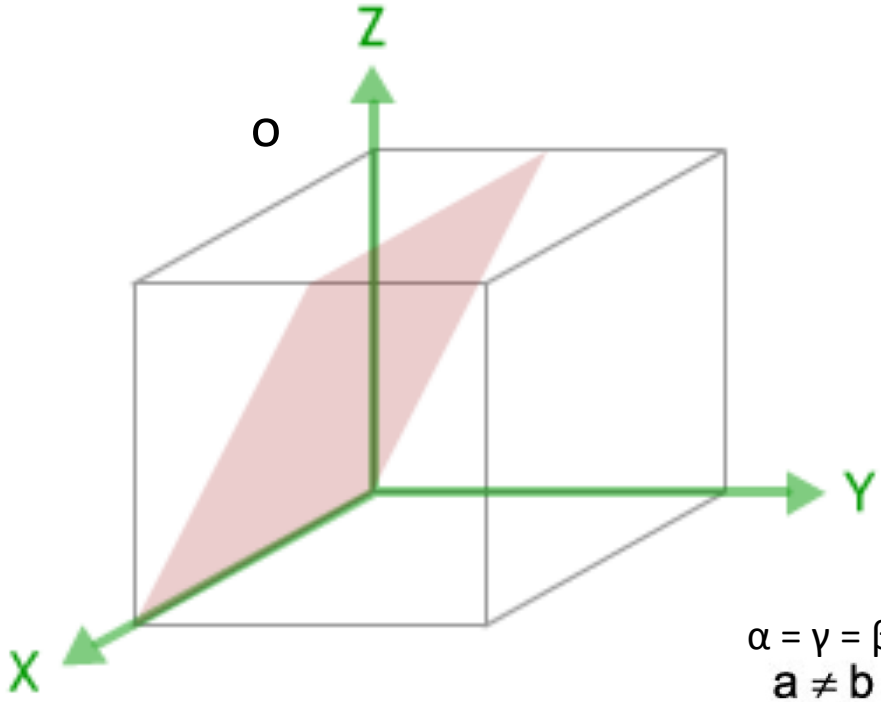




Deep drawn cup where plastic anisotropy in the sheet plane resulted in non-uniform deformations ("ears").

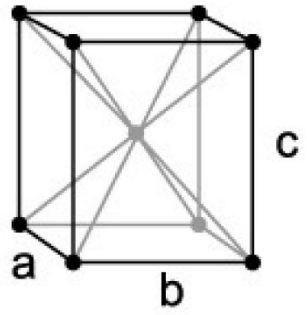
3. Sketch the $[2\bar{1}1]$ direction and the $(02\bar{1})$ plane in an orthorhombic cell.





$\alpha = \gamma = \beta = 90^{o}$

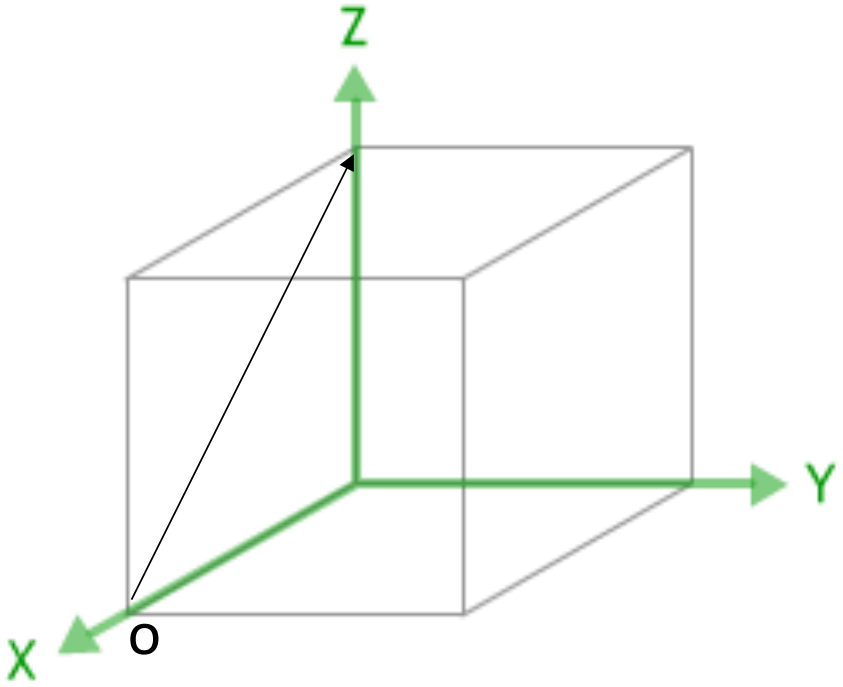
$a \neq b \neq c$

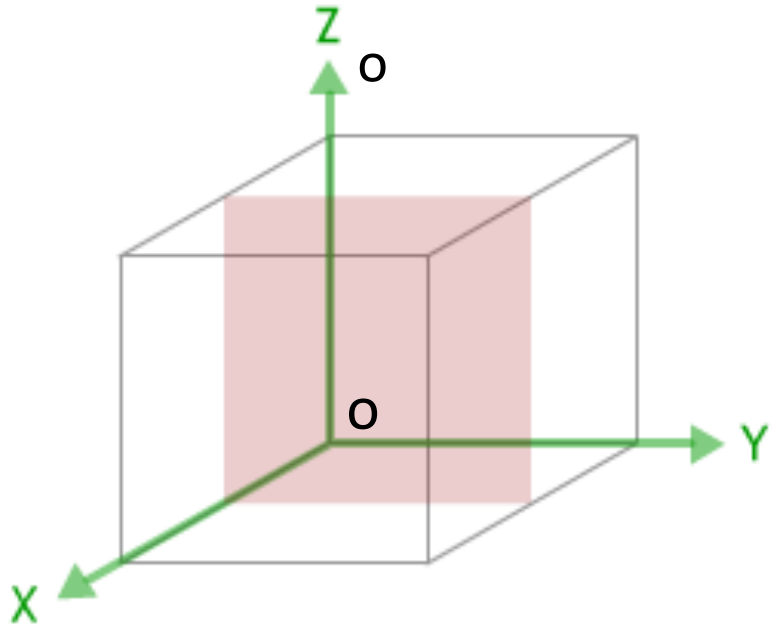


Same way as in a cubic cell…

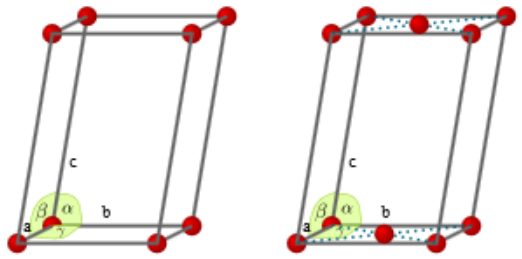
I centering in this drawing

4. Sketch the $[\bar{1}01]$ direction and the (200) plane in an monoclinic cell.





Same way as in a cubic cell…

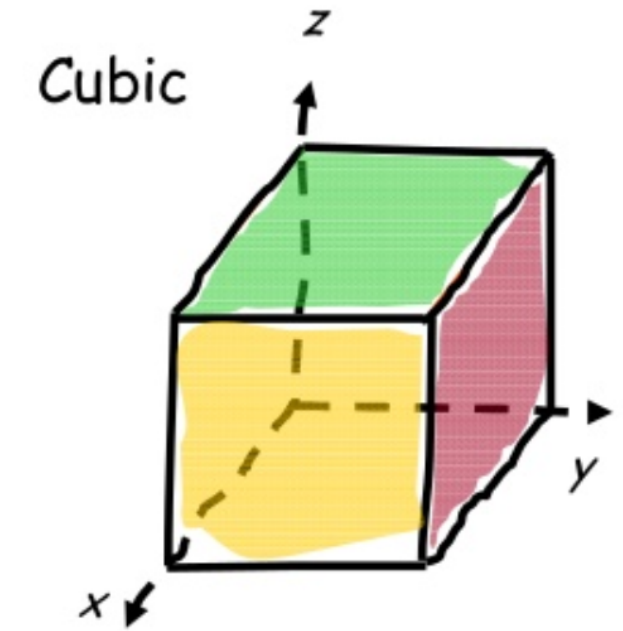


$\alpha = \gamma = 90^{o} \neq \beta$

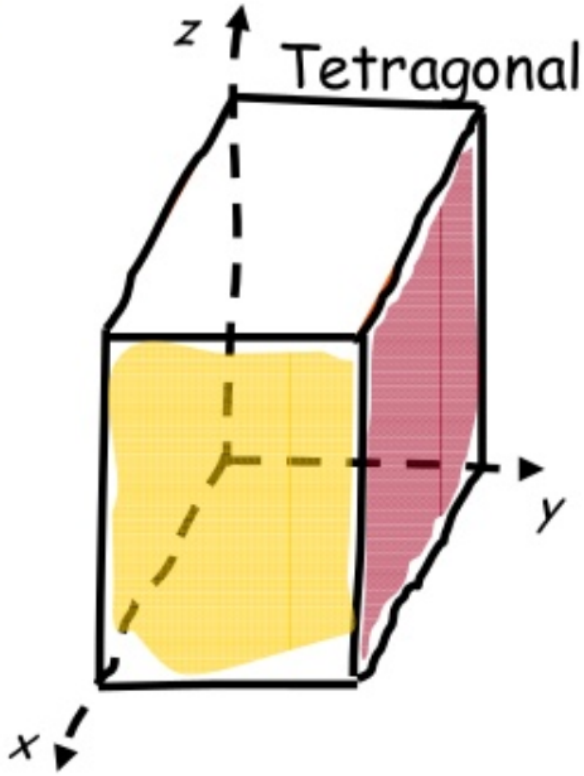
5. Planes and directions of a form in tetragonal cells

Be wary of different designations (of a form)…

Miller indices of a family of symmetry related planes



$\{100\}_{cubic}$ = (100), (010), (001)



$\{100\}_{tetragonal}$ = (100), (010)

~~(001)~~

5.a In tetragonal crystals which are the directions of the [011] form?

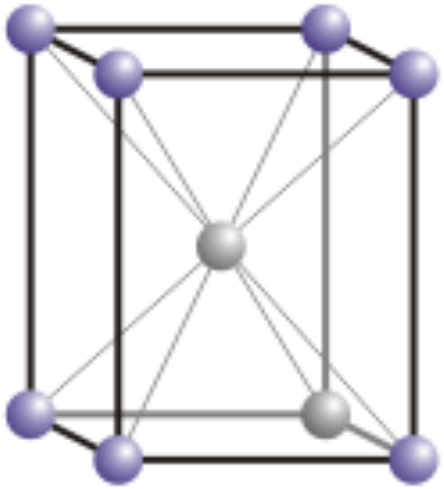
[011] [01$\bar{1}$]

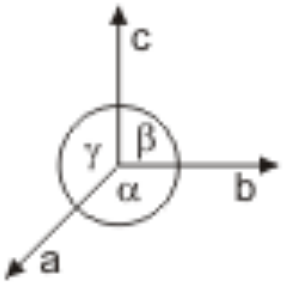
[0$\bar{1}$1] [0$\bar{1}\bar{1}$]

[101] [10$\bar{1}$]

[$\bar{1}$01] [$\bar{1}$0$\bar{1}$]

$\in$ <011>





a=b≠c

α=β=γ=90°

I centering in this drawing

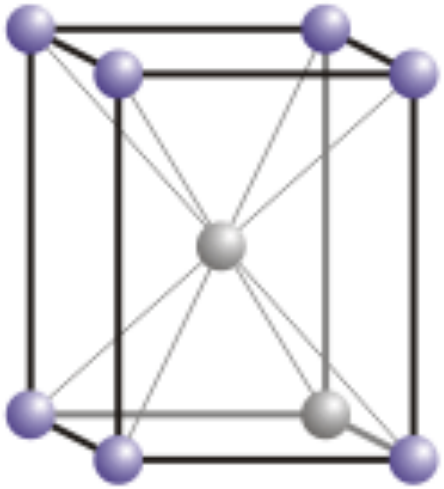
From hkl only h and k are permutable

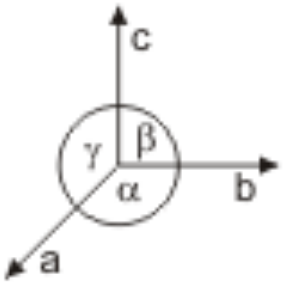
5.b In tetragonal crystals which are the planes of the (100) form?

(100) $(\bar{1}00)$

(010) $(0\bar{1}0)$

$\in$ {100}





a=b≠c

α=β=γ=90°

I centering in this drawing

From hkl only h and k are permutable

6.(a) Determine the relation between zone axis indices (3-D) and Weber indices (4-D, expressly defined for hexagonal unit cells)

Be wary of different designations (Weber)…

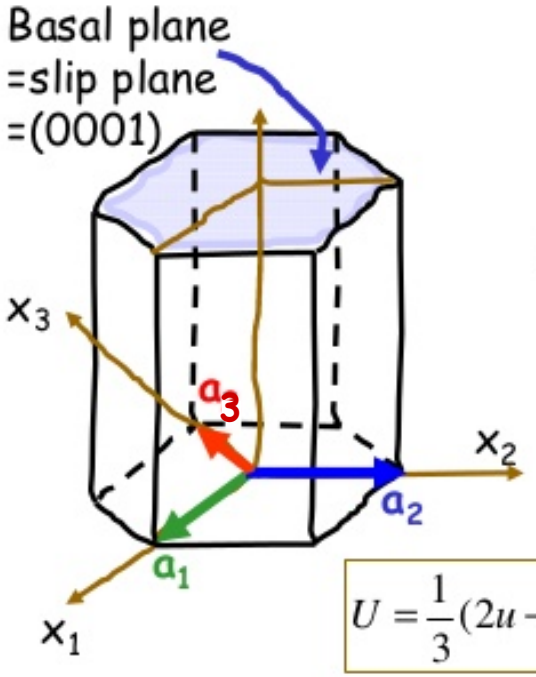
Miller-Bravais Indices of Directions in hexagonal crystals

$$[uvw] \equiv [UVTW]$$

Vectorially $\mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3 = \mathbf{0}$

Replace $\mathbf{a}_3$ and T

Require that: $U + V + T = 0$



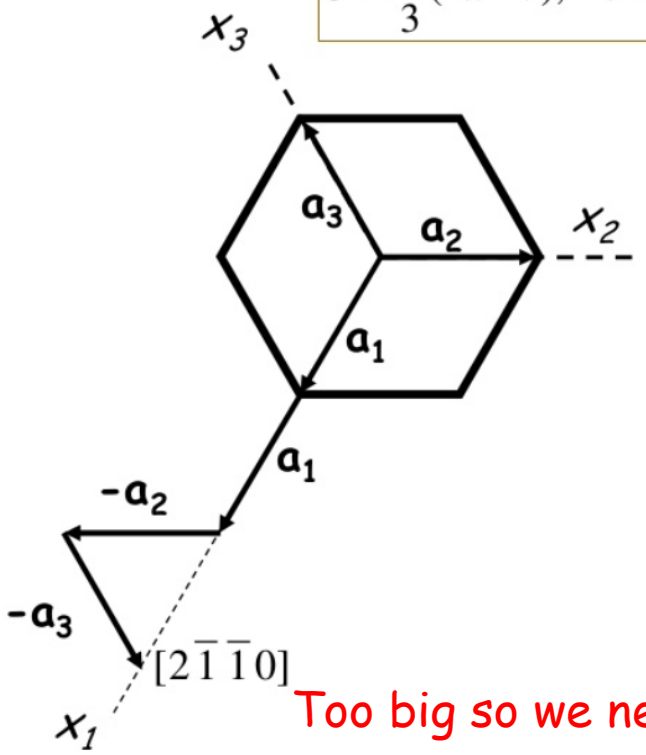
$$U\mathbf{a}_1 + V\mathbf{a}_2 + T\mathbf{a}_3 + W\mathbf{c} = u\mathbf{a}_1 + v\mathbf{a}_2 + w\mathbf{c}$$

$$U = \frac{1}{3}(2u - v); \quad V = \frac{1}{3}(2v - u); \quad T = -(u + v); \quad W = w$$

6.(b) Convert the zone axis indices $[1\,1\,0]$ and $[0\,0\bar{1}]$ into Weber indices. Convert the $(1\,1\,1)$ and $(0\bar{1}2)$ Miller indices into Miller-Bravais indices.

For the axes:

$$U=\frac{1}{3}(2u-v);\quad V=\frac{1}{3}(2v-u);\quad T=-(u+v);\quad W=w$$



x_1: $[100]\Rightarrow\left[\frac{2}{3}\ -\frac{1}{3}\ -\frac{1}{3}\ 0\right]\equiv[2\,\bar{1}\,\bar{1}\,0]$

x_2: $[010]\Rightarrow\left[-\frac{1}{3}\ \frac{2}{3}\ -\frac{1}{3}\ 0\right]\equiv[\bar{1}\,2\,\bar{1}\,0]$

x_3: $[\bar{1}\,\bar{1}\,0]\Rightarrow\left[-\frac{1}{3}\ -\frac{1}{3}\ \frac{2}{3}\ 0\right]\equiv[\bar{1}\,\bar{1}\,2\,0]$

Too big so we need to divide by 3!

For the directions:

$[110]\equiv[11\bar{2}0]$

$[00\bar{1}]\equiv[000\bar{1}]$

For the planes:

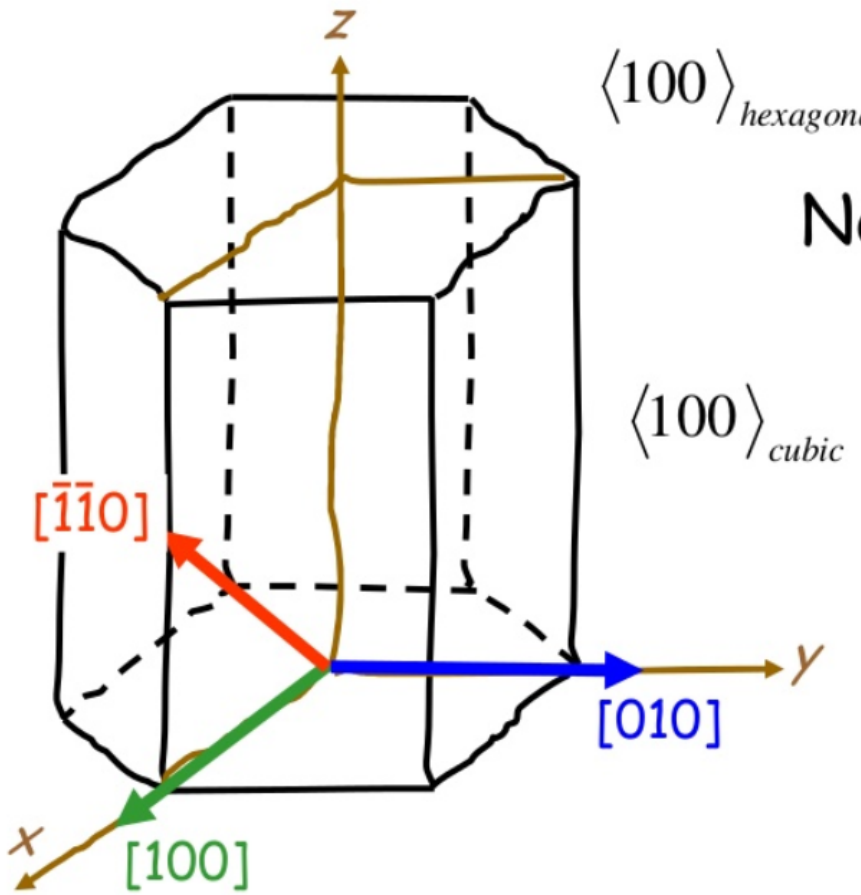
$(111)\equiv(11\bar{2}1)$

$(0\bar{1}2)\equiv(0\bar{1}12)$

6.(c) What is the utility of the 4 indices?

Or why the additional complication?!

Symmetry related directions in the hexagonal crystal system



$\langle 100 \rangle_{hexagonal}$ = [100], [010], [$\bar{1}\bar{1}$0]

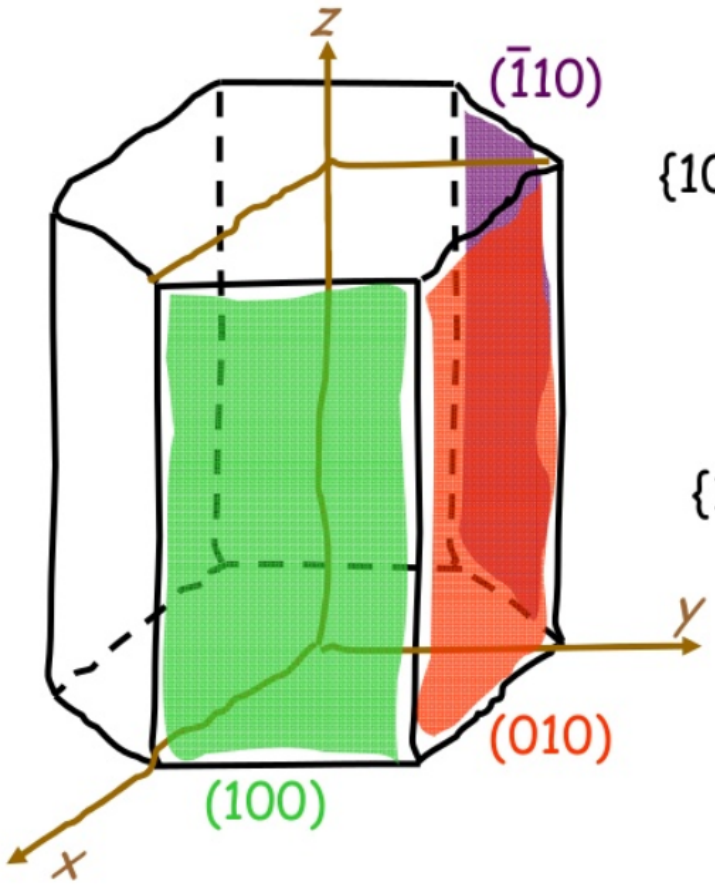
Not permutations

$\langle 100 \rangle_{cubic}$ = [100], [010], [001]

Permutations

6.(c) What is the utility of the 4 indices?

Symmetry related planes in the hexagonal crystal system



$\{100\}_{hexagonal}$ = (100), (010),(1̄10)

Not permutations

$\{100\}_{cubic}$ = (100), (010), (001)

Permutations

6.(c) What is the utility of the 4 indices?

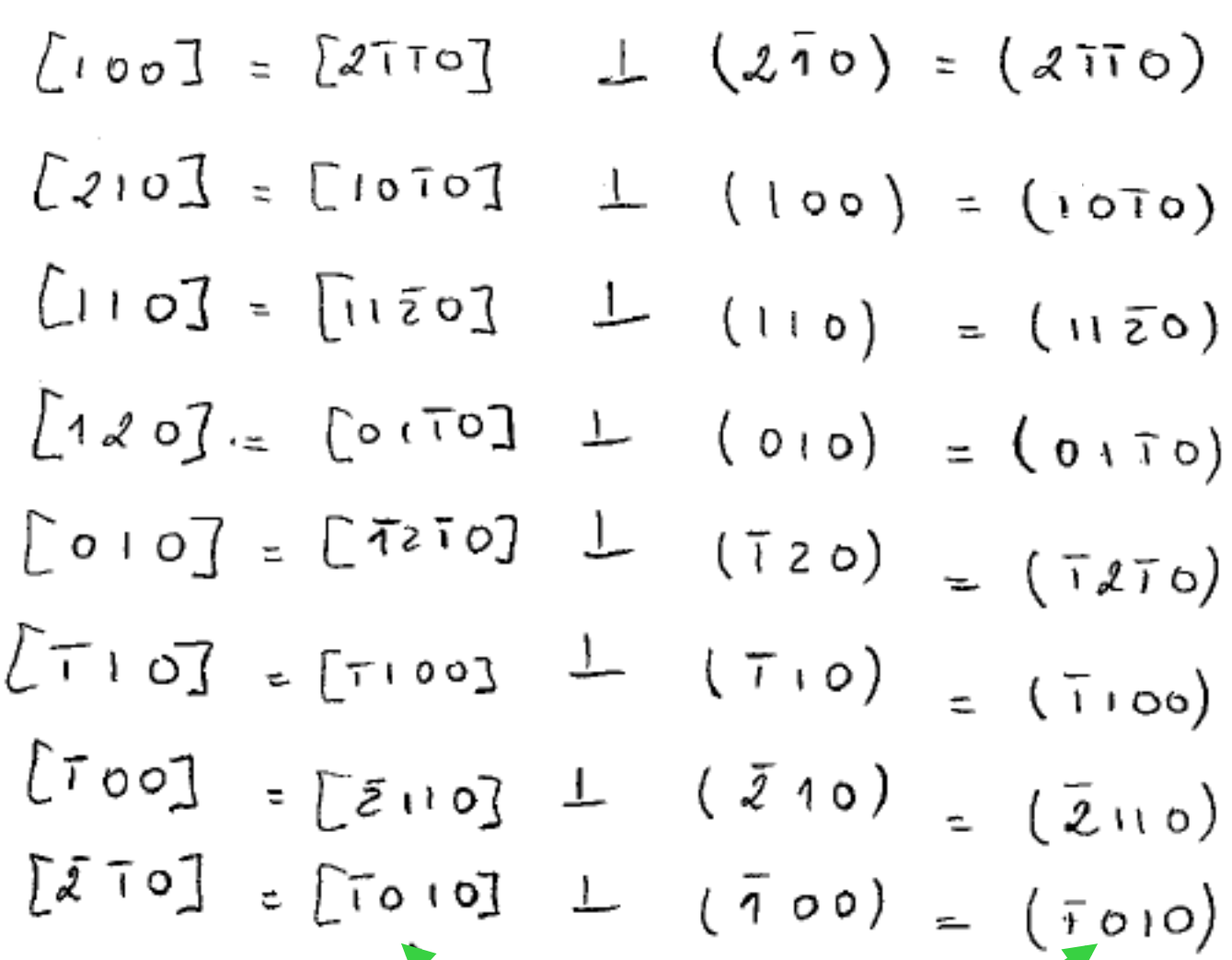
Problem:

In hexagonal system symmetry related planes and directions do ***NOT*** have Miller indices which are *permutations*

Solution:

Use the four-index Miller-Bravais Indices instead

6.(c) What is the utility of the 4 indices?



Planes or directions 'of the form'?

Only permutations of the first 3 indices are allowed.

Normals to planes? As in cubic as long as l is zero.

[1$\bar{2}$13] ✗ (1$\bar{2}$13)

i.e. valid only for prismatic planes not for pyramidal ones.

relations?

easy to see in 4 indices...

To practice

http://www.doitpoms.ac.uk/tlplib/miller_indices/index.php