

MEAM/MSE 507

Fundamentals of Materials

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Week 4, Lecture 4: Crystallographic notation (part 2)
Asynchronous

Space group notation

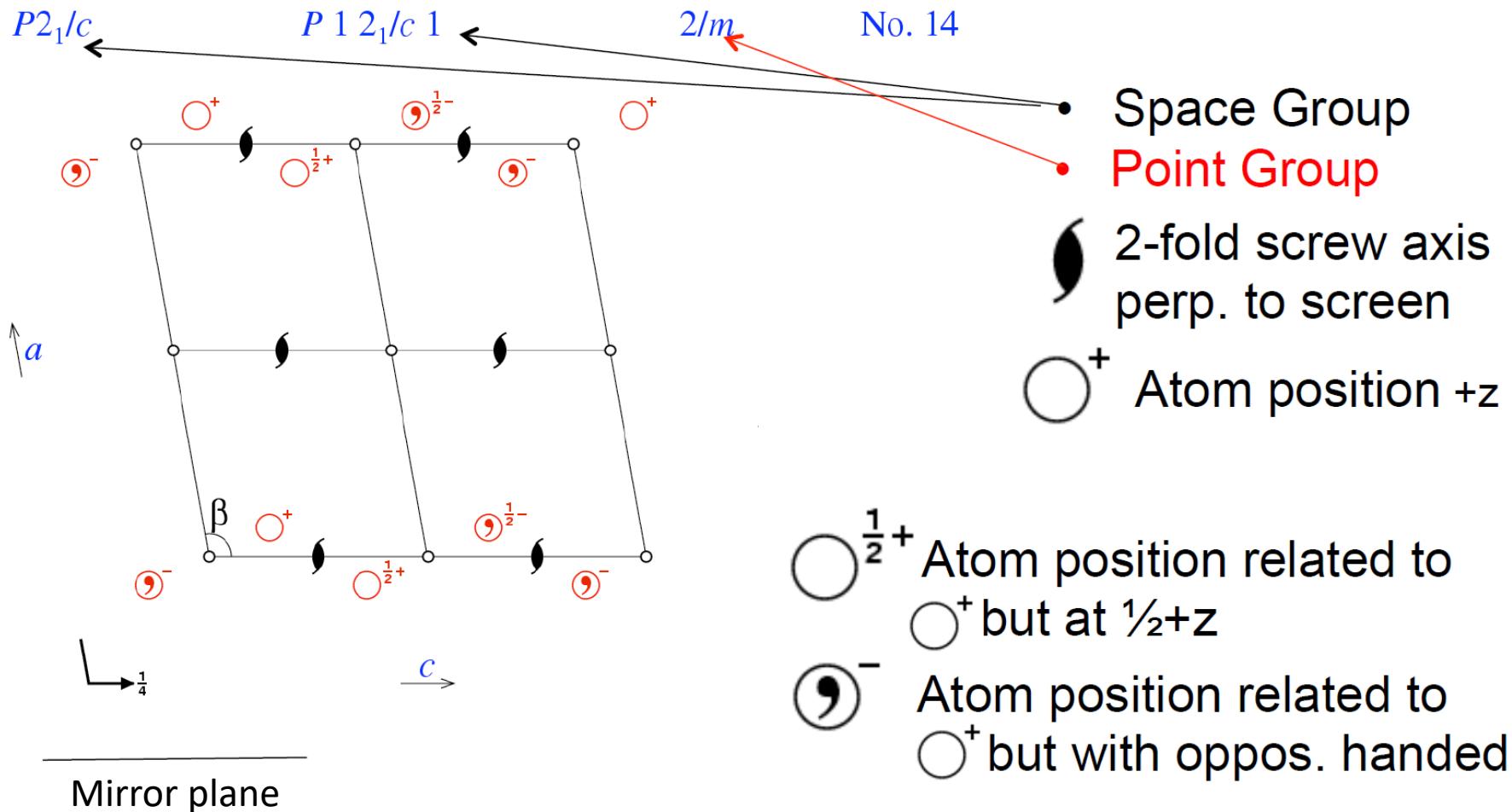
Space group =

- Point group + translations (including screws & glides)
- Several different systems (use Hermann-Mauguin)
- 1st letter: P (primitive), A,B,C (single face centered), F (all face centered), I (body centered), R (rhombohedrally centered)
- Triclinic P1, P $\overline{1}$
- Monoclinic P2, Pm, P2/m
 - the space group symbol indicates the symmetry with respect to the unique axis direction
- Orthorhombic P222, Pmm2, Pm2m, P2mm, Pmmm
 - the 3 indices indicate symmetry w.r.t. x, y, and z-axes

Space group notation

- Tetragonal $P4$, $P\bar{4}$, $P4/m$, $P422$, $P4mm$, $P4\bar{2}m$, $P4\bar{m}2$, $P4/mmm$
 - the 4-fold symmetry is always chosen to lie parallel to the z-axis (1st index)
 - the second and third indices refer to the x and y-axes
 - the remaining symbol refers to symmetry with respect to both of the diagonals between the x and y-axes
- Trigonal / Rhombohedral $P3$, $P\bar{3}$, $P321$, $P312$, $P31m$, $P\bar{3}m1$, $P\bar{3}\bar{1}m$
 - the 3-fold symmetry lies parallel to the z-axis
 - additional elements lie parallel to the x, y-axes or perpendicular to them
- Hexagonal $P6$, $P\bar{6}$, $P6/m$, $P622$, $P6mm$, $P\bar{6}2m$, $P\bar{6}m2$, $P6/mmm$
 - like trigonal except that the symmetry w.r.t., z-axis is order 6
- Cubic $P23$, $Pm\bar{3}$, $P432$, $P\bar{4}3m$, $Pm3m$
 - 1st index is parallel to x,y,z-axes
 - 2nd index refers to body diagonals
 - 3rd index, refers to face diagonals

International Tables for Crystallography



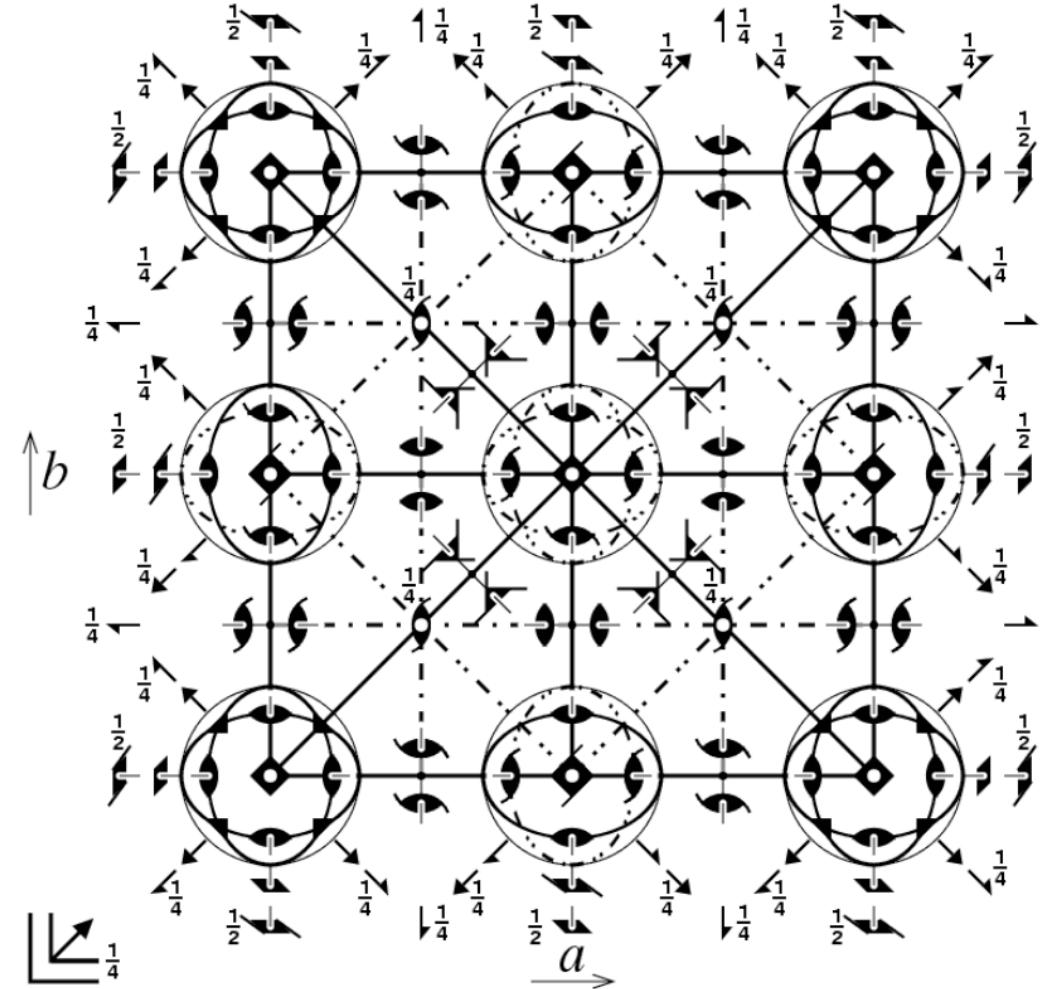
Body Centered Cubic

$Im\bar{3}m$

$I4/m \bar{3}2/m$

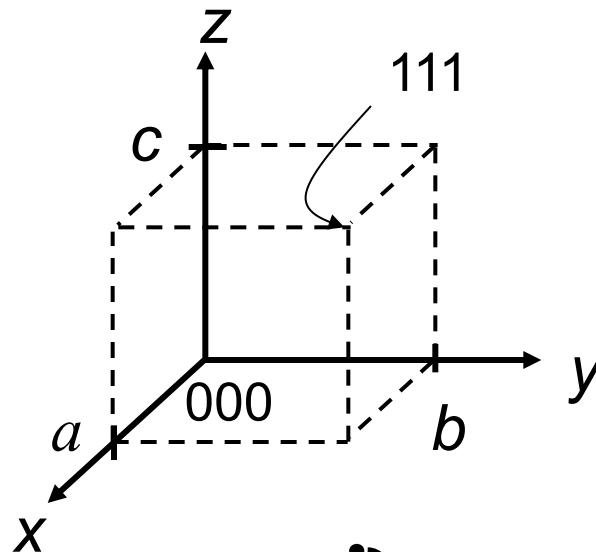
$m\bar{3}m$

No. 229



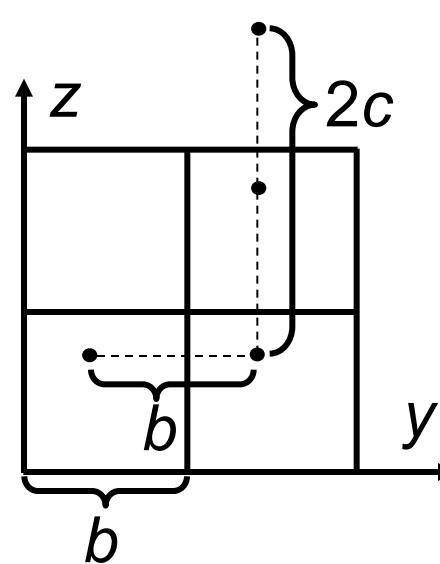
E.g., number 229 – You can look up specific symmetries in international crystallography catalogs.

Point coordinates



Point coordinates for unit cell center are

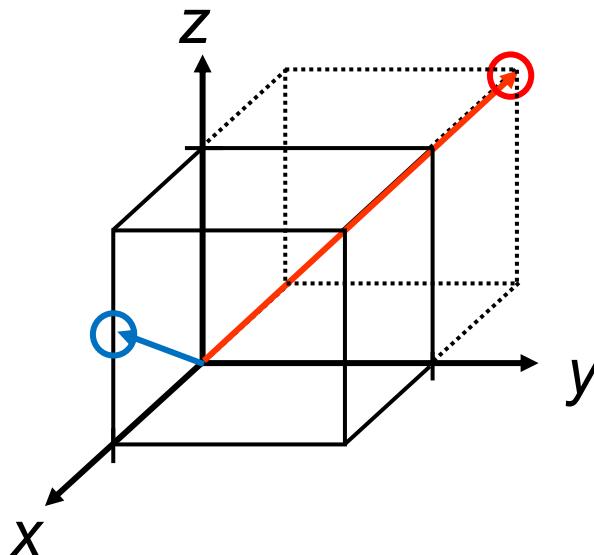
$$a/2, b/2, c/2 \quad \frac{1}{2} \frac{1}{2} \frac{1}{2}$$



Point coordinates for unit cell corner are 111

Under translation: integer multiple of lattice constants \rightarrow 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: $1, 0, \frac{1}{2} \rightarrow 2, 0, 1 \rightarrow [201]$

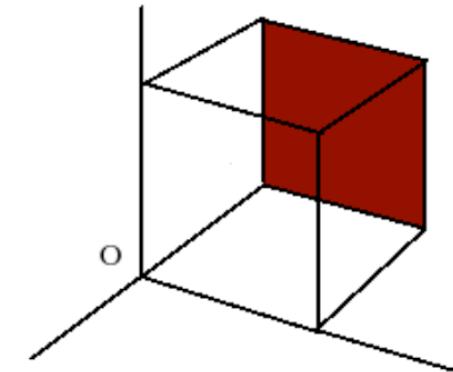
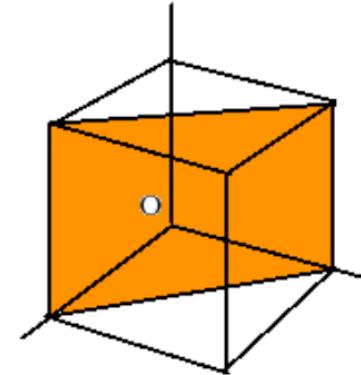
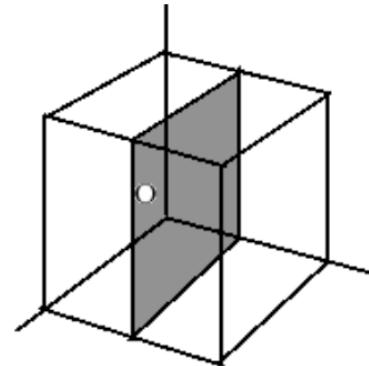
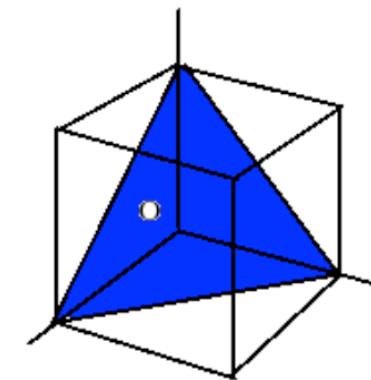
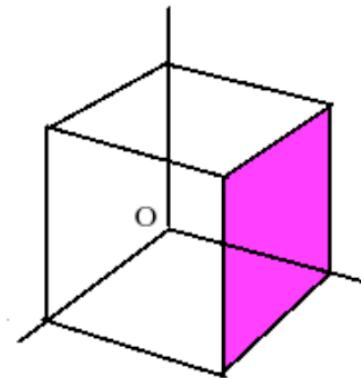
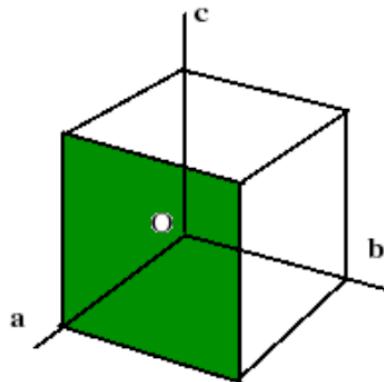
$-1, 1, 1 \rightarrow [\bar{1}\bar{1}1]$ bar represents a negative index

families of directions $\langle uvw \rangle$

NOTE: all members of a family of directions are equivalent. In a cubic crystal $\langle 110 \rangle$ includes $[110]$, $[101]$, $[011]$, $[1\bar{1}0]$, $[10\bar{1}]$, $[01\bar{1}]$ but in a tetragonal crystal $a=b \neq c$, $\langle 101 \rangle$ includes only $[101]$, $[011]$, $[01\bar{1}]$ and $[10\bar{1}]$ or $\langle 110 \rangle : [110] \text{ and } [\bar{1}\bar{1}0]$

Crystallographic planes

- A plane is indexed (hkl) according to its normal direction [hkl]



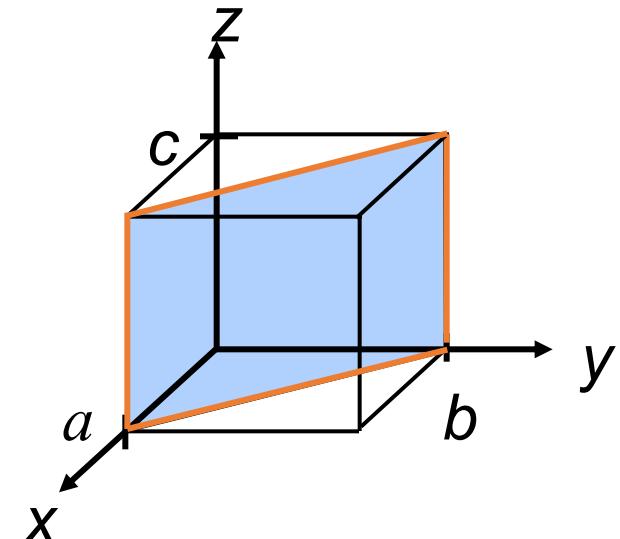
Crystallographic planes

- Miller Indices: Reciprocals of the (three) axial intercepts for a plane, cleared of fractions & common multiples.
- 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 i.e., (hkl)

Crystallographic planes

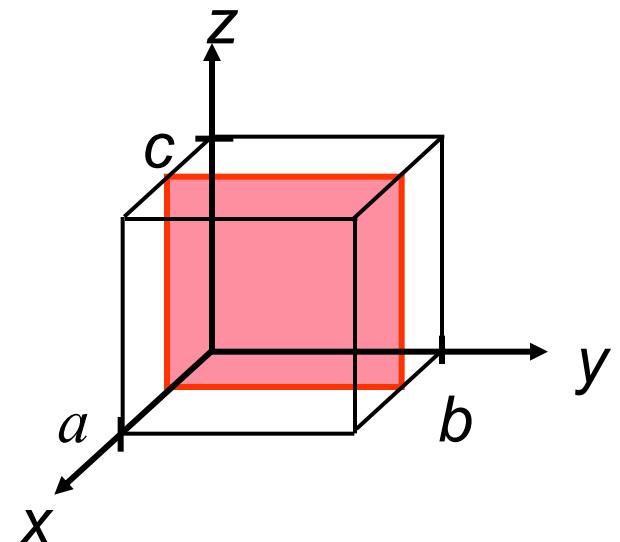
example

	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

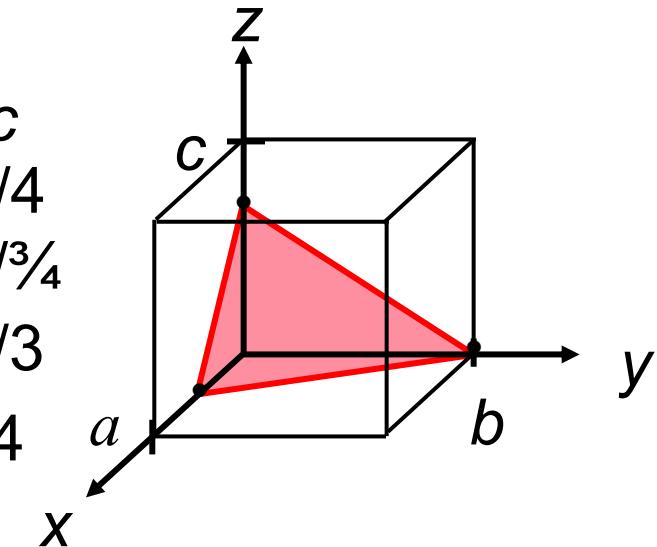
	a	b	c
1. Intercepts	1/2	∞	∞
2. Reciprocals	1/½	1/ ∞	1/ ∞
	2	0	0
3. Reduction	2	0	0
4. Miller Indices	(200)		



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)		



Family of Planes $\{hk\}$

Ex: $\{110\} = (101), (110), (011), (10\bar{1}), (\bar{1}\bar{1}0), (0\bar{1}\bar{1})$

Why no $(\bar{1}0\bar{1})$ or $(\bar{1}01)$?

