PHY 745 Group Theory
11-11:50 AM MWF Olin 102

Plan for Lecture 16:

Introduction to space groups

Reading: Chapter 9 in DDJ

1. **Definition and scope of space groups**
2. **Terminology**
3. **Examples**

This lecture contains some materials from an electronic version of the DDJ text.

9	Wed: 02/01/2017	Chap. 8	Vibrational excitations	#7	02/03/2017
10	Fri: 02/03/2017	Notes	Continuous groups	#8	02/06/2017
11	Mon: 02/06/2017	Notes	Group of three-dimensional rotations	#9	02/08/2017
12	Wed: 02/08/2017	Notes	Continuous groups	#10	02/10/2017
13	Fri: 02/10/2017	Chap. 5	Atomic orbitals	#11	02/13/2017
14	Mon: 02/13/2017	Chap. 6	Direct product groups	#12	02/15/2017
15	Wed: 02/15/2017	Chap. 7	Molecular orbital	#13	02/17/2017
16	Fri: 02/17/2017	Chap. 9	Introduction to Space Groups	#14	02/20/2017
17	Mon: 02/20/2017				
18	Wed: 02/22/2017				
19	Fri: 02/24/2017				
20	Mon: 02/27/2017				Exam
21	Wed: 03/01/2017				Exam
22	Fri: 03/03/2017				Exam Due
	Mon: 03/06/2017		*Spring break - no class*		
	Wed: 03/08/2017		*Spring break - no class*		
	Fri: 03/10/2017		*Spring break - no class*		
	Mon: 03/13/2017		*APS Meeting - no class*		
	Wed: 03/15/2017		*APS Meeting - no class*		
	Fri: 03/17/2017		*APS Meeting - no class*		
23	Mon: 03/20/2017				
24	Wed: 03/22/2017				

Comment on character analysis of iC_n for angular momentum basis functions

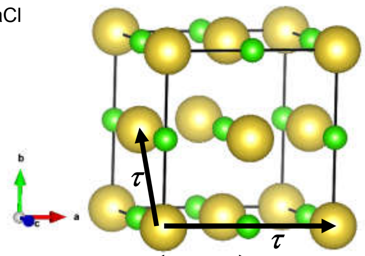
$$Y_{lm}(-\hat{\mathbf{r}}) = (-1)^l Y_{lm}(\hat{\mathbf{r}})$$

$$\Rightarrow \chi^l(C_n) = \left.\frac{\sin\left(\left(l+\frac{1}{2}\right)\alpha\right)}{\sin(\alpha/2)}\right]_{\alpha=2\pi/n}$$

$$\Rightarrow \chi^l(iC_n) = (-1)^l \left.\frac{\sin\left(\left(l+\frac{1}{2}\right)\alpha\right)}{\sin(\alpha/2)}\right]_{\alpha=2\pi/n}$$

Space groups

NaCl



$$\left\{R_\alpha|\boldsymbol{\tau}\right\}$$

Point operation

Translation

Space group operation on position vector **r**

$\left\{R_\alpha|\boldsymbol{\tau}\right\}\mathbf{r}=\mathbf{r}'=R_\alpha\mathbf{r}+\boldsymbol{\tau}$

Multiplication of space group elements

$\left\{R_\beta|\boldsymbol{\tau}'\right\}\left\{R_\alpha|\boldsymbol{\tau}\right\}\mathbf{r}=R_\beta\left(R_\alpha\mathbf{r}\right)+R_\beta\boldsymbol{\tau}+\boldsymbol{\tau}'=\left\{R_\beta R_\alpha|R_\beta\boldsymbol{\tau}+\boldsymbol{\tau}'\right\}\mathbf{r}$

Special elements

Identity: $\left\{\varepsilon|0\right\}$

Pure point group operation: $\left\{R_\alpha|0\right\}$

Pure translation: $\left\{\varepsilon|\boldsymbol{\tau}\right\}$

Inverse: $\left\{R_\alpha|\boldsymbol{\tau}\right\}^{-1}=\left\{R_\alpha^{-1}|-R_\alpha^{-1}\boldsymbol{\tau}\right\}$

More details

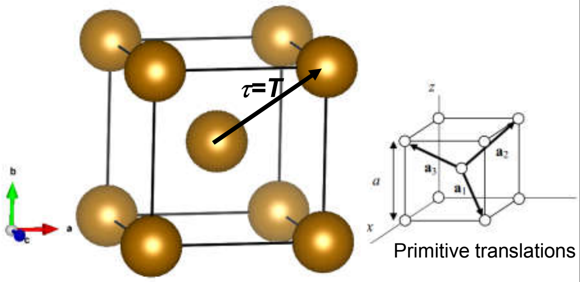
$$\boldsymbol{\tau}=\boldsymbol{\tau}_\alpha+\mathbf{T}$$

Non primitive translation

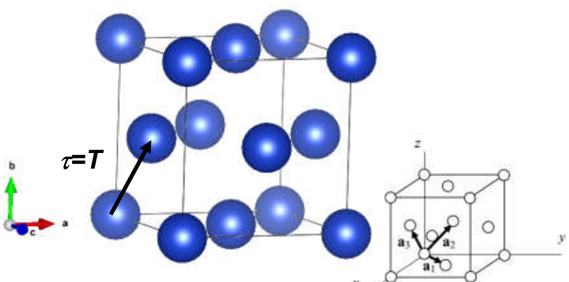
Lattice translation

If, for a suitable choice of the origin in the lattice, all of the group tranlation vectors are lattice translations **T**, the group is called "symmorphic", otherwise the group is called "non-symmorphic".

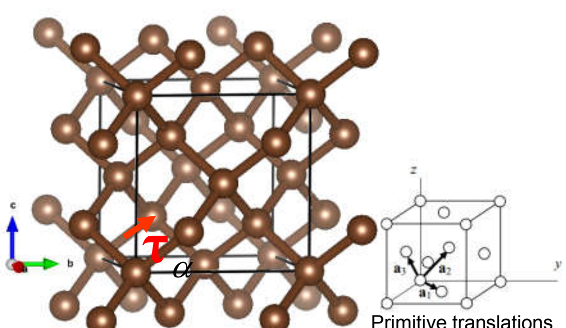
Example of symmorphic lattice Fe (body centered cubic lattice)



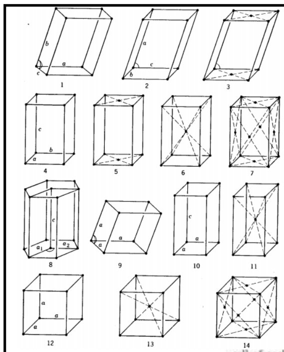
Example of symmorphic lattice Cu (face centered cubic lattice)



Non-symmorphic space group -- diamond



$(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ center of symmetry



The fourteen Bravais space lattices illustrated by a unit cell of each: (1) triclinic, simple; (2) monoclinic, simple; (3) monoclinic, base centered; (4) orthorhombic, simple; (5) orthorhombic, base centered; (6) orthorhombic, body centered; (7) orthorhombic, face centered; (8) hexagonal; (9) rhombohedral; (10) tetragonal, simple; (11) tetragonal, body centered; (12) cubic, simple; (13) cubic, body centered; and (14) cubic, face centered.

2/17/2017 PHY 745 Spring 2017 -- Lecture 16 10

Table 12.1: The 73 symmorphic space groups. Here P, I, F, and B, respectively, denote primitive, body centered, face centered and base centered Bravais lattices (see Fig. 12.1).

Crystal system	Bravais lattice	Space group
Triclinic	P	$P1$, $P\bar{1}$
Monoclinic	P	$P2$, Pm, $P2/m$
	B or A	$B2$, Bm, $B2/m$ (1st setting)
Orthorhombic	P	$P222$, $Pmm2$, $Pmmm$
	C, A, or B	$C222$, $Cmm2$, $Amm2^*$, $Cmmm$
	I	$I222$, $Imm2$, $Immm$
	F	$F222$, $Fmm2$, $Fmmm$
Tetragonal	P	$P4$, $P\bar{4}$, $P4/m$, $P422$, $P4mm$, $P42m$, $P\bar{4}m2^*$, $P4/mmm$
	I	$I4$, $I\bar{4}$, $I4/m$, $I422$, $I4mm$ $I\bar{4}2m$, $I\bar{4}m2^*$, $I4/mmm$
Cubic	P	$P23$, $Pm3$, $P432$, $P\bar{4}3m$, $Pm3m$
	I	$I23$, $Im3$, $I432$, $I\bar{4}3m$, $Im3m$
	F	$F23$, $Fm3$, $F432$, $F\bar{4}3m$, $Fm3m$
Trigonal	P	$P3$, $P\bar{3}$ $P312$, $P321^*$, $P\bar{3}m1$, $P1$, $P\bar{1}$
(Rhombohedral)	R	$R3$, $R\bar{3}$ $R32$, $R3m$, $R\bar{3}m$,
Hexagonal	P	$P6$, $P\bar{6}$, $P6/m$, $P622$, $P6mm$, $P\bar{6}m2$, $P\bar{6}m2^*$, $P6/mmm$

* The asterisks mark the seven extra space groups that are generated with the orientation of the point group operations is taken into account with respect to the Bravais cell.

2/17/2017 PHY 745 Spring 2017 -- Lecture 16 11

Some non-symmorphic operations and their descriptions

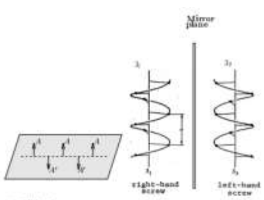


Figure 12.4: (a) The glide plane operation: (b) Right and left-hand screw axes. The right and left hand screw axes belong to closely related but different space groups.

2/17/2017 PHY 745 Spring 2017 -- Lecture 16 12

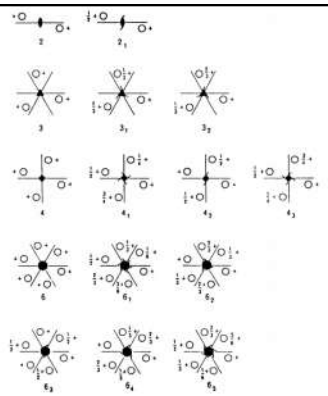
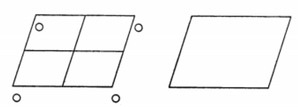


Figure 12.5: A summary of all possible screw axes.

Some examples in 2 dimensions

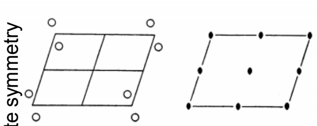
*p*1 No. 1 *p* 1 1 Oblique



Origin on 1

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
1	*a*	1	*x*,*y*.	General: No conditions

*p*2 No. 2 *p* 2 1 1 2 Oblique

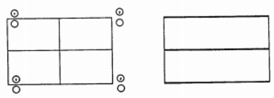


Origin at 2

Multiplicity	Wyckoff letter	Site symmetry		
2	*e*	1	$x,y;\ \bar{x},\bar{y}$.	General: No conditions
1	*d*	2	½,½.	Special: No conditions
1	*c*	2	½,0.	
1	*b*	2	0,½.	
1	*a*	2	0,0.	

Oblique

Rectangular *m* $p\,1\,m\,1$ No. 3 *pm*



Origin on *m*

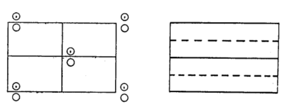
limiting lections

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
2	*c*	1	$x,y;\ \bar{x},y.$	General: No conditions
1	*b*	*m*	$\frac{1}{2},y.$	Special: No conditions
1	*a*	*m*	$0,y.$	

Oblique

Centered cell

cm No. 5 $c\,1\,m\,1$ *m* Rectangular

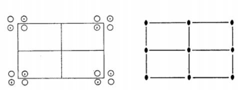


Origin on *m*

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0;\ \frac{1}{2},\frac{1}{2})+$	Conditions limiting possible reflections
4	*b*	1	$x,y;\ \bar{x},y.$	General: hk: $h+k=2n$
2	*a*	*m*	$0,y.$	Special: as above only

Example with higher symmetry

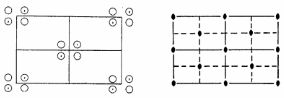
Rectangular *m m* $p\,2\,m\,m$ No. 6 *pmm*



Origin at 2*mm*

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
4	*i*	1	$x,y;\ \bar{x},y;\ \bar{x},\bar{y};\ x,\bar{y}.$	General: No conditions
2	*h*	*m*	$\frac{1}{2},y;\ \frac{1}{2},\bar{y}.$	Special: No conditions
2	*g*	*m*	$0,y;\ 0,\bar{y}.$	
2	*f*	*m*	$x,\frac{1}{2};\ \bar{x},\frac{1}{2}.$	
2	*e*	*m*	$x,0;\ \bar{x},0.$	
1	*d*	*mm*	$\frac{1}{2},\frac{1}{2}.$	
1	*c*	*mm*	$\frac{1}{2},0.$	
1	*b*	*mm*	$0,\frac{1}{2}.$	
1	*a*	*mm*	$0,0.$	

c m m No. 9 *c* 2 *m m* *m m* Rectangular

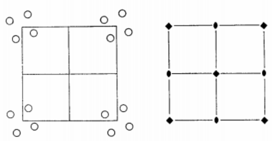


Origin at 2*mm*

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0;\ \frac{1}{2},\frac{1}{2})+$	Conditions limiting possible reflections
				General:
8	*f*	1	$x,y;\ \bar{x},y;\ \bar{x},\bar{y};\ x,\bar{y}.$	hk: $h+k=2n$
				Special: as above, plus
4	*e*	*m*	$0,y;\ 0,\bar{y}.$	no extra conditions
4	*d*	*m*	$x,0;\ \bar{x},0.$	no extra conditions
4	*c*	2	$\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\frac{3}{4}.$	hk: $h=2n$; $(k=2n)$
2	*b*	*mm*	$0,\frac{1}{2}.$	no extra conditions
2	*a*	*mm*	$0,0.$	no extra conditions

Square lattice

Square 4 *p* 4 No. 10 *p* 4

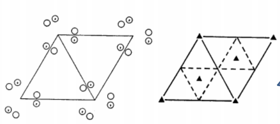


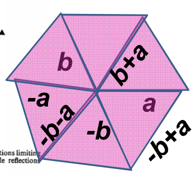
Origin at 4

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
4	*d*	1	$x,y;\ \bar{x},\bar{y};\ y,\bar{x};\ \bar{y},x.$	No conditions
				Special:
2	*c*	2	$\frac{1}{2},0;\ 0,\frac{1}{2}.$	hk: $h+k=2n$
1	*b*	4	$\frac{1}{2},\frac{1}{2}.$	No conditions
1	*a*	4	$0,0.$	No conditions

Hexagonal

p 3 1 *m* No. 15 *p* 3 1 *m* 3 *m* Hexagonal

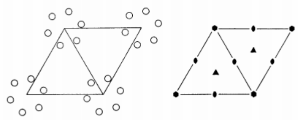




Origin at 31*m*

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
6	*d*	1	$x,y;\ \bar{y},x-y;\ y-x,\bar{x};$ $y,x;\ \bar{x},y-x;\ x-y,\bar{y}.$	No conditions
				Special:
3	*c*	*m*	$x,0;\ 0,x;\ \bar{x},\bar{x}.$	No conditions
2	*b*	3	$\frac{1}{3},\frac{2}{3};\ \frac{2}{3},\frac{1}{3}.$	
1	*a*	3*m*	$0,0.$	

Hexagonal 6 $p6$ No. 16 $p6$



Origin at 6

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
6	*d*	1	x,y; $\bar{y},x-y$; $y-x,\bar{x}$; $\bar{x},\bar{y}$; $y,y-x$; $x-y,x$.	No conditions
				Special:
3	*c*	2	$\frac{1}{2},0$; $0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2}$.	No conditions
2	*b*	3	$\frac{1}{3},\frac{2}{3}$; $\frac{2}{3},\frac{1}{3}$.	
1	*a*	6	$0,0$.	

2/17/2017 PHY 745 Spring 2017 -- Lecture 16 22