PHY 752 Solid State Physics
11-11:50 AM MWF Olin 103

Plan for Lecture 5:

Reading: Chapter 2 in GGGPP;

Crystal structures and brief introduction to group theory

1. Survey of crystal structures
2. Elements of symmetry
3. Some ideas of group theory

PHY 752 Solid State Physics

MWF 11 AM-11:50 PM	OPL 103	http://www.wfu.edu/~natalie/f15phy752/

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Course schedule

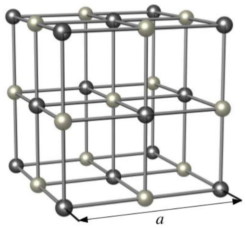
(Preliminary schedule -- subject to frequent adjustment.)

	Date	F&W Reading	Topic	Assignment
1	Wed, 8/26/2015	Chap. 1.1-1.2	Electrons in a periodic one-dimensional potential	#1
2	Fri, 8/28/2015	Chap. 1.3	Electrons in a periodic one-dimensional potential	#2
3	Mon, 8/31/2015	Chap. 1.4	Tight binding models	#3
4	Wed, 9/02/2015	Chap. 1.6, 2.1	Crystal structures	#4
5	Fri, 9/04/2015	Chap. 2	Group theory	#5
6	Mon, 9/07/2015	Chap. 2	Group theory	#6
7	Wed, 9/09/2015	Chap. 2	Group theory	
8	Fri, 9/11/2015			
9	Mon, 9/14/2015			
10	Wed, 9/16/2015			

Some common crystal forms found in nature quick review using some materials from Marder's text book

- Rocksalt—Sodium Chloride
- Cesium Chloride
- Fluorite—Calcium Fluoride
- Zincblende—Zinc Sulfide
- Wurtzite—Zinc Oxide
- Perovskite—Calcium Titanate

NaCl

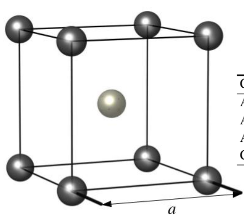


Example materials

Crystal	*a*	Crystal	*a*	Crystal	*a*	Crystal	*a*	Crystal	*a*
AgBr	5.77	CrN	4.14	LiI	6.00	NiO	4.17	SrS	6.02
AgCl	5.55	CsF	6.01	MgO	4.21	PbS	5.93	SrSe	6.23
AgF	4.92	FeO	4.31	MgS	5.20	PbSe	6.12	SrTe	6.47
BaO	5.52	KBr	6.60	MgSe	5.45	PbTe	6.45	TiC	4.32
BaS	6.39	KCl	6.30	MnO	4.44	RbBr	6.85	TiN	4.24
BaSe	6.60	KF	5.35	MnS	5.22	RbCl	6.58	TiO	4.24
BaTe	6.99	KI	7.07	MnSe	5.49	RbF	5.64	VC	4.18
CaS	5.69	LiBr	5.50	NaBr	5.97	RbI	7.34	VN	4.13
CaSe	5.91	LiCl	5.13	NaCl	5.64	SnAs	5.68	ZrC	4.68
CaTe	6.35	LiF	4.02	NaF	4.62	SnTe	6.31	ZrN	4.61
CdO	4.70	LiH	4.09	NaI	6.47	SrO	5.16		

Face-centered-cubic
with basis

CsCl

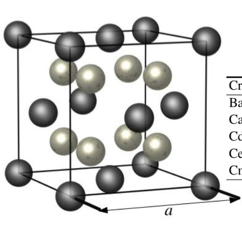


Example materials

Crystal	*a*	Crystal	*a*	Crystal	*a*
AgCd	3.33	CsCl	4.12	NiAl	2.88
AgMg	3.28	CuPd	2.99	TiCl	3.83
AgZn	3.16	CuZn	2.95	TlI	4.20
CsBr	4.29	NH_4Cl	3.86	TlSb	3.84

Simple cubic structure
with basis

CaF_2

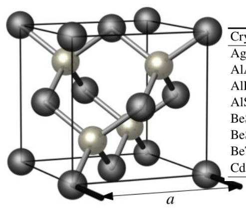


Example materials

Crystal	*a*	Crystal	*a*	Crystal	*a*
BaF_2	6.20	$CoSi_2$	5.36	Mg_2Si	6.39
CaF_2	5.46	HfO_2	5.12	Mg_2Sn	6.77
CdF_2	5.39	Li_2O	4.62	Na_2S	6.53
CeO_2	5.41	Li_2S	5.71	$SrCl_2$	6.98
CmO_2	5.37	Mg_2Pb	6.84	UO_2	5.47

Face-centered-cubic
with basis

Zincblende

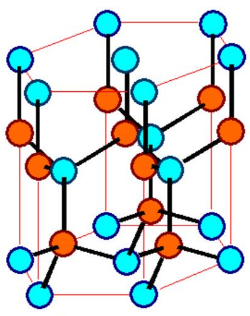


Example materials

Crystal	a	Crystal	a	Crystal	a
AgI	6.47	CdTe	6.48	HgSe	6.08
AlAs	5.62	CuBr	5.69	HgTe	6.43
AlP	5.45	CuCl	5.41	InAs	6.04
AlSb	6.13	CuI	6.04	InP	5.87
BeS	4.85	GaAs	5.63	InSb	6.48
BeSe	5.07	GaP	5.45	SiC	4.35
BeTe	5.54	GaSb	6.12	ZnS	5.41
CdS	5.82	HgS	5.85	ZnTe	6.09

Face-centered-cubic with basis

ZnS - Wurtzite

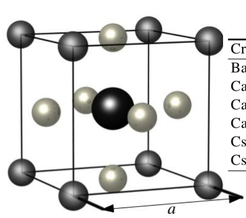


Example materials

Crystal	a	c	Crystal	a	c
AlN	3.11	4.98	MgTe	4.52	7.33
BeO	2.70	4.38	NH_4F	4.39	7.02
CdS	4.13	6.75	SiC	3.08	5.05
CdSe	4.30	7.02	ZnO	3.25	5.23
CuH	2.89	4.61	ZnS	3.81	6.23

Hexagonal structure with basis

Perovskite



Example materials

Crystal	a	Crystal	a		
$BaTiO_3$	4.01	$CsHgCl_3$	5.44	$LaAlO_3$	3.78
$CaSnO_3$	3.92	$CsIO_3$	4.66	$LaGaO_3$	3.88
$CaTiO_3$	3.84	KIO_3	4.41	$RbIO_3$	4.52
$CaZrO_3$	4.02	$KMgF_3$	3.97	$SrTiO_3$	3.91
$CsCdBr_3$	5.33	$KNiF_3$	4.01	$SrZrO_3$	4.10
$CsHgBr_3$	5.77	$KZnF_3$	4.05	$YAlO_3$	3.68

Cubic lattice with basis

Systemization of crystal forms

- 14 Bravais lattices
- 32 Point groups
- 230 Space groups

Short digression on abstract group theory

- What is group theory ?
- What is it doing in the course ?

Short digression on abstract group theory

What is group theory ?

A group is a collection of "elements" – $A, B, C, \ldots$ and a "multiplication" process. The abstract multiplication $(\cdot)$ pairs two group elements, and associates the "result" with a third element. (For example $(A \cdot B = C)$.) The elements and the multiplication process must have the following properties.

1. The collection of elements is closed under multiplication. That is, if elements A and B are in the group and $A \cdot B = C$, element C must be in the group.
2. One of the members of the group is a "unit element" (E). That is, for any element A of the group, $A \cdot E = E \cdot A = A$.
3. For each element A of the group, there is another element A^{-1} which is its "inverse". That is $A \cdot A^{-1} = A^{-1} \cdot A = E$.
4. The multiplication process is "associative". That is for sequential mulplication of group elements A, B, and C, $(A \cdot B) \cdot C = A \cdot (B \cdot C)$.

Short digression on abstract group theory

What is group theory doing in a solid

Example of group theory applied to space groups

Ref: L. P. Bouckaert, R. Smoluchowski, and E. Wigner, *Phys. Rev.* **50**, 58 (1936) – "Theory of Brillouin zones and symmetry properties of wave functions in crystals"

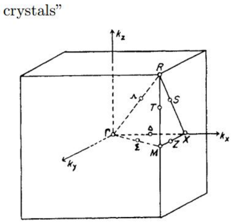
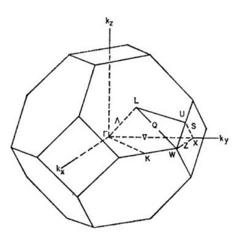


FIG. 2.

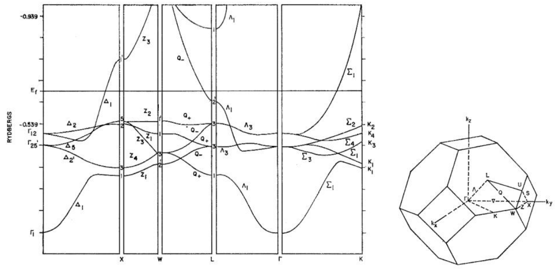
Brillouin zone of simple cubic lattice



Brillouin zone of face centered cubic lattice

Example of space group theory in band structure analysis

Ref: G. A. Burdick, *Phys. Rev.* **129**, 138 (1963) – "Energy band structure of copper"



Example of group theory applied to space groups – continued

Ref: BSW – Some appropriate "character tables"

TABLE I. *Characters of small representations of* Γ, *R*, *H*.

Γ, R, H	E	$3C_4^2$	$6C_4$	$6C_2$	$8C_3$	J	$3JC_4^2$	$6JC_4$	$6JC_2$	$8JC_3$
Γ_1	1	1	1	1	1	1	1	1	1	1
Γ_2	1	1	−1	−1	1	1	1	−1	−1	1
Γ_{12}	2	2	0	0	−1	2	2	0	0	−1
Γ_{15}'	3	−1	1	−1	0	3	−1	1	−1	0
Γ_{25}'	3	−1	−1	1	0	3	−1	−1	1	0
Γ_1'	1	1	1	1	1	−1	−1	−1	−1	−1
Γ_2'	1	1	−1	−1	1	−1	−1	1	1	−1
Γ_{12}'	2	2	0	0	−1	−2	−2	0	0	1
Γ_{15}	3	−1	1	−1	0	−3	1	−1	1	0
Γ_{25}	3	−1	−1	1	0	−3	1	1	−1	0

TABLE II. *Characters for the small representations of* Δ, *T*.

Δ, T	E	C_4^2	$2C_4$	$2JC_4^2$	$2JC_2$
Δ_1	1	1	1	1	1
Δ_2	1	1	−1	1	−1
Δ_2'	1	1	−1	−1	1
Δ_1'	1	1	1	−1	−1
Δ_5	2	−2	0	0	0

TABLE V. *Characters of small representations of* M, X.

M X	E E	$2C_4^2$ $2C_4^2\perp$	$C_4^2\perp$ $C_4^2\parallel$	$2C_4\perp$ $2C_4\parallel$	$2C_2$ $2C_2$	J J	$2JC_4^2$ $2JC_4^2\perp$	$JC_4^2\perp$ $JC_4^2\parallel$	$2JC_4\perp$ $2JC_4\parallel$	$2JC_2$ $2JC_2$
M_1	1	1	1	1	1	1	1	1	1	1
M_2	1	1	1	−1	−1	1	1	1	−1	−1
M_3	1	−1	1	−1	1	1	−1	1	−1	1
M_4	1	−1	1	1	−1	1	−1	1	1	−1
M_1'	1	1	1	1	1	−1	−1	−1	−1	−1
M_2'	1	1	1	−1	−1	−1	−1	−1	1	1
M_3'	1	−1	1	−1	1	−1	1	−1	1	−1
M_4'	1	−1	1	1	−1	−1	1	−1	−1	1
M_5	2	0	−2	0	0	2	0	−2	0	0
M_5'	2	0	−2	0	0	−2	0	2	0	0

Example of group theory applied to space groups – continued

Ref: BSW – Some appropriate "compatability tables"

TABLE VII. *Compatibility relations between* Γ *and* Δ, Λ, Σ.

Γ_1	Γ_2	Γ_{12}	Γ_{15}'	Γ_{25}'
Δ_1	Δ_2	$\Delta_1\Delta_2$	$\Delta_1'\Delta_5$	$\Delta_2'\Delta_5$
Λ_1	Λ_2	Λ_3	$\Lambda_2\Lambda_3$	$\Lambda_1\Lambda_3$
Σ_1	Σ_4	$\Sigma_1\Sigma_4$	$\Sigma_2\Sigma_3\Sigma_4$	$\Sigma_1\Sigma_2\Sigma_3$
Γ_1'	Γ_2'	Γ_{12}'	Γ_{15}	Γ_{25}
Δ_1'	Δ_2'	$\Delta_1'\Delta_2'$	$\Delta_1\Delta_5$	$\Delta_2\Delta_5$
Λ_2	Λ_1	Λ_3	$\Lambda_1\Lambda_3$	$\Lambda_2\Lambda_3$
Σ_2	Σ_3	$\Sigma_2\Sigma_3$	$\Sigma_1\Sigma_3\Sigma_4$	$\Sigma_1\Sigma_2\Sigma_4$

TABLE IX. *Compatibility relations between X and* Δ, *Z*, *S*.

X_1	X_2	X_3	X_4	X_1'	X_2'	X_3'	X_4'	X_5	X_5'
Δ_1	Δ_2	Δ_2'	Δ_1'	Δ_1'	Δ_2'	Δ_2	Δ_1	Δ_5	Δ_5

Example of group theory applied to space groups – continued

Analysis of transitions between quantum mechanical states

$$(\text{Transition probability}) \propto |\mathcal{M}|^2 \equiv \left| \int d^3r \;\; \Psi_f^*(\mathbf{r})\mathcal{O}\Psi_i(\mathbf{r}) \right|^2 .$$

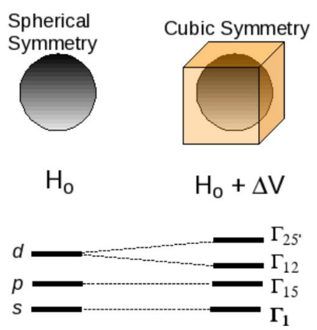
$$\mathcal{M} \propto \sum_C N_C \chi_f(C)\chi_{\mathcal{O}}(C)\chi_i(C).$$

Some examples:

- Optical transitions (absorption, emission, polarization effects)
- Analysis of phonon modes; Infrared transitions, Raman transitions

Example of group theory applied to point groups

Analysis of "crystal field effects" on atomic states

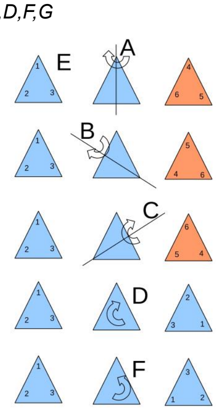


Example of a 6-member group *E,A,B,C,D,F,G*

Group multiplication table

Group of order 6

	E	A	B	C	D	F
E	E	A	B	C	D	F
A	A	E	D	F	B	C
B	B	F	E	D	C	A
C	C	D	F	E	A	B
D	D	C	A	B	F	E
F	F	B	C	A	E	D



	E	A	B	C	D	F
E	E	A	B	C	D	F
A	A	E	D	F	B	C
B	B	F	E	D	C	A
C	C	D	F	E	A	B
D	D	C	A	B	F	E
F	F	B	C	A	E	D

Check on group properties:
1. Closed; multiplication table uniquely generates group members.
2. Unit element included.
3. Each element has inverse.
4. Multiplication process is associative.

Definitions

Subgroup: members of larger group which have the property of a group

Class: members of a group which are generated by the construction

$$\mathcal{C} = X_i^{-1} Y X_i \quad \text{where } X_i \text{ and } Y \text{ are group elements}$$

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