PHY 752 Electrodynamics
9-9:50 AM MWF Olin 107

Plan for Lecture 2:

Reading: Chapter 1 & 2 in MPM;

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 11-11:50 AM | OPL 107 | http://www.wfu.edu/~natalie/s15phy752/

Instructor: Natalie Holzwarth | Phone:758-5510 | Office:300 OPL | e-mail:natalie@wfu.edu

Course schedule for Spring 2015

(Preliminary schedule -- subject to frequent adjustment.)

	Lecture date	MPM Reading	Topic	Assign.	Due date
1	Mon: 01/12/2015	Chap. 1 & 2	Crystal structures	#1	01/23/2015
2	Wed: 01/14/2015	Chap. 1 & 2	Some group theory	#2	01/23/2015
	Fri: 01/16/2015	No class	NAWH out of town		
	Mon: 01/19/2015	No class	MLK Holiday		
3	Wed: 01/21/2015	Chap. 1 & 2	Some group theory		01/23/2015

WFU Physics Colloquium

TITLE: Carbon Nanotube-Based Polymer Composite Thermoelectric Generators

SPEAKER: Dr. Corey Hewitt ,

Department of Physics
Wake Forest University

TIME: Wednesday January 14, 2015 at 4:00 PM

PLACE: Room 101 Olin Physical Laboratory

Refreshments will be served at 3:30 PM in the Olin Lounge. All interested persons are cordially invited to attend.

ABSTRACT

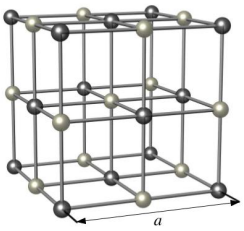
Carbon nanotube-based polymer composites possess several properties that make them ideal for use in low powered waste heat recovery applications not suitable to nonorganic crystalline materials, such as their light weight and flexible physical structure and ease of fabrication. Additionally, the favorable thermoelectric properties of the carbon nanotubes

Some common crystal forms found in nature

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

Note: Materials from Marder used in preparing this lecture.

NaCl

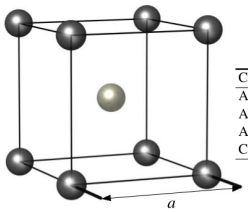


Example materials

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

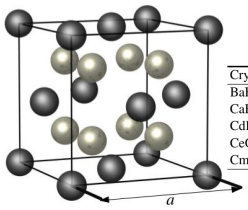


Example materials

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

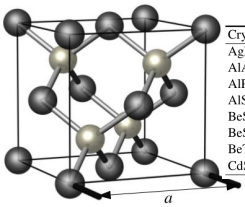


Example materials

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

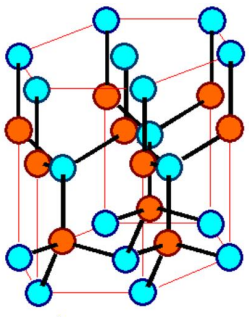


Example materials

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

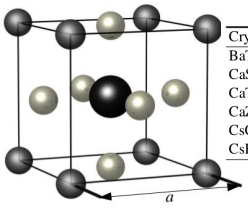


Example materials

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"

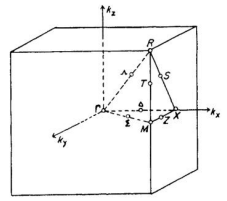
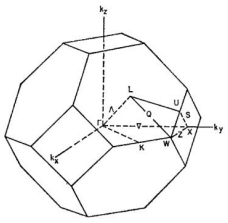


FIG. 2.

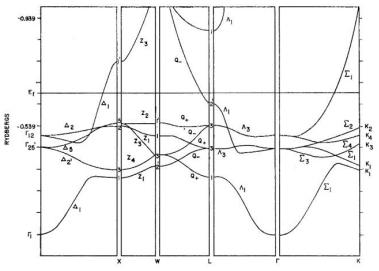
Brillouin zone of simple cubic lattice

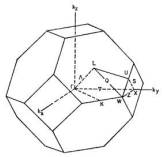


Brillouin zone of face centered cubic lattice

Example of space group theory in band structure analysis

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





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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_2^z	$2C_4$	$2JC_2^z$	$2JC_4$
Δ_1	1	1	1	1	1
Δ_2	1	1	−1	1	−1
Δ_1'	1	1	−1	−1	1
Δ_2'	1	1	1	−1	−1
Δ_5	2	−2	0	0	0

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

M, X	E	$2C_2^z$	$2C_4^2$	$C_2^xC_2^y$	$2C_4C_2^{xy}$	$2C_4^3$	J	$2JC_2^z$	$2JC_4^2$	$JC_2^xC_2^y$	$2JC_4C_2^{xy}$	$2JC_4^3$
M_1	1	1	1	1	1	1	1	1	1	1	1	1
M_2	1	1	1	−1	−1	1	1	1	1	−1	−1	1
M_3	1	−1	1	−1	1	−1	1	−1	1	−1	1	−1
M_4	1	−1	1	1	−1	−1	1	−1	1	1	−1	−1
M_1'	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1
M_2'	1	1	1	−1	−1	−1	−1	−1	−1	1	1	1
M_3'	1	−1	1	−1	1	−1	−1	1	−1	1	−1	1
M_4'	1	−1	1	1	−1	−1	−1	1	−1	−1	1	1
M_5	2	0	−2	0	0	2	0	−2	0	0	0	0
M_5'	2	0	−2	0	0	−2	0	2	0	0	0	0

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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}	$\Gamma_{25'}$
Δ_1	Δ_2	$\Delta_1\Delta_2$	$\Delta_1\Delta_3$	$\Delta_2\Delta_3$
Λ_1	Λ_2	Λ_2	$\Lambda_2\Lambda_3$	$\Lambda_1\Lambda_3$
Σ_1	Σ_4	$\Sigma_1\Sigma_4$	$\Sigma_2\Sigma_3\Sigma_4$	$\Sigma_1\Sigma_3\Sigma_4$
Γ_1'	Γ_2'	Γ_{12}'	Γ_{15}	Γ_{25}
Δ_1'	Δ_2'	$\Delta_1'\Delta_2'$	$\Delta_1\Delta_3$	$\Delta_2\Delta_3$
Λ_2	Λ_1	Λ_2	$\Lambda_1\Lambda_3$	$\Lambda_2\Lambda_3$
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

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

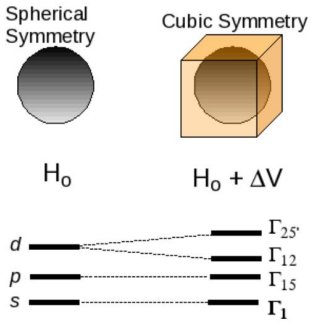
$$\mathcal{M} \propto \sum_C N_C \chi_f(C) \chi_{\mathcal{O}}(C) \chi_i(C).$$

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

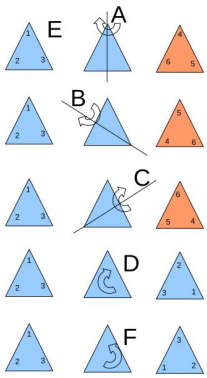


Example of a 6-member group *E,A,B,C,D,F,G*

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

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