Survey of Materials. Lecture 2
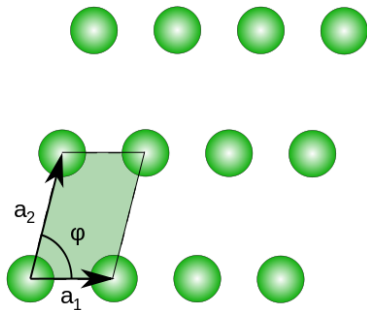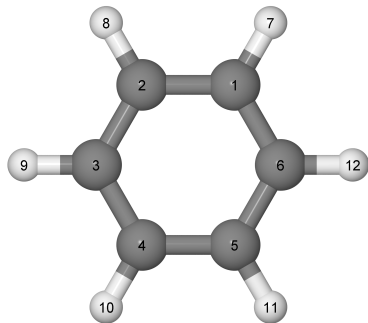
Atomistic structure

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October 2, 2018

Outline

- Why symmetry is important
- 2D crystallography
- 3D crystallography
- Nonperiodic solids
- Structure characterization and determination
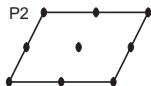
2D crystallography

Space group = point group + translation symmetry

- Determine all 2D point groups

- Determine all 2D Bravais lattices

2D crystallography

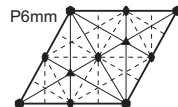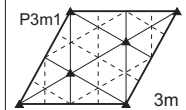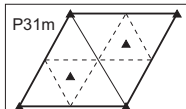2D space groups (17), point groups, Bravais lattices, and crystal systems (4)

P1

P2

Bravais lattices:
P2   oblique
Pmm2   rectangular
Cmm2   rhombic
P4mm   square
P6mm   hexagonal

Point groups:
1-6 C_{1-6}
m D_1
mm2 D_2
3m D_3
4mm D_4
6mm D_6

Symmetries:
● ▲ ◆ ●
- - - - - -

Pm

Cm

Pb

m

Pmm2

Cmm2

Pma2

Pba2

mm2

P4

P4mm

P4bm

4mm

P3

P6

P31m

P3m1

3m

P6mm
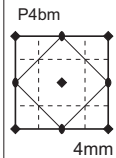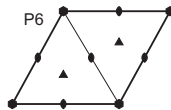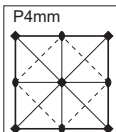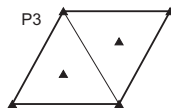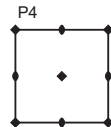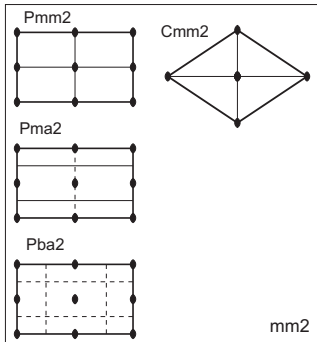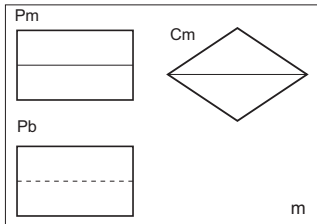
2D glide plane
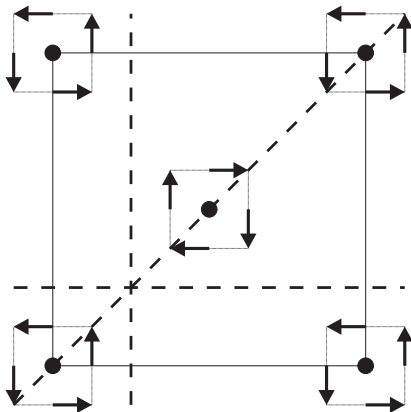
2D materials

- graphene, BN
- organic networks
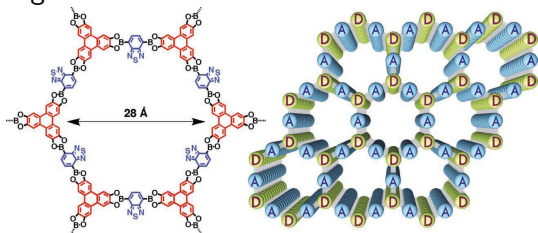
- MoS$_2$
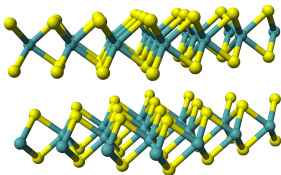
- P, As

3D point groups
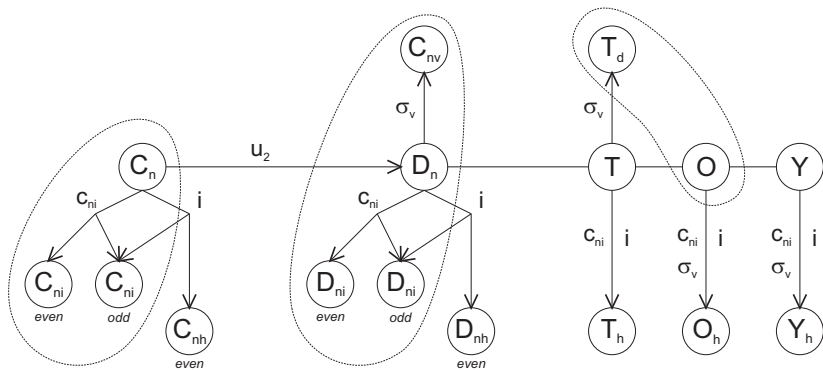
3D symmetry elements

Axes							Planes	
	n	-n	n_1	n_2	n_3	n_4	n_5	
1	○							m
2	●		◗					a,b
3	▲	△	▲	▲				c
4	◆	◈	◆	◆	◆			n
6	⬣	⬡	⬣	⬣	⬣	⬣	⬣	d
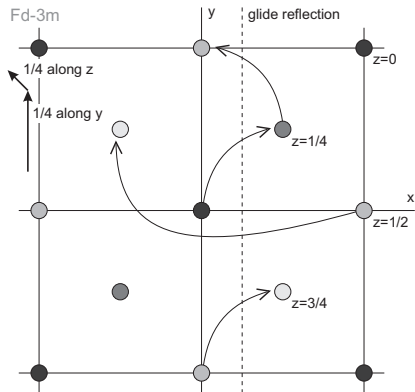
3D crystallography

Lecture of Artem Abakumov or any textbook

Classification of space groups

structural type	A4 (dia)	A3 (hcp)	A7 (α-As)
space group	Fd-3m	P63/mmc	R-3m
arithmetic crystal class	Fm-3m	P6/mmm	R-3m
lattice centering	F	P	R
crystal class	m-3m	6/mmm	-3m
crystal family	c	h	h*

* Lattice system is rhombohedral, crystal system is trigonal

Lattice system vs crystal system, crystal family

	space groups		lattice system	crystal family	crystal system
P1	...	P-1	anorthic*	a	anorthic
P2	...	C2/c	monoclinic	m	monoclinic
P222	...	Imma	orthorhombic	o	orthorhombic
P4	...	I4$_1$/acd	tetragonal	t	tetragonal
R3	...	R-3c	rhombohedral	**h**	trigonal
P3	...	P-3c1	**hexagonal**	**h**	**trigonal**
P6	...	P6$_3$/mmc	hexagonal	**h**	hexagonal
P23	...	Ia-3d	cubic	c	cubic

* anorthic is also called triclinic

Structure factor and radial distribution function

$$S(\boldsymbol{q}) = \frac{1}{N} \left| \sum_i e^{-i\boldsymbol{q}\boldsymbol{r}_i} \right| \equiv 1 + \rho \int_V e^{-i\boldsymbol{q}\boldsymbol{r}} g(\boldsymbol{r}) \, dV, \ g(\boldsymbol{r}) = \sum_{i \neq 0} \delta \left(\boldsymbol{r} - \boldsymbol{r}_i \right)$$
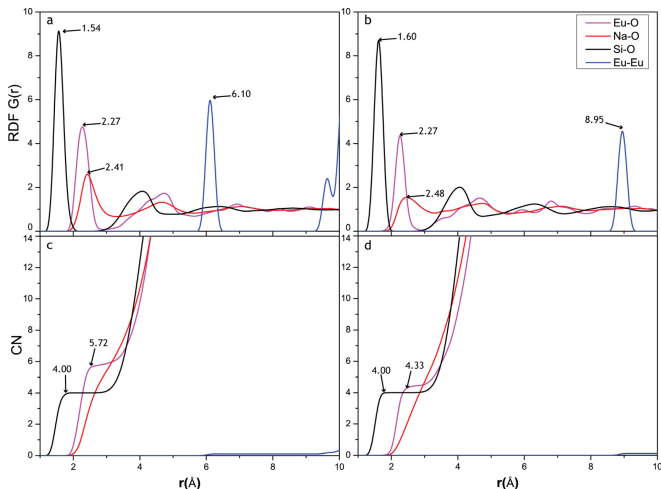
Summary and Resources

See summary here

- Wikipedia
- Bilbao Crystallographic Server
- Crystal structures
- References: crystallography, symmetry
- Textbooks (sections General, Crystallography, Symmetry)

Visualization software:
- Jmol
- Mercury
- Surface explorer (online tool)