

Survey of Materials. Lecture 2

Atomistic structure

Andriy Zhugayevych

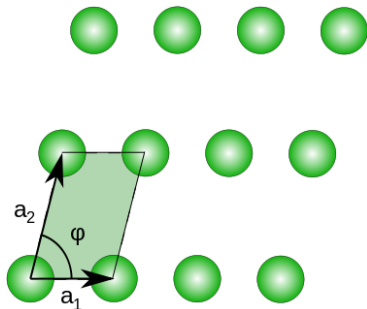
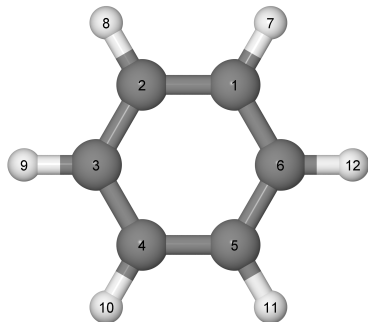
October 30, 2018

Outline

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

2D crystallography

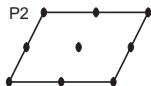
Space group = point group + translation symmetry



- Determine all 2D point groups
- Determine all 2D Bravais lattices

2D crystallography

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

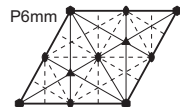
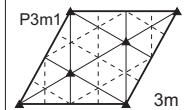
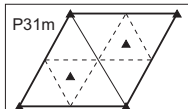
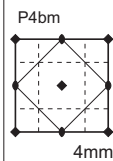
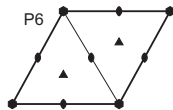
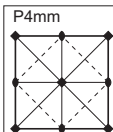
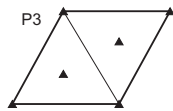
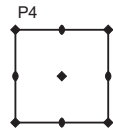
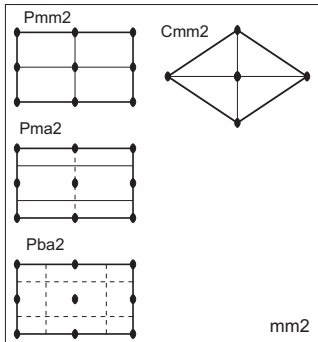
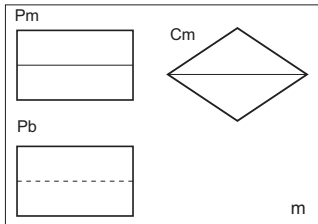


Bravais lattices:
 P2 oblique
 Pmm2 rectangular
 Cmm2 rhombic
 P4mm square
 P6mm hexagonal

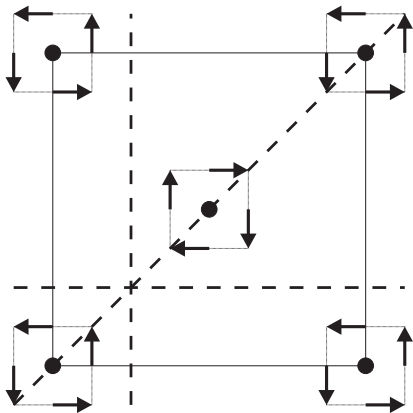
Point groups:

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

Symmetries:

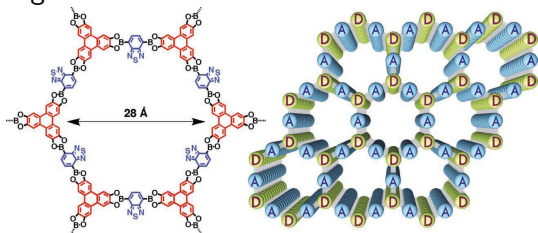


2D glide plane

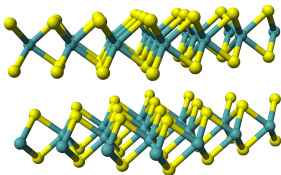


2D materials

- graphene, BN
- organic networks

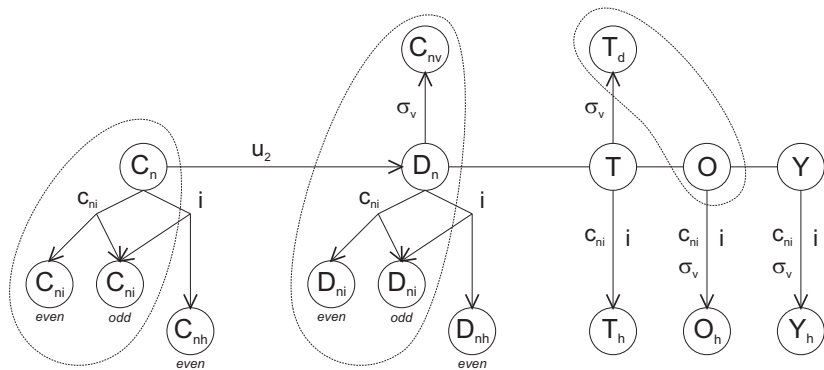


- MoS₂



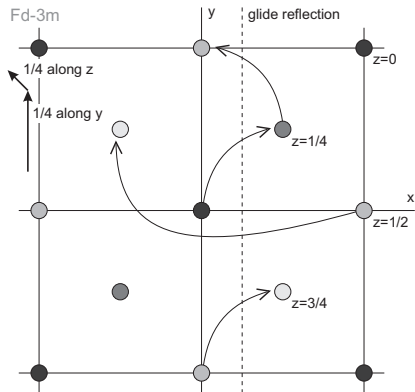
- P, As

3D point groups



3D symmetry elements

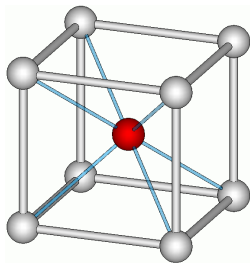
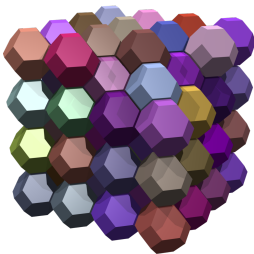
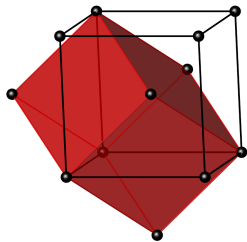
Axes								Planes	
	n	-n	n_1	n_2	n_3	n_4	n_5		
1	o							m	_____
2	●	●	●					a,b	-----
3	▲	▲	▲	▲				c
4	◆	◆	◆	◆	◆			n	-----
6	⬢	⬢	⬢	⬢	⬢	⬢	⬢	d	----->



3D crystallography

Lecture of Artem Abakumov or any textbook

Unit cell



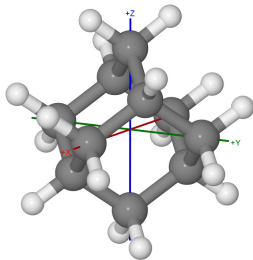
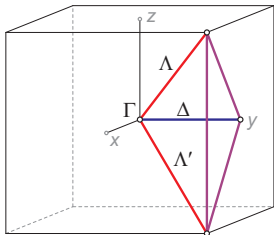
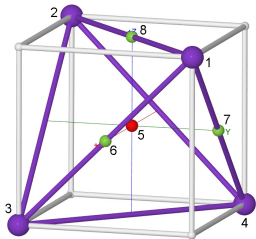
	min.size	parallelepiped	symmetric
primitive	+	+	-
Wigner-Seitz	+	-	+
Bravais	-	+	+

Generators, fundamental domain (asymmetric unit)

also orbits (Wyckoff positions), stabilizers etc.

$$T_d \equiv -43m = \{1, 8c_3, 3c_2, 6c_{4i}, 6\sigma_v\} \sim O$$

Generators: $c_3(1)$ and $\sigma_v(34)$, e.g. $c_3(1)\sigma_v(34) = c_{4i}^{-1}(7)$, $c_{4i}^2 = c_2$



	orbit	WP	stab.	atoms
000	Γ	1a	-43m	
xxx	Λ	4e	3m	CH
x00	Δ	6f	2mm	C
xxz	$\Lambda\Delta$	12i	m	H
xyz		24j	1	

Fundamental domain is $\Lambda\Delta\Lambda'$ -pyramid ($V = 1/24$)

Asymmetric unit is HCCH

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

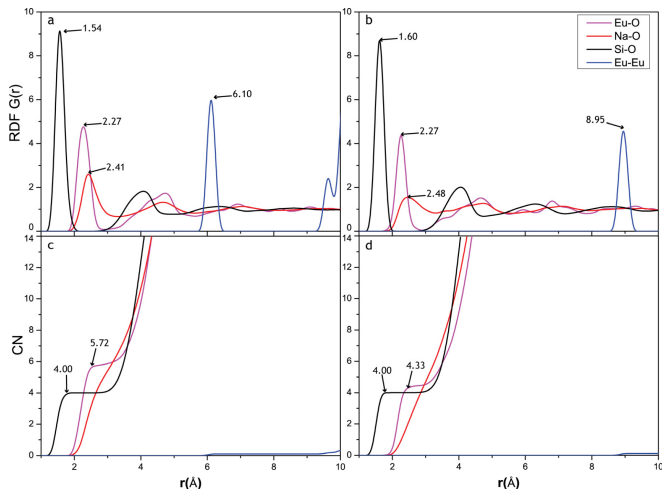
Lattice system vs crystal system, crystal family

	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

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



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)