I. The Basics and What we are interested in

A. A baby-level encounter

An early triumph of quantum mechanics was its applications to crystalline solids, and its success in understanding[+] why there are conductors, insulators, and semiconductors. The success was built on how QM could be applied to understand much of atoms and molecules. After all, a solid can be regarded as a huge molecule (with some nice features such as periodicity).

[+] The understanding of superconductors has to wait for 30 more years (1956-57), again using quantum mechanics.

- ρ or $\sigma = \frac{1}{\rho}$ spans 24 orders of magnitude!
- Even so, quantum physics can explain almost all of these!

Electrical Resistivity (ohm-m)	(log)		Electrical Conductivity (S/m)
	–8	8	
* intercalated graphite	–7	7	copper, silver iron
	–6	6	stainless steel, metallic glass
graphite (in-plane) graphite (out of plane)	–5	5	$YBa_2Cu_3O_7$ (ab plane)
* polyacetylene (doped)	–4	4	$YBa_2Cu_3O_7$ (c-axis)
	–3	3	silicon (doped) * ZnO (doped)
TTF-TCNQ	–2	2	seawater
	–1	1	Fe_3O_4
	0	0	germanium
	1	–1	
	2	–2	silicon
	3	–3	InSb
	4	–4	
	5	–5	water AgCl
* polyacetylene (undoped)	6	–6	
	7	–7	
	8	–8	* ZnO (undoped)
	9	–9	
	10	–10	
Bakelite	11	–11	NaCl
polypyrrole	12	–12	
	13	–13	
Lucite (PMMA)	14	–14	Al_2O_3
polyvinyl chloride	15	–15	mica silica
polyethylene, teflon	16	–16	diamond

Resistivity and conductivity of a variety of materials at room temperature. (Note: values are approximate, and for insulators and semiconductors, *very* sensitive to impurities.)

* and ⬭ are related to semiconductors

- Sensitive to presence of impurities

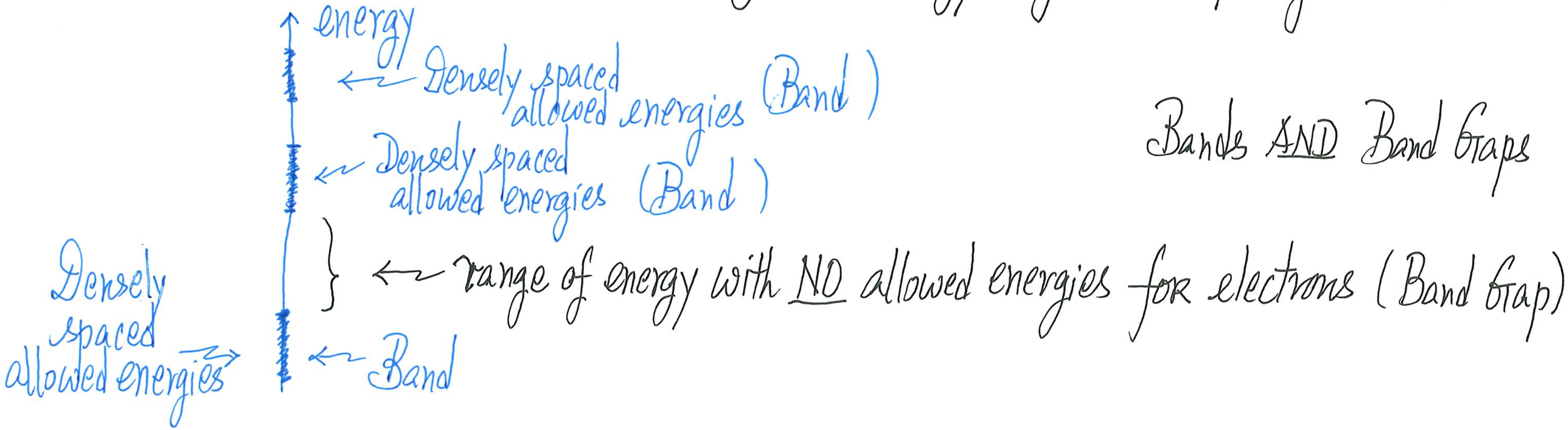
[impurites help increase σ!]

diamond has the same structure as Si and Ge, but 10^{13} times less conducting!

[Taken from Livingston, "Electronic Properties of Engineering Materials"]

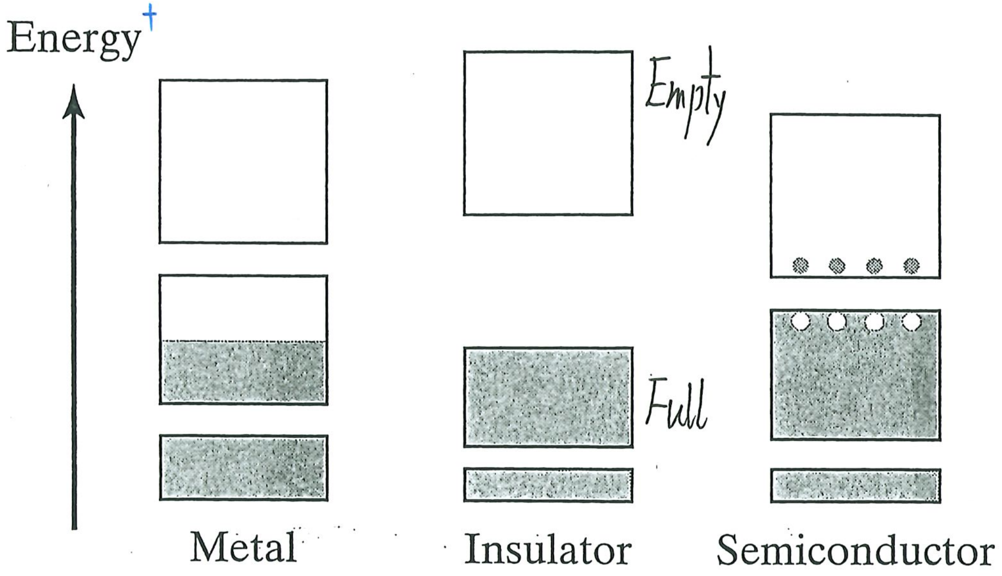
Key Problems

- How electrons (electronic states) behave in a periodic potential energy function in QM?
  - What does the question mean?
  - How complicated/easy is the problem?
- Solutions to the (Time-independent) Schrödinger Equation give how the allowed energies (energy eigenvalues/eigenstates)



Bands AND Band Gaps

Filling in Electrons (How?)



Metal: Partially filled band(s)

Insulator: Big Gap between highest completely filled band and lowest completely empty band (e.g. diamond (carbon))

Semiconductor: Small gap allows thermal ($T \neq 0$) excitations of electrons across the gap ⇒ resistivity drops with T

like an insulator but having a smaller energy gap (e.g. Silicon, gap ~ 1.1eV)

$E_g < 3.2$ eV (semiconductors) [not well-defined][‡]

[†] What is the x-axis? Who knows! Such figures are often used, but one should be careful about whether the x-axis carries some meaning.

[‡] 3.2 eV includes ZnO into the class

Semiconductors

- Large impurity effects
- ρ vs T

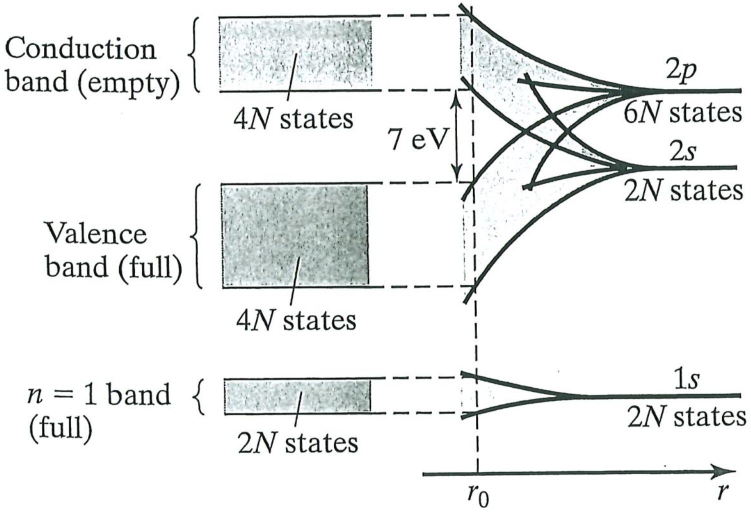
different from metals

- Negative charge carriers (those electrons in nearly empty upper band)

  AND Positive charge carriers (due to missing electrons in nearly filled lower band)
- (Some semiconductors) Sensitive to Light (light can alter carrier densities)
- (Consequences) Non-ohmic I-V, junction devices

- How do atoms form a solid when they come together?

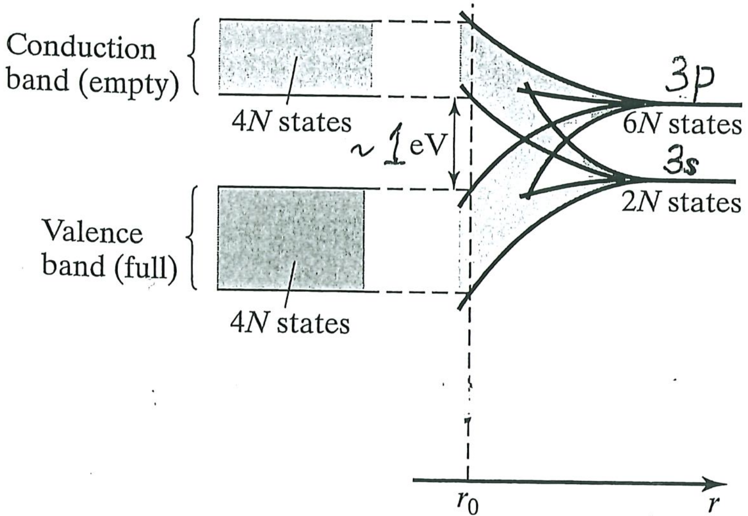
Diamond (insulator)



atoms come closer in a solid

Separated atoms

Silicon (semiconductor)

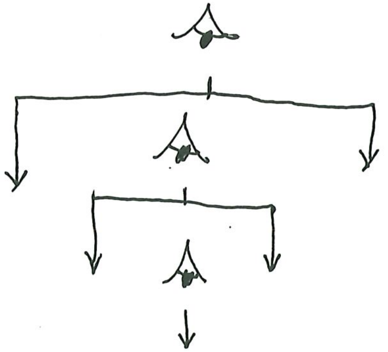


- Why? (QM)
- Bonding and Hydribization (QM)

- What do these pictures convey?

[Q: Do we need periodicity to have energy bands and band gaps?]

Periodic Table of the Elements



Key
atomic mass — 12.011
electronegativity — 2.5
electronic configuration — [He]$2s^22p^2$ (atomic physics)
symbol — C
atomic number — 6
name — Carbon

Periods ↓	Group I A	II A	III B	IV B	V B	VI B	VII B	VII			I B	II B	III A	IV A	V A	VI A	VII A	Noble Gases 0
1	1.0079 2.2 $1s$ H 1 Hydrogen																	4.0026 $1s^2$ He 2 Helium
2	6.941 1.0 [He]$2s$ Li 3 Lithium	9.01218 1.5 [He]$2s^2$ Be 4 Beryllium											10.81 2.0 [He]$2s^22p$ B 5 Boron	12.011 2.5 [He]$2s^22p^2$ C 6 Carbon	14.0067 3.1 [He]$2s^22p^3$ N 7 Nitrogen	15.9994 3.5 [He]$2s^22p^4$ O 8 Oxygen	18.9984 4.1 [He]$2s^22p^5$ F 9 Fluorine	20.179 [He]$2s^22p^6$ Ne 10 Neon
3	22.98977 1.0 [Ne]$3s$ Na 11 Sodium	24.305 1.2 [Ne]$3s^2$ Mg 12 Magnesium											26.9815 1.5 [Ne]$3s^23p$ Al 13 Aluminum	28.0855 1.7 [Ne]$3s^23p^2$ Si 14 Silicon	30.97376 2.1 [Ne]$3s^23p^3$ P 15 Phosphorus	32.06 2.4 [Ne]$3s^23p^4$ S 16 Sulfur	35.453 2.8 [Ne]$3s^23p^5$ Cl 17 Chlorine	39.948 [Ne]$3s^23p^6$ Ar 18 Argon
4	39.0983 0.9 [Ar]$4s$ K 19 Potassium	40.08 1.0 [Ar]$4s^2$ Ca 20 Calcium	44.9559 1.2 [Ar]$3d4s^2$ Sc 21 Scandium	47.88 1.3 [Ar]$3d^24s^2$ Ti 22 Titanium	50.9415 1.5 [Ar]$3d^34s^2$ V 23 Vanadium	51.996 1.6 [Ar]$3d^54s$ Cr 24 Chromium	54.9380 1.6 [Ar]$3d^54s^2$ Mn 25 Manganese	55.847 1.6 [Ar]$3d^64s^2$ Fe 26 Iron	58.9332 1.7 [Ar]$3d^74s^2$ Co 27 Cobalt	58.70 1.8 [Ar]$3d^84s^2$ Ni 28 Nickel	63.546 1.8 [Ar]$3d^{10}4s$ Cu 29 Copper	65.38 1.7 [Ar]$3d^{10}4s^2$ Zn 30 Zinc	69.72 1.8 [Ar]$3d^{10}4s^24p$ Ga 31 Gallium	72.59 2.0 [Ar]$3d^{10}4s^24p^2$ Ge 32 Germanium	74.9216 2.2 [Ar]$3d^{10}4s^24p^3$ As 33 Arsenic	78.96 2.5 [Ar]$3d^{10}4s^24p^4$ Se 34 Selenium	79.904 2.7 [Ar]$3d^{10}4s^24p^5$ Br 35 Bromine	83.80 [Ar]$3d^{10}4s^24p^6$ Kr 36 Krypton
5	85.4678 0.9 [Kr]$5s$ Rb 37 Rubidium	87.62 1.0 [Kr]$5s^2$ Sr 38 Strontium	88.9059 1.1 [Kr]$4d5s^2$ Y 39 Yttrium	91.22 1.2 [Kr]$4d^25s^2$ Zr 40 Zirconium	92.9064 1.2 [Kr]$4d^45s$ Nb 41 Niobium	95.94 1.3 [Kr]$4d^55s$ Mo 42 Molybdenum	98.906 1.4 [Kr]$4d^65s$ Tc 43 Technetium	101.07 1.4 [Kr]$4d^75s$ Ru 44 Ruthenium	102.9055 1.5 [Kr]$4d^85s$ Rh 45 Rhodium	106.4 1.4 [Kr]$4d^{10}$ Pd 46 Palladium	107.868 1.4 [Kr]$4d^{10}5s$ Ag 47 Silver	112.41 1.5 [Kr]$4d^{10}5s^2$ Cd 48 Cadmium	114.82 1.5 [Kr]$4d^{10}5s^25p$ In 49 Indium	118.69 1.7 [Kr]$4d^{10}5s^25p^2$ Sn 50 Tin	121.75 1.8 [Kr]$4d^{10}5s^25p^3$ Sb 51 Antimony	127.60 2.0 [Kr]$4d^{10}5s^25p^4$ Te 52 Tellurium	126.9045 2.2 [Kr]$4d^{10}5s^25p^5$ I 53 Iodine	131.30 [Kr]$4d^{10}5s^25p^6$ Xe 54 Xenon
6	132.9054 0.9 [Xe]$6s$ Cs 55 Cesium	137.33 1.0 [Xe]$6s^2$ Ba 56 Barium	138.9055 1.1 [Xe]$5d6s^2$ *La 57 Lanthanum	178.49 1.2 [Xe]$4f^{14}5d^26s^2$ Hf 72 Hafnium	180.9479 1.3 [Xe]$4f^{14}5d^36s^2$ Ta 73 Tantalum	183.85 1.4 [Xe]$4f^{14}5d^46s^2$ W 74 Tungsten	186.207 1.5 [Xe]$4f^{14}5d^56s^2$ Re 75 Rhenium	190.2 1.5 [Xe]$4f^{14}5d^66s^2$ Os 76 Osmium	192.22 1.6 [Xe]$4f^{14}5d^76s^2$ Ir 77 Iridium	195.09 1.4 [Xe]$4f^{14}5d^96s$ Pt 78 Platinum	196.9665 1.4 [Xe]$4f^{14}5d^{10}6s$ Au 79 Gold	200.59 1.5 [Xe]$4f^{14}5d^{10}6s^2$ Hg 80 Mercury	204.37 1.4 [Xe]$4f^{14}5d^{10}6s^26p$ Tl 81 Thallium	207.2 1.6 [Xe]$4f^{14}5d^{10}6s^26p^2$ Pb 82 Lead	208.9804 1.7 [Xe]$4f^{14}5d^{10}6s^26p^3$ Bi 83 Bismuth	(209) 1.8 [Xe]$4f^{14}5d^{10}6s^26p^4$ Po 84 Polonium	(210) 2.0 [Xe]$4f^{14}5d^{10}6s^26p^5$ At 85 Astatine	(222) [Xe]$4f^{14}5d^{10}6s^26p^6$ Rn 86 Radon
7	(223) 0.9 [Rn]$7s$ Fr 87 Francium	226.0254 1.0 [Rn]$7s^2$ Ra 88 Radium	227.0278 1.0 [Rn]$6d7s^2$ †Ac 89 Actinium	(261) [Rn]$5f^{14}6d^27s^2$ Unq 104 Unnilquadium	(262) [Rn]$5f^{14}6d^37s^2$ Unp 105 Unnilpentium	(263) [Rn]$5f^{14}6d^47s^2$ Unh 106 Unnilhexium												

* Lanthanides	6	140.12 1.1 [Xe]$4f^26s^2$ Ce 58 Cerium	140.9077 1.1 [Xe]$4f^36s^2$ Pr 59 Praseodymium	144.24 1.1 [Xe]$4f^46s^2$ Nd 60 Neodymium	145 1.1 [Xe]$4f^56s^2$ Pm 61 Promethium	150.4 1.1 [Xe]$4f^66s^2$ Sm 62 Samarium	151.96 1.0 [Xe]$4f^76s^2$ Eu 63 Europium	157.25 1.1 [Xe]$4f^75d6s^2$ Gd 64 Gadolinium	158.9254 1.1 [Xe]$4f^96s^2$ Tb 65 Terbium	162.50 1.1 [Xe]$4f^{10}6s^2$ Dy 66 Dysprosium	164.9304 1.1 [Xe]$4f^{11}6s^2$ Ho 67 Holmium	167.26 1.1 [Xe]$4f^{12}6s^2$ Er 68 Erbium	168.9342 1.1 [Xe]$4f^{13}6s^2$ Tm 69 Thulium	173.04 1.1 [Xe]$4f^{14}6s^2$ Yb 70 Ytterbium	174.967 1.1 [Xe]$4f^{14}5d6s^2$ Lu 71 Lutetium
† Actinides	7	232.0381 1.1 [Rn]$6d^27s^2$ Th 90 Thorium	231.0359 1.1 [Rn]$5f^26d7s^2$ Pa 91 Protactinium	238.029 1.2 [Rn]$5f^36d7s^2$ U 92 Uranium	237.0482 1.2 [Rn]$5f^46d7s^2$ Np 93 Neptunium	(244) 1.2 [Rn]$5f^67s^2$ Pu 94 Plutonium	(243) 1.2 [Rn]$5f^77s^2$ Am 95 Americium	(247) ≈1.2 [Rn]$5f^76d7s^2$ Cm 96 Curium	(247) ≈1.2 [Rn]$5f^97s^2$ Bk 97 Berkelium	(251) ≈1.2 [Rn]$5f^{10}7s^2$ Cf 98 Californium	(254) ≈1.2 [Rn]$5f^{11}7s^2$ Es 99 Einsteinium	(257) ≈1.2 [Rn]$5f^{12}7s^2$ Fm 100 Fermium	(258) ≈1.2 [Rn]$5f^{13}7s^2$ Md 101 Mendelevium	259 [Rn]$5f^{14}7s^2$ No 102 Nobelium	260 [Rn]$5f^{14}6d7s^2$ Lr 103 Lawrencium

Everyone working on physics of materials & matter [atoms/molecules/nuclei] should have an image of the periodic table in mind!

Some Semiconductors

- Group IV : Si , Ge
- III-V : GaAs , InSb , GaSb , InP , InAs
- II-VI : CdS , CdTe , ZnSe , CdSe

- IV-VI : PbS , PbTe , SnTe

Questions

- Crystal Structures and descriptions
- Consequences of periodicity in crystals
- Understanding of energy bands/band gaps
- Electronic structure/Band structure
- Modelling of important bands
- Physics of charge carriers

⋮

[Assumed basic knowledge in undergraduate quantum physics, statistical physics, and solid state physics]

Approach and Goals

- Big Picture and Systematic Way to approach physics problems related to Solids

Key Concepts/Ideas

[not necessarily with many equations]

Know what to learn/path to learn when the need arises

Logical sequence of ideas

What Basic Physics (Theories) can do to understand electronic, transport, optical properties

What are so special about solids (using semiconductors as the context for learning)?

[Jump into new research when new materials come up!]

PHYS5660: An intermediate-level solid state physics course using semiconductors and their applications as the context to build up a systematic view on solids.

For students more inclined to theories...

- Try "Solid State Theory"
- Try "Many-Body Physics"

Main Textbook:

M. Balkanski and R.F. Wallis, "Semiconductor Physics and Applications", Oxford Univ. Press. [Refer to as "BW" henceforth]

References:

See course webpage list

B. Structure of Crystalline Solids

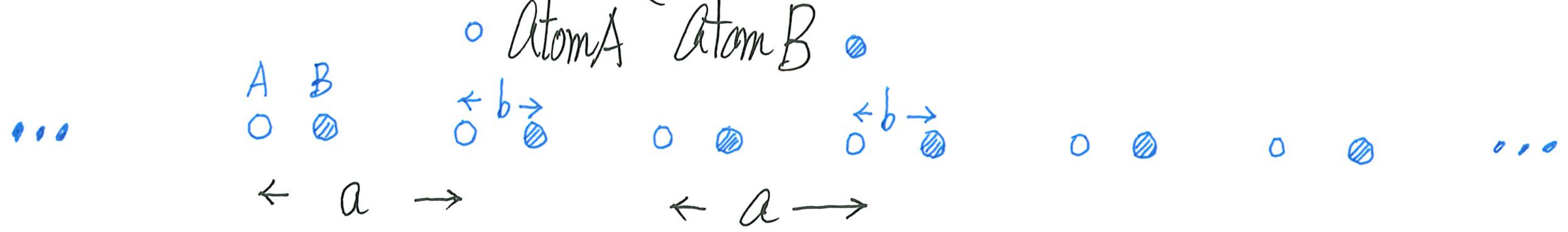
$$\boxed{\text{Crystal Structure} = \text{Lattice} + \text{Basis}} \quad \text{(Key Concept)} \qquad (1)$$

Crystal Structure → Real Stuff! (e.g. Si, Ge, GaAs)

Lattice → Mathematical construction (involves lattice points, not real atoms; introduces Lattice Vectors $\vec{R}$'s for describing periodicity)

Basis → Where a small group of atoms sit (real stuff) relative to a lattice point

Eg. 1D solid† (AB solid)



- Lattice [an abstract construction] (there is only one lattice possible in 1D)

permitive translation vector $\vec{a}_1$

[a = lattice constant ; "x" are lattice points] $\vec{R} = n\vec{a}_1 = n\overbrace{a\hat{x}}^{\vec{a}_1}$

$(n = 0, \pm 1, \pm 2, \dots)$

are lattice vectors

- Basis of Two Atoms
  - Atom A sits on a lattice point ($\vec{\rho}_A = 0$ relative to lattice point)

    Atom B sits at $\vec{\rho}_B = b\hat{x} = b/a\ (a\hat{x}) = \underbrace{(b/a)}_{(<1)}\vec{a}_1$

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† It is always useful to have 1D pictures in mind, as it is easier to think about the physics without the troubles of geometry in higher dimensions.

2D lattices

- Need two Primitive Translation Vectors $\vec{a}_1$ and $\vec{a}_2$ to generate lattice

$$\vec{R} = l_1 \vec{a}_1 + l_2 \vec{a}_2 \quad ; \quad l_1, l_2 \text{ are integers } (0, \pm 1, \pm 2, \ldots)$$

$$\equiv \vec{R}_{l_1 l_2} \equiv \vec{R}_l \quad \text{(subscript "}l\text{" includes } (l_1, l_2))$$

Lattice Vectors (infinitely many in principle (for an infinite solid))

3D Lattices

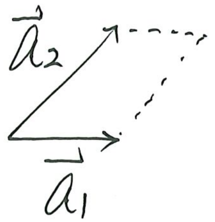
- Need $\vec{a}_1, \vec{a}_2, \vec{a}_3$;

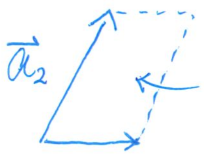
$$\boxed{\vec{R}_l = \vec{R}_{l_1,l_2,l_3} = l_1 \vec{a}_1 + l_2 \vec{a}_2 + l_3 \vec{a}_3} \qquad (2)$$

Lattice vectors

Starting from one lattice point "x", from "x" and using $\vec{R}$'s map out a lattice

2D Bravais Lattices

- $\vec{a}_1$, $\vec{a}_2$ define a parallelogram  (a tile)
- How many fundamental tiles of different shapes that can cover a 2D wall without leaving some voids OR without overlapping tiles?
- "Different shapes" mean "Different symmetry elements in the lattice generated"



a permitive unit cell (a tile)

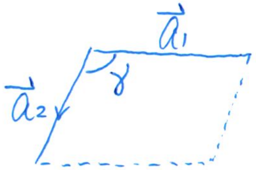
Five Bravais Lattices in 2D (no more)

○ $\frac{2\pi}{2}$ (180°) rotation with axis into paper

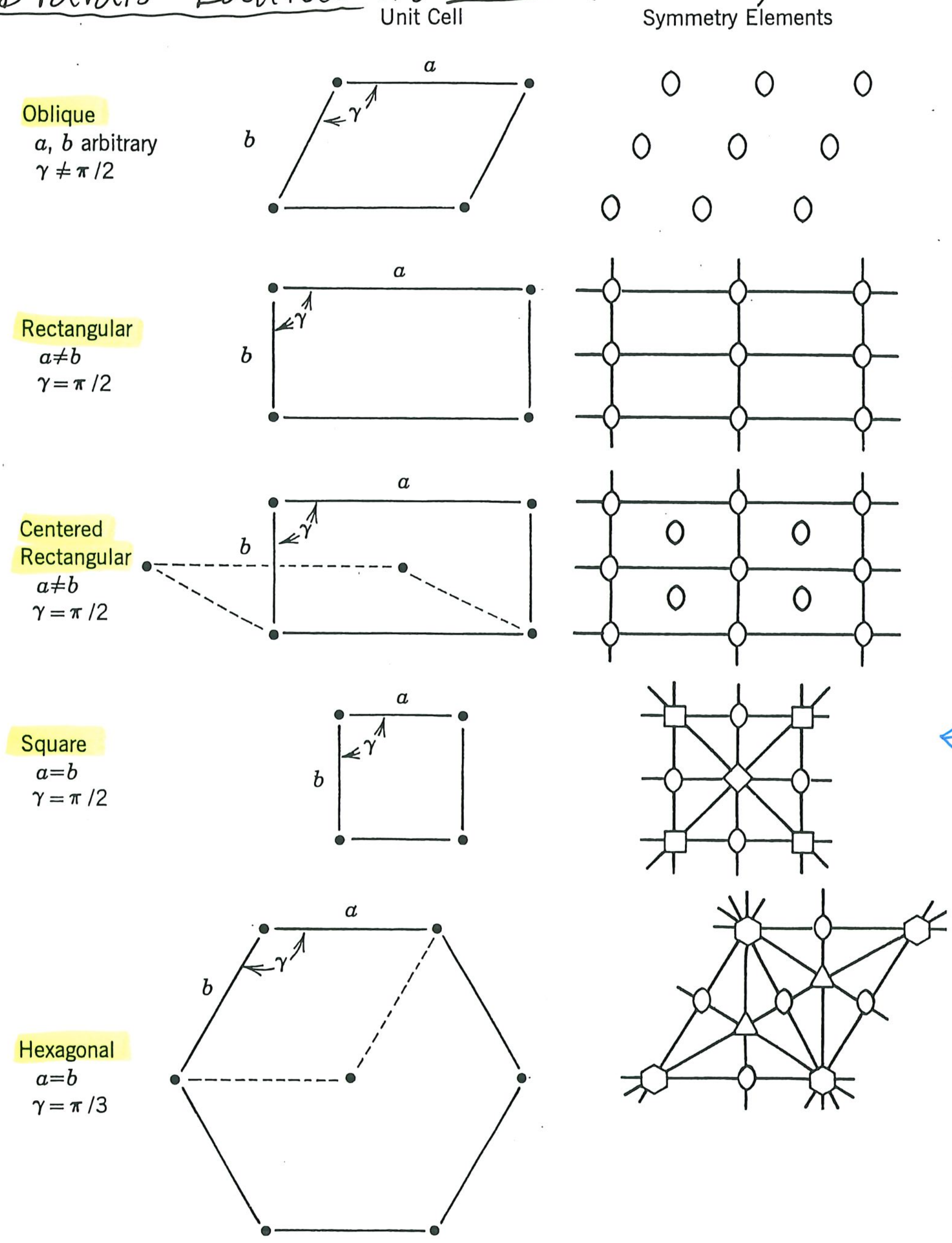
□ $\frac{2\pi}{4}$ (90°) rotation with axis into paper

△ $\frac{2\pi}{3}$ (120°) rotation with axis into paper

/ π (180°) rotation about line (mirror line)



Relationship between $|\vec{a}_1|$ and $|\vec{a}_2|$, and the angle γ matter



Two-dimensional lattices: unit cells and symmetry elements.

primitive unit cell (dashed lines) vs conventional unit cell

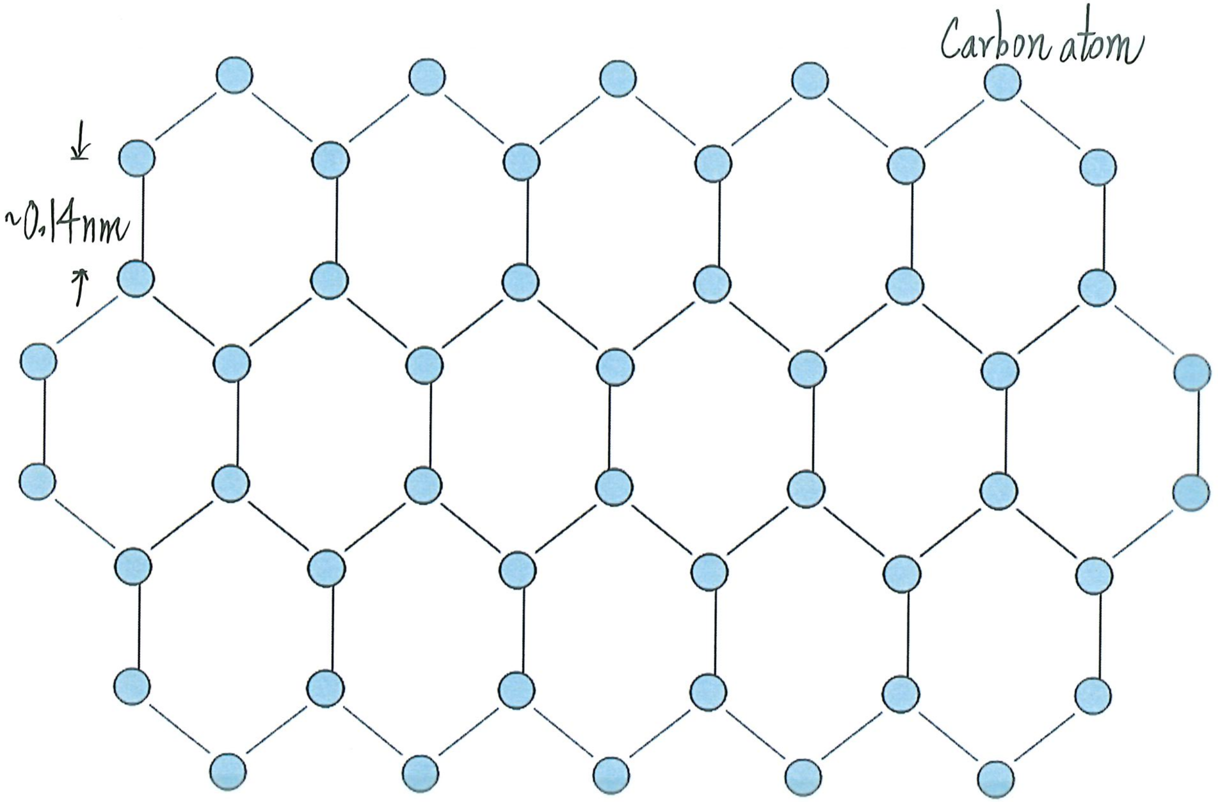
← lattice has high symmetry (many symmetry elements/operations)

primitive unit cell vs conventional unit cell

[From Christman, "Fundamentals of Solid State Physics"]

Meaning: All 2D crystalline solids must belong to one of the five Bravais Lattices

Graphene (one layer of graphite) [hottest material in recent 15 years]



"Gapless"
OR
"zero-gap"
Semiconductor

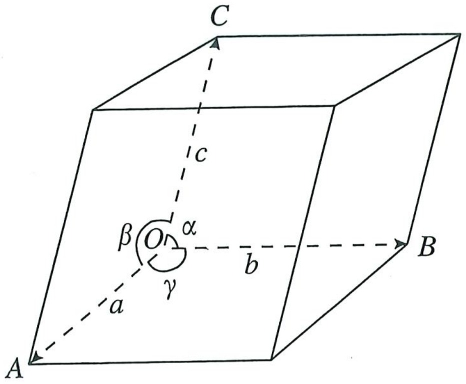
How to describe the structure of Graphene?

3D Bravais Lattices

- $\vec{a}_1$, $\vec{a}_2$, $\vec{a}_3$ primitive translation vectors (not orthogonal in general)
- define a parallelepiped[†], use $\vec{R}$'s can "tile" a volume (no voids)
- Symmetry of lattices generated ⇒ 14 Possible Bravais lattices in 3D
- $\underbrace{\text{Primitive unit cell}}_{\text{contains only one lattice point}}$ vs $\underbrace{\text{Conventional Unit Cell}}_{\text{contains more than one lattice points but more convenient}}$ (thus NOT primitive)

[†] defines a primitive unit cell (contains one lattice point)

Parallelepiped



Crystal axes ***a***, ***b***, ***c*** and angles α, β, γ.

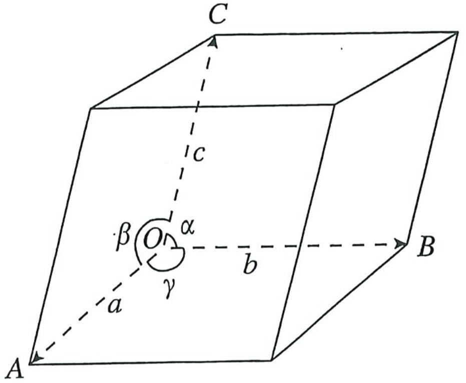
If conventional cell is the same as the primitive unit cell, thus $\vec{a}=\vec{a}_1$, $\vec{b}=\vec{a}_2$, $\vec{c}=\vec{a}_3$; and $a=|\vec{a}|$, $b=|\vec{b}|$, $c=|\vec{c}|$.

If conventional cell ≠ primitive unit cell, thus $\vec{a}$, $\vec{b}$, $\vec{c}$ ("crystal axes here) are different from $\vec{a}_1$, $\vec{a}_2$, $\vec{a}_3$.

This is the case for semiconductors!

Volume of Conventional unit cell > Volume of Primitive unit cell

$$\Omega_c = \Omega_{cell} = |\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)| \quad (3)$$



Crystal axes ***a***, ***b***, ***c*** and angles α, β, γ.

The 14 Bravais lattices for the 7 crystal systems

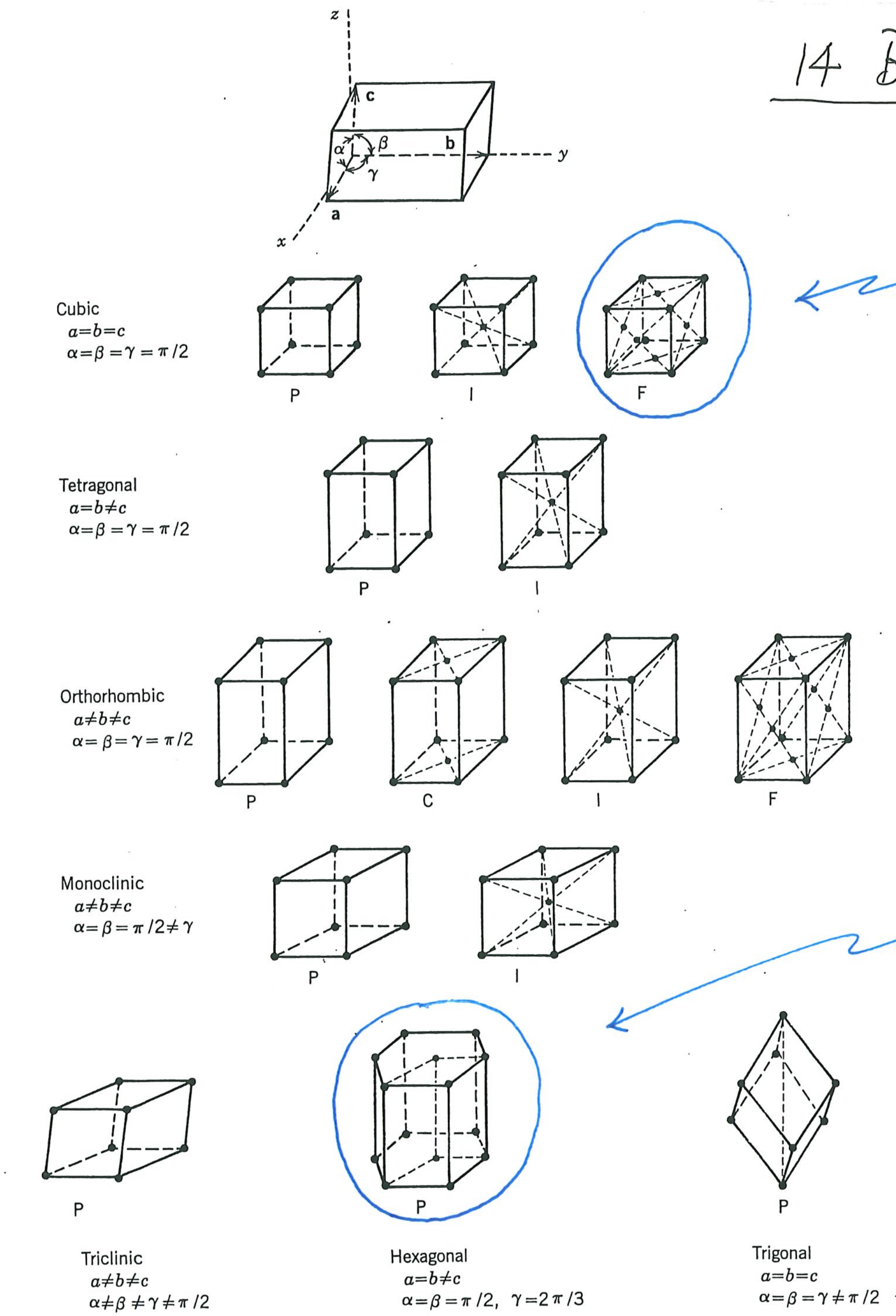
System		Bravais lattice	Restrictions on conventional cells
cubic	(3)	simple or primitive	$a = b = c$ $\alpha = \beta = \gamma = 90°$
		face-centered	
		body-centered	
tetragonal	(2)	primitive	$a = b \neq c$
		body-centered	$\alpha = \beta = \gamma = 90°$
orthorhombic	(4)	primitive	$a \neq b \neq c$
		base-centered	$\alpha = \beta = \gamma = 90°$
		face-centered	
		body-centered	
hexagonal	(1)	primitive	$a = b \neq c$ $\alpha = \beta = 90°,\ \gamma = 120°$
trigonal	(1)	primitive	$a = b = c$ $\alpha = \beta = \gamma < 120° \neq 90°$
monoclinic	(2)	primitive	$a \neq b \neq c$
		base-centered	$\alpha = \gamma = 90° \neq \beta$
triclinic	(1)	primitive	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$
	(14)		

Semiconductors: fcc and hexagonal lattices are most relevant

(recall: there are basis atoms to be attached to each point)

[Figure and Table taken from BW]

14 Bravais Lattices in 3D



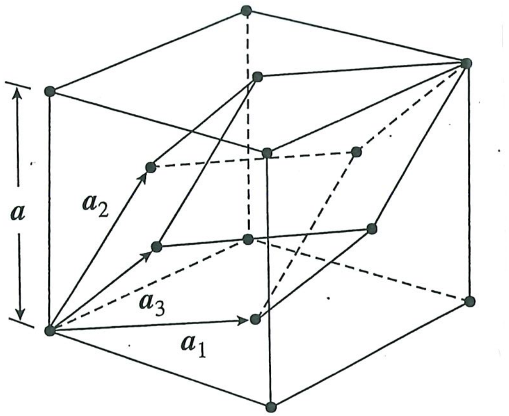
The 7 three-dimensional lattice systems and 14 Bravais lattices.

most important in semiconductor physics

Also important

[From Christman, "Fundamentals of Solid State Physics"]

Diamond, Si, Ge belong to the face-centered cubic lattice



Conventional and primitive unit cells of the face-centered cubic lattice.

The "a" is the lattice constant given in data book

Si: $\underbrace{a = 5.43\,\text{Å}}$; Ge: $\underbrace{a = 5.65\,\text{Å}}$

this is the convention (live with it!)

"a" is <u>NOT</u> separation between neighboring atoms, but referring to the cubic conventional unit cell

$$\left.\begin{aligned} \vec{a}_1 &= \frac{a}{2}(\hat{x}+\hat{y}) \\ \vec{a}_2 &= \frac{a}{2}(\hat{y}+\hat{z}) \\ \vec{a}_3 &= \frac{a}{2}(\hat{z}+\hat{x}) \end{aligned}\right\}$$

permitive translation vectors (a popular choice)

(see figure)

Ω_c = volume of primitive unit cell†

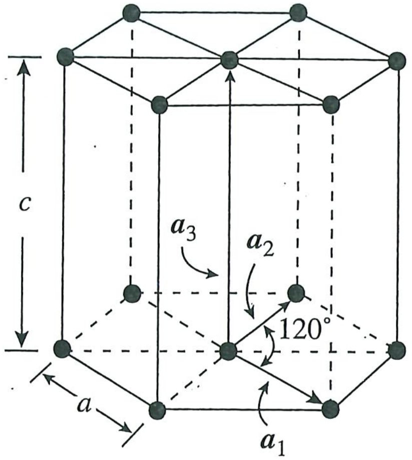
$$= |\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)| = \frac{1}{4}\underbrace{a^3}$$

← Volume of conventional cell

⇒ There are 4 lattice points in conventional cell

†see parallelepiped formed by $\vec{a}_1, \vec{a}_2, \vec{a}_3$ in figure

II-VI compounds (e.g. CdS) have Hexagonal Lattice (it also has a cubic form)



Conventional and primitive unit cells of the hexagonal lattice.

[From BW]

$a = 4.207$ Å, $c = 6.843$ Å (see figure)

(Related to hexagonal close-packed structure)

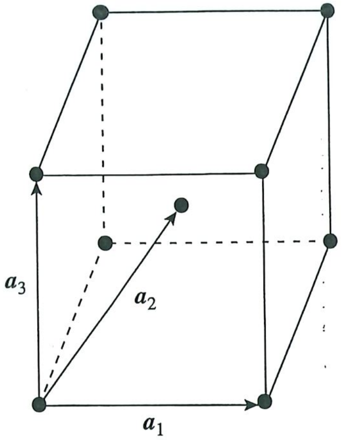
The underlying lattice of Wurtzite structures

Characteristic parameters of face-centered cubic and hexagonal lattices

	Face-centered	Hexagonal
Conventional cell volume	a^3	$(3\sqrt{3}/2)a^2c$
Lattice points per cell	4	3
Primitive cell volume	$\frac{1}{4}a^3$	$(\sqrt{3}/2)a^2c$
Lattice points per unit volume	$4/a^3$	$2/\sqrt{3}a^2c$
Numbers of nearest neighbors	12	6 $(c > a)$
Nearest neighbor distance	$a/\sqrt{2}$	$a(c > a)$
Number of second neighbors	6	$2(c < \sqrt{3}a)$
Second neighbor distance	a	$c(c < \sqrt{3}a)$

Up to here, it is about the Mathematical Construction of Lattices

Ex: Study the Primitive unit cell and conventional unit cell of BCC.



Primitive translation vectors for the body-centered cubic Bravais lattice which connect the lattice point at the origin to lattice points at two cube corners and one cube center.

$$\vec{a}_1 = a\hat{x}$$

$$\vec{a}_2 = \frac{a}{2}(\hat{x}+\hat{y}+\hat{z})$$

$$\vec{a}_3 = a\hat{z}$$

↑

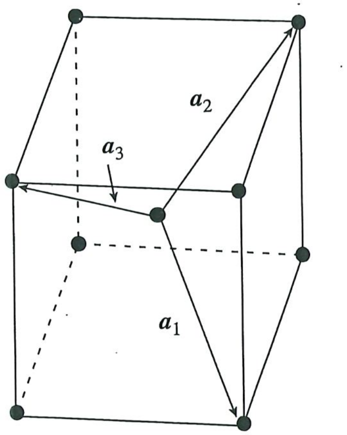
Both work OK! (Why?)

↓

$$\vec{a}_1 = \frac{a}{2}(\hat{x}-\hat{y}-\hat{z})$$

$$\vec{a}_2 = \frac{a}{2}(\hat{x}+\hat{y}+\hat{z})$$

$$\vec{a}_3 = \frac{a}{2}(-\hat{x}-\hat{y}-\hat{z})$$



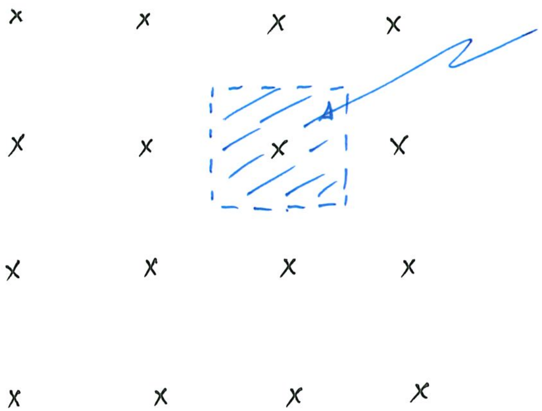
Primitive translation vectors of the body-centered cubic lattice connecting the lattice point at the origin to lattice points at three cube centers.

Body-centered cubic lattice is important to semiconductors because it is the Reciprocal Lattice of FCC.

Volume nearest to a lattice point : The Wigner-Seitz Cell

- Take a point, find volume that is nearest to the point than any other point
- Volume gives Wigner-Seitz cell of the lattice
- One lattice point in W-S cell ⇒ Volume = Ω_c ← also has one lattice point in it
- Shape of W-S cell best represents the symmetry of the lattice
- W-S cell is also a primitive cell (can be used as a "tile")

2D square lattice

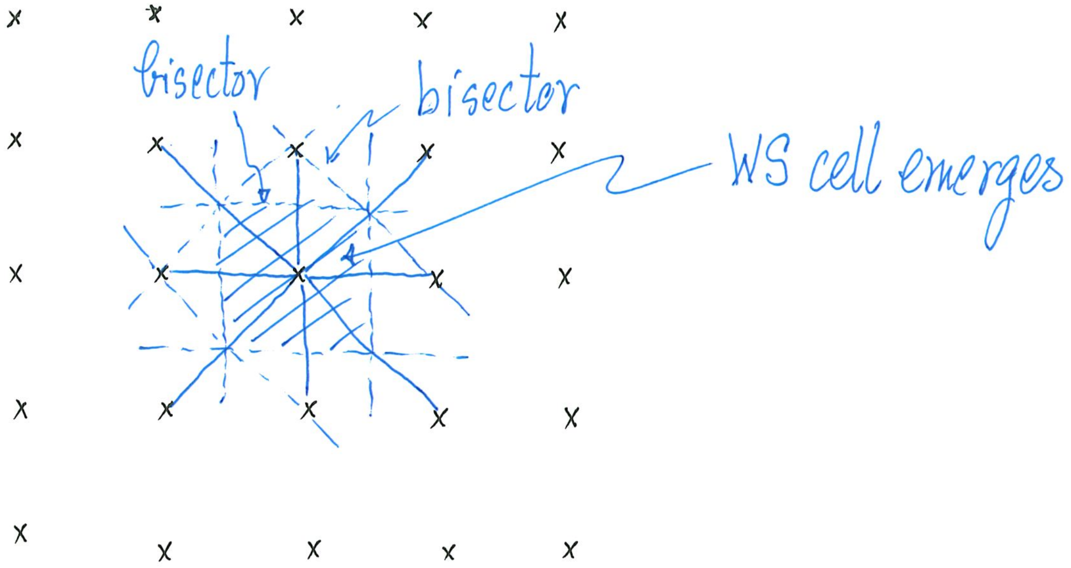


Wigner-Seitz cell of square lattice

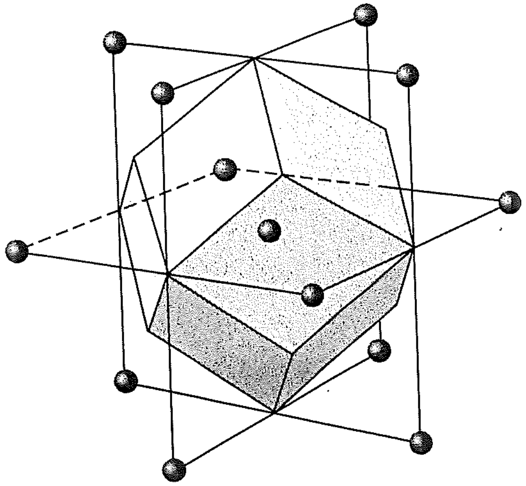
(every point is nearer to lattice point at the center than other lattice points)

Procedure

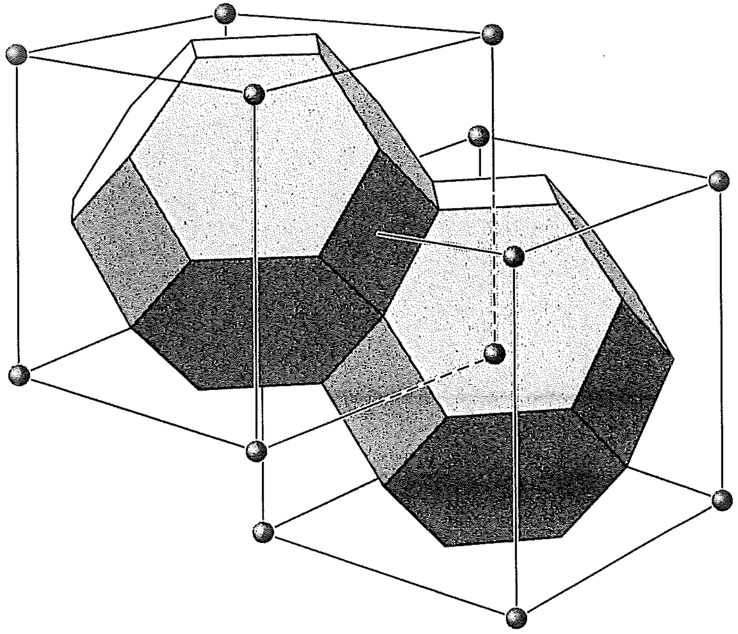
- Draw lines from lattice point to other lattice points
- Drop perpendicular lines (planes) to bisect the lines
- Wigner-Seitz cell emerges as area (2D) [volume (3D)] enclosed by bisecting planes



Some Wigner-Seitz Cells in 3D



Face-centered Cubic Lattice
Wigner-Seitz Cell

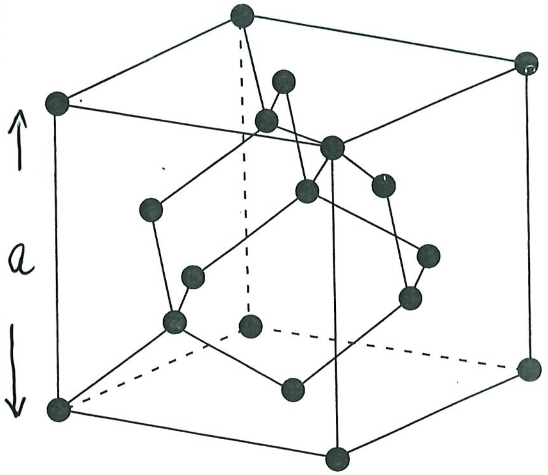


Body-centered Cubic Lattice
Wigner-Seitz Cell

[From Kittel, "Introduction to Solid State Physics"]

Real Semiconductors (With Atoms)

- Si, Ge takes on the Diamond Structure



Conventional unit cell of the diamond structure.

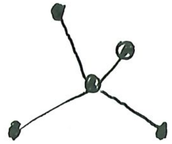
- Carbon atoms ⇒ Diamond (insulator)
- Silicon atoms ⇒ Semiconductor
- Germanium ⇒ Semiconductor

2 atoms decorating every lattice point
⇒ a basis of 2 atoms (identical atoms for Si, Ge)

Referring to the lattice constant a

- one atom at $\vec{\rho}_1 = 0$ (on a lattice point)
- another atom at $\vec{\rho}_2 = \frac{a}{4}(\hat{x} + \hat{y} + \hat{z})$ from a lattice point

or $\left(\frac{a}{4}, \frac{a}{4}, \frac{a}{4}\right)$

Note that  structure (109°28′ between "bonds")

each atom has 4 nearest neighbors in a tetrahedron

Referring to picture on last page:

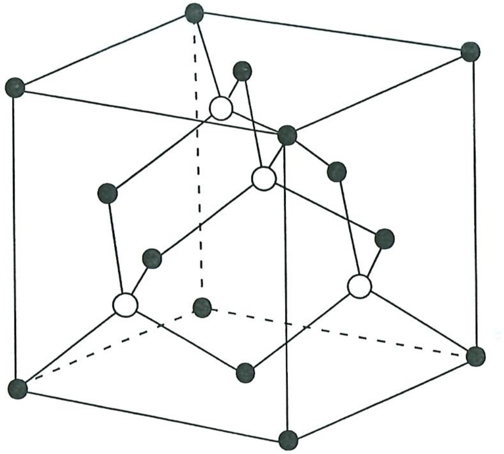
Atom at (0,0,0) has 4 nearest neighbors at $\begin{cases} a(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}) \\ a(-\frac{1}{4}, -\frac{1}{4}, \frac{1}{4}) \\ a(-\frac{1}{4}, \frac{1}{4}, -\frac{1}{4}) \\ a(\frac{1}{4}, -\frac{1}{4}, -\frac{1}{4}) \end{cases}$

Atom at $a(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ has 4 nearest neighbors at $\begin{cases} a(0,0,0) \\ a(\frac{1}{2}, \frac{1}{2}, 0) \\ a(\frac{1}{2}, 0, \frac{1}{2}) \\ a(0, \frac{1}{2}, \frac{1}{2}) \end{cases}$

[remind you of sp^3 hybridization? What is it?]

- Many III - V compounds have Zincblende structure

  e.g. GaAs, InSb, ...



Conventional unit cell of the zincblende structure.

- ● Atom A ○ Atom B

locations of A and B like those in diamond structure

Atom A at $a(0,0,0)$; Atom B at $a\left(\frac{1}{4},\frac{1}{4},\frac{1}{4}\right)$

Since $A \neq B$, Zincblende structure has lower symmetry than diamond structure

$$\text{Atoms A form FCC}, \underbrace{\text{Atoms B form FCC}}_{\text{Displaced by } \left(\frac{a}{4},\frac{a}{4},\frac{a}{4}\right) \text{ from FCC of A atoms}}$$

Lattice constants a in Å for representative cubic semiconductors at room temperature

Material	Structure	a	Material	Structure	a
Si	diamond	5.43			
Ge	diamond	5.65	ZnS	zincblende	5.423
AlP	zincblende	5.431	ZnSe	zincblende	5.661
AlAs	zincblende	5.631	ZnTe	zincblende	6.082
AlSb	zincblende	6.142	CdS	zincblende	5.832
GaP	zincblende	5.447	CdSe	zincblende	6.052
GaAs	zincblende	5.646	CdTe	zincblende	6.423
GaSb	zincblende	6.130	PbS	rocksalt	5.935
InAs	zincblende	6.048	PbSe	rocksalt	6.152
InSb	zincblende	6.474	PbTe	rocksalt	6.353

Common Sense: $a \sim 5\text{-}6$ Å (Why so? Atomic Physics)

a refers to conventional unit cell (cube)

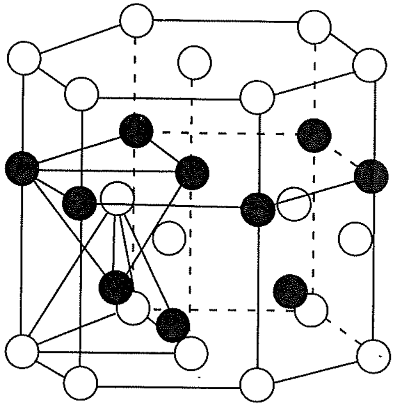
Wurtzite Structure

- II- VI compounds such as CdS

Hexagonal Lattice

\+

Basis of $\underbrace{\text{4 atoms}}_{\text{two A atoms + two B atoms}}$ (decorating each point)



Wurtzite structure showing the tetrahedral environment of each type of atom.

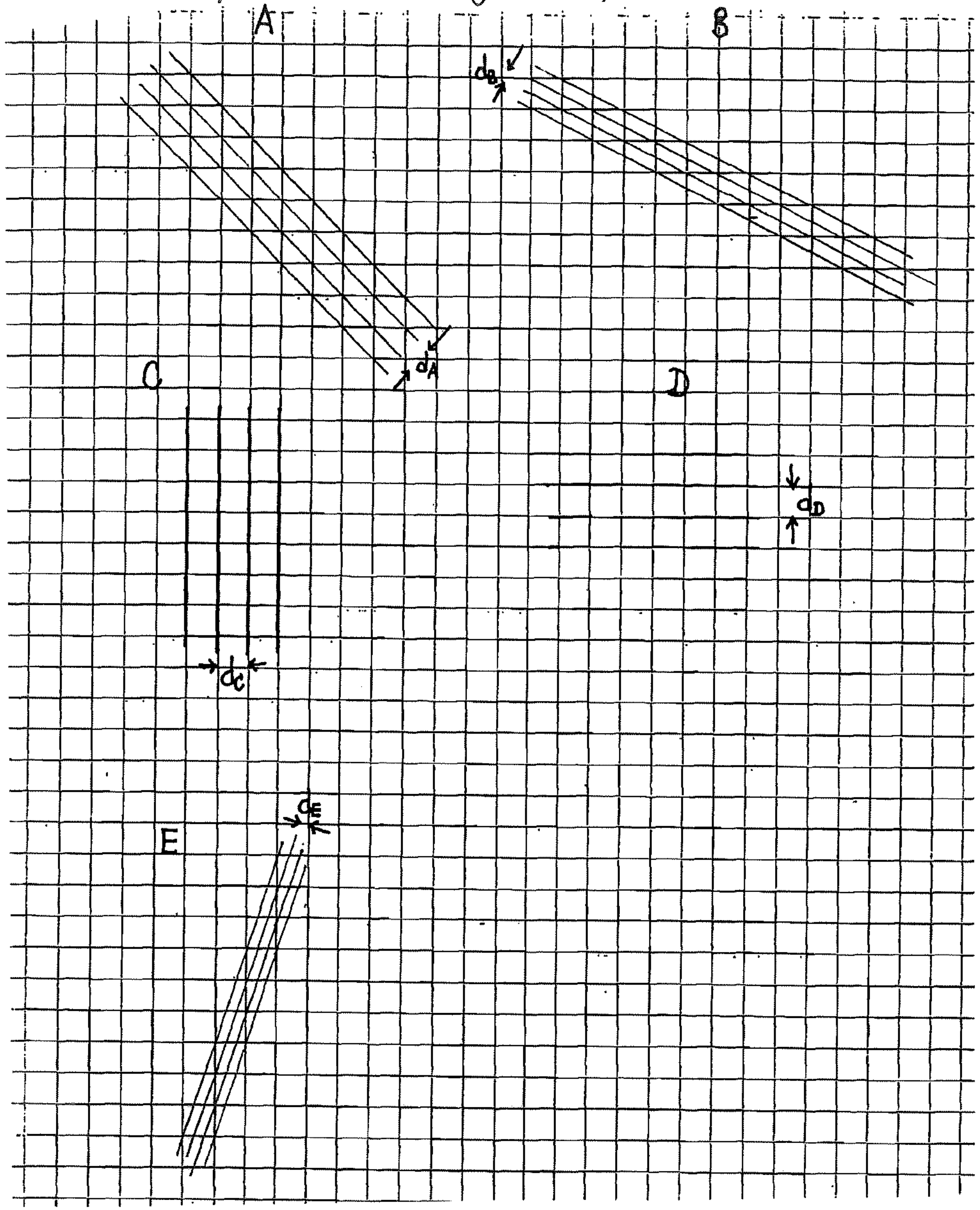
Lattice constant a and the c/a ratio for representative wurtzite structure semiconductors at room temperature

Material	a	c/a
ZnS	3.819	1.64
CdS	4.139	1.62
CdSe	4.309	1.63

[From "BW"]

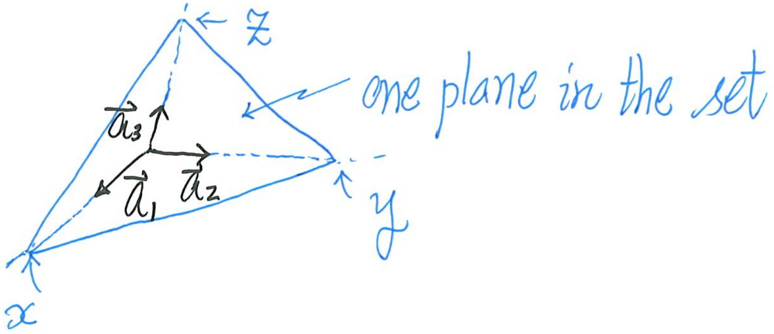
Crystal Planes (formal)

- Many sets of crystal planes that contain all lattice points



- A crystal has many sets of parallel planes that cover all lattice points (see 2D example)
- Set of planes is important for X-ray analysis
- How to label crystal planes?

- Has $\vec{a}_1, \vec{a}_2, \vec{a}_3$



- Read out intercepts x, y, z
- Find smallest integers such that $\frac{1}{x} : \frac{1}{y} : \frac{1}{z} = \overset{\text{integers}}{h : k : l}$

(no intercept means intercept is at ∞, $\frac{1}{\infty} = 0$)

(hkl) (Miller indices) labels the set of planes

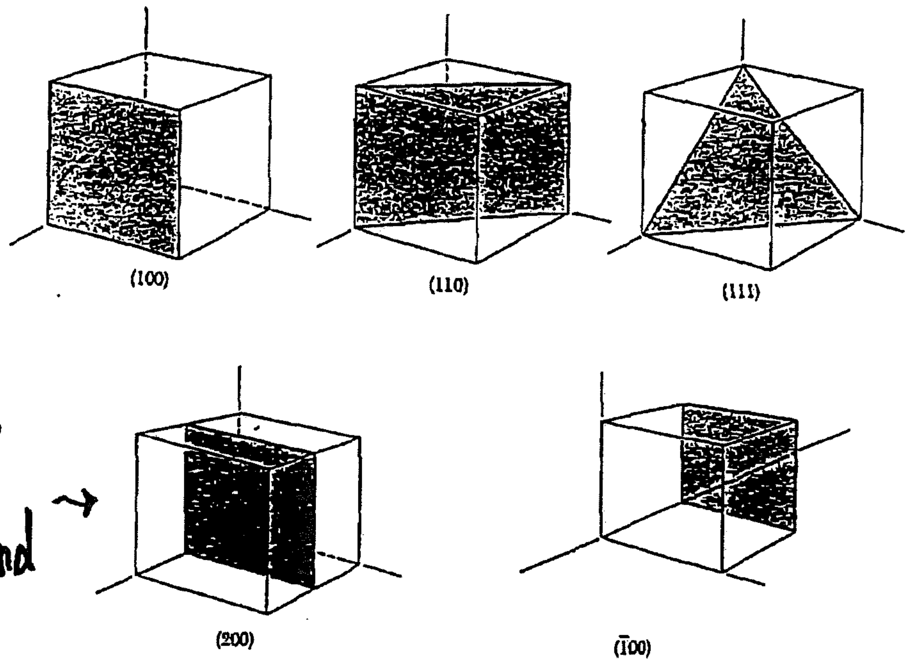
By symmetry, there are other sets of planes that are equivalent
(e.g. cubic ($x \to y$, $y \to z$, $z \to x$))

$\{hkl\}$ represents the family of these sets of planes

This is the recipe.

But there are conventions to follow besides the standard procedure

Cubic lattices



(100) (110) (111)

(200) ($\bar{1}00$)

useful for bcc and fcc →

Indices of important planes in a cubic crystal. The plane (200) is parallel to (100) and to ($\bar{1}00$).

- Here, the (200) plane means a plane parallel to (100) but cutting the x-axis at a/2. (Useful in bcc and fcc)

- Given $\vec{a}_1, \vec{a}_2, \vec{a}_3$, can construct $(\vec{a}_2\times\vec{a}_3)$, $(\vec{a}_3\times\vec{a}_1)$, $(\vec{a}_1\times\vec{a}_2)$
- Set of planes described by (hkl)
- $\boxed{\begin{array}{l}\vec{g} \equiv h(\vec{a}_2\times\vec{a}_3) + k(\vec{a}_3\times\vec{a}_1) + l(\vec{a}_1\times\vec{a}_2) \\ \text{is a vector } \underline{\text{NORMAL to the planes}}\end{array}}^{+}$ (4)

(Ex: Show this)

$$d \equiv \text{distance between adjacent planes (labelled by } (hkl))$$

$$= \frac{\Omega_c}{|\vec{g}|} \leftarrow \text{volume of primitive unit cell } |\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)|$$

e.g. simple cubic (hkl) planes $(\vec{a}_1 = a\hat{x},\ \vec{a}_2 = a\hat{y},\ \vec{a}_3 = a\hat{z})$, $\vec{g} = ha^2\hat{x} + ka^2\hat{y} + la^2\hat{z}$

$$d(hkl) = \frac{a^3}{a^2\sqrt{h^2+k^2+l^2}} = \frac{a}{\sqrt{h^2+k^2+l^2}}$$

[+] Started to see that constructing $(\vec{a}_2\times\vec{a}_3)$, $(\vec{a}_3\times\vec{a}_1)$, $(\vec{a}_1\times\vec{a}_2)$ will be useful. Indeed, this is a reason of constructing the Reciprocal Lattice.

Summary

- Lattice + Basis (General)
- face-centered cubic lattice [diamond and zincblende structures have fcc Bravais lattice]
- $\vec{R}_\ell = l_1 \vec{a}_1 + l_2 \vec{a}_2 + l_3 \vec{a}_3$ maps out lattice
- $\vec{\rho}_i$ locates basis atoms relative to a lattice point
- $\vec{\rho}_1 = 0$, $\vec{\rho}_2 = a(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ for diamond (Si, Ge) and zincblende (GaAs, InSb)
- Primitive unit cell, Conventional unit cell, Wigner-Seitz cell
- Lattice planes, $(hk\ell)$ labelling, $\{hk\ell\}$ labelling
- $\vec{g} = h(\vec{a}_2 \times \vec{a}_3) + k(\vec{a}_3 \times \vec{a}_1) + \ell(\vec{a}_1 \times \vec{a}_2)$ is normal to $(hk\ell)$ set of planes

(Other basic language of crystal structures will be introduced when needed)