Day 1 Phys 58

~~Need substitute for 2 Mondays!~~

- Introduce myself
- Introductions of class.
- Syllabus,
  - textbook (cover 1–8, part of 9, part of 14)
  - HW
  - exam

What is a solid?, resist shear

- crystalline ☆ This class!
- amorphous

- infinite ☆
- finite (surfaces)

Crystal: periodicity (atoms)

1D: • • • •

what about •• •• •• •• ?

period — yes, is crystal

lattice details of periodicity (abstract pts)

basis details of atoms that are found at the lattice pts

Note lattice choice is not unique

lattice × × × ×
basis ••

=

lattice × × × ×
basis |→••

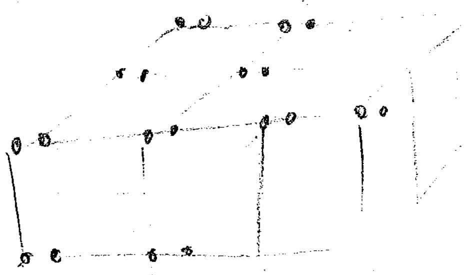
(but some choices are better than others)

best choice? × × × ×
•|•

basis is symmetric, possibly best choice.

Symmetry! Mathematical technique for analyzing symm. = Group Theory (beyond this class)

3D



← could be crystal

lattice = "simple cubic"

basis? atom 1 at $(0,0,0)$
atom 2 at $(0,\frac{1}{4},0)$

Lattice vectors - Defn: Any vector which causes (infinite) crystal to be unchanged after translation
— Vectors that join lattice pts

(translates into itself)

What are some L.V.s for cube above?

Primitive lattice vectors: (1) the 3 ones (non unique choice) that form basis for all L.V.s

Example: for cube above,

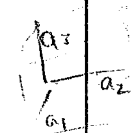
$\vec{a}_1 = (1,0,0)$
$\vec{a}_2 = (0,1,0)$
$\vec{a}_3 = (0,0,1)$

(2) and are as "small as possible"
(a consequence of (1), really. See Fig 3 pg 5)

ones that minimize area (volume) will all work

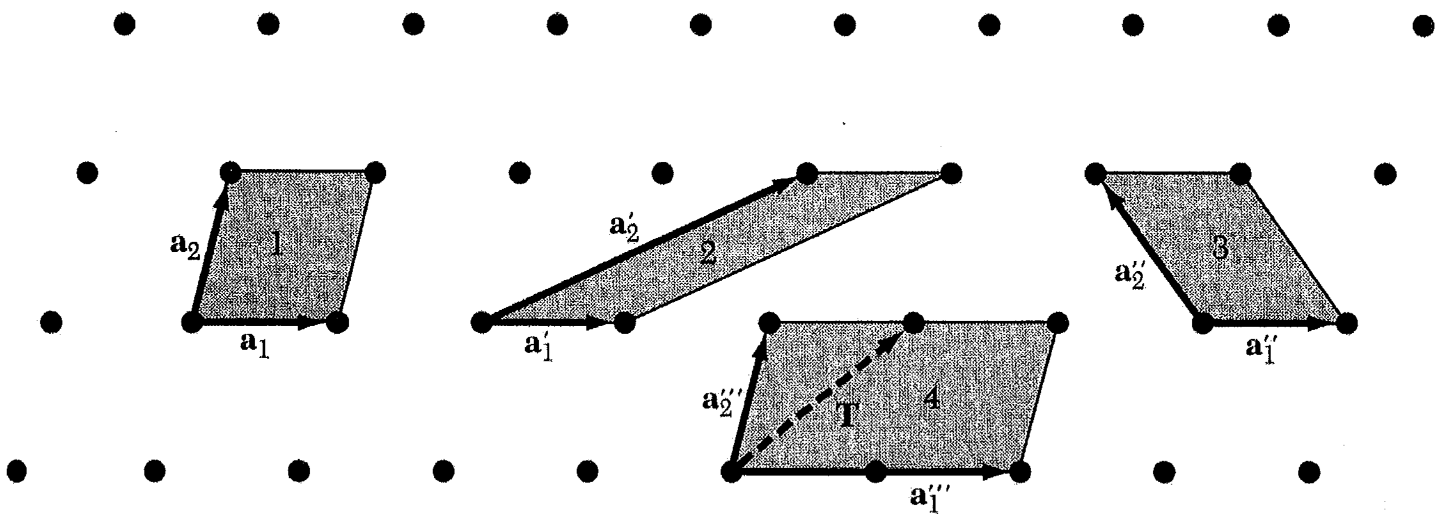
Small as possible: defined by volume of space of parallelepiped defined by $\vec{a}_1, \vec{a}_2, \vec{a}_3$

$$\text{volume} = |\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)|$$



any lattice vector $\vec{R} = n\vec{a}_1 + m\vec{a}_2 + l\vec{a}_3$

K'ttel, Fig. 3a (page 5)



(a)

Basis vectors – vectors from origin to basis atoms
↳ position of lattice point

j atoms: $\vec{r}_j = x_j \vec{a}_1 + y_j \vec{a}_2 + z_j \vec{a}_3$

if desired, can pick origin so

x_j, y_j, z_j all between 0 + 1.

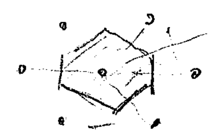
day 2

Wigner-Seitz cell

– a "primitive lattice cell" = parallelepiped formed by $\vec{a}_1, \vec{a}_2, \vec{a}_3$

→ How many will there be in a given volume?
Answer: the same as # of lattice pts.

– the WS cell = a specially chosen primitive cell



region enclosed by perpendicular bisectors.

primitive basis

– a basis that's based on a set of primitive L.V.s.

14 Bravais Lattices – handout, see notes on next page

Symmetry, again

day 2 Notation

1) translation (already discussed)

2) rotation — defn by axis about which x'tal can be rotated

simple cubic: $90°$, $180°$, $270°$ about x
C_4, C_2, C_4^3
C_2^2

also about y, z

Notation.. let's not bother (?)

C_{YX}^- = 270° rotation about x-axis C_{YX}^+ = 90° rotation

3) reflection: defined by plane about which x'tal atoms can be reflected σ_x

4) combo: rotation + reflection labeled "S"

5) inversion: if pt exists through which all atoms can be inverted "I"

group of pt symmetries together form a "group"

Symmetry of crystal vs symmetry of lattice rev

3D lattices

14 Bravais lattices! (I expected more)

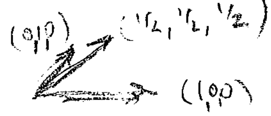
→ handout from Stokes' book

Note on bcc and fcc : like 2D "centered rectangular" have a choice

→ Mostly use the "conventional cell", cubic and not the primitive cell

Skipped

one choice of lattice vectors



(units of a)

another choice, Kittel Fig 1.10 pg 10

$\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}$

$-\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

$\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}$

fcc

primitive basis vectors

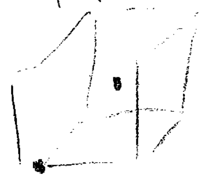
$\frac{1}{2}, \frac{1}{2}, 0$

$0, \frac{1}{2}, \frac{1}{2}$

$\frac{1}{2}, 0, \frac{1}{2}$

Fig 11 pg 11

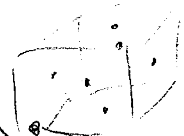
bcc : How many pts in conventional cell?



two

$\frac{1}{8} \times 8 + 1 = 2$

volume of primitive cell $= \frac{a^3}{2}$



four

corner : 8, each shared by 8

face : 6, each shared by 2

$\frac{1}{8} \times 8 + \frac{1}{2} \times 6 = 4$

volume of primitive cell $\frac{a^3}{4}$

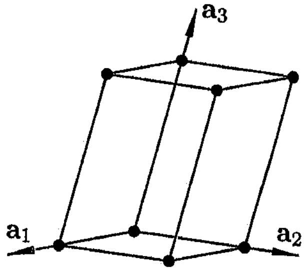
This class :

I think all materials we will study are lattice types

1) cubic (sc)
2) bcc
3) fcc
4) hexagonal (?)

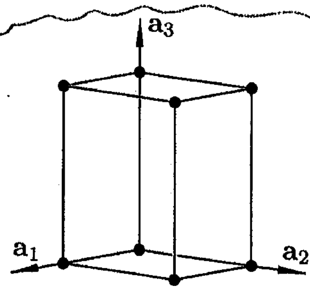
From Stokes, Solid State Physics for Advanced Undergrad Students.

14 Bravais Lattices in 3D



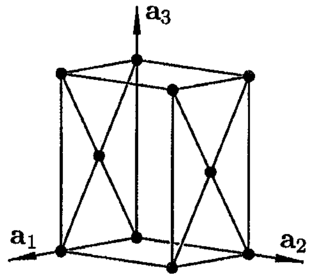
Triclinic P

$a_1 \neq a_2 \neq a_3$
$\alpha \neq \beta \neq \gamma$

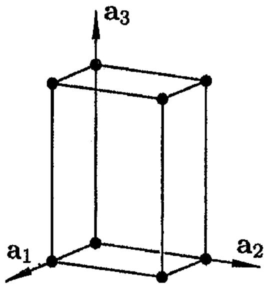


Monoclinic P

$a_1 \neq a_2 \neq a_3$
$\alpha = \gamma = 90° \neq \beta$

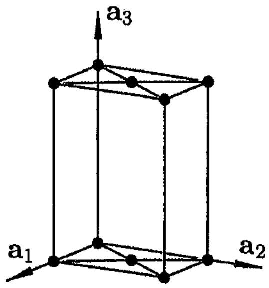


Monoclinic B

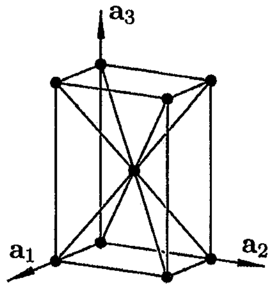


Orthorhombic P

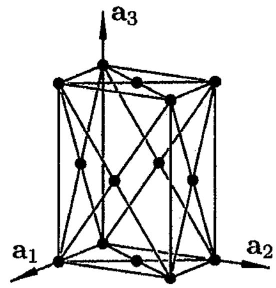
$a_1 \neq a_2 \neq a_3$
$\alpha = \beta = \gamma = 90°$



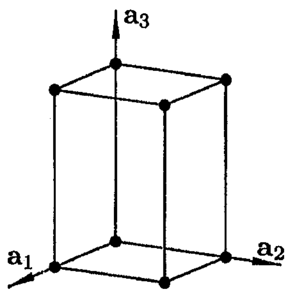
Orthorhombic C



Orthorhombic I

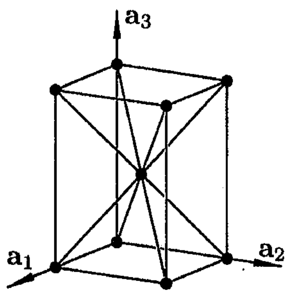


Orthorhombic F

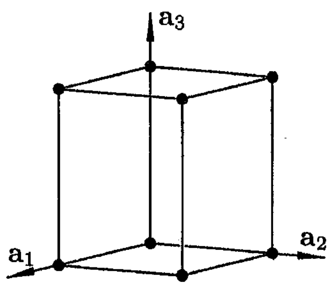


Tetragonal P

$a_1 = a_2 \neq a_3$
$\alpha = \beta = \gamma = 90°$

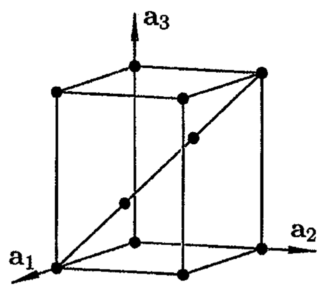


Tetragonal I



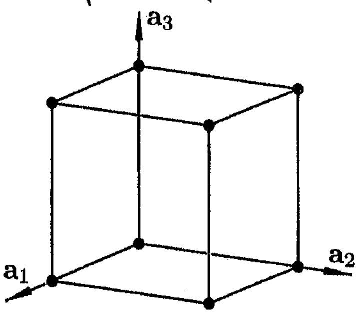
Hexagonal P

$a_1 = a_2 \neq a_3$
$\alpha = \beta = 90°, \gamma = 120°$



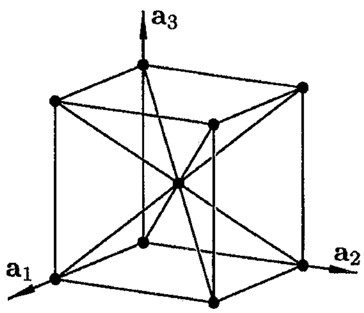
Hexagonal R

aka "Trigonal"
(with different $\vec{a}_1, \vec{a}_2, \vec{a}_3$ vectors)



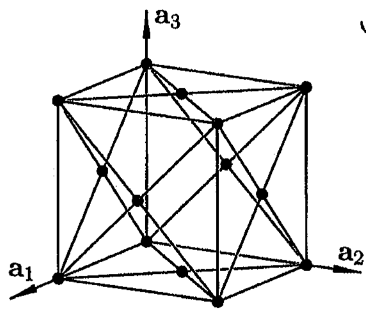
Cubic P

$a_1 = a_2 = a_3$
$\alpha = \beta = \gamma = 90°$



Cubic I

"body centered"



Cubic F

"face centered"

(Not mentioned in Kittel)

There are an infinite # of possible crystals
(because basis atoms could be anywhere)

However, there are not an infinite # of ways of classifying the crystals by symmetry.

→ 230 different "space groups"
(of which the Bravais lattices are 14)
dividing into full symmetry of translations + pt group

→ usually ~~the~~ categorized in
32 different "crystal classes"
when ~~or~~ sorted only by pt group symmetries

sc, fcc, bcc (and diamond)
all in same crystal class
but are different space groups

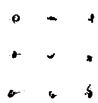
Lattice always has at least as much (if not more) symm. than crystal

Focus now on <u>lattices</u>

Group lattices by symmetry properties

 = same class as 

but different than

 ← this one more symmetric

Consider <u>all possible lattices</u>, turns out only so many distinct classes.

→ called the "Bravais lattices"

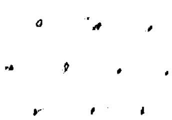
<u>2D</u> - 5 Bravais lattices

1) oblique → $a_1 \neq a_2$, ϕ = no special angle

2) rectangular → $a_1 \neq a_2$ $\phi = 90°$

3) square → $a_1 = a_2$, $\phi = 90°$

4) hexagonal



$a_1 = a_2$, $\phi = 120°$

(why not 60°?) → arbitrary

Harold: obtuse angles generally used when given a choice

~~Day 2~~ ~~Why not pentagonal?~~

5) centered rectangular

rectangular, but w/extra
dot in middle of rectangle