

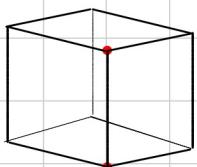
unit cell: volume with which the whole space can be covered without voids or overlap. Not unique for a crystal.
May contain any number of points

primitive (unit) cell: single point inside

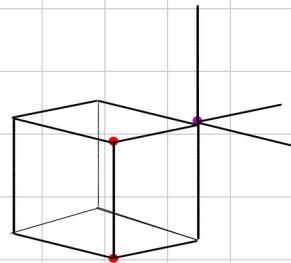
Coordination number: number of nearest neighbors

Some special lattices

SC. simple cubic

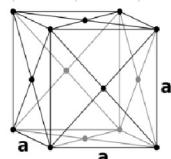
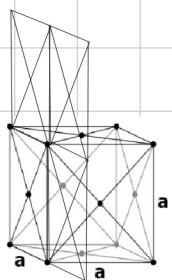


coord.#: 6



- fcc - cube with lattice points at the corners and in the middle of all faces

coord.# = 12

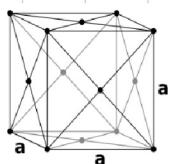


3 parallel planes, 4 points
on each

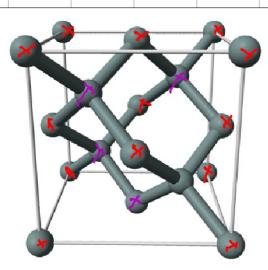
only one plane shown

Diamond lattice:

fcc with 2 atom basis, $\frac{1}{4}$ body diagonal distant



\equiv on two fcc lattice w. 1 atom basis
 $\frac{1}{4}$ body diagonal displaced by $\frac{1}{4}$ of the body diagonal:



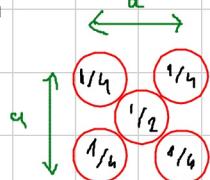
the bonds
are shown
here

red - fcc

purple - fcc (displaced by $\frac{1}{4}$ b.d.)

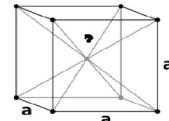
Question:

surface density of points
when $a = 5 \text{ nm}$



$$S_{\text{point}} = \frac{1.5}{a^2} = \frac{1.5}{25} \frac{1}{\text{nm}^2} = 0.6 \frac{1}{\text{nm}^2} = 6 \cdot 10^{17} \frac{1}{\text{m}^2}$$

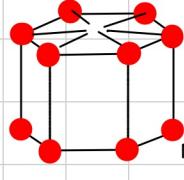
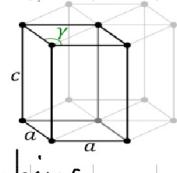
- bcc - cube with lattice points at the corners and in the middle of the cube



- hcp - not a cubic system

$\gamma = 120^\circ$

hexagonal close packing

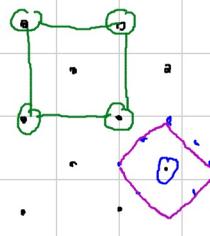


point lattice + basis
put basis here

1 point / cell \rightarrow primitive (unit) cell

1 point $< N$ / cell \rightarrow unit cell

\searrow conventional unit cell
(has all symmetries)



primitive cell
Wigner - Seitz cell

Symmetries

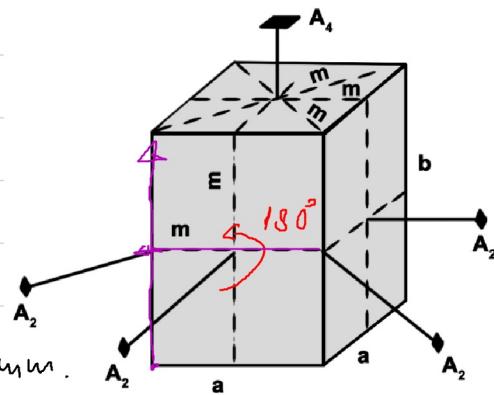
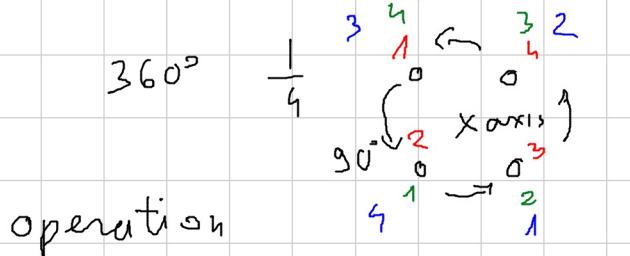
translational symmetry

\leftarrow every crystal
must have it

$$\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$$

\vec{a} lattice vector

rotational symmetry



180°

2 - fold

3 - fold?

2, 3, 4, ~~1~~, 6

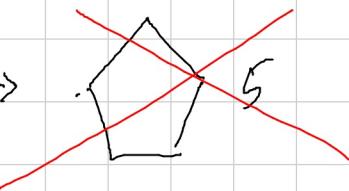
2-fold

3-fold

4-fold

6-fold

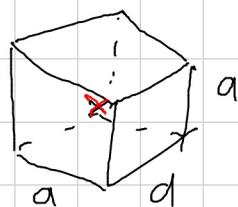
not in
crystals \rightarrow



fullerenes \leftarrow not a crystal
 C_{-80}

mirror plane

reflections to a point
inversion center



$i \uparrow \rightarrow$ rotointversion

categorization of crystals based on symmetries

Bravais lattice

14

monoclinic (right prism with parallelogram base; here seen from above)	simple $\alpha = 90^\circ$ $\beta, \gamma = 90^\circ$	base-centered $\alpha = 90^\circ$ $\beta, \gamma = 90^\circ$
orthorhombic (cuboid)	simple $a \neq b \neq c$	base-centered $a \neq b \neq c$
tetragonal (square cuboid)	simple $a = c$	body-centered $a = c$
rhombohedral (trigonal trapezohedron)	$\alpha \neq 90^\circ$	
hexagonal (centered regular hexagon)		
cubic (isometric; cube)	simple	body-centered
		face-centered

1) lattice with given symmetries
2) all points

$$\text{set of } R \rightarrow \left\{ R = \sum_{l=1}^3 u_l g_l \right\}$$

basis

diamond (C)
fcc with 2 atom bases

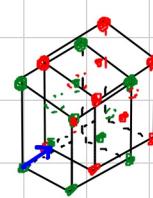
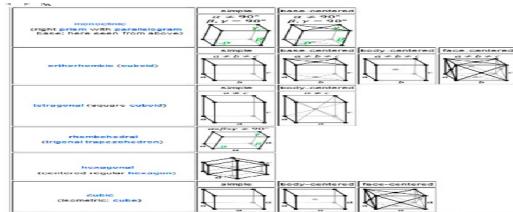


Figure 10.13: The 14 Bravais lattices

→ $\frac{1}{3}$ body diagonal

Crystallographic systems

$$N = 230$$



perfect crystal

translational sym.

infinite
no defects

Crystallographic defects

point defects

vacancy

thermodynamics

S - maximum

$$N_V, N_A$$

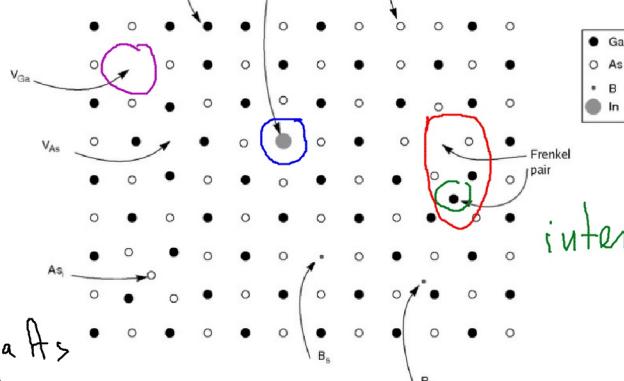
$$\alpha = \frac{N_V}{N_V + N_A} = e^{-\frac{\varepsilon_V}{k_B T}}$$

GaAs

$$T = 300 \text{ K}$$

$$1000 \text{ K}$$

substitutional atom



interstitial

$$\alpha = 10^{-17}$$

$$\alpha = 10^{-5}$$

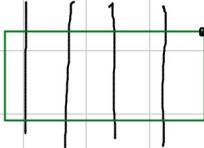
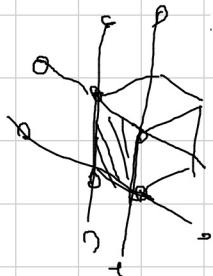
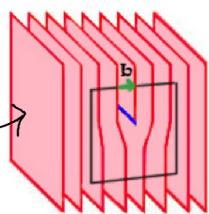
antisite



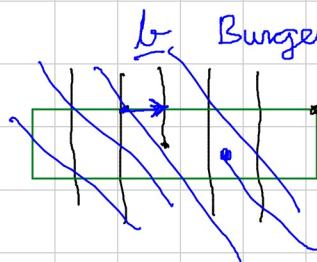
line defects

dislocations

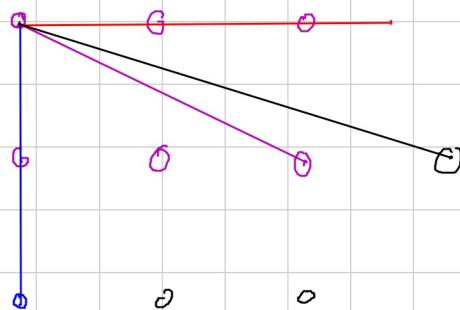
lattice
planes



edge dislocation



Burgers vector



screw
dislocation

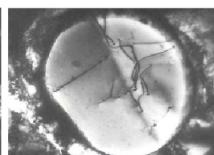
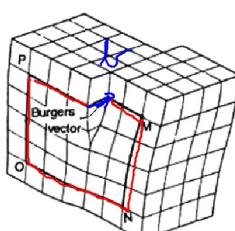
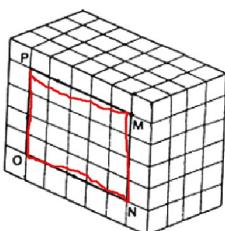
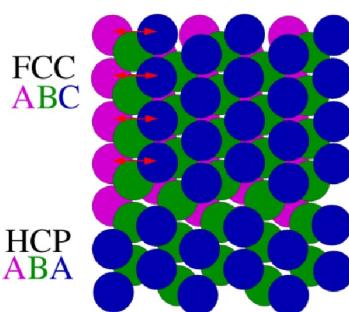
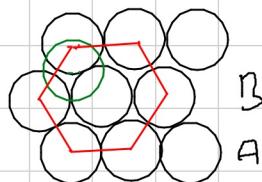


Figure 10.21: Transmission Electron Micrograph of dislocations

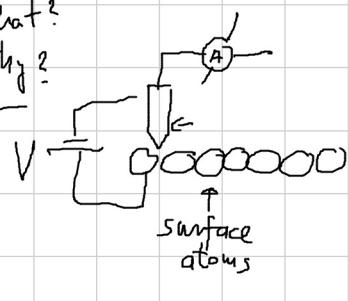
Bulk defects

stacking fault



Determination of lattices

Reciprocal lattice \leftarrow what?
 \leftarrow why?

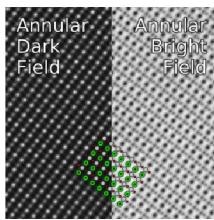


$$QM \Rightarrow$$

tunneling
↑
↓

$$\lambda = \frac{h}{p}$$

Scanning
Tunneling
Microscope



STM

EM waves

X-rays

$\lambda \sim$ distance
interference patterns