# 2. Solid State Physics – unit cells, symmetries, Bravais lattice, defects

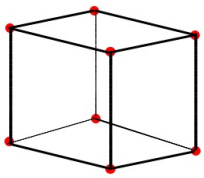
**unit cell**: volume with which the whole space can be covered without voids or overlap. Not unique for a crystal. May contain any number of points

**primitive (unit) cell**: single point inside

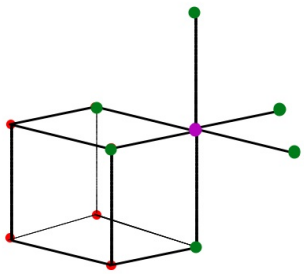
**Coordination number**: number of nearest neighbors

## Some special lattices

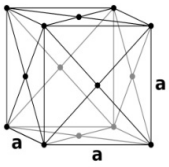
SC: simple cubic



coord.#: 6

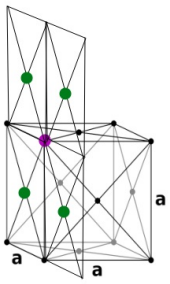


- fcc - cube with lattice points at the corners and in the middle of all faces




coord.# = 12

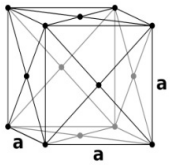
3 ⊥ planes, 4 points on each




only one plane shown

Diamond lattice:

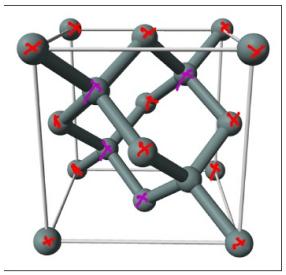
fcc with 2 atom basis, $\frac{1}{4}$ × body diagonal distant




$\cdot \equiv$ 

1/4 body diagonal

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



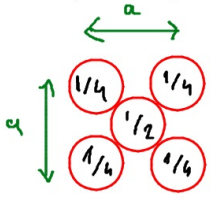
← the bonds are shown here

red – fcc

purple – fcc (displaced by $\frac{1}{2}$ b.d.)

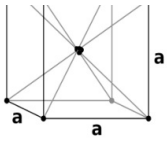
Question:

surface density of points when a = 5nm

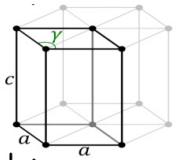



$$S_{point} = \frac{1.5}{a^2} = \frac{1.5}{25}\frac{1}{nm^2} = 0{,}6\frac{1}{nm^2} = 6 \cdot 10^{17}\frac{1}{m^2}$$

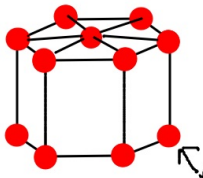
- bcc - cube with lattice points at the corners and in the middle of the cube




- hcp - not a cubic system
  $\gamma = 120°$




hexagonal close packing



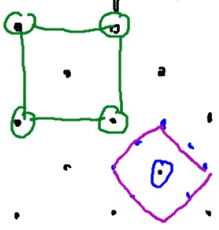
point lattice + basis

↖ put basis here

1 point / cell → primitive (unit) cell

1 point < N / cell → unit cell

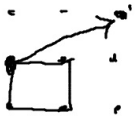
↘ conventional unit cell (has all symmetries)




← primitive all Wigner - Seitz cell

Symmetries

**translational symmetry** ← every crystal must have it

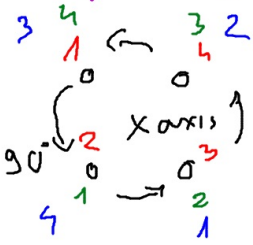


$\underline{R} = n_1 \underline{a}_1 + n_2 \underline{a}_2 + n_3 \underline{a}_3$

↑ lattice vector

rotational symmetry

360° 1/4

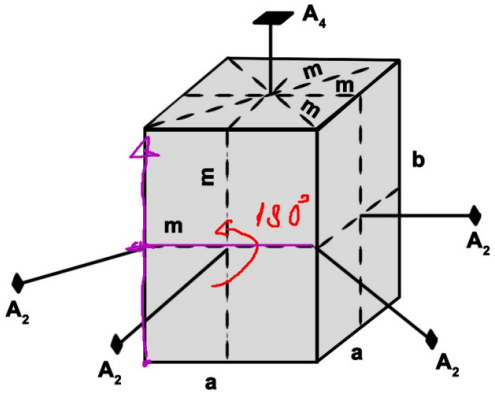



operation

90° 4-fold rot. symm.

180° 2-fold —11—

3-fold?




2-fold | 3-fold △ | 4 fold | ~~5-fold~~ | 6-fold

not in crystals

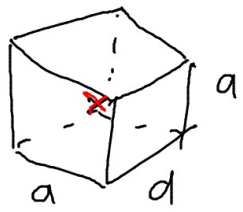
2, 3, 4, ~~5~~, 6

C-80 → fullerenes ← not a crystal

mirror plane

reflection to a point

inversion center




$i \uparrow^n$ rotoinversion

categorization of crystals based on symmetries

## Bravais lattice

1) lattice with given symmetries
2) all points

set of $\underline{R}$ → $\left\{ \underline{R} = \sum_{i=1}^{3} n_i \underline{a}_i \right\}$

14

Crystallographic systems

$N = 230$

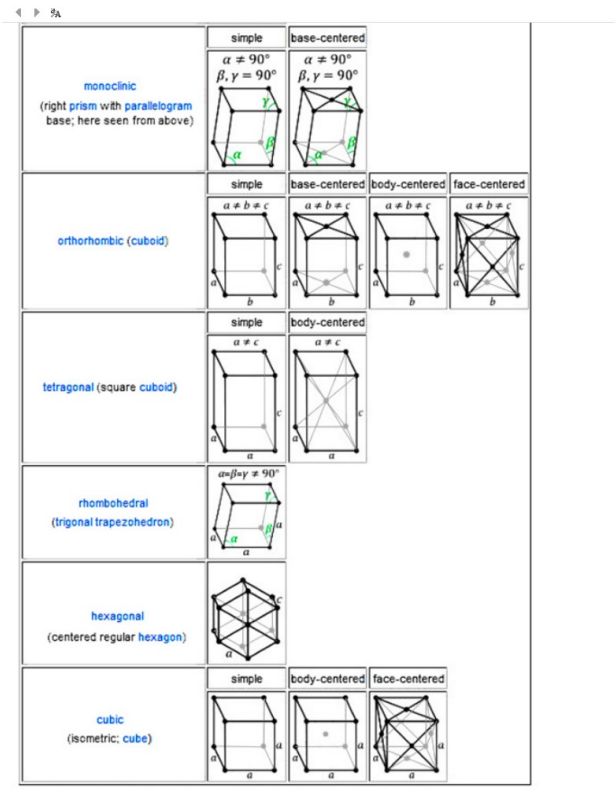
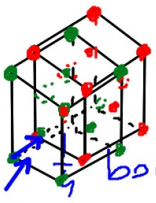



**Figure 10.13:** The 14 Bravais lattices

diamond (C) basis — fcc with 2 atom bases or not a Bravais lattice



body diagonal

## Crystallographic defects

Perfect crystal: translational symmetry

defects and thermal vibrations destroy this

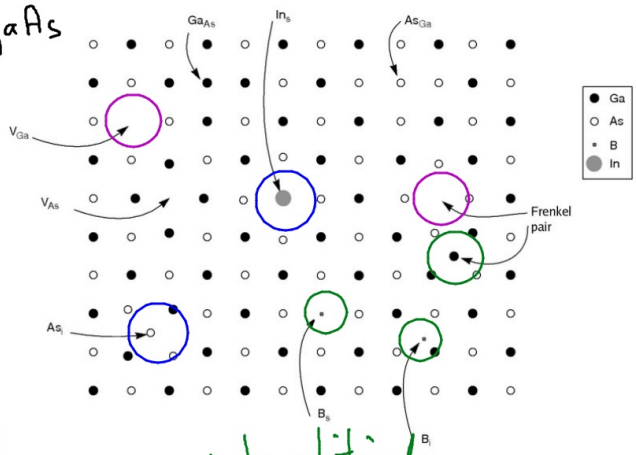
1D — point defects
2D — line defects

3D – planar defects
bulk defects

## Point defects:

substitutional atom

example: GaAs




vacancy

thermodynamics ⇒ in equilibrium vacancies must be present

S – maximum

$N_V, N_A$

vacancy creation

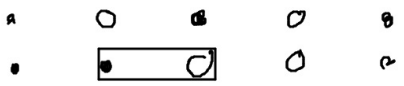
$$\alpha := \frac{N_V}{N_V + N_A} = e^{-\varepsilon_V / k_B T}$$

e.g. GaAs $T = 300$ K $\quad \alpha = 10^{-17}$

1000 K $\quad \alpha = 10^{-5}$

interstitials

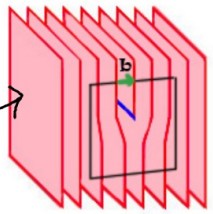
antisite



## line defects

## dislocations

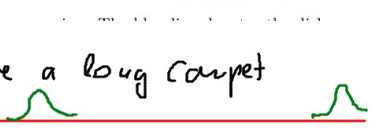
lattice planes

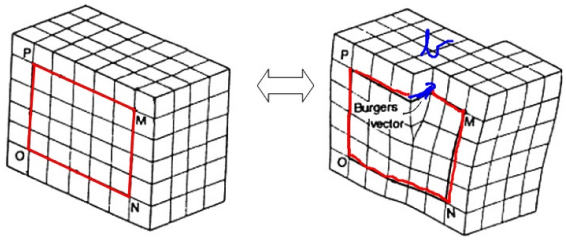



edge dislocation

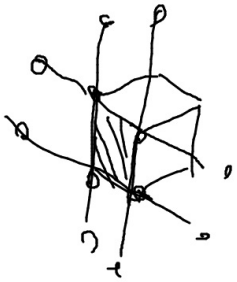
b Burgers vector

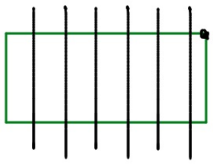
how to move a long carpet

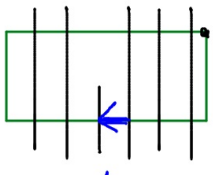





screw dislocation








– stress creates dislocations

– dislocations

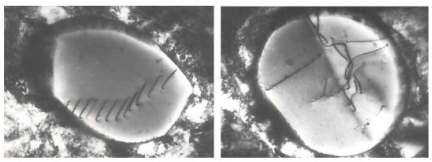
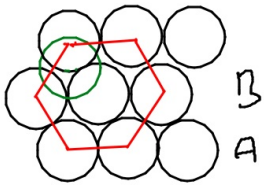


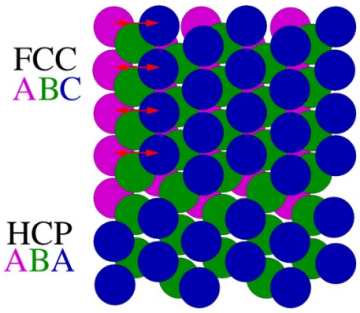
Figure 10.21: Transmission Electron Micrograph of dislocations

- dislocations may move and intersect
- when intersected they cannot move freely

## planar defects

stacking fault



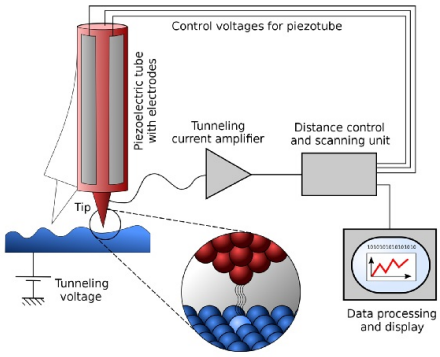

## Bulk defects

---

Determination of lattices

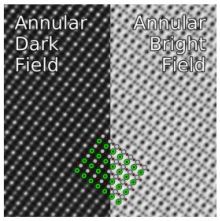
non-conventional microscopy

Scanning Tunneling Microscope (STM)




By Michael Schmid and Grzegorz Pietrzak - Rastertunnelmikroskop-schema.svg, CC BY-SA 2.0 at, https://commons.wikimedia.org/w/index.php?curid=8919417O

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




others: Atomic Force Microscope

---

X-ray spectroscopy (E.M. waves)

$\lambda \sim d_{atomic}$

interference patterns

Reciprocal lattice ← what? why?