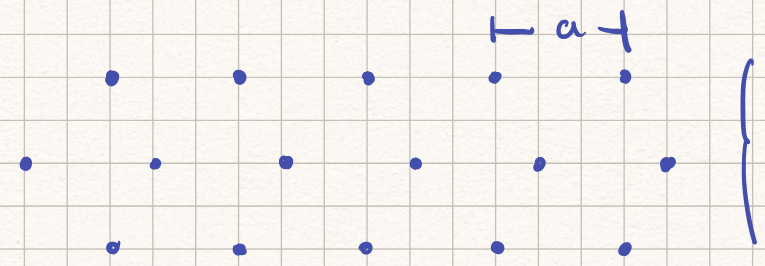
Lattices and Crystal structures

Crystal = basis + lattice



lattice: collection of mathematical points

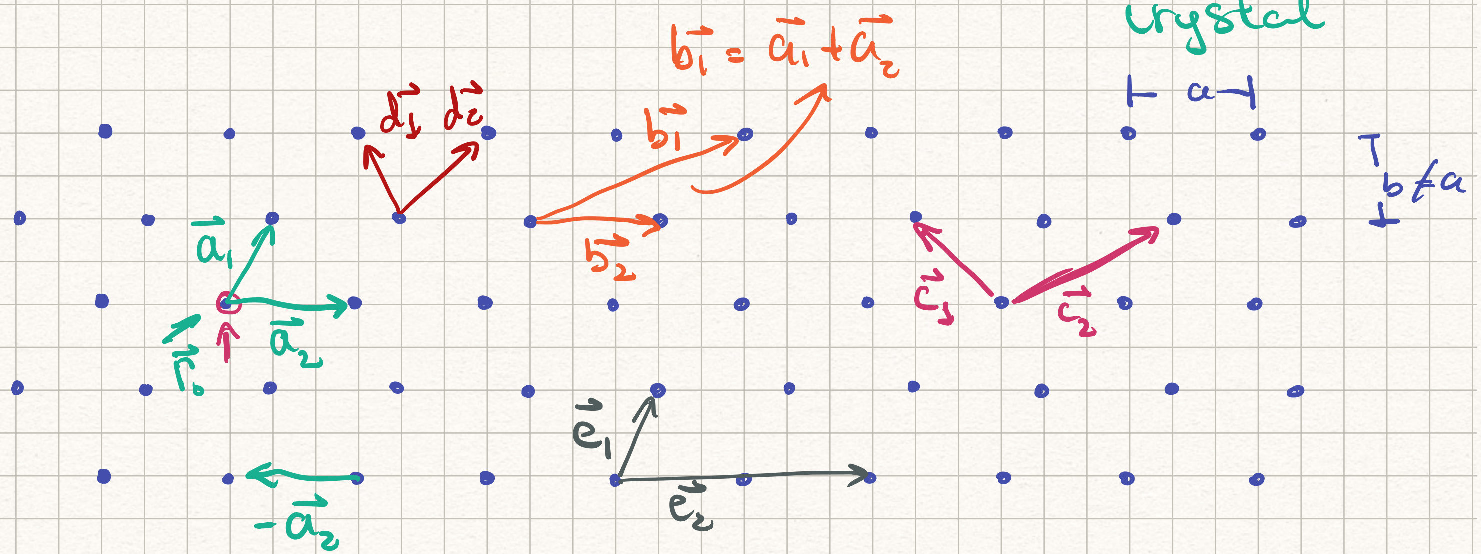
Position of atoms / molecules

C
- Diamonds
- Graphene (2D)
- Graphite

NaCl → Salt

Na^+ Cl^-

Basis of the salt crystal



•: lattice point

$\vec{a_1}, \vec{a_2}$: Translation vector ← $\{\vec{c_1}, \vec{c_2}\}$

$\vec{b_1}, \vec{b_2}$ ↗

← $\{\vec{d_1}, \vec{d_2}\}$

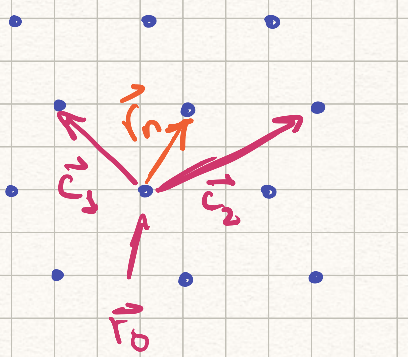
← $\{\vec{e_1}, \vec{e_2}\}$

$\vec{r_n}$: the position of n-th lattice point

$\vec{r_n} = \vec{r_0} + \mu_n \vec{a_1} + \nu_n \vec{a_2}$ $\qquad \{\mu_n, \nu_n\} \in$ Integers

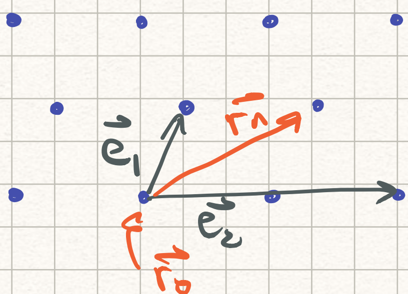
Holds for any $\vec{r_0}$ and for any $\vec{r_n}$ with $\{a_1, a_2\}$ $\{\vec{b_1}, \vec{b_2}\}$

Find $\vec{d_1}$ and $\vec{d_2}$ in terms of $\vec{a_1}$ and $\vec{a_2}$.



There's no μ_n and ν_n such that $\vec{r_n} = \vec{r_0} + \mu_n \vec{c_1} + \nu_n \vec{c_2}$

We cannot explore the <u>entire</u> lattice using the vectors $\{\vec{c_1}, \vec{c_2}\}$ and $\{\vec{e_1}, \vec{e_2}\}$

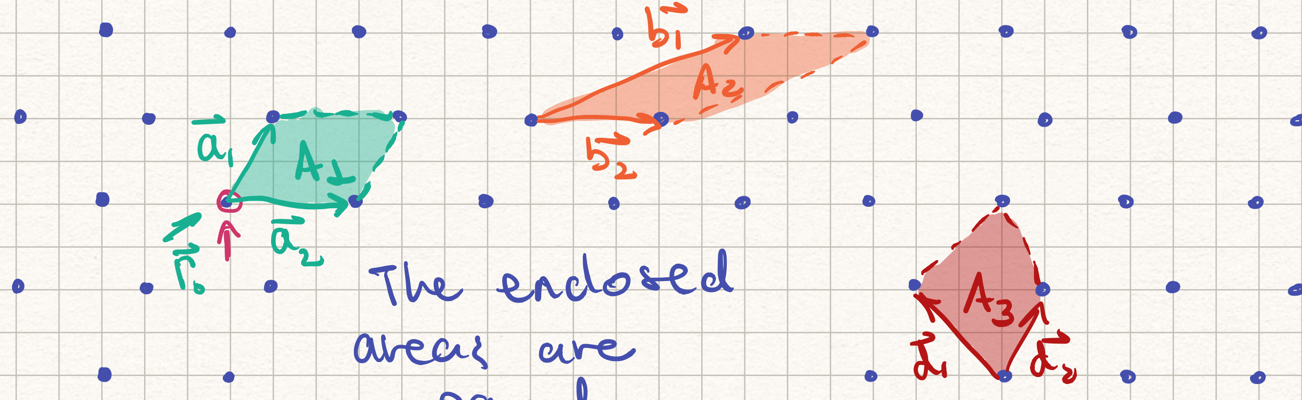


$\vec{r_n} = \vec{r_0} + \mu_n \vec{e_1} + \nu_n \vec{e_2}$

If the translation vector allows to explore the entire lattice $\Rightarrow$ Translation vectors are "primitive"

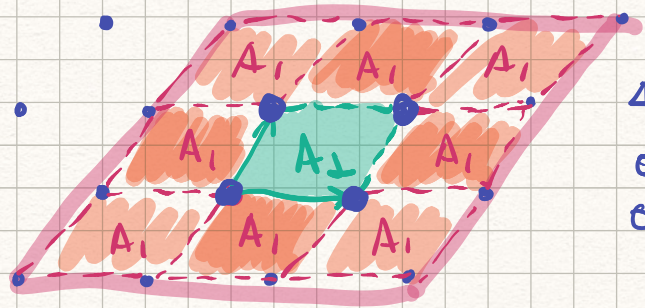
$\{\vec{a_1}, \vec{a_2}\}$, $\{\vec{b_1}, \vec{b_2}\}$ and $\{\vec{d_1}, \vec{d_2}\}$ are primitive Trans. vectors.

$\{\vec{c_1}, \vec{c_2}\}$ and $\{\vec{e_1}, \vec{e_2}\}$ are <u>not</u> primitive trans. vectors



The enclosed areas are equal. $A_1 = A_2 = A_3$

A_1 (A_2 and A_3): primitive cell

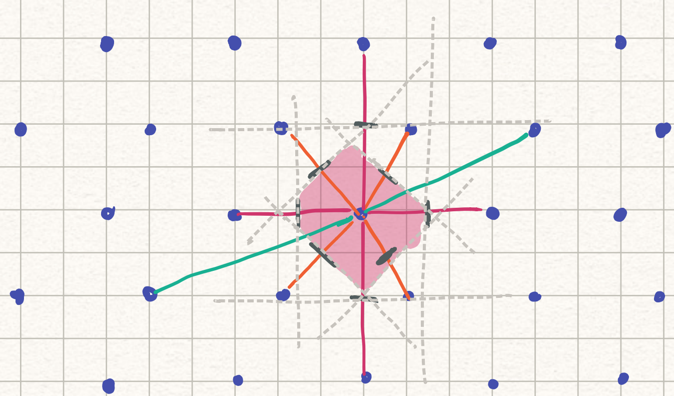


4 lattice points on the corners of the "green" cell $\times \dfrac{1}{4 \text{ cells}}$

= 1 lattice point per cell

primitive cell:
→ minimum area enclosed from a lattice
→ 1 (and only 1) lattice point inside

Wigner-Seitz cell



1. Connect nearest neighbours
2. Cut the connections midway
3. Extend these lines
4. Highlight the area enclosed ↑ minimum