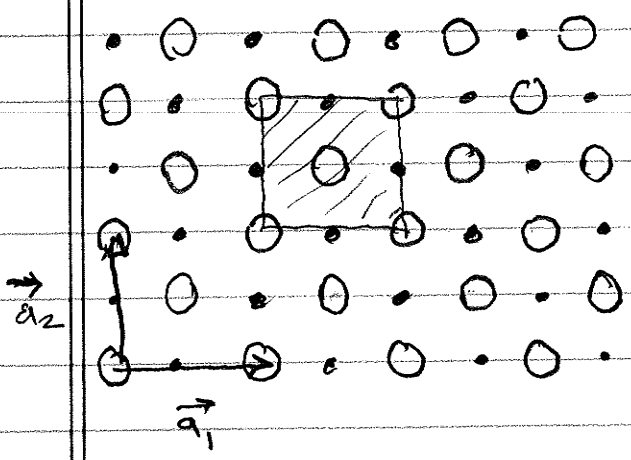
Crystal Structure - Sidebottom

If we look at many solids we notice the nuclei's positions form a pattern. (This is the chief distinction between a solid and a liquid!)

How do we describe such a pattern mathematically? Consider an example (in 2D so I can draw it)



Two types of atoms • and ○

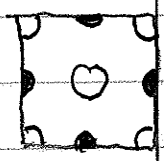
repeating unit is shaded square

Describe by position of lower left corner

$$\vec{T} = h\vec{a}_1 + k\vec{a}_2 \qquad h, k \text{ integers}$$

and also the contents of tile

repeating unit →



central ○ atom $\quad \vec{R}_1 = \frac{1}{2}\vec{a}_1 + \frac{1}{2}\vec{a}_2$

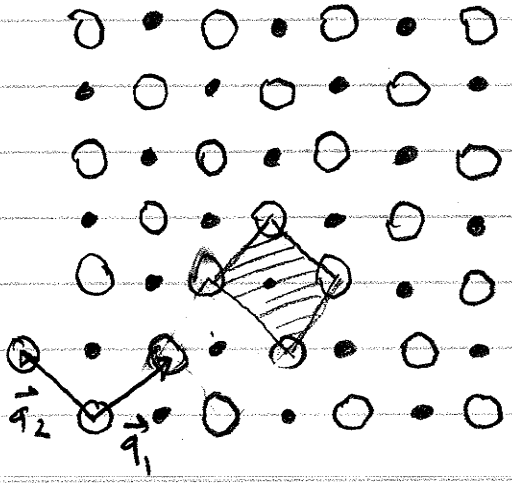
four corner ○ atoms $\quad \left\{ \begin{array}{l} R_2 = 0\vec{a}_1 + 0\vec{a}_2 \\ R_3 = 1\vec{a}_1 + 0\vec{a}_2 \\ R_4 = \\ R_5 = \end{array} \right\}$ 1/4 atom each

four side • atoms $\quad \left\{ \begin{array}{l} R_6 = \frac{1}{2}\vec{a}_1 + 0\vec{a}_2 \\ R_7 = 0\vec{a}_1 + \frac{1}{2}\vec{a}_2 \end{array} \right\}$ 1/2 atom each

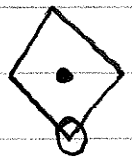
TOTAL : 2 ○ atoms + 2 • atoms

SB
CS-2

But this is more complicated than necessary
(we were prejudiced by our love for horizontal + vertical!)



Use tilted $\vec{a}_1, \vec{a}_2$



← repeating unit

$\vec{T} = h\vec{a}_1 + k\vec{a}_2$ gives location of lowest point of tile

$\vec{R}_1 = 0\vec{a}_1 + 0\vec{a}_2$ location of O atom
$\vec{R}_2 = \frac{1}{2}\vec{a}_1 + \frac{1}{2}\vec{a}_2$ " " • atom

Total 1 O and 1 • atoms

"Primitive cell": the smallest tile that can fill space with desired pattern

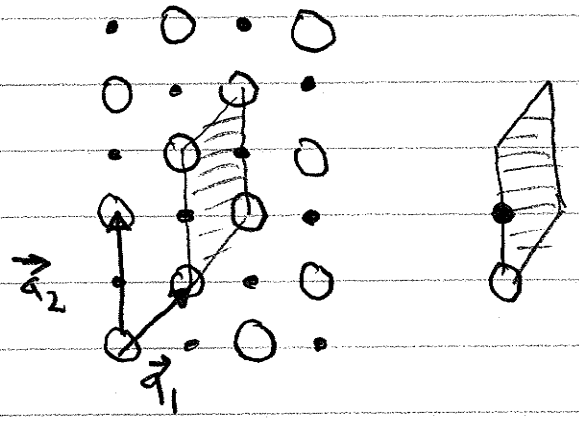
(1) only 1 lattice point $h\vec{a}_1 + k\vec{a}_2$

(2) smallest area $|\vec{a}_1 \times \vec{a}_2|$

(3) basis set of just single molecular unit
(O • in example above)

SB
CS-3

Primitive cell is not unique

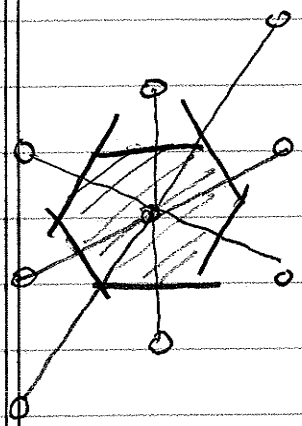


also works.

○ at $0\vec{a}_1 + 0\vec{a}_2$

• at $0\vec{a}_1 + \frac{1}{2}\vec{a}_2$

Wigner-Seitz primitive cell is a particularly nice choice. It is constructed by drawing lines from 1 lattice point $T = h\vec{a}_1 + k\vec{a}_2$ to all neighbours, and then bisecting those lines and taking enclosed area

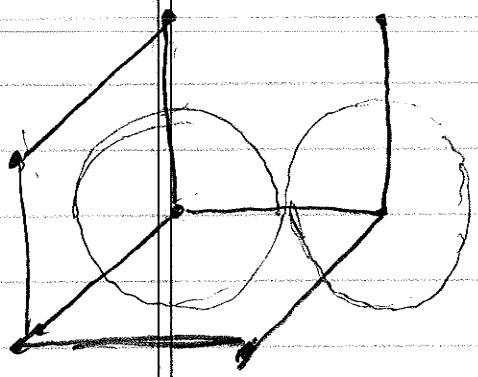


SB
CS-4

Sometimes a primitive cell, although smallest volume, makes it harder to visualize the crystal structure. Consider bcc and fcc. They are easily understood by laying out a cubic cell and then putting additional atoms at the center or at the center of the faces. Such an "easier to visualize" cell is called a conventional cell.

Packing fraction: How much space is occupied if identical balls are placed on lattice sites so they just touch?

Simple cubic



Cubic cell $V = a^3$

spheres occupy $8 \cdot \frac{1}{8} \cdot \pi \frac{4}{3}\left(\frac{a}{2}\right)^3$

$$PF = \frac{4\pi}{24} = .524$$

BCC PF = .680

FCC PF = .740