Solid State Theory

Literature

J. M. Ziman: Principles of the Theory of Solids

C. Kittel: Introduction to Solid State Physics

N. W. Ashcroft and N. D. Mermin: Solid State Physics

A. A. Abrikosov: Fundamentals of the Theory of Metals

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Manfred Sigrist lectures:

www.itp.phys.ethz.ch/education/fs14/sst

Our web page:

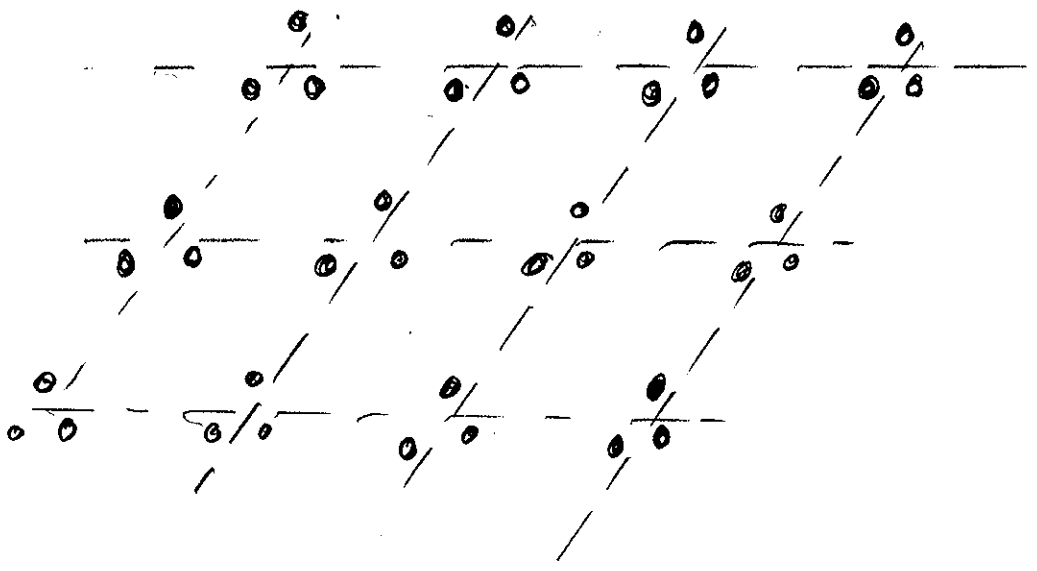
www.itp.phys.ethz.ch/education/fs15/sst

Crystal lattice

An ideal crystal is constructed by the infinite repitition of identical structure units in space. In the simple solids the structural unit is a simple atom as for nobel and alkali metals, iron, aluminum. For other crystal it may comprise many atoms or molecules.

The structure of all crystals can be described as a lattice with a group of atoms attached to every lattice point. This group of atoms is called the <u>basis</u>

Crystal structure = lattice + basis



The lattice brings periodicity.

Whereas liquid is translational invariant, e.g. its density is constant $\rho(r) = const$, in crystals continuous translational symmetry is <u>broken</u> and reduced to the discrete translation by lattice vectors

$$\rho(\vec{r}) = \rho(\vec{r} + \vec{T})$$

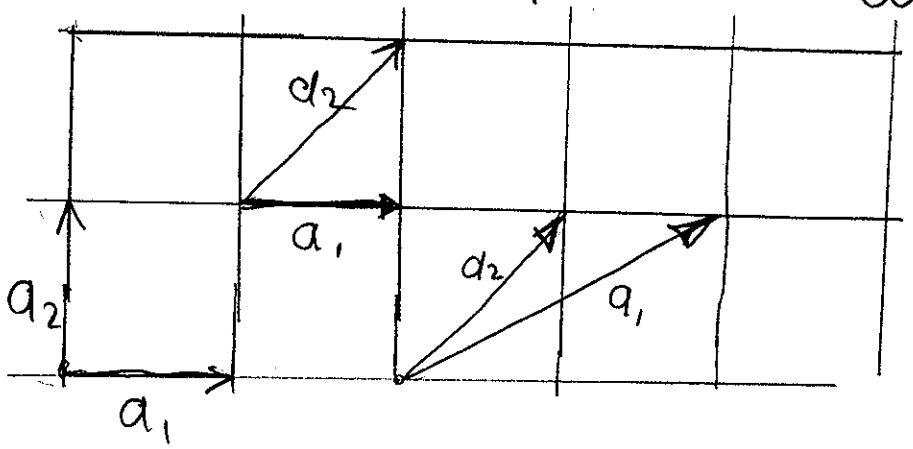
$$\vec{T} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$$

This lattice is called <u>Bravais</u> lattice (Auguste Bravais 1850)

All points of this lattice are equivalent and can be connected by translation $\vec{T}$

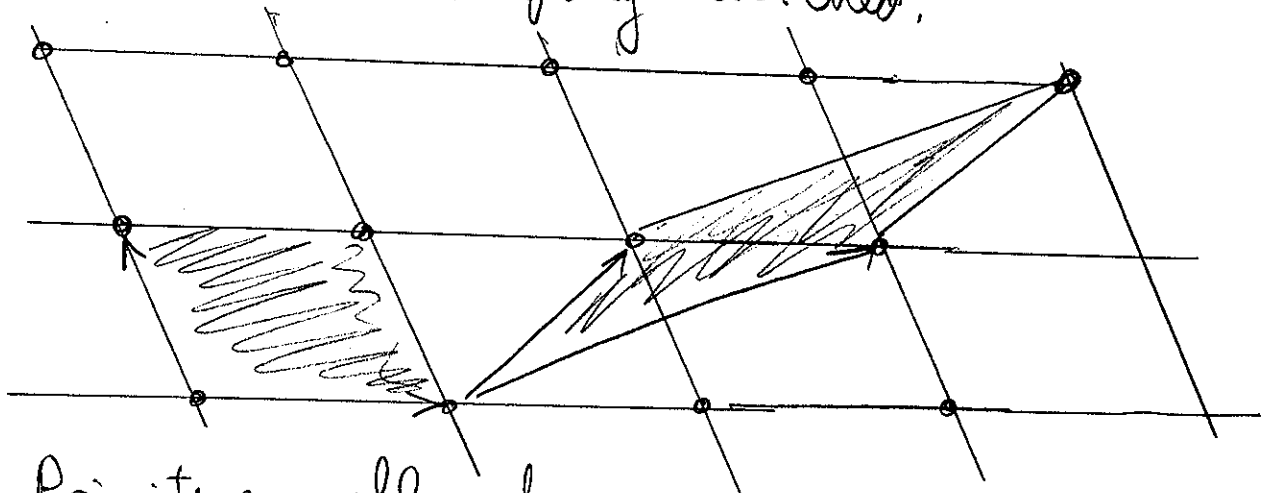
Vectors $\vec{a}_1, \vec{a}_2, \vec{a}_3$ are called <u>primitive vectors</u> or basic vectors

The choice of $\vec{a}_i$ is not unique:

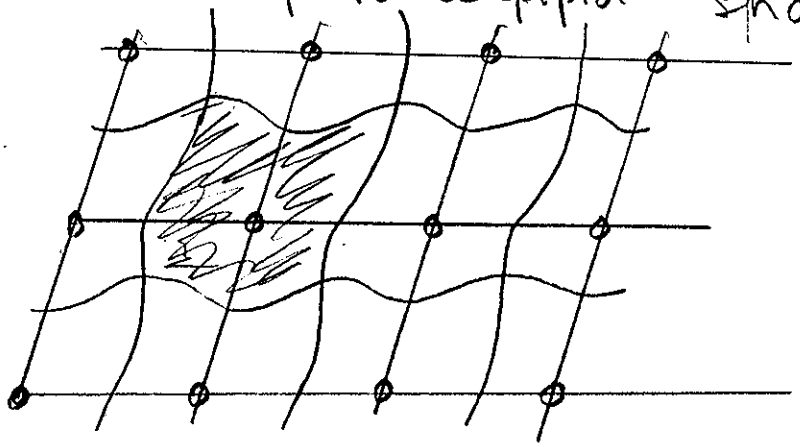


A volume of space, that, when translated through all the vectors in a Bravais lattice fills all the space without leaving voids or overlapping is called primitive cell of the lattice.

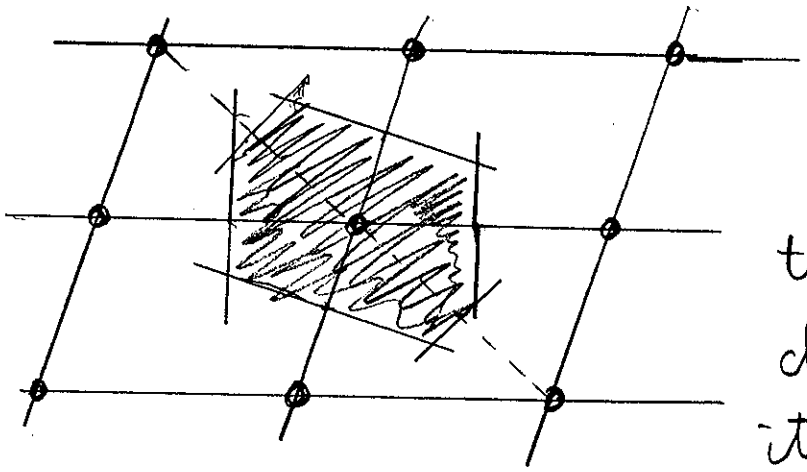
An obvious choice for the primitive cell would be the parallelepipid based on the primitive vectors $\vec{a}_1, \vec{a}_2, \vec{a}_3$. Since there is no unique way to define these vectors the primitive cell is not uniquely defined.



Primitive cell doesn't have to be of the parallelepipid shape



One typical choice of the primitive cell is the Wigner-Seitz cell. This cell is defined as one site and all the points that are closer to that site than to any other lattice sites

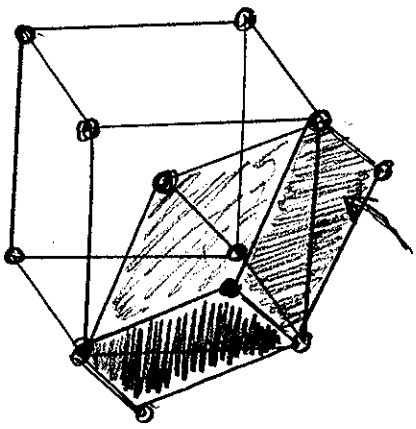


The six sides of this cell bisect the lines that connect chosen point to its neighbours

In general Wigner-Seitz cell is either rectangle or hexagon.

All the primitive cells contain exactly one lattice point (unless they are on its surface)
It follows from the volume consideration
For the lattice with N sites there N translations $\vec{T}$
Thus total volume $V = N v_0$, where v_0 is the unit cell volume => number of cells = number of particles => each cell has exactly 1 particle
Primitive cell volume is given by $v_0 = \vec{a}_1 \cdot [\vec{a}_2 \times \vec{a}_3]$

One can also fill space with nonprimitive unit cells by translations that form some subset of the vectors of a Bravais lattice. These unit cells may have higher symmetry than the primitive cell. A typical example is the Body centered cubic Bravais lattice



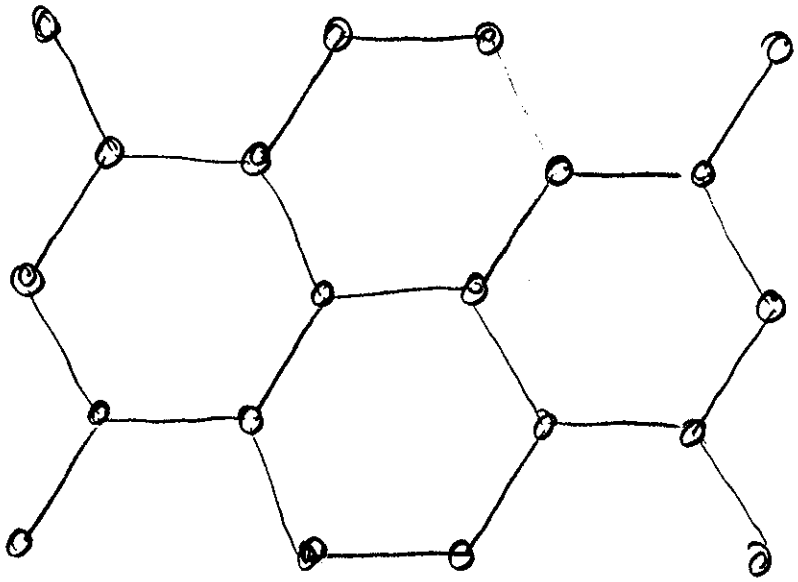
Primitive cell

The volume of the cube is twice larger than of the primitive cell it has basis of two atoms (center of the cube and one of its vertexes)

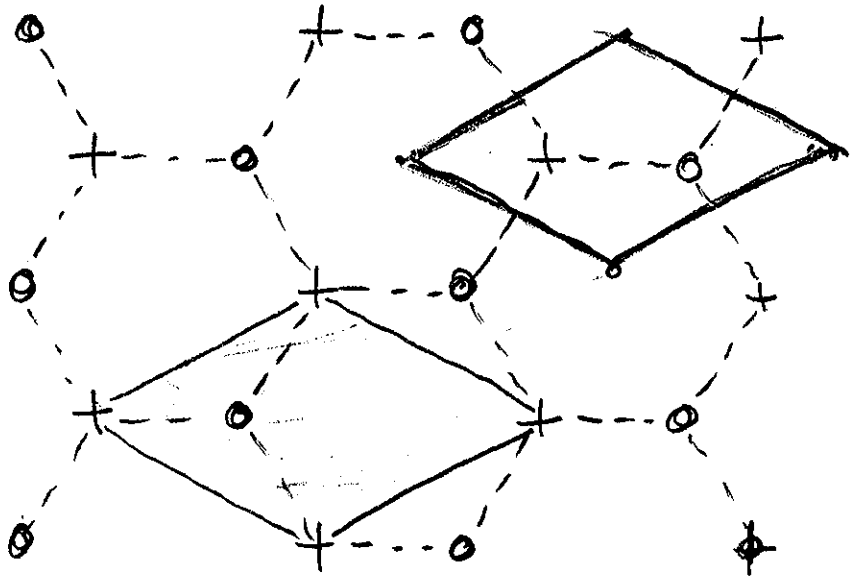
Non Bravais lattices

Not every lattice is Bravais lattice

An important example is the honeycomb lattice (graphene).

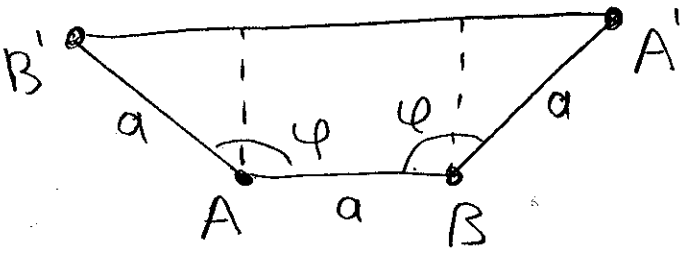


It can be viewed as bipartite lattice formed by two hexgonal lattices => it is hexagonal Bravais lattice with the basis



In addition to translational symmetry crystal lattice may have symmetry with respect to rotation or mirror reflection. All Bravais lattices have inversion center.

Not all rotations are allowed. Consider rotation by $\varphi = \frac{2\pi}{n}$. If A is one of the lattice sites with the rotation axis going through it and B is its neighbor in the plane ortogonal to the rotation axis



Then B' and A' are also the lattice points

Then $|A'B'|$ should be integer number of periods a

$|A'B'| = na$. But $|A'B'| = a + 2a\cos\left(\frac{\pi}{2} - \varphi\right) =$

$= a - 2a\cos\varphi = na \Rightarrow$

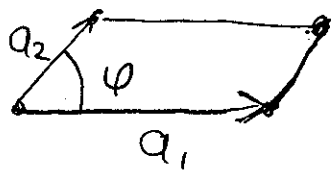
$\cos\varphi = \frac{1-n}{2} \Rightarrow n = 0, 1, 2, 3$ and

$\varphi = \frac{2\pi}{n}$ with $n = 2, 3, 4, 6$

A fivefold rotation symmetry <u>can not exist in a lattice</u>

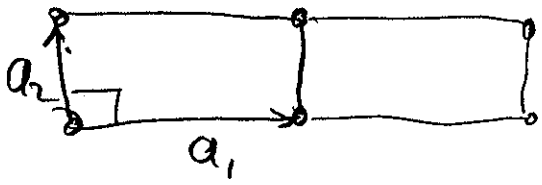
Two-Dimensional lattice types

We choose primitive cell as parallelogram



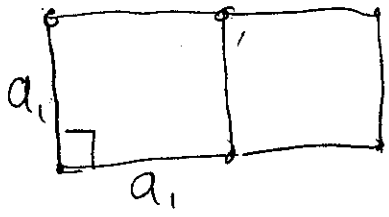
If no other symmetry is present — oblique lattice

For $\varphi = 90°$ we get rectangular lattice



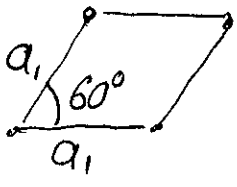
It have reflection planes and 180° rotations

If $\varphi = 90°$, $a_1 = a_2$ we have square lattice



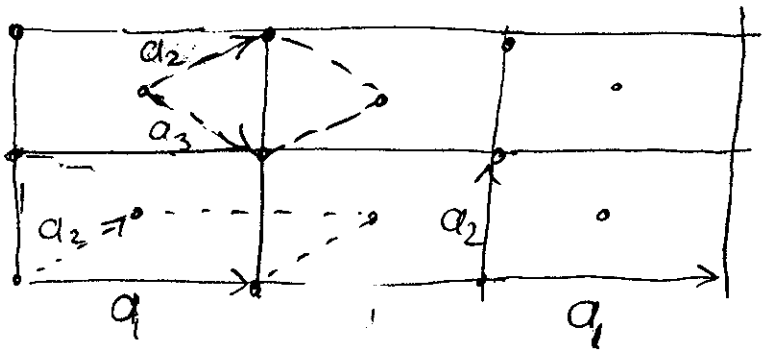
Here we have 90° rotations

If $\varphi = 60°$, $a_1 = a_2$ we have hexagonal lattice

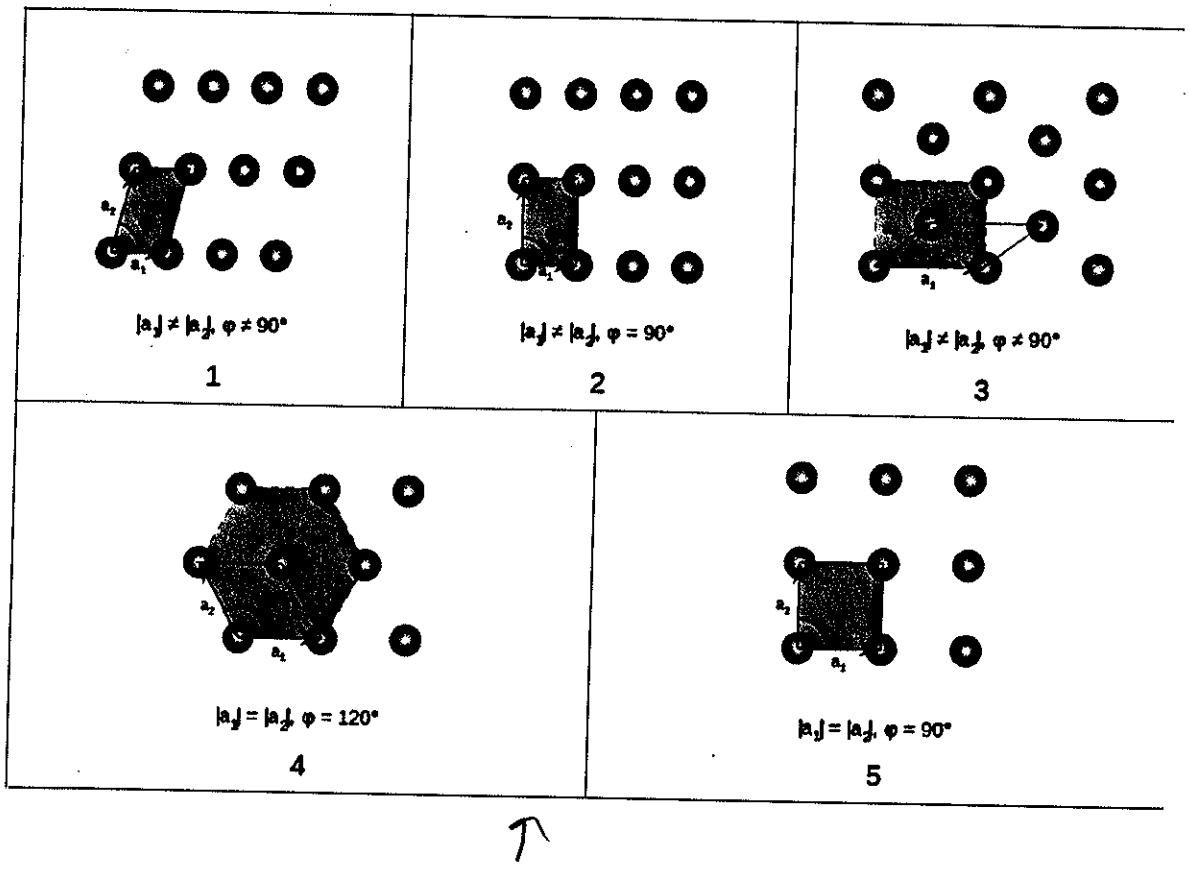


It also has reflection planes but 60° rotation

The fifth lattice is centered rectangular lattice



If primitive parallelogram a_1, a_2 doesn't have required symmetry. One can take unit cell with the basis — centered rectangle. Or one can take another set of primitive vectors ; a_2, a_3 that make rhombus, thus it is also called rhombic



2d Bravais lattices