

FYS3400 - Vår 2024 (Kondenserte fasers fysikk)

<https://www.uio.no/studier/emner/matnat/fys/FYS3400/v24/index.html>

**Pensum: Introduction to Solid State Physics
by Charles Kittel (Chapters 1-9 and 17 - 20)**

David Rivas Gongora, Joakim Bergli, and Andrej Kuznetsov

delivery address: Department of Physics, PB 1048 Blindern, 0316 OSLO

Tel: +4745502842

e-post: d.r.gongora@smn.uio.no

visiting address: MiNaLab, Gaustadaleen 23a

2024 FYS3400 Lecture Plan (based on C.Kittel's Introduction to Solid State Physics, Chapters 1-9, 17-20)

Module I – Periodicity and Disorder (Chapters 1-3, 19, 20)

calender week

Mo 15/1 10-12 Introduction. Crystal bonding. Periodicity and lattices. Lattice planes and Miller indices. Reciprocal space.

3

Th 18/1 10-11 Bragg diffraction and Laue condition

Mo 22/1 10-12 Ewald construction, interpretation of a diffraction experiment, Bragg planes and Brillouin zones

4

Th 25/1 10-11 Surfaces and interfaces. Disorder. Defects crystals. Equilibrium concentration of vacancies

Mo 29/1 10-12 Mechanical properties of solids. Diffusion phenomena in solids

5

Th 1/2 10-11 Summary of Module I

Module II – Phonons (Chapters 4, 5, and 18 pp.557-561)

Mo 5/2 10-12 Vibrations in monoatomic and diatomic chains of atoms; examples of dispersion relations in 3D

6

Th 8/2 10-11 Periodic boundary conditions (Born – von Karman); phonons and its density of states (DOS)

Mo 12/2 10-12 Effect of temperature - Planck distribution; Lattice heat capacity: Dulong-Petit, Einstein, and Debye models

7

Th 15/2 10-11 Comparison of different lattice heat capacity models

Mo 19/2 10-12 Thermal conductivity and thermal expansion

8

Th 22/2 12-13 Summary of Module II

Module III – Electrons (Chapters 6, 7, 11 - pp 315-317, 18 - pp.528-530, 19, and Appendix D)

Mo 26/2 10-12 Free electron gas (FEG) versus free electron Fermi gas (FEFG); DOS of FEFG in 3D

9

Th 29/2 10-11 Effect of temperature – Fermi-Dirac distribution; Heat capacity of FEFG in 3D

Mo 4/3 10-12 DOS of FEFG in 2D - quantum wells, DOS in 1D – quantum wires, and in 0D – quantum dots

10

Th 7/3 10-11 Transport properties of electrons

Module IV – Disordered systems (guest lecture slides - Joakim Bergli)

Mo 11/3 10-12 Thermal properties of glasses: Model of two level systems

11

Th 14/3 10-11 Electron transport in disordered solids: wave localization and hopping

Mo 18/3 10-12 Advanced theory of disordered systems

12

Th 21/3 10-11 Summary of Module IV

Easter

Module V – Semiconductors (Chapters 8, 9 pp 223-231, and 17, 19)

Th 4/4 10-11 Recap of Module III

14

Mo 8/4 10-12 Origin of the band gap; Nearly free electron model; Kronig-Penney model

15

Th 11/4 10-11 Effective mass method for calculating localized energy levels for defects in crystals

Mo 15/4 10-12 Intrinsic and extrinsic electrons and holes in semiconductors

16

Th 18/4 10-11 Carrier statistics in semiconductors

Mo 22/4 10-12 p-n junctions

17

Th 25/5 10-11 Optical properties of semiconductors

Mo 29/4 10-12 Advanced photonic devices including quantum tech

18

Th 2/5 10-11 Summary of Module V

Summary and repetition

Mo 6/5 10-12 Repetition - course in a nutshell

19

Exam: oral examination

tentatively during week 20 or 21

FYS3400: Lectures 1-2

**Introduction. Crystal bonding. Periodicity and lattices.
Brag diffraction and Laue condition. Reciprocal space.**

- **Condensed Matter Physics à la FYS3400;**
- **Relevance of condensed matter physics fundamentals to modern technologies;**
- **Why elements bond together? Why in crystals? Survey of crystal bonding;**
- **Lattice planes and Miller indices;**
- **Use of waves to study crystals explaining the idea of using the reciprocal space;**
- **Introduction of the reciprocal space;**
- **Formal description of crystal structures.**

FYS3400: Lectures 1-2

**Introduction. Crystal bonding. Periodicity and lattices.
Brag diffraction and Laue condition. Reciprocal space.**

- **Condensed Matter Physics à la FYS3400;**
- **Relevance of condensed matter physics fundamentals to modern technologies;**
- **Why elements bond together? Why in crystals? Survey of crystal bonding;**
- **Lattice planes and Miller indices;**
- **Use of waves to study crystals explaining the idea of using the reciprocal space;**
- **Introduction of the reciprocal space;**
- **Formal description of crystal structures.**

Condensed Matter Physics

Condensed Matter Physics



Solid State Physics of Crystals

Condensed Matter Physics



Solid State Physics of Crystals



Properties of Waves in Periodic Lattices

Condensed Matter Physics



Solid State Physics of Crystals



Properties of Waves in **Periodic Lattices**

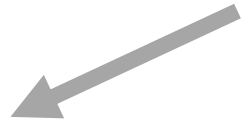
Condensed Matter Physics



Solid State Physics of Crystals



Properties of Waves in Periodic Lattices



Elastic waves in lattices

Vibrations

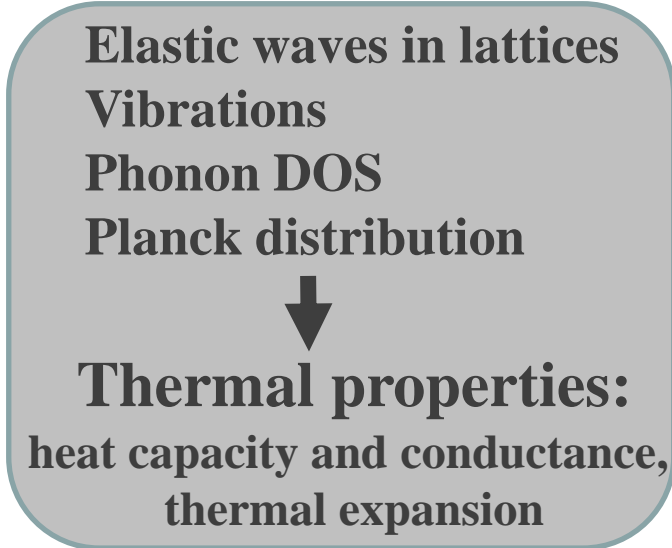
Phonon DOS

Planck distribution



Thermal properties:

heat capacity and conductance,
thermal expansion



Condensed Matter Physics



Solid State Physics of Crystals



Properties of Waves in Periodic Lattices



Elastic waves in lattices

Vibrations

Phonon DOS

Planck distribution



Thermal properties:

heat capacity and conductance,
thermal expansion

Electron waves in lattices

Free electrons

Electron DOS

Fermi-Dirac distribution



Electronic properties:

Electron concentration and transport,
contribution to the heat capacity

Condensed Matter Physics



Solid State Physics of Crystals



Properties of Waves in Periodic Lattices



Elastic waves in lattices

Vibrations

Phonon DOS

Planck distribution



Thermal properties:

heat capacity and conductance,
thermal expansion

Electron waves in lattices

Free electrons

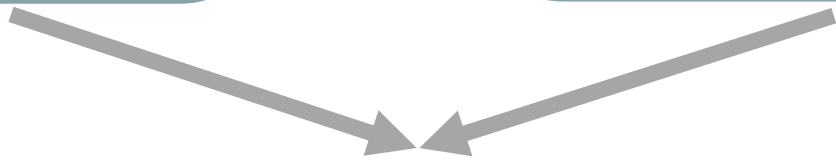
Electron DOS

Fermi-Dirac distribution



Electronic properties:

Electron concentration and transport,
contribution to the heat capacity



Advanced theory and novel materials properties

Condensed Matter Physics

Solid State Physics of Crystals

Disordered systems

Properties of Waves in Periodic Lattices

Elastic waves in lattices
Vibrations
Phonon DOS
Planck distribution

Disordered systems

Thermal properties:
heat capacity and conductance,
thermal expansion

Electron waves in lattices
Free electrons
Electron DOS
Fermi-Dirac distribution

Disordered system

Electronic properties:
Electron concentration and transport,
contribution to the heat capacity

Advanced theory and novel materials properties

Disordered systems

Why «physics of solid state» may be understood by studying waves in periodic lattices

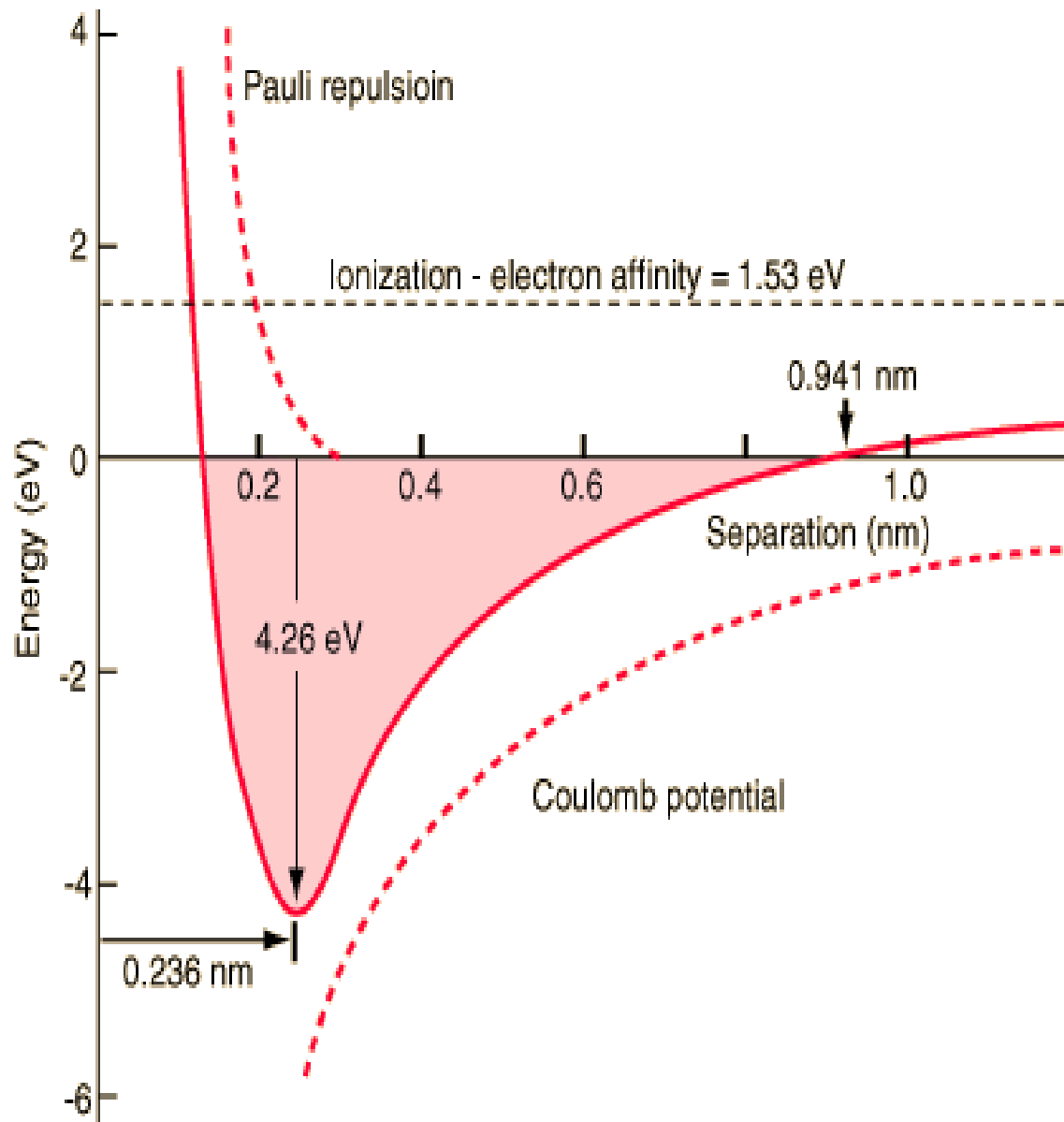
**Two questions: (i) why in periodic lattices?
 (ii) why waves?**

Firstly, let's discuss (i):

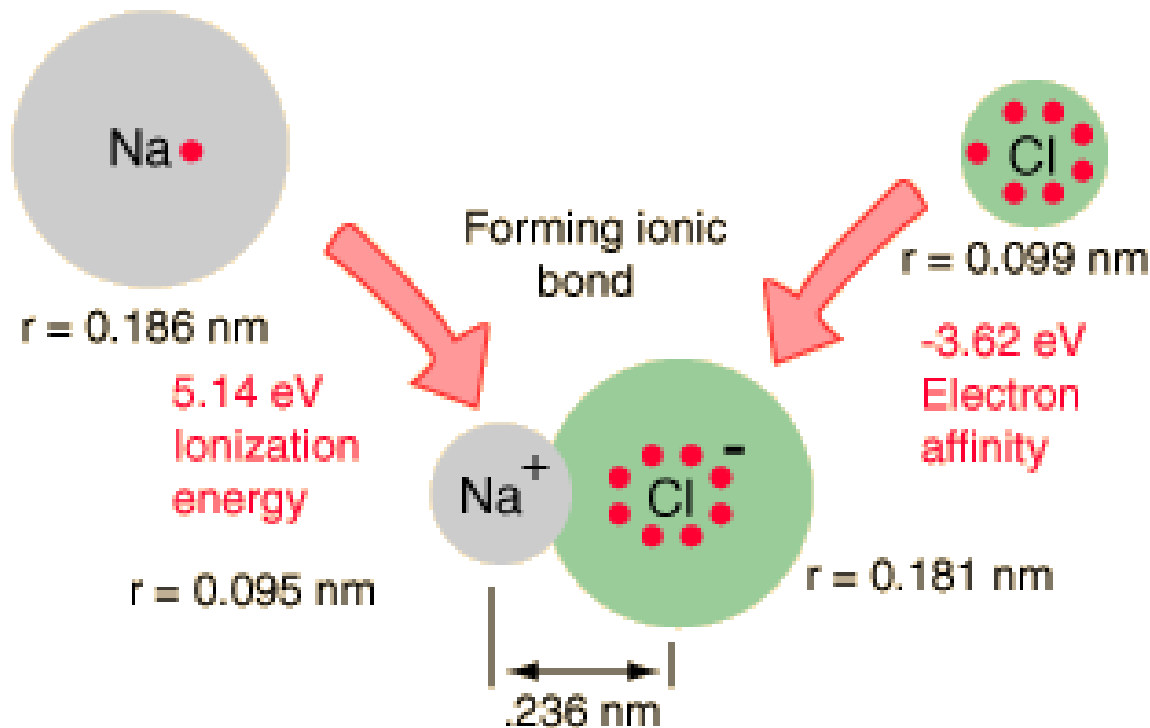
- What is known from previous courses how atoms form solids?**
- Do atoms form a periodic lattice or distributed chaotically?**
- What are the criteria for solids being amorphous or crystalline?**
- What does the intuition tell? What are the scientific insights?**

Use NaCl as an example to explain the atom ordering.

NaCl as an example of atomic ordering



NaCl as an example of atomic ordering



Energy balance

5.14 eV Ionization energy
 -3.62 eV Electron affinity
 -6.10 eV Coulomb attraction

 -4.58 eV

But the dissociation energy of NaCl is measured to be -4.26 eV . The difference is $+0.32 \text{ eV}$ attributed to Pauli repulsion.

Electric potential energy

$$\frac{-Ke^2}{r} = \frac{-1.44 \text{ eV nm}}{0.236 \text{ nm}} = -6.1 \text{ eV}$$

Why «physics of solid state» may be understood by studying waves in periodic lattices

Two questions: (i) why in periodic lattices?
 (ii) why waves?

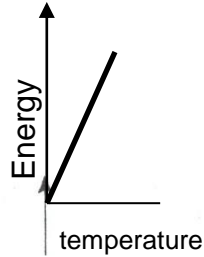
Secondly, let's discuss (ii):

- Why talking about waves, are there waves inside the crystals?
- Or we are after waves exposed on crystals to be used as probes?
- The principles for waves - lattice interactions are common; x-rays, vibrations, electrons, all obey Bragg's diffraction!

Wave vector $k = 2\pi/\lambda$, given in units of the reciprocal length; How to plot k at lattice points, than?

Use the reciprocal space to visualize the wave-lattice interactions !!

Example on how the structure determines thermal properties – to be followed within Module II

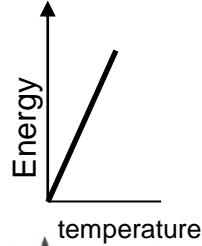


**Classical
oscillators**

Any energy state is accessible for any oscillator in form of $k_B T$, i.e. no distribution function is applied and the total energy is

$$\bar{E} = N\bar{E}_1 = 3Nk_B T$$

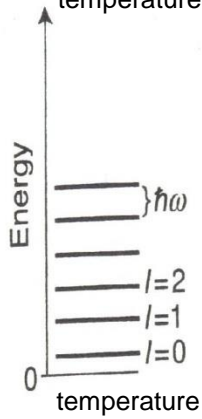
Example on how the structure determines thermal properties – to be followed within Module II



Classical oscillators

Any energy state is accessible for any oscillator in form of $k_B T$, i.e. no distribution function is applied and the total energy is

$$\bar{E} = N\bar{E}_1 = 3Nk_B T$$



Quantum oscillators

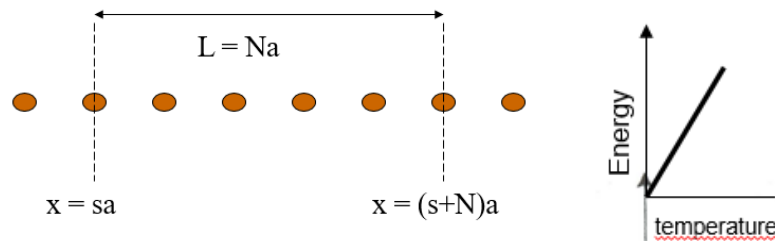
Not all energies are accessible, but only those in quanta of $\hbar\omega n$, and Planck distribution is employed to calculate the occupancy at temperature T , so that

$$E = 3N \cdot \langle n \rangle \cdot \hbar\omega$$

$$E = 3N \sum_{n=0}^{\infty} f(E_n) E_n = 3N \frac{\sum_{n=0}^{\infty} E_n e^{-E_n/k_B T}}{\sum_{n=0}^{\infty} e^{-E_n/k_B T}} = 3N \frac{1}{e^{\hbar\omega/k_B T} - 1} \cdot \hbar\omega$$

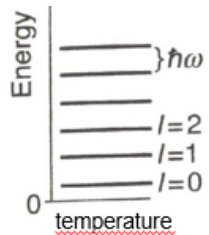
Example on how the structure determines thermal properties

– to be followed within Module II



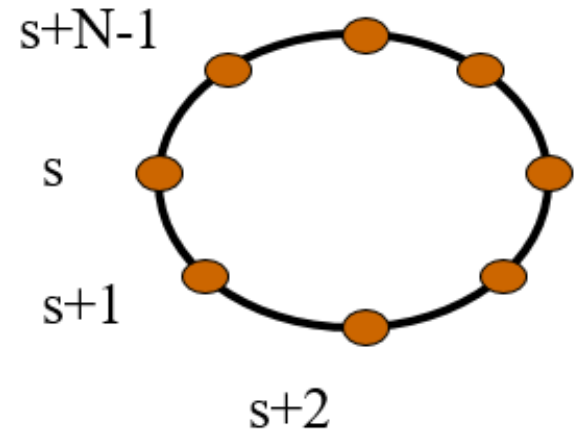
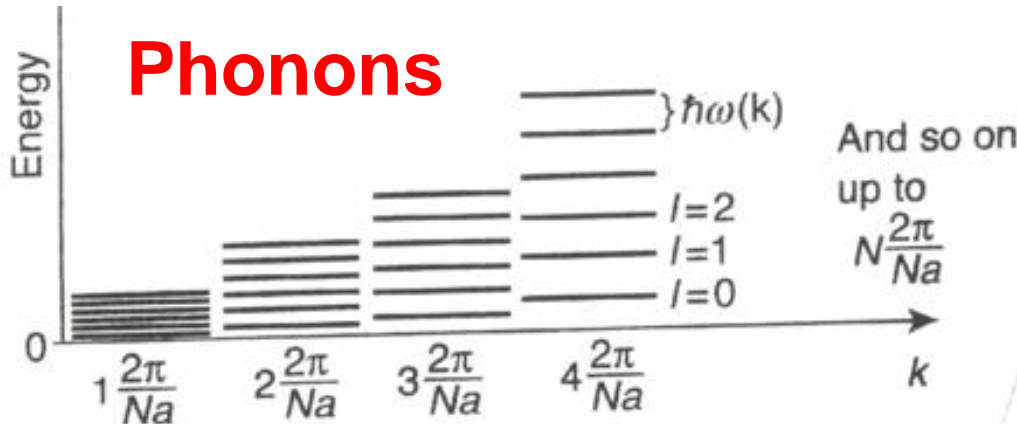
Classical oscillators

Any energy state is accessible for any oscillator in form of $k_B T$, i.e. no distribution function is applied and the total energy is $\bar{E} = N\bar{E}_1 = 3Nk_B T$



Quantum oscillators

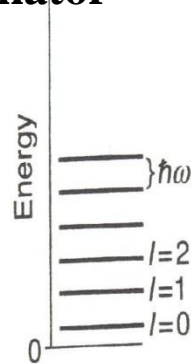
Not all energies are accessible, but only those in quants of $\hbar\omega$, and Planck distribution is employed to calculate the occupancy at temperature T , so that $E = 3N \cdot \langle n \rangle \cdot \hbar\omega$



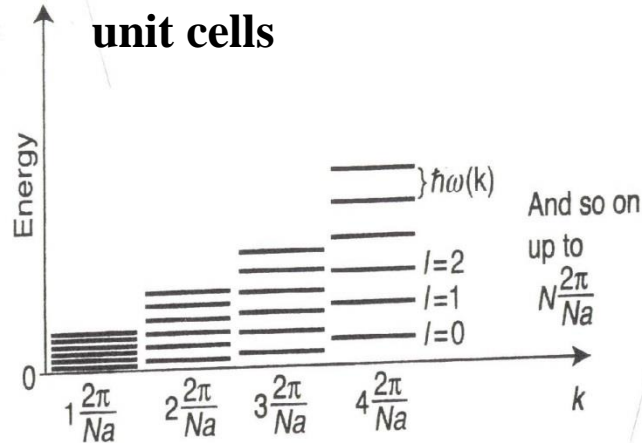
Example on how the structure determines thermal properties

– to be followed within Module II

Energy level diagram for one harmonic oscillator



Energy level diagram for a chain of atoms with one atom per unit cell and a length of N unit cells



$$E = 3N \cdot \langle n \rangle \cdot \hbar \omega$$

$$E = 3 \int_{\omega_{\min}}^{\omega_{\max}} d\omega D(\omega) \langle n \rangle \hbar \omega$$

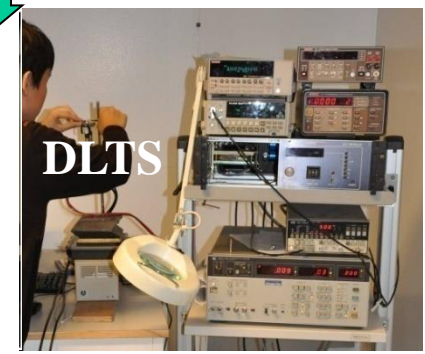
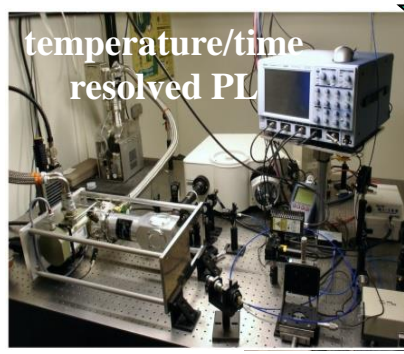
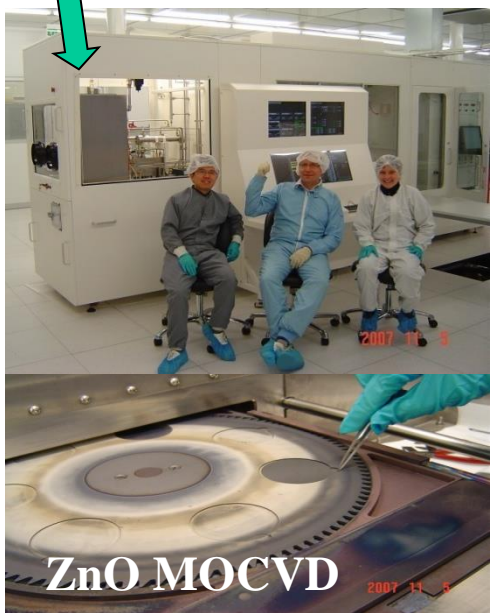
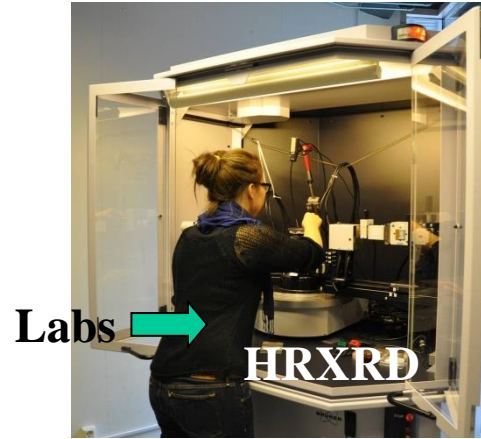
FYS3400: Lectures 1-2

**Introduction. Crystal bonding. Periodicity and lattices.
Brag diffraction and Laue condition. Reciprocal space.**

- Condensed Matter Physics à la FYS3400;
- **Relevance of condensed matter physics fundamentals to modern technologies;**
- Why elements bond together? Why in crystals? Survey of crystal bonding;
- Lattice planes and Miller indices;
- Use of waves to study crystals explaining the idea of using the reciprocal space;
- Introduction of the reciprocal space;
- Formal description of crystal structures.

Semiconductor physics at UiO

Micro- and Nanotechnology Laboratory (MiNaLab)

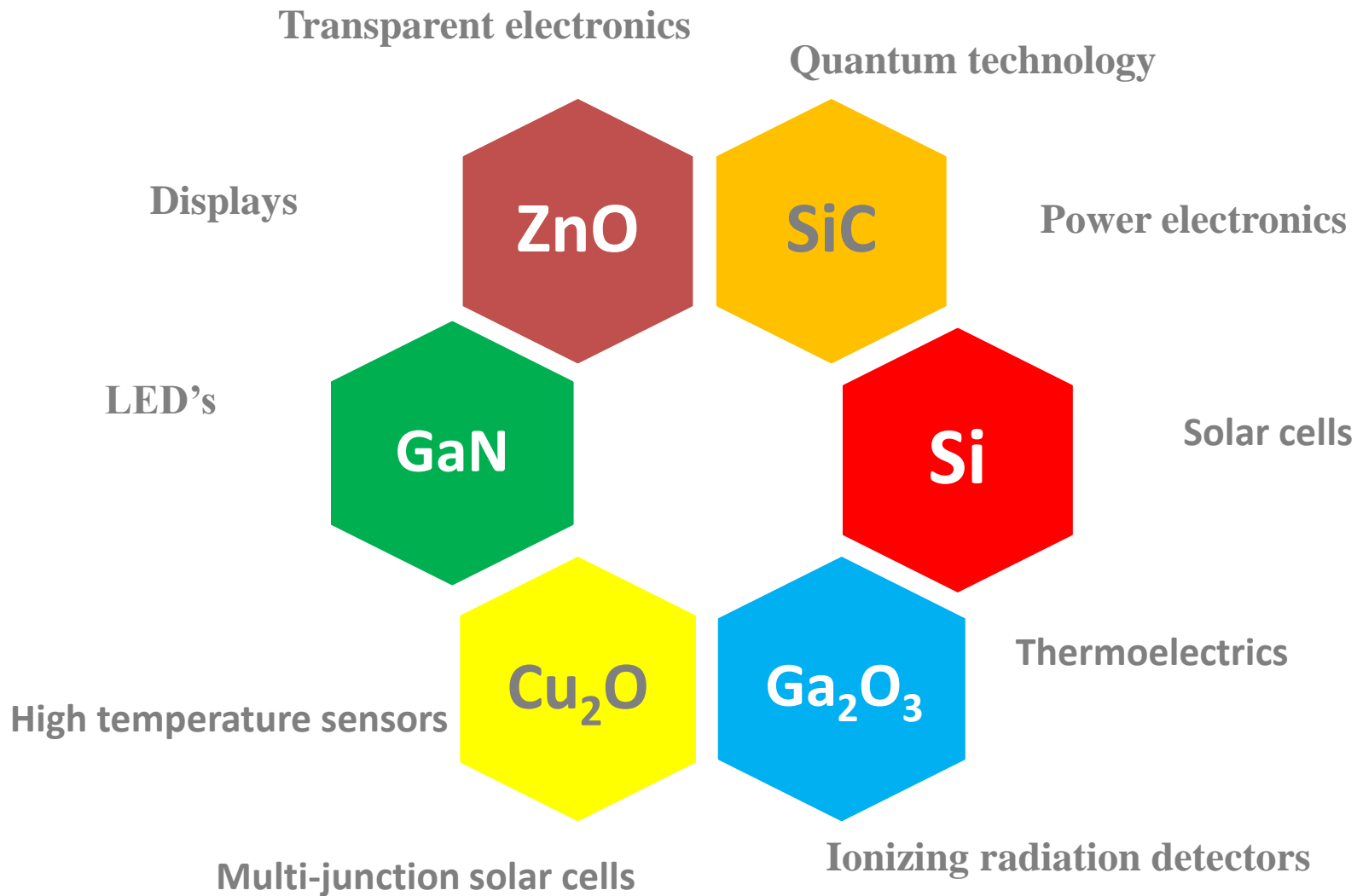


Halvlederfysikk ved UiO / MiNa-Lab

- 6 Professors
- 4 Adm/technical staff
- ~ 10 Post docs
- ~ 15 PhD students and ~ 10 Msc students

Semiconductor Physics at UiO

...application-motivated basic research...



Research highlights: Radiation tolerance

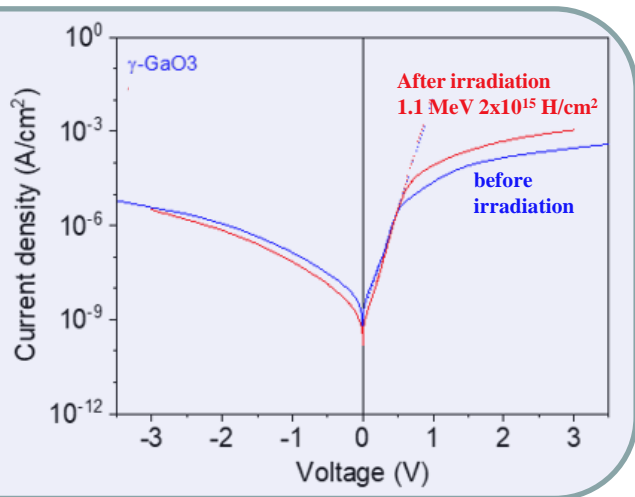
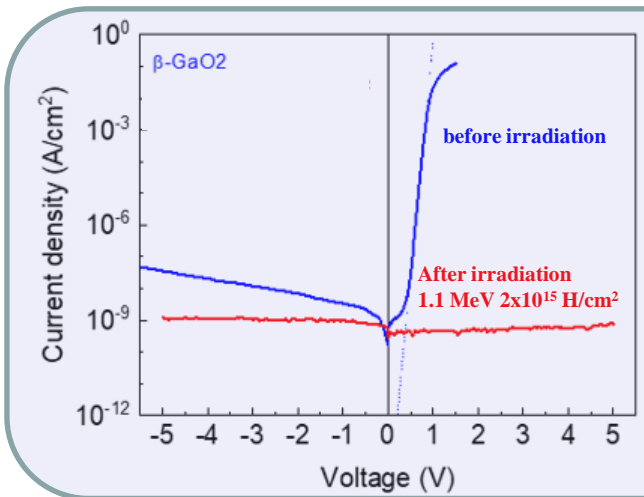
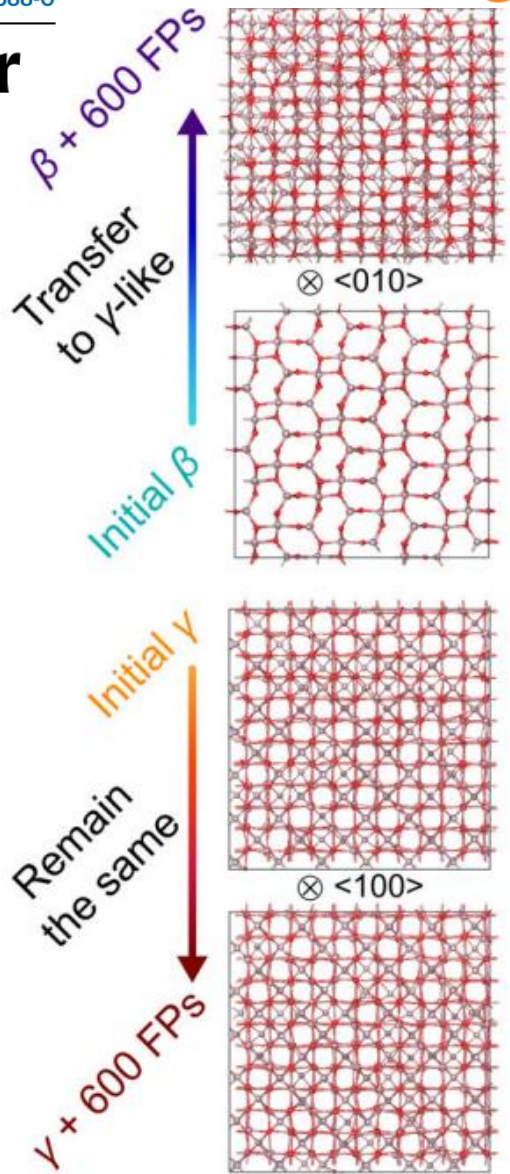
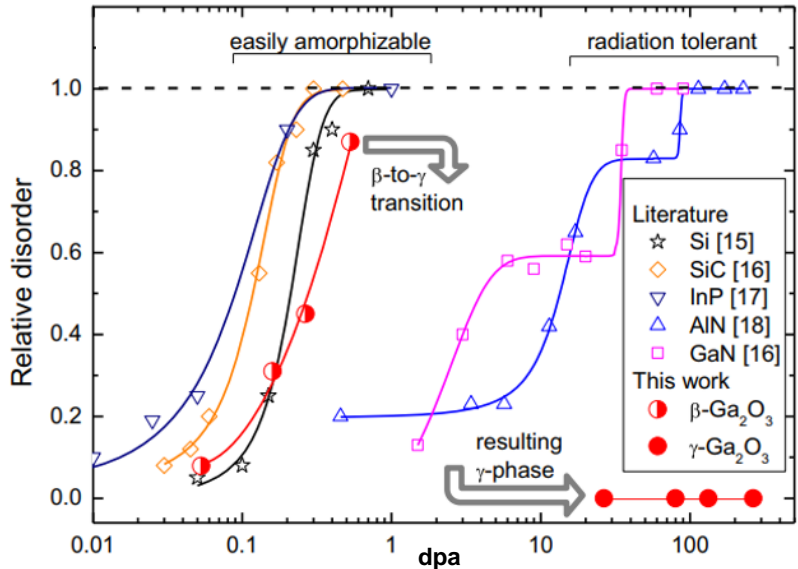
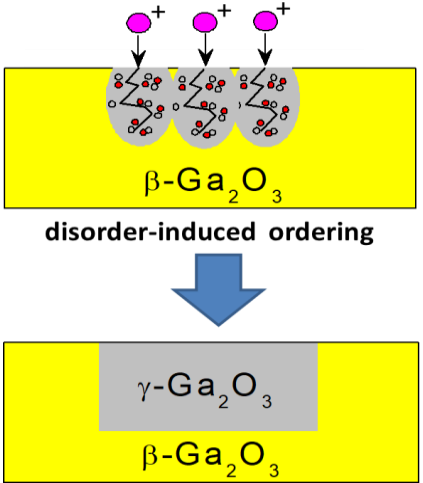
nature communications

Nat Commun **14**, 4855 (2023)

<https://doi.org/10.1038/s41467-023-40588-0>



Universal radiation tolerant semiconductor



Research highlights: Quantum defects in silicon

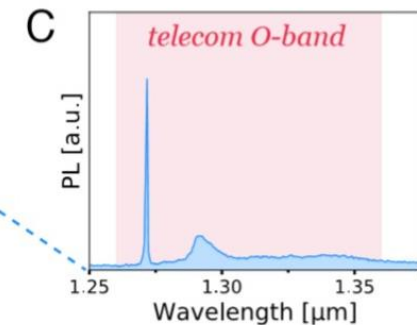
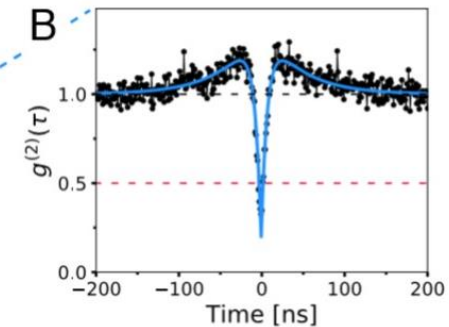
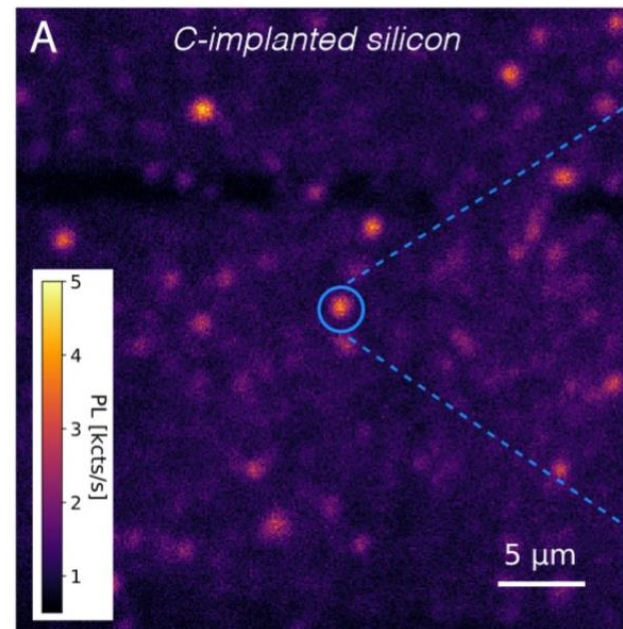
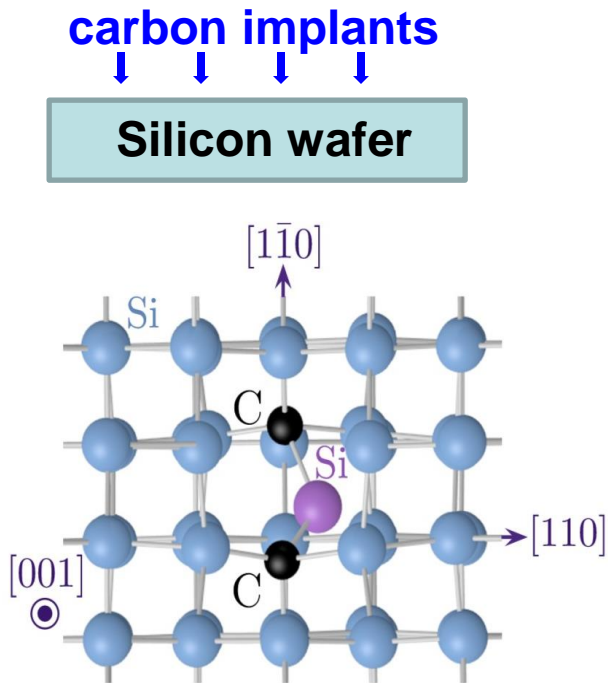
nature
electronics

ARTICLES

<https://doi.org/10.1038/s41928-020-00499-0>



Single artificial atoms in silicon emitting at telecom wavelengths *Nature Electronics* volume 3, pages 738–743 (2020)



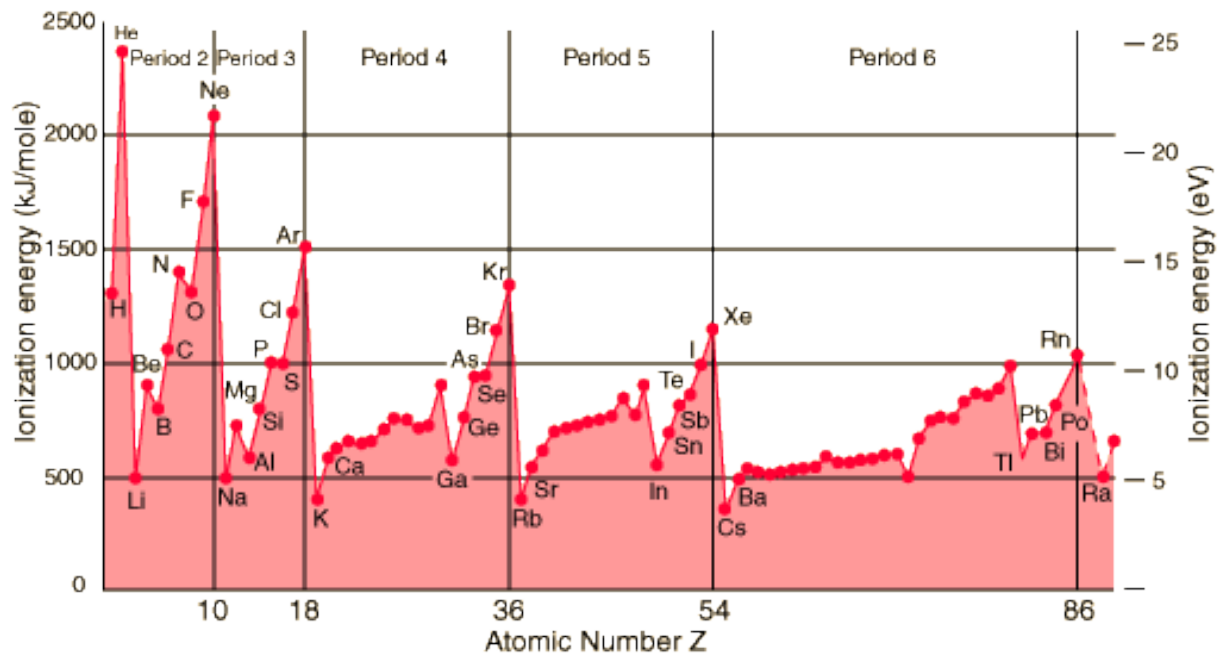
This observation constitutes the first demonstration of single-photon emission from an isolated defect embedded in the silicon lattice.

FYS3400: Lectures 1-2

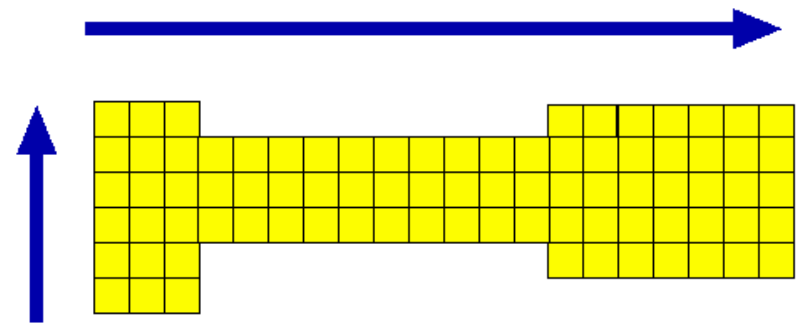
**Introduction. Crystal bonding. Periodicity and lattices.
Brag diffraction and Laue condition. Reciprocal space.**

- Condensed Matter Physics à la FYS3400;
- Relevance of condensed matter physics fundamentals to modern technologies;
- **Why elements bond together? Why in crystals? Survey of crystal bonding;**
- Lattice planes and Miller indices;
- Use of waves to study crystals explaining the idea of using the reciprocal space;
- Introduction of the reciprocal space;
- Formal description of crystal structures.

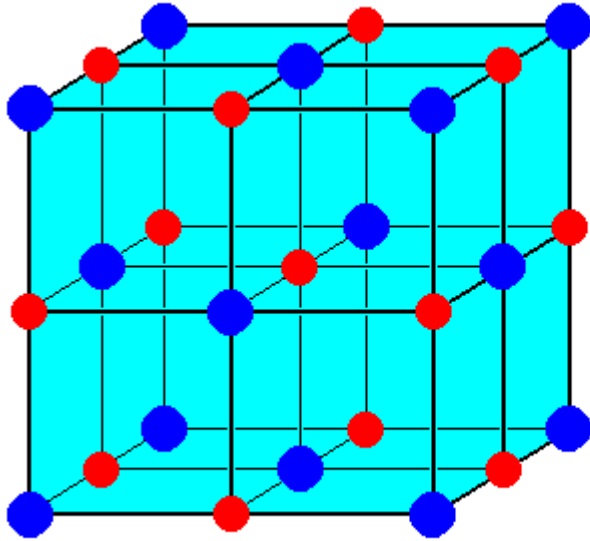
Ionic bonding



Electron Affinity Increases With Arrows



Ionic bonding



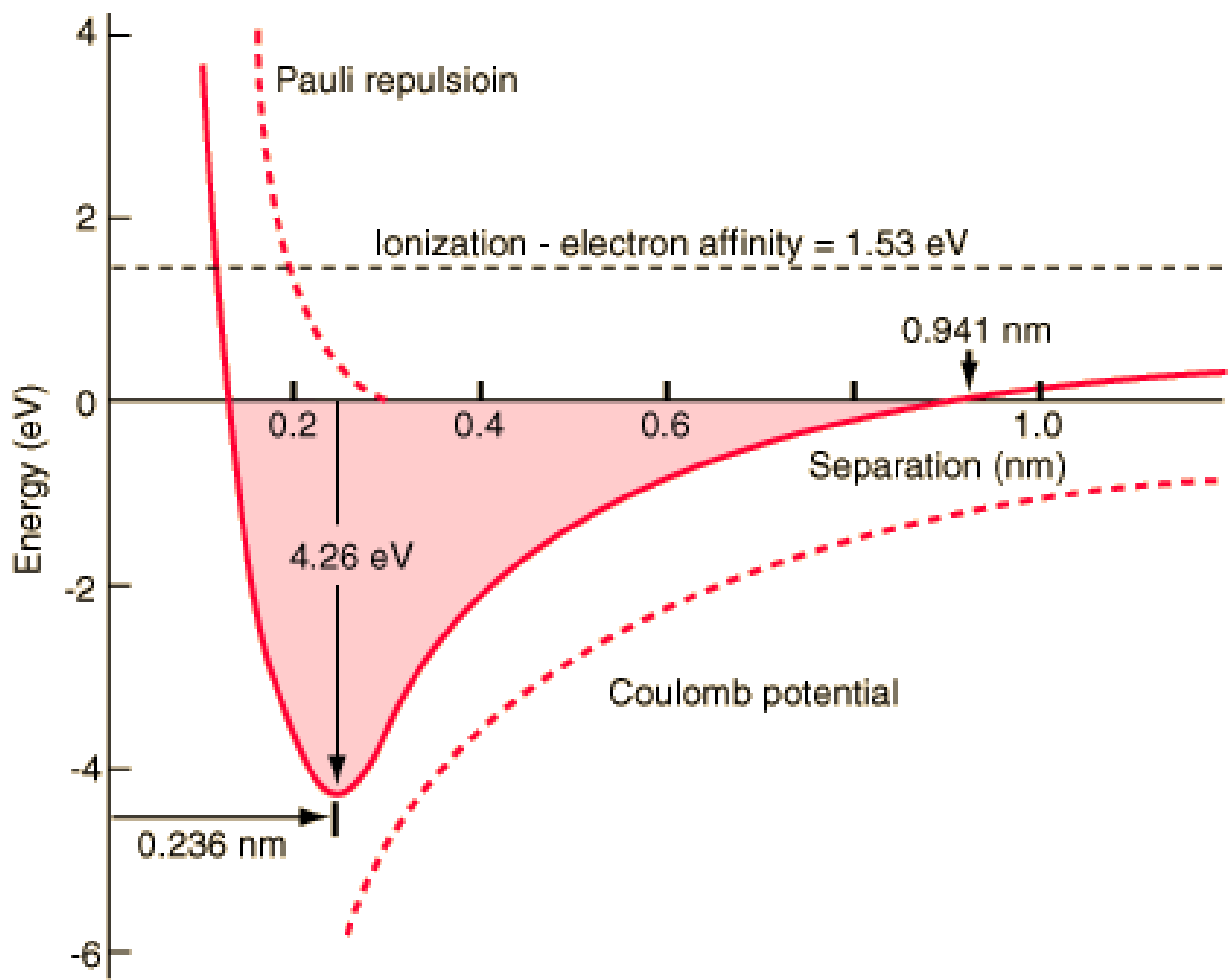
It costs 5.1 eV for Na to ionize and 3.6 eV for Cl to accommodate an extra electron so that the "balance" is:
 $5.1 - 3.6 = 1.5 \text{ eV}.$

What is the driving force for the bonding than?!

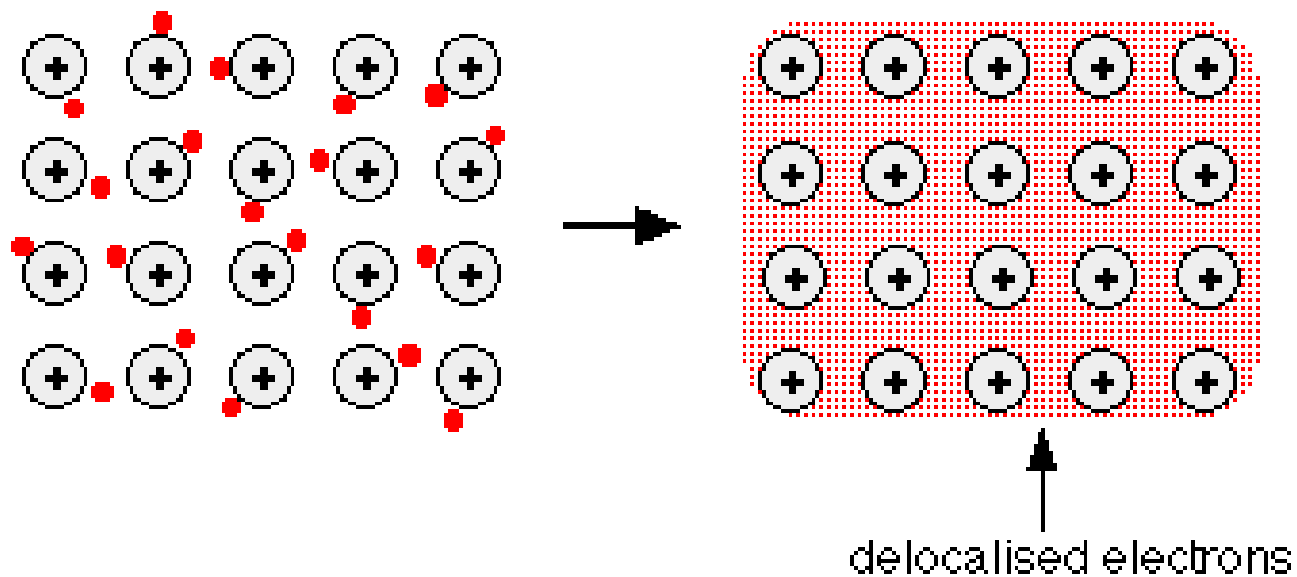
Coulomb attraction, of course!

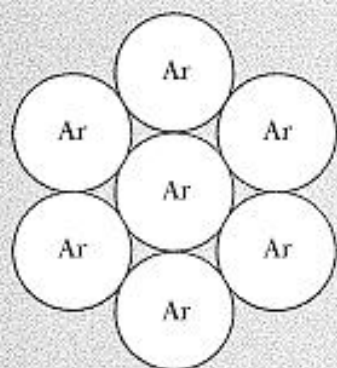
$$E = -e^2 / 4\pi\epsilon_0 a$$

Ionic bonding

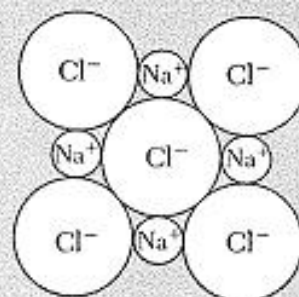


Metallic bonding

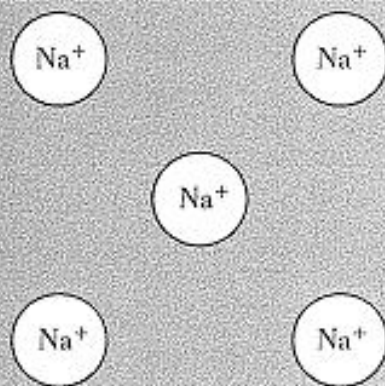




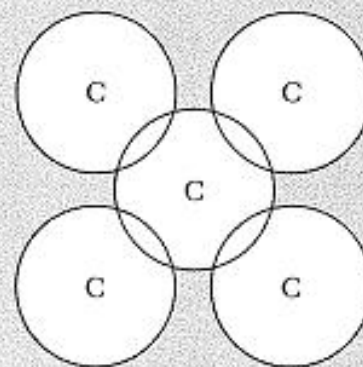
Crystalline argon
(van der Waals)
(a)



Sodium chloride
(ionic)
(b)



Sodium
(metallic)
(c)



Diamond
(covalent)
(d)

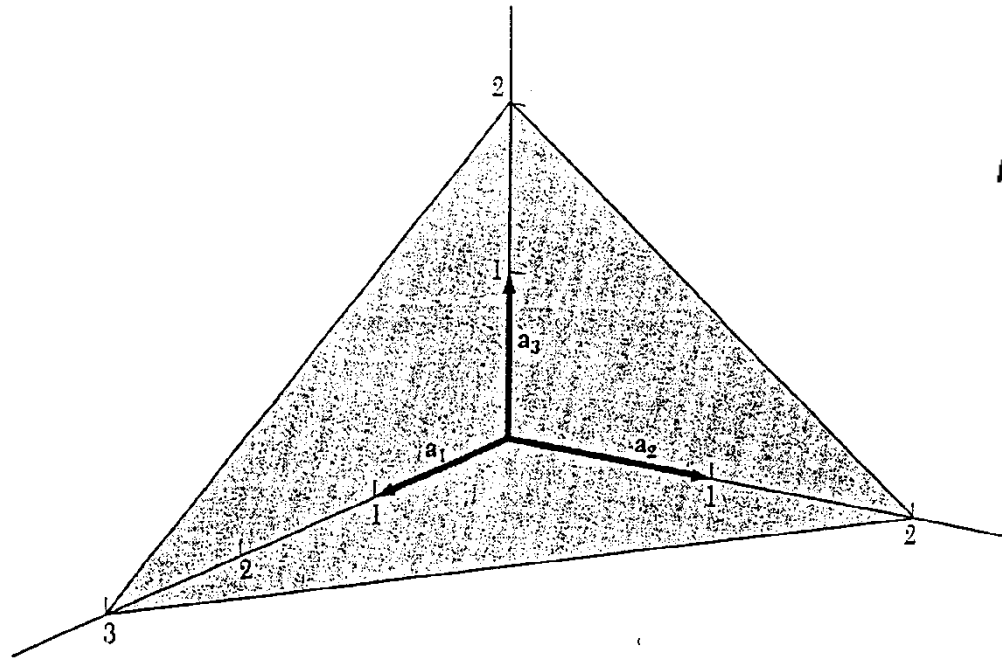
FYS3400: Lectures 1-2

**Introduction. Crystal bonding. Periodicity and lattices.
Brag diffraction and Laue condition. Reciprocal space.**

- Condensed Matter Physics à la FYS3400;
- Relevance of condensed matter physics fundamentals to modern technologies;
- Why elements bond together? Why in crystals? Survey of crystal bonding;
- **Lattice planes and Miller indices;**
- Use of waves to study crystals explaining the idea of using the reciprocal space;
- Introduction of the reciprocal space;
- Formal description of crystal structures.

Miller indices of lattice planes

- The indices of a crystal plane (h,k,l) are defined to be a set of integers with no common factors, inversely proportional to the intercepts of the crystal plane along the crystal axes:



$$h:k:l = \frac{1}{x_1} : \frac{1}{x_2} : \frac{1}{x_3}$$

Figure 15 This plane intercepts the a_1 , a_2 , a_3 axes at $3a_1$, $2a_2$, $2a_3$. The reciprocals of these numbers are $\frac{1}{3}$, $\frac{1}{2}$, $\frac{1}{2}$. The smallest three integers having the same ratio are 2, 3, 3, and thus the indices of the plane are (233).

Indices of Planes: Cubic Crystal

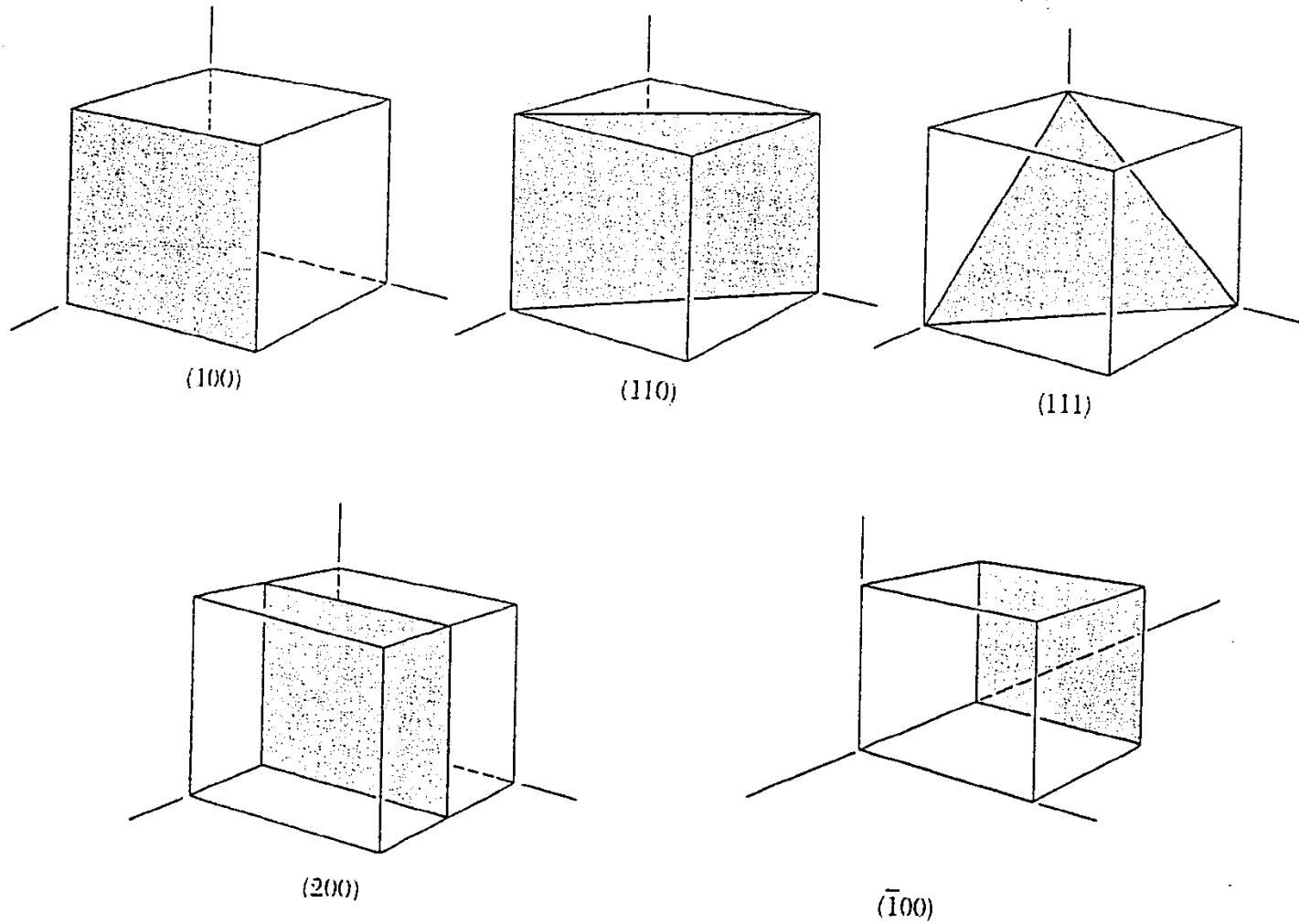
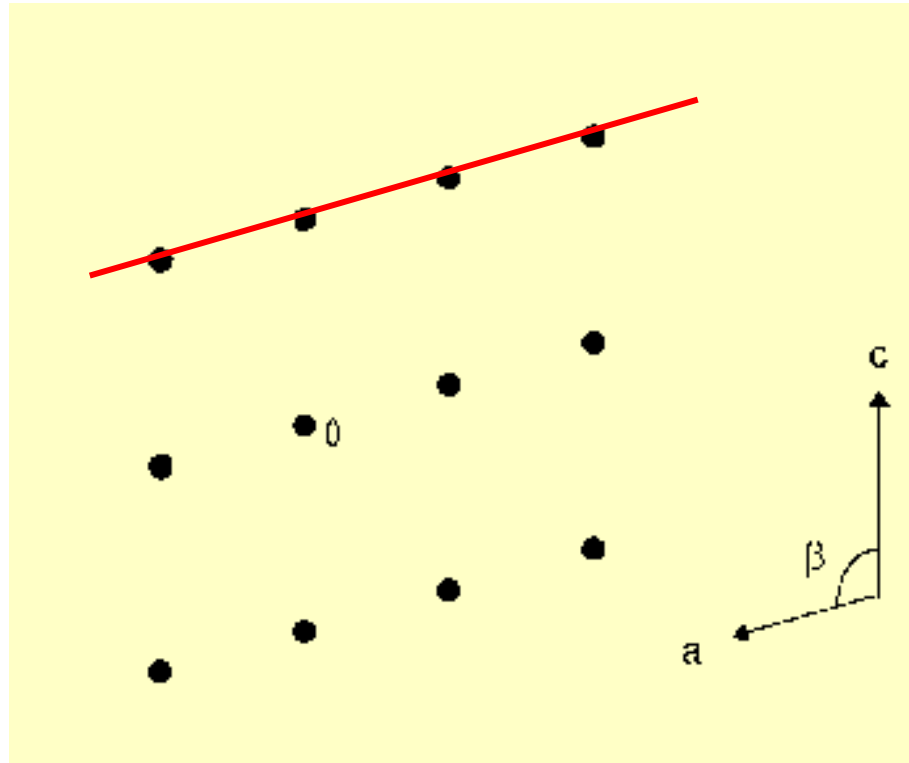


Figure 16 Indices of important planes in a cubic crystal. The plane (200) is parallel to (100) and to $(\bar{1}00)$.

Miller indices of lattice planes

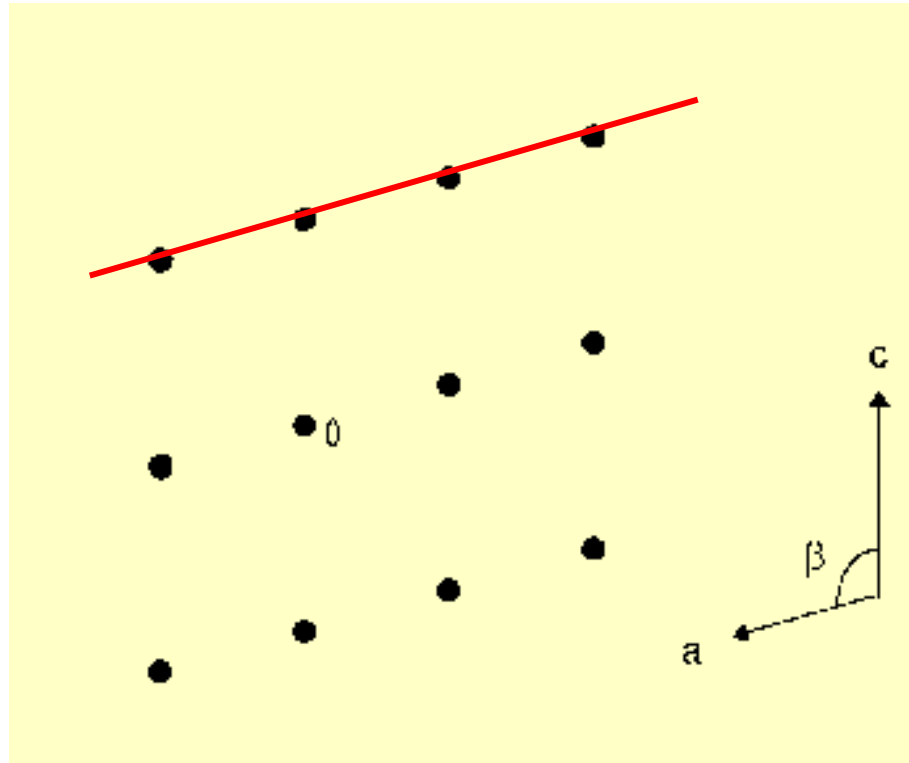
We will use a monoclinic unit cell to avoid orthogonal axes; define a plane and consider some lattice planes



Miller indices of lattice planes

We will use a monoclinic unit cell to avoid orthogonal axes; define a plane and consider some lattice planes

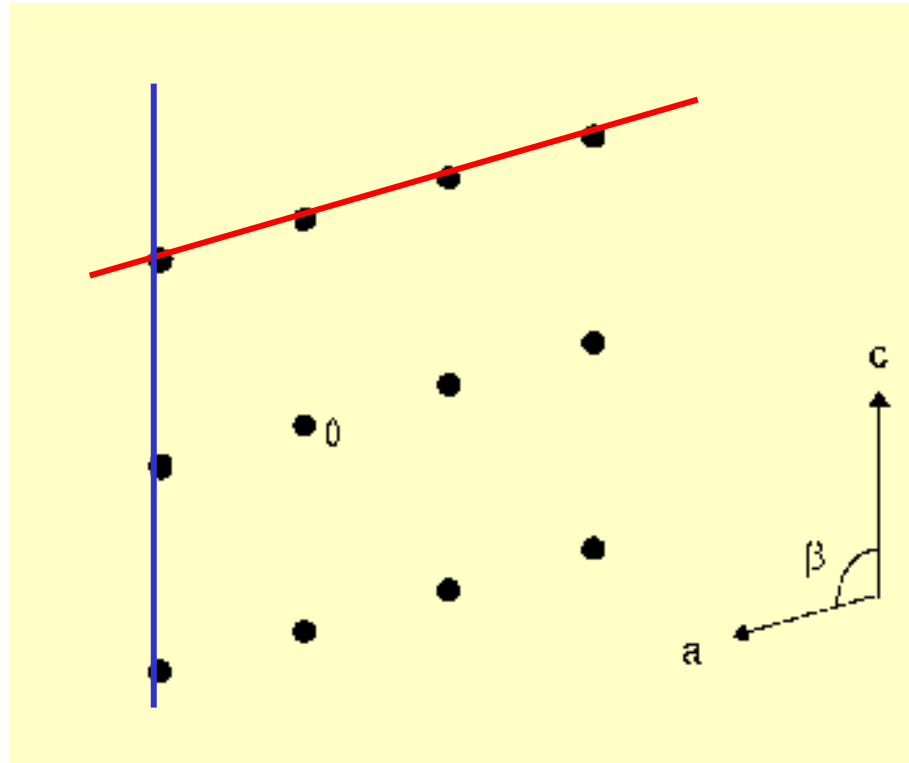
(001)



Miller indices of lattice planes

We will use a monoclinic unit cell to avoid orthogonal axes; define a plan and consider some lattice planes

(001)

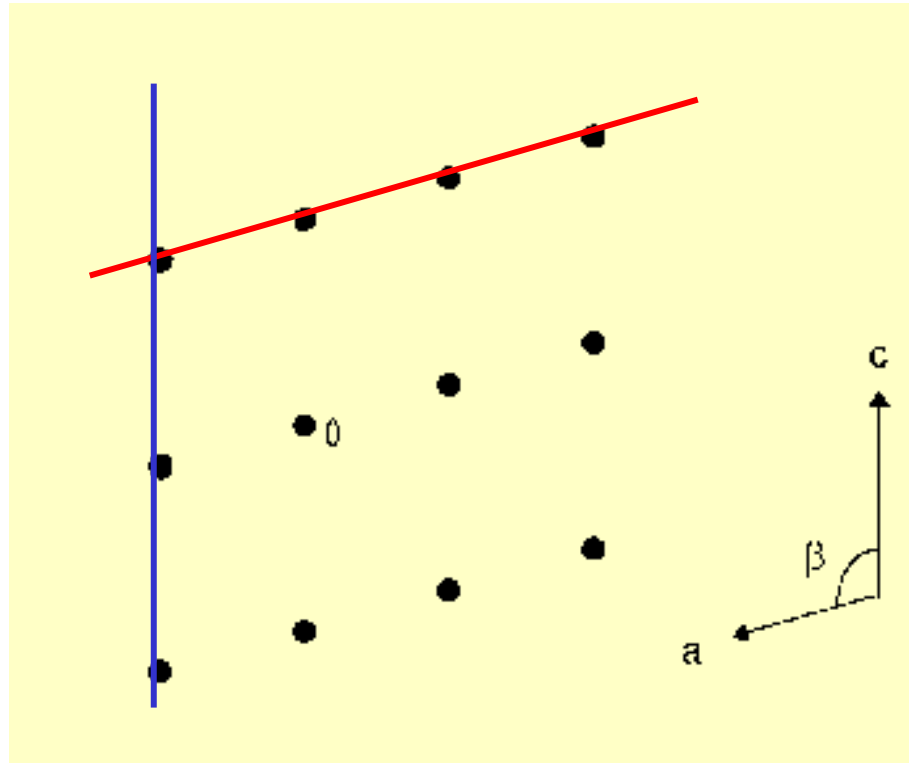


Miller indices of lattice planes

We will use a monoclinic unit cell to avoid orthogonal axes; define a plan and consider some lattice planes

(001)

(100)

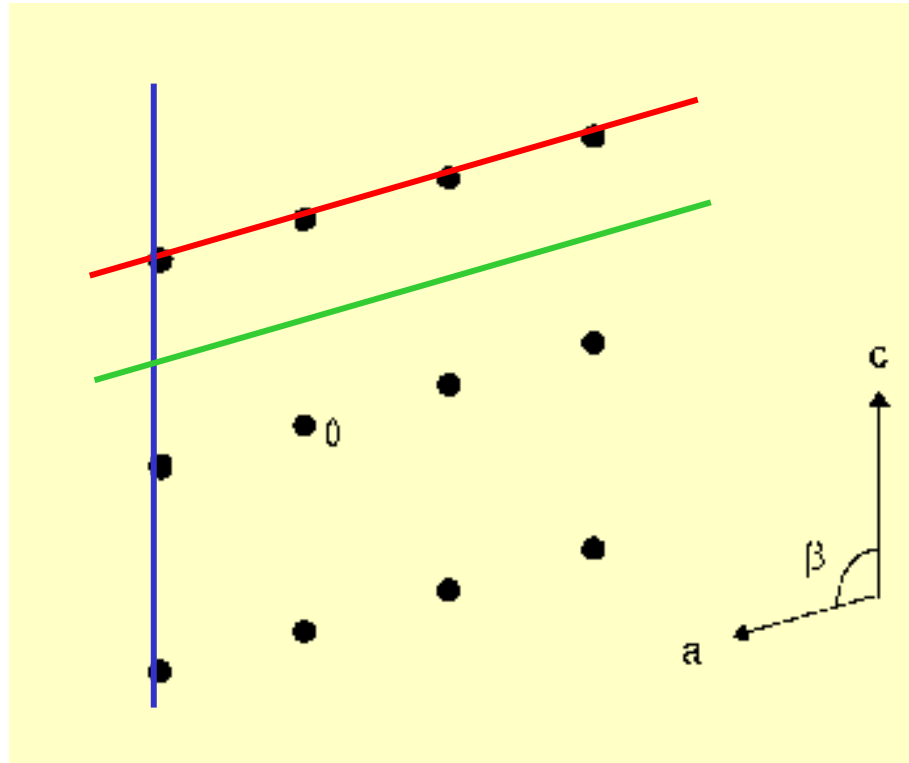


Miller indices of lattice planes

We will use a monoclinic unit cell to avoid orthogonal axes; define a plan and consider some lattice planes

(001)

(100)



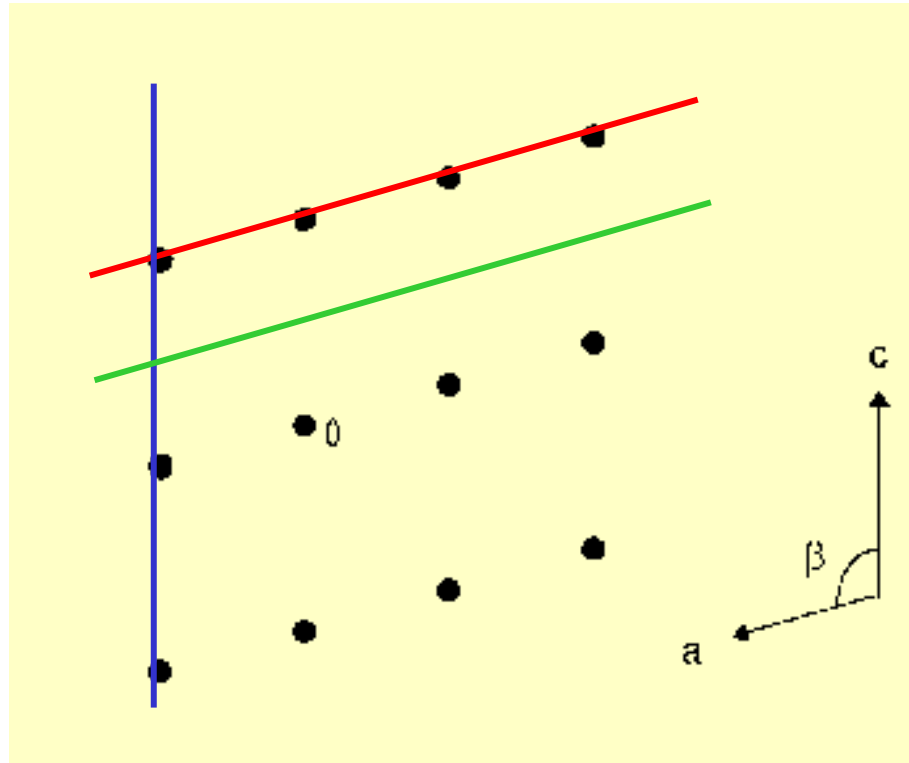
Miller indices of lattice planes

We will use a monoclinic unit cell to avoid orthogonal axes; define a plan and consider some lattice planes

(001)

(100)

(002)



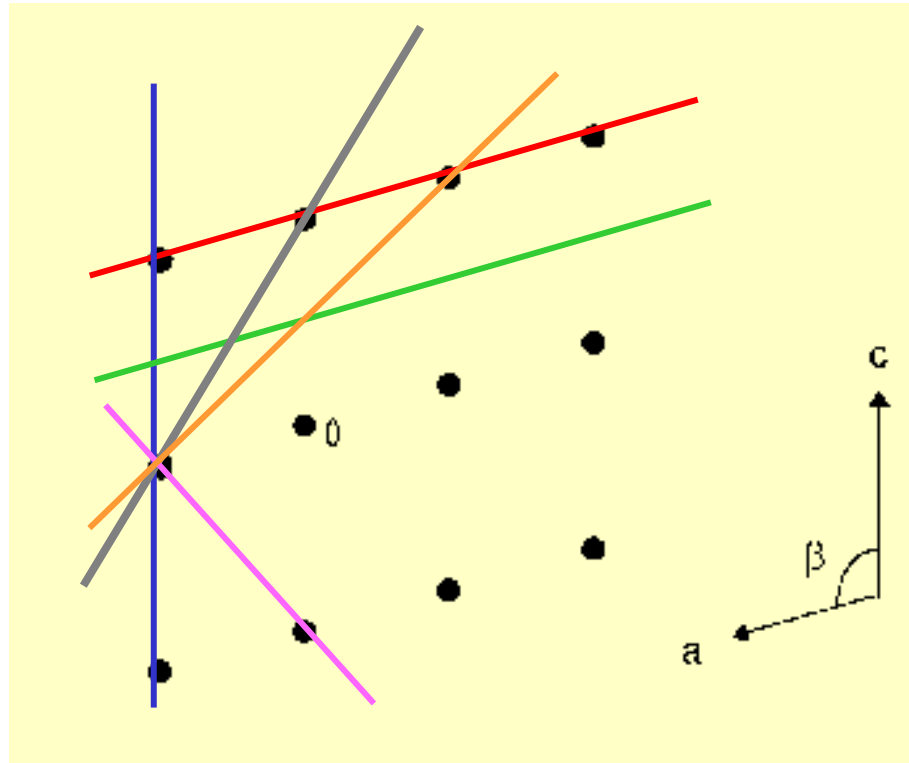
Miller indices of lattice planes

We will use a monoclinic unit cell to avoid orthogonal axes; define a plan and consider some lattice planes

(001)

(100)

(002)



Miller indices of lattice planes

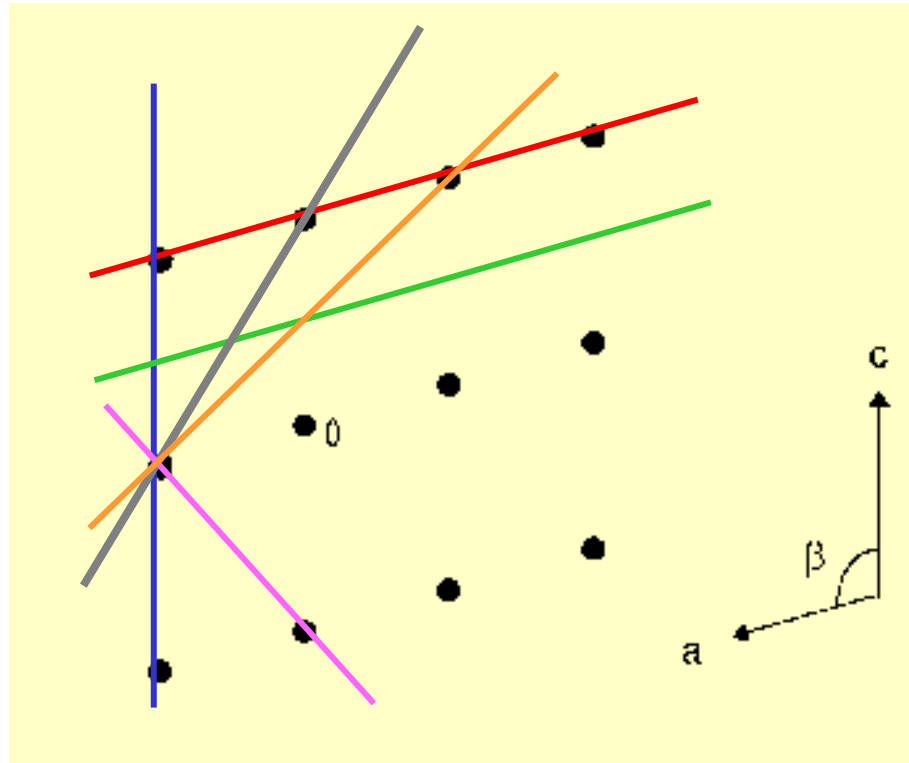
We will use a monoclinic unit cell to avoid orthogonal axes; define a plan and consider some lattice planes

(001)

(100)

(002)

(101)



Miller indices of lattice planes

We will use a monoclinic unit cell to avoid orthogonal axes; define a plan and consider some lattice planes

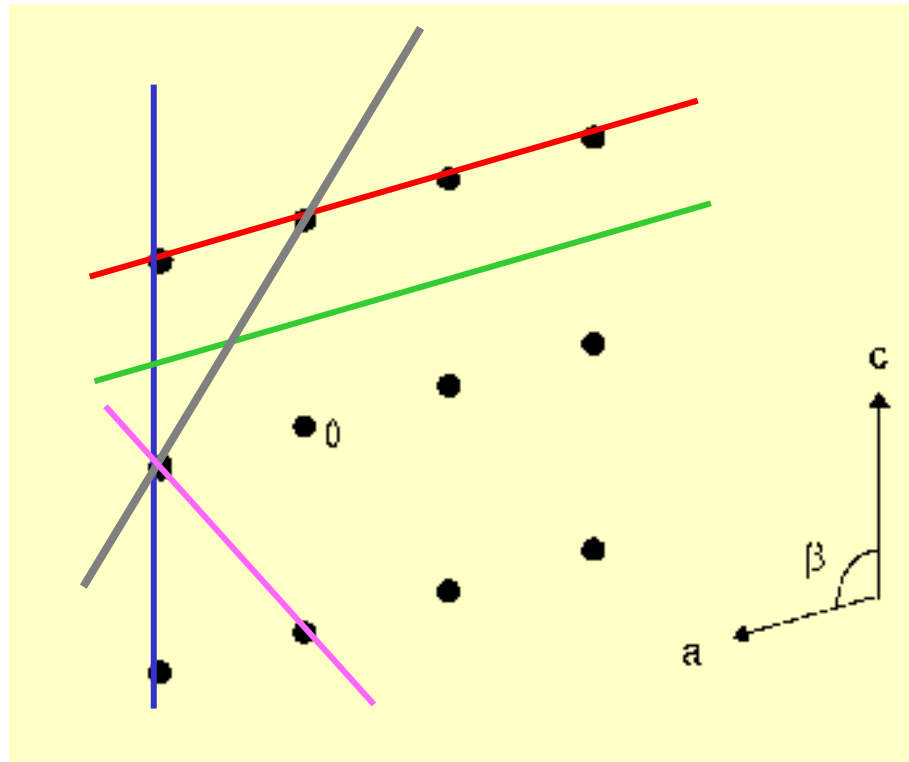
(001)

(100)

(002)

(101)

(10 $\bar{1}$)



Miller indices of lattice planes

We will use a monoclinic unit cell to avoid orthogonal axes; define a plan and consider some lattice planes

(001)

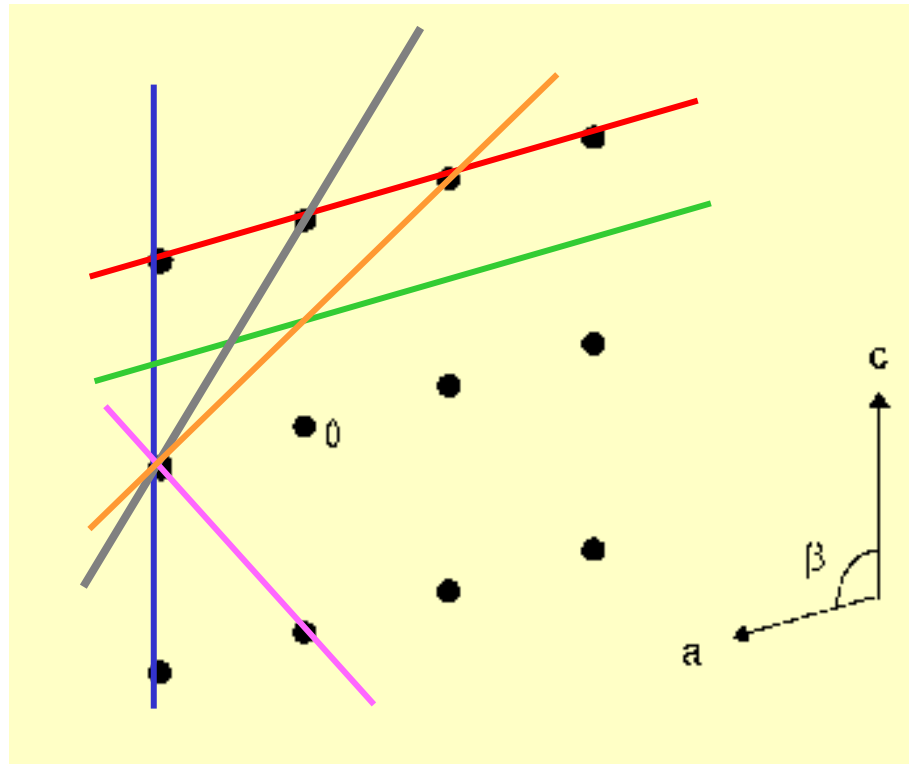
(100)

(002)

(101)

(10 $\bar{1}$)

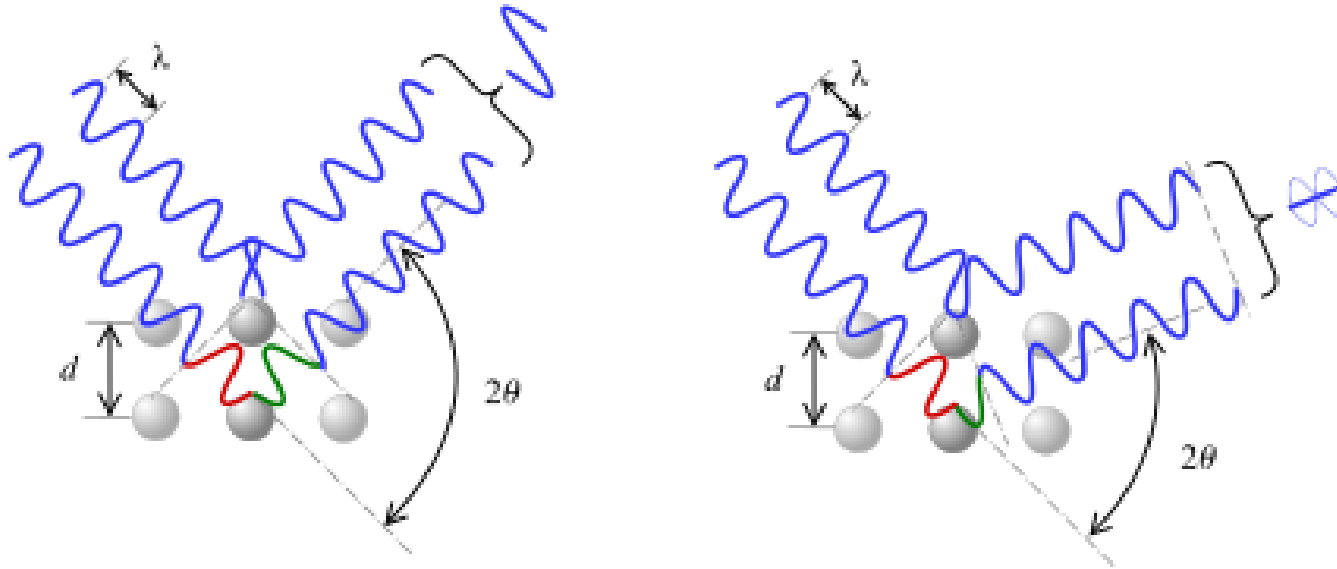
(102)



FYS3400: Lectures 1-2
Introduction. Crystal bonding. Periodicity and lattices.
Brag diffraction and Laue condition. Reciprocal space.

- Condensed Matter Physics à la FYS3400;
- Relevance of condensed matter physics fundamentals to modern technologies;
- Why elements bond together? Why in crystals? Survey of crystal bonding;
- Lattice planes and Miller indices;
- **Use of waves to study crystals explaining the idea of using the reciprocal space;**
- Introduction of the reciprocal space;
- Formal description of crystal structures.

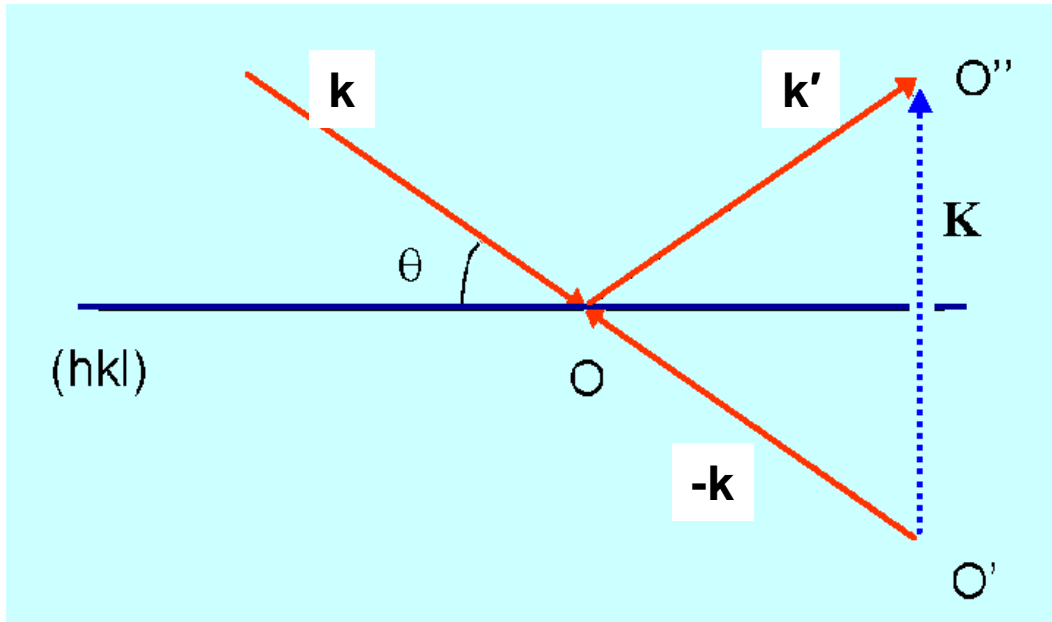
Bragg diffraction – constructive interference for the wave interacting with crystal planes



The conditions leading to diffraction are given by the Bragg's law, relating the angle of incidence of the radiation (θ) to the wavelength (λ) of the incident radiation and the spacing between the crystal lattice planes (d):

$$2 d \sin (\theta) = n \lambda$$

Laue condition

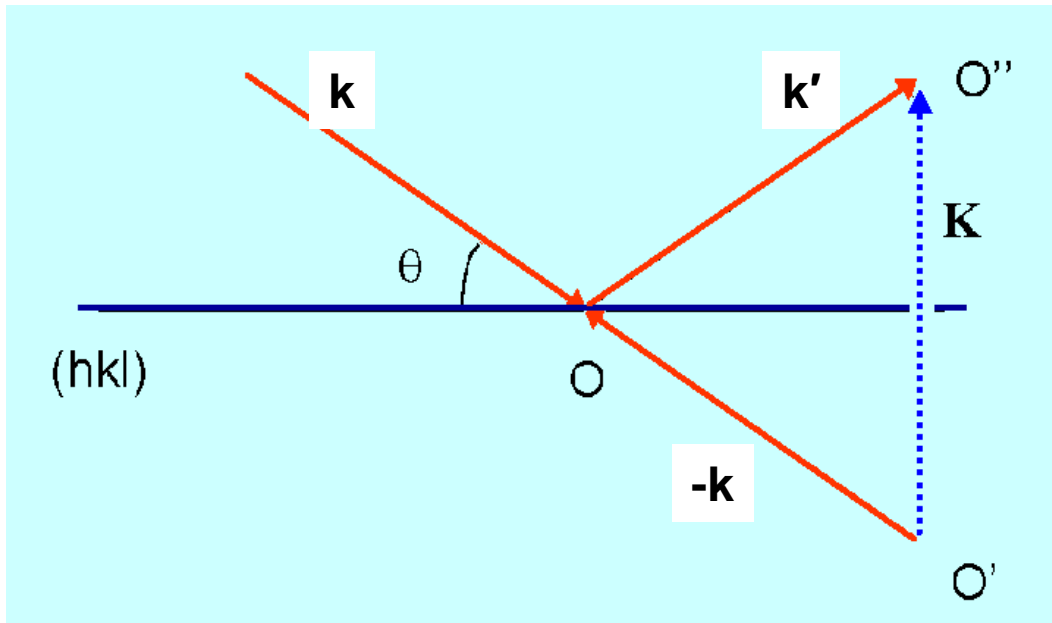


$$|\mathbf{K}| = 2|k|\sin\theta_{hkl} = \frac{2\sin\theta_{hkl}}{\lambda}$$

$\vec{\mathbf{K}}$ is perpendicular to the (hkl) plane, so can be defined as:

$$\vec{\mathbf{K}} = \left[\frac{2\sin\theta_{hkl}}{\lambda} \right] \hat{\mathbf{n}}$$

Laue condition



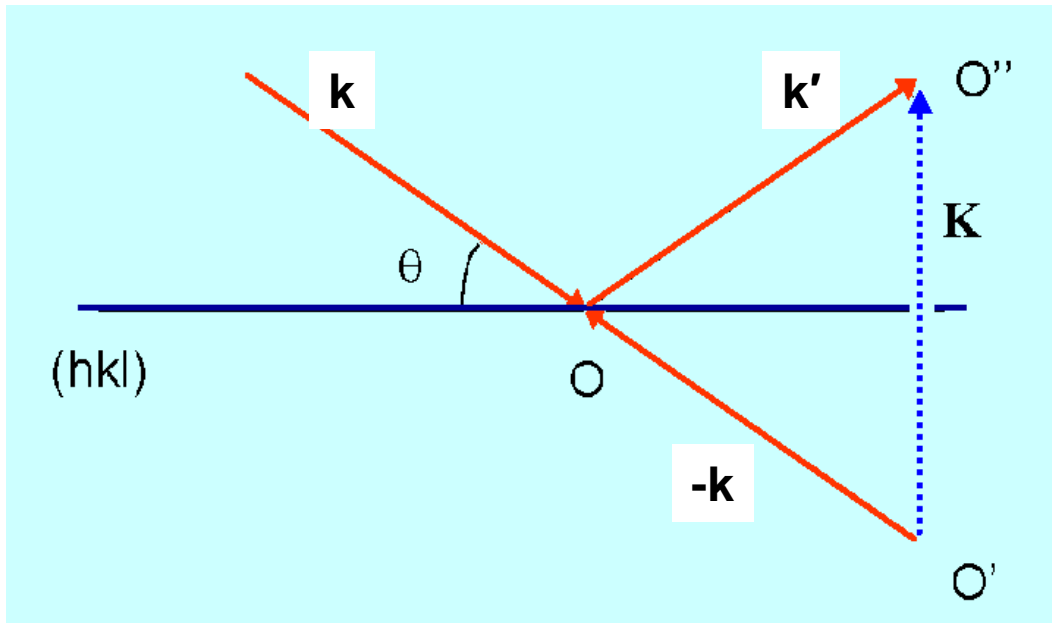
$$|\mathbf{K}| = 2|k|\sin\theta_{hkl} = \frac{2\sin\theta_{hkl}}{\lambda}$$

$\vec{\mathbf{K}}$ is perpendicular to the (hkl) plane, so can be defined as:

$$\vec{\mathbf{K}} = \left[\frac{2\sin\theta_{hkl}}{\lambda} \right] \hat{\mathbf{n}}$$

\mathbf{G} is also perpendicular to (hkl) so $\hat{\mathbf{n}} = \frac{\mathbf{G}_{hkl}}{|\mathbf{G}_{hkl}|}$

Laue condition



$$|\mathbf{K}| = 2|k| \sin \theta_{hkl} = \frac{2 \sin \theta_{hkl}}{\lambda}$$

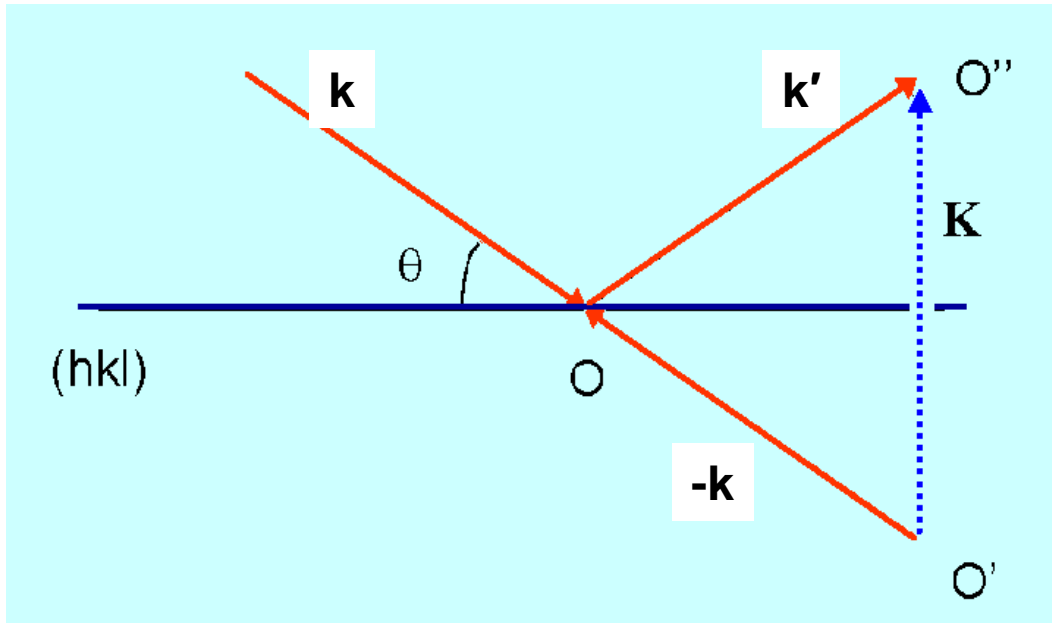
$\vec{\mathbf{K}}$ is perpendicular to the (hkl) plane, so can be defined as:

$$\vec{\mathbf{K}} = \left[\frac{2 \sin \theta_{hkl}}{\lambda} \right] \hat{\mathbf{n}}$$

\mathbf{G} is also perpendicular to (hkl) so $\hat{\mathbf{n}} = \frac{\mathbf{G}_{hkl}}{|\mathbf{G}_{hkl}|}$

$$\Rightarrow \mathbf{K} = \frac{2}{\lambda |\mathbf{G}_{hkl}|} \sin \theta_{hkl} \mathbf{G}_{hkl} \quad \text{and} \quad |\mathbf{G}_{hkl}| = \frac{1}{d_{hkl}} \quad \text{from previous}$$

Laue condition



$$|\mathbf{K}| = 2|k| \sin \theta_{hkl} = \frac{2 \sin \theta_{hkl}}{\lambda}$$

$\vec{\mathbf{K}}$ is perpendicular to the (hkl) plane, so can be defined as:

$$\vec{\mathbf{K}} = \left[\frac{2 \sin \theta_{hkl}}{\lambda} \right] \hat{\mathbf{n}}$$

\mathbf{G} is also perpendicular to (hkl) so $\hat{\mathbf{n}} = \frac{\mathbf{G}_{hkl}}{|\mathbf{G}_{hkl}|}$

$$\Rightarrow \mathbf{K} = \frac{2}{\lambda |\mathbf{G}_{hkl}|} \sin \theta_{hkl} \mathbf{G}_{hkl}$$

and $|\mathbf{G}_{hkl}| = \frac{1}{d_{hkl}}$ from previous

$$\Rightarrow \mathbf{K} = \frac{2d_{hkl} \sin \theta_{hkl}}{\lambda} \mathbf{G}_{hkl}$$

But Bragg: $2d \sin \theta = \lambda$

$$\mathbf{K} = \mathbf{G}_{hkl}$$

the Laue condition

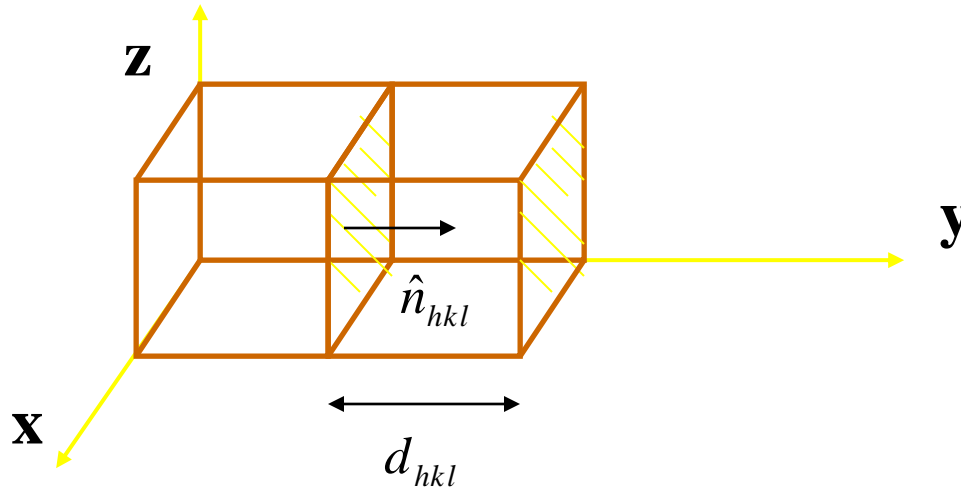
FYS3400: Lectures 1-2

**Introduction. Crystal bonding. Periodicity and lattices.
Brag diffraction and Laue condition. Reciprocal space.**

- Condensed Matter Physics à la FYS3400;
- Relevance of condensed matter physics fundamentals to modern technologies;
- Why elements bond together? Why in crystals? Survey of crystal bonding;
- Lattice planes and Miller indices;
- Use of waves to study crystals explaining the idea of using the reciprocal space;
- **Introduction of the reciprocal space;**
- Formal description of crystal structures.

Reciprocal lattice

Crystal planes (hkl) in the real-space or direct lattice are characterized by the normal vector \hat{n}_{hkl} and the interplanar spacing d_{hkl} :



Defining a different lattice in reciprocal space whose points lie at positions given by the vectors

$$\bar{G}_{hkl} \equiv \frac{2\pi\hat{n}_{hkl}}{d_{hkl}}$$

These vectors are parallel to the [hkl] direction but has magnitude $2\pi/d_{hkl}$, which is a reciprocal distance

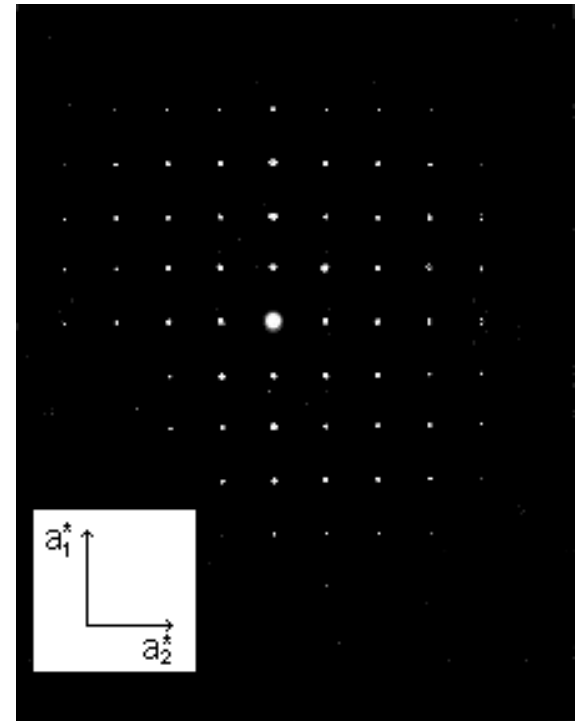
Reciprocal lattice

The reciprocal lattice is composed of all points lying at positions \vec{G}_{hkl} from the origin, so that there is one point in the reciprocal lattice for each set of planes (hkl) in the real-space lattice.

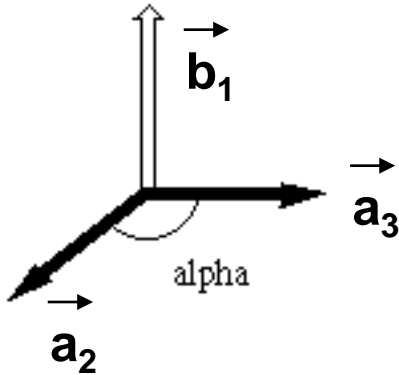
This seems like an unnecessary abstraction. Is there a benefit for defining such a reciprocal lattice?

YES, the reciprocal lattice simplifies the interpretation of x-ray diffraction from crystals because:

- Diffraction pattern is not a direct representation of the crystal lattice
 - Diffraction pattern is a representation of the *reciprocal lattice*



Reciprocal lattice



Generallizing, we introduce a set of new unit vectors so that they are normal to the plains determined by the previously introduced translation vectors

Definition of reciprocal translation vectors

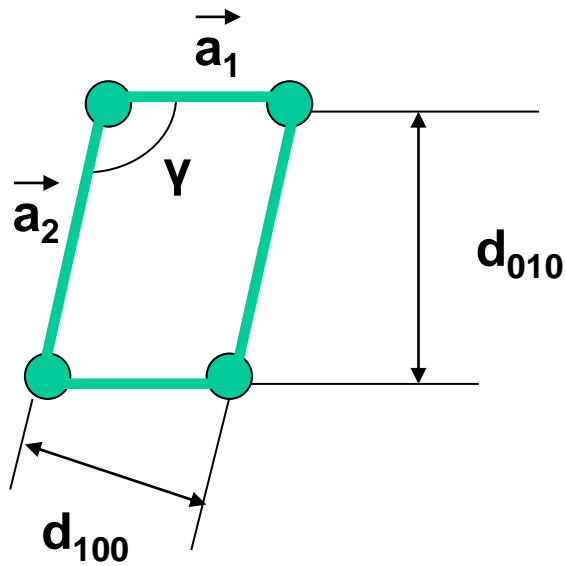
$$\vec{b}_1 = (\vec{a}_2 \times \vec{a}_3) 2\pi/V_c \quad \vec{b}_2 = (\vec{a}_3 \times \vec{a}_1) 2\pi/V_c \quad \vec{b}_3 = (\vec{a}_1 \times \vec{a}_2) 2\pi/V_c$$

$$V_c = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) - \text{volume of a unit cell}$$

$$\vec{G} = v_1 \vec{b}_1 + v_2 \vec{b}_2 + v_3 \vec{b}_3$$

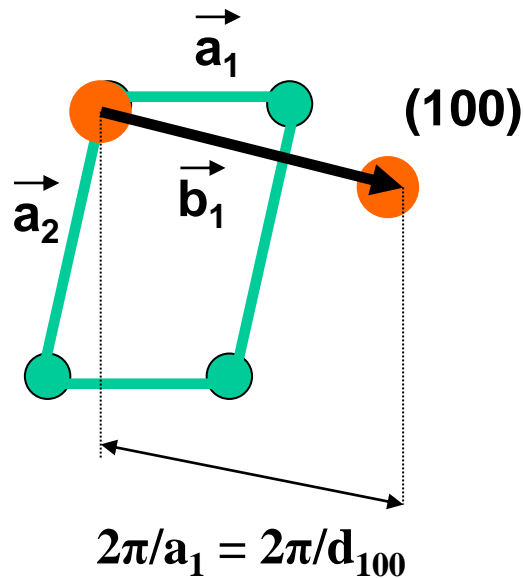
Reciprocal lattice

Reciprocal lattice is nothing with "anti-matter" or "black holes" to do – it is determined by a set of vectors with specific magnitudes just having a bit unusual dimensions – $1/\text{length}$. It is actually relatively straightforward – as long as we understand the definitions – to sketch the reciprocal lattice.



Reciprocal lattice

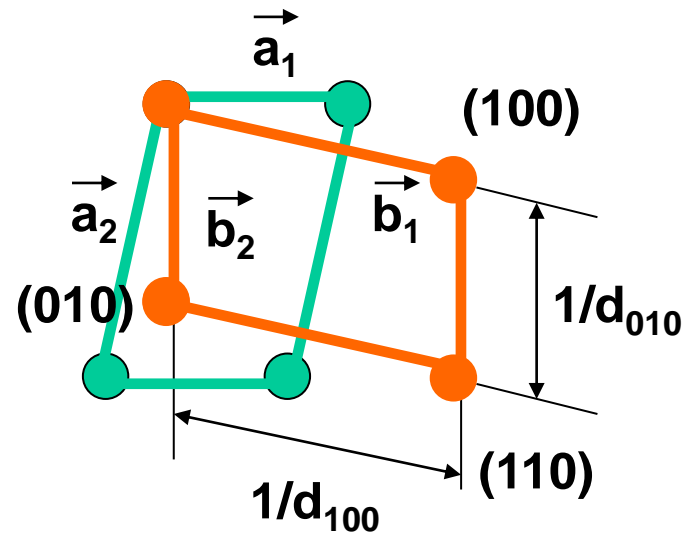
Reciprocal lattice is nothing with "anti-matter" or "black holes" to do – it is determined by a set of vectors with specific magnitudes just having a bit unusual dimensions – $1/\text{length}$. It is actually relatively straightforward – as long as we understand the definitions – to sketch the reciprocal lattice.



The important part is that b_1 should be normal to a plain determined by $[a_2 \times a_3]$ and having a magnitude of $1/a_1$ – just by definition - or $1/d_{100}$, where d_{100} is the interplain distance between (100) family of plains. NB, for any plain from (100) family the point in the reciprocal space is exactly the same meaning that any reciprocal lattice point represents its own family of plains in the real space.

Reciprocal lattice

Reciprocal lattice is nothing with "anti-matter" or "black holes" to do – it is determined by a set of vectors with specific magnitudes just having a bit unusual dimensions – $1/\text{length}$. It is actually relatively straightforward – as long as we understand the definitions – to sketch the reciprocal lattice.



The important part is that b_1 should be normal to a plain determined by $[\vec{a}_2 \times \vec{a}_3]$ and having a magnitude of $1/a_1$ – just by definition - or $1/d_{100}$, where d_{100} is the interplain distance between (100) family of plains. NB, for any plain from (100) family the point in the reciprocal space is exactly the same meaning that any reciprocal lattice point represents its own family of plains in the real space.

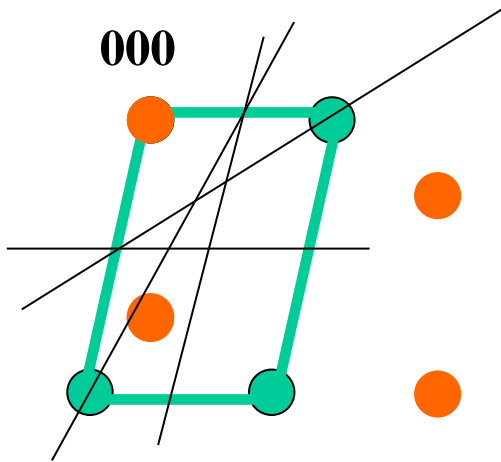
Similar excercise can be done with vector b_2 which points out to a reciprocal lattice point representing (010) family of plains.

In adition (110) family of plaines in the real space would naturally result in to (110)-points in the reciprocal space.

The procedure can be repeated any type of plain cuts in the real space

Reciprocal lattice

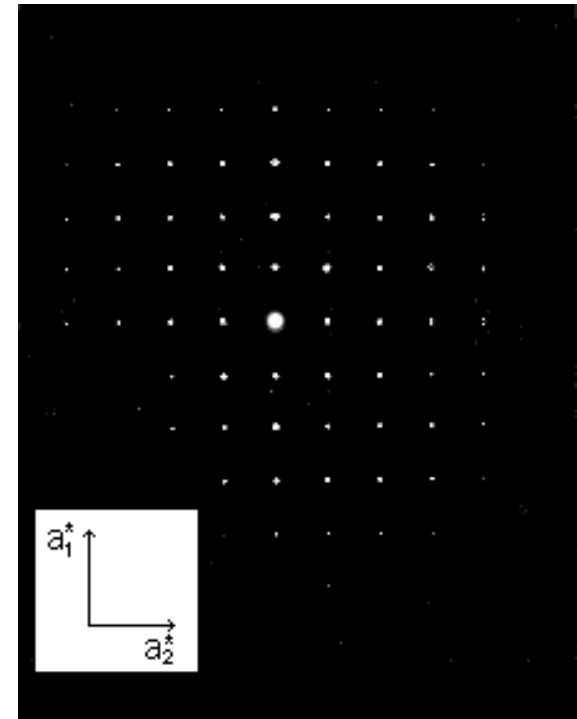
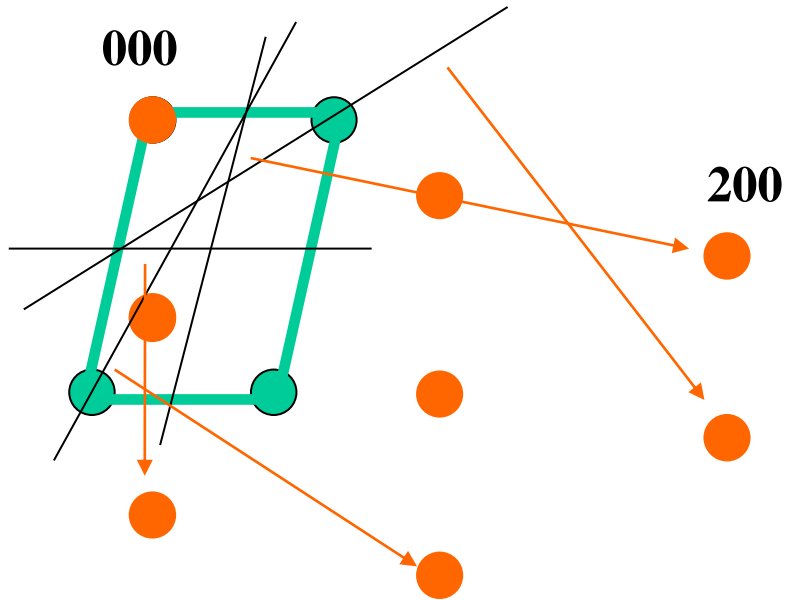
Reciprocal lattice is nothing with "anti-matter" or "black holes" to do – it is determined by a set of vectors with specific magnitudes just having a bit unusual dimensions – 1/length. It is actually relatively straightforward – as long as we understood the definitions – to sketch the reciprocal lattice.



$$d_{hkl} = \frac{a}{\sqrt{(h^2 + k^2 + l^2)}}$$

Reciprocal lattice

Reciprocal lattice is nothing with "anti-matter" or "black holes" to do – it is determined by a set of vectors with specific magnitudes just having a bit unusual dimensions – $1/\text{length}$. It is actually relatively straightforward – as long as we understood the definitions – to sketch the reciprocal lattice.



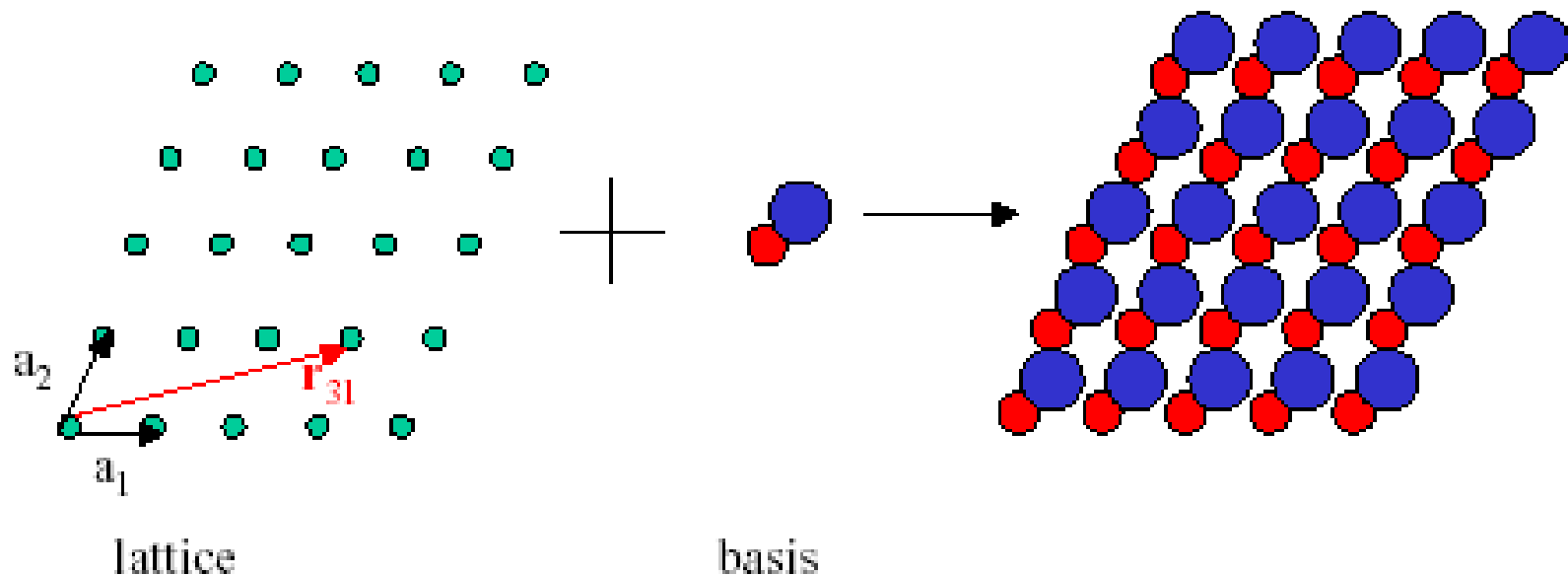
FYS3400: Lectures 1-2

**Introduction. Crystal bonding. Periodicity and lattices.
Brag diffraction and Laue condition. Reciprocal space.**

- Condensed Matter Physics à la FYS3400;
- Relevance of condensed matter physics fundamentals to modern technologies;
- Why elements bond together? Why in crystals? Survey of crystal bonding;
- Lattice planes and Miller indices;
- Use of waves to study crystals explaining the idea of using the reciprocal space;
- Introduction of the reciprocal space;
- **Formal description of crystal structures.**

Crystal structure I

- In bulk, many solids are crystalline.
- Have discrete translational and rotational symmetries.
- Real-space structure is periodic - repetitions of a single *unit cell*.
- Smallest unit cell that gives full structure: *primitive unit cell*
- Can describe structure by a *lattice* and a *basis*.



Ideal Crystal

- An ideal crystal is a periodic array of structural units, such as atoms or molecules.
- It can be constructed by the *infinite repetition* of these identical structural units in space.
- Structure can be described in terms of a *lattice*, with a group of atoms attached to each lattice point. The group of atoms is the basis.

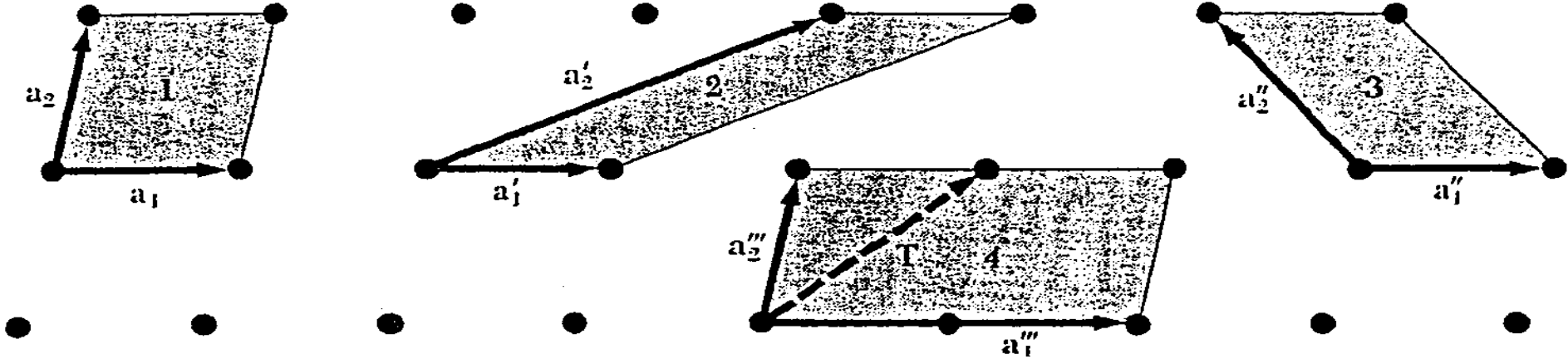
Bravais Lattice

- An infinite array of discrete points with an arrangement and orientation that appears exactly the same, from any of the points the array is viewed from.
- A three dimensional Bravais lattice consists of all points with position vectors \mathbf{R} that can be written as a linear combination of *primitive vectors*. The expansion coefficients must be *integers*.

Primitive Unit Cell

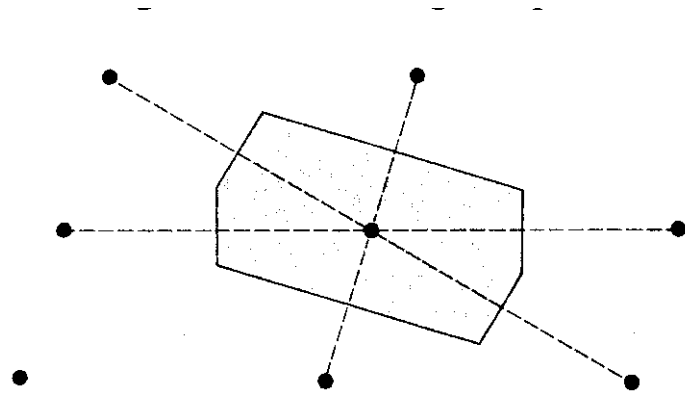
- A *primitive cell* or primitive unit cell is a volume of space that when translated through all the vectors in a Bravais lattice just fills all of space without either overlapping itself or leaving voids.
- A primitive cell must contain precisely one lattice point.

Crystal structure II



Primitive (a_1, a_2) and not primitive (a'''_1, a'''_2) translation vectors

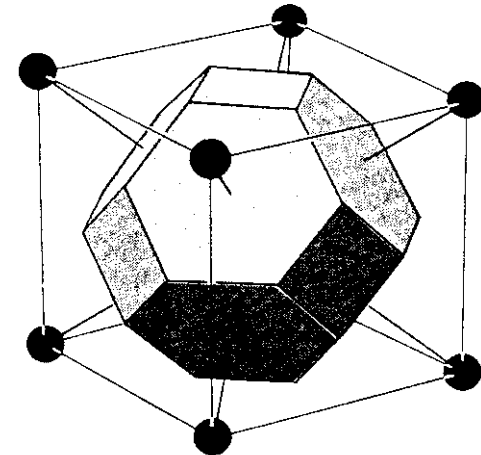
Wigner-Seitz Primitive Cell: Full symmetry of Bravais Lattice

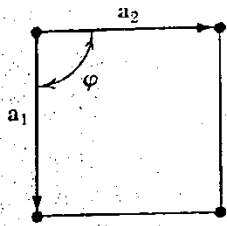


- **Figure 4.14**
The Wigner-Seitz cell for a two-dimensional Bravais lattice. The six sides of the cell bisect the lines joining the central points to its six nearest neighboring points (shown as dashed lines). In two dimensions the Wigner-Seitz cell is always a hexagon unless the lattice is rectangular (see Problem 4a).

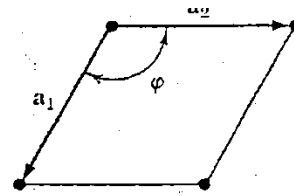
Figure 4.15

The Wigner-Seitz cell for the body-centered cubic Bravais lattice (a “truncated octahedron”). The surrounding cube is a conventional body-centered cubic cell with a lattice point at its center and on each vertex. The hexagonal faces bisect the lines joining the central point to the points on the vertices (drawn as solid lines). The square faces bisect the lines joining the central point to the central points in each of the six neighboring cubic cells (not drawn). The hexagons are regular (see Problem 4d).

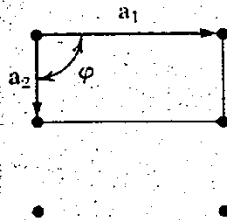




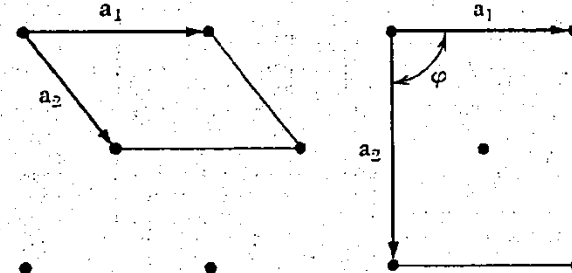
(a) Square lattice
 $|a_1| = |a_2|$; $\varphi = 90^\circ$



(b) Hexagonal lattice
 $|a_1| = |a_2|$; $\varphi = 120^\circ$



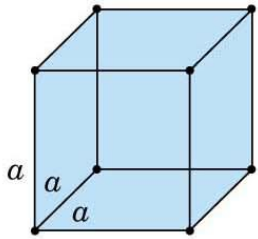
(c) Rectangular lattice
 $|a_1| \neq |a_2|$; $\varphi = 90^\circ$



(d) Centered rectangular lattice;
 axes are shown for both the
 primitive cell and for the
 rectangular unit cell, for
 which $|a_1| \neq |a_2|$; $\varphi = 90^\circ$.

2-D lattices

3-D lattices



Cubic

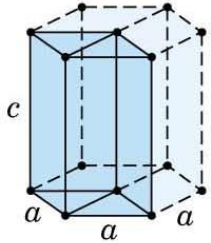
$$a=b=c$$

$$\alpha=\beta=\gamma=90^\circ$$

Orthorhombic

$$a \neq b \neq c$$

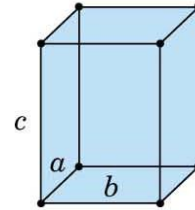
$$\alpha=\beta=\gamma=90^\circ$$



Hexagonal

$$a=b \neq c$$

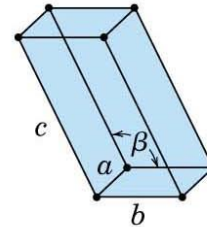
$$\alpha=\beta=90^\circ ; \gamma=120^\circ$$



Monoclinic

$$a \neq b \neq c$$

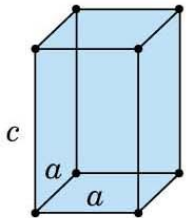
$$\alpha=\gamma=90^\circ \neq \beta$$



Tetragonal

$$a=b \neq c$$

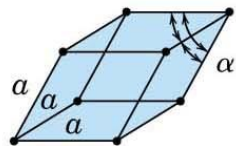
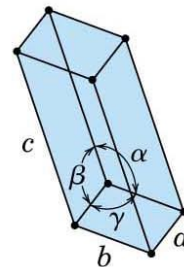
$$\alpha=\beta=\gamma=90^\circ$$



Triclinic

$$a \neq b \neq c$$

$$\alpha \neq \beta \neq \gamma \neq 90^\circ$$



Rhombohedral

$$a=b=c$$

$$\alpha=\beta=\gamma \neq 90^\circ$$

Primitive Cell: FCC Lattice

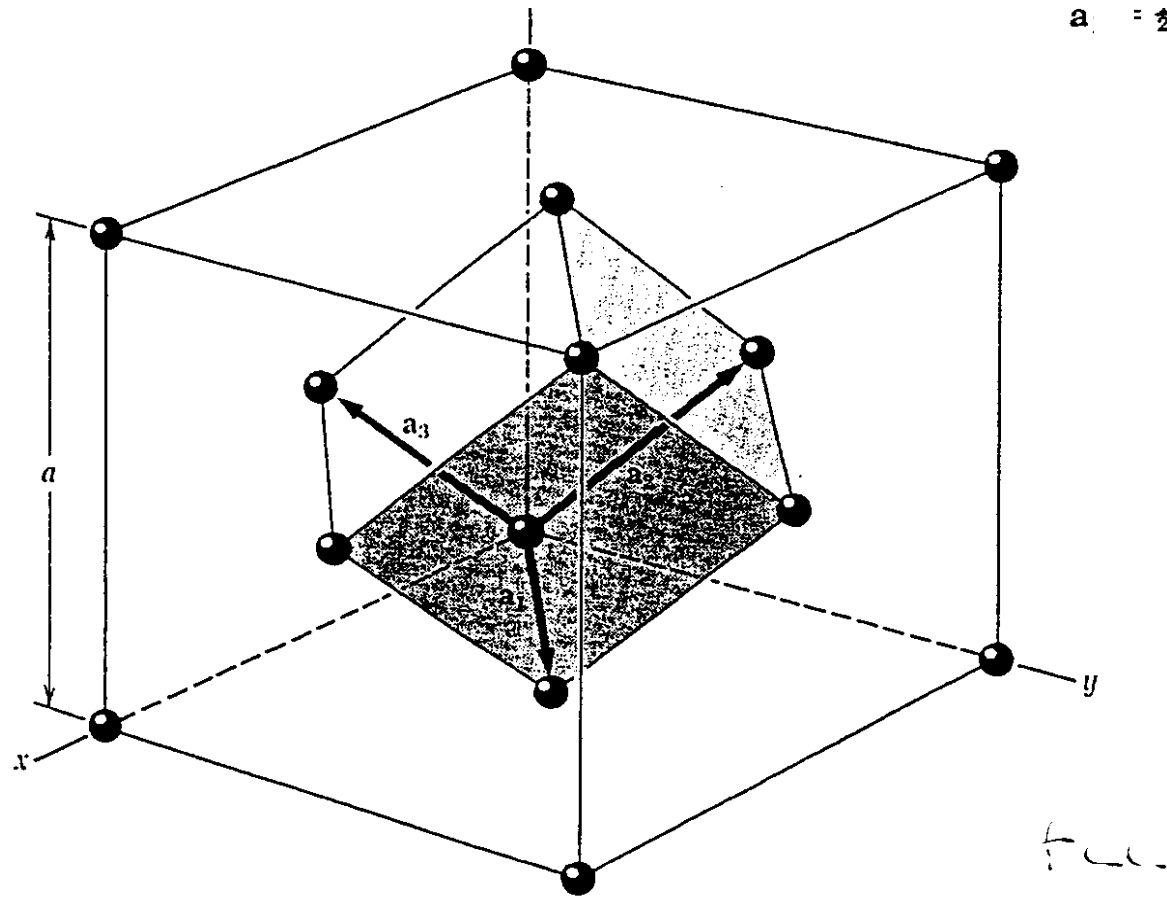


Figure 13 The rhombohedral primitive cell of the face-centered cubic crystal. The primitive translation vectors \mathbf{a}_1 , \mathbf{a}_2 , \mathbf{a}_3 connect the lattice point at the origin with lattice points at the face centers. As drawn, the primitive vectors are:

$$\mathbf{a}_1 = \frac{1}{2}a(\hat{x} + \hat{y}) ; \quad \mathbf{a}_2 = \frac{1}{2}a(\hat{y} + \hat{z}) ; \quad \mathbf{a}_3 = \frac{1}{2}a(\hat{z} + \hat{x}) .$$

The angles between the axes are 60° . Here \hat{x} , \hat{y} , \hat{z} are the Cartesian unit vectors.