FYS3410 - Vår 2010 (Kondenserte fasers fysikk)

http://www.uio.no/studier/emner/matnat/fys/FYS3410/index-eng.xml

Based on Introduction to Solid State Physics by Kittel

Course content

- Periodic structures, understanding of diffraction experiment and reciprocal lattice
- Imperfections in crystals: diffusion, point defects, dislocations
- Crystal vibrations: phonon heat capacity and thermal conductivity
- Free electron Fermi gas: density of states, Fermi level, and electrical conductivity
- Electrons in periodic potential: energy bands theory classification of metals, semiconductors and insulators
- Semiconductors: band gap, effective masses, charge carrier distributions, doping, pn-junctions
- Metals: Fermi surfaces, temperature dependence of electrical conductivity

Andrej Kuznetsov, Dept of Physics and Centre for Material Science and Nanothechnology
Postboks 1048 Blindern, 0316 OSLO
Tel: +47-22852870, e-post: andrej.kuznetsov@fys.uio.no
visiting address: MiNaLab, Gaustadaleen 23b

FYS3410 lecture schedule and exams: Spring 2010

M/18/1/2010:	Introduction and motivation. Periodicity and lattices	2h
W/20/1/2010:	Index system for crystal planes. Crystal structures	1h
M/25/1/2010:	Reciprocal space, Laue condition and Ewald construction	2h
W/27/1/2010:	Interpretation of a diffraction experiment	1h
M/01/2/2010:	Crystal binding and introduction to elastic strain	2h
W/03/2/2010:	Point defects, case study – vacancies	1h
M/08/2/2010:	Point defects and atomic diffusion	2h
W/10/2/2010:	Diffusion (continuation); dislocations	1h
M/15/2/2010:	Crystal vibrations and phonons	2h
W/17/2/2010:	Crystal vibrations and phonons	1h
M/22/2/2010:	Planck distribution and density of states	2h
W/24/2/2010:	Debye model	1h
M/01/3/2010:	Einstein model and general result for density of states	2h
W/03/3/2010:	Thermal conductivity	1h
M/08/3/2010:	Free electron Fermi gas in 1D and 3D – ground state	2h
W/10/3/2010:	Density of states, effect of temperature – FD distribution	1h
M/15/3/2010:	Heat capacity of FEFG	2h
W/17/3/2010:	Repetition	1h
22/3/2010:	Mid-term exam	

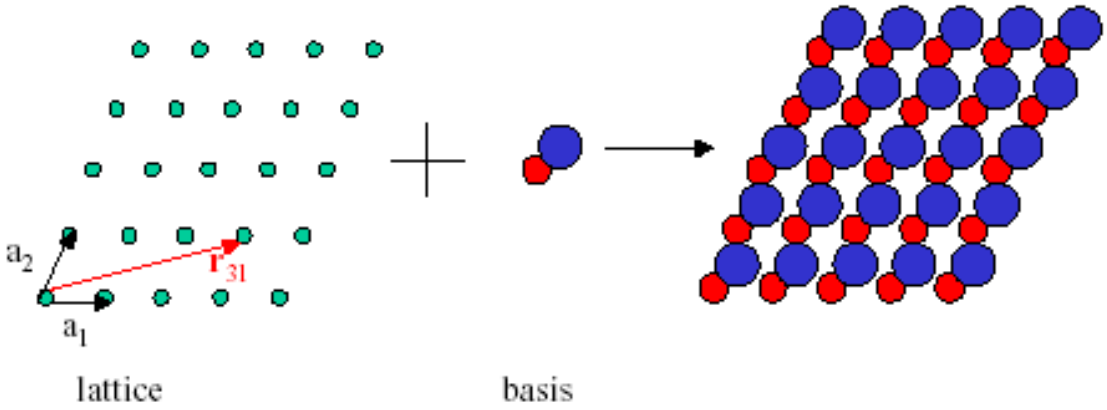
M/14/4/2010:	Electrical and thermal conductivity in metals	2h
W/12/4/2010:	Bragg reflection of electron waves at the boundary of BZ	1h
M/19/4/2010:	Energy bands, Kronig - Penny model	2h
W/21/4/2010:	Empty lattice approximation; number of orbitals in a band	1h
M/26/4/2010:	Semiconductors, effective mass method, intrinsic carriers	2h
W/28/4/2010:	Impurity states in semiconductors and carrier statistics	1h
M/03/5/2010:	p-n junctions and heterojunctions	2h
W/05/5/2010:	surface structure, surface states, Schottky contacts	2h
M/10/5/2010:	no lectures	
W/12/5/2010:	no lectures	
W/19/5/2010:	Repetition	2h
W26/5/2010:	Repetition	2h

28/5/2010: Final Exam (sensor: Prof. Arne Nylandsted Larsen at the Århus University, Denmark, http://person.au.dk/en/anl@phys.au.dk)

Lecture 2: Periodicity, lattices, and index system for crystal planes

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.**

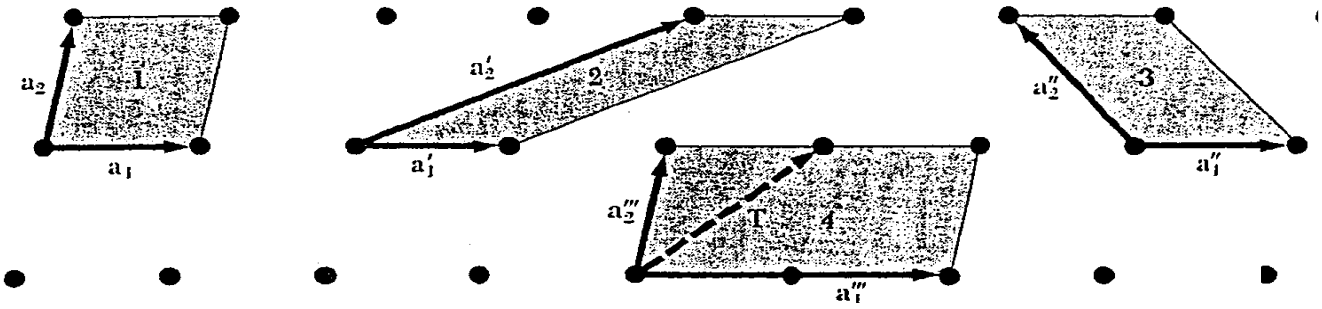
Bravais Lattice

- **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 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

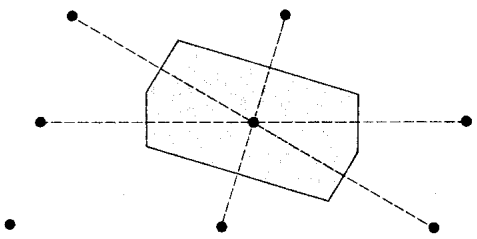
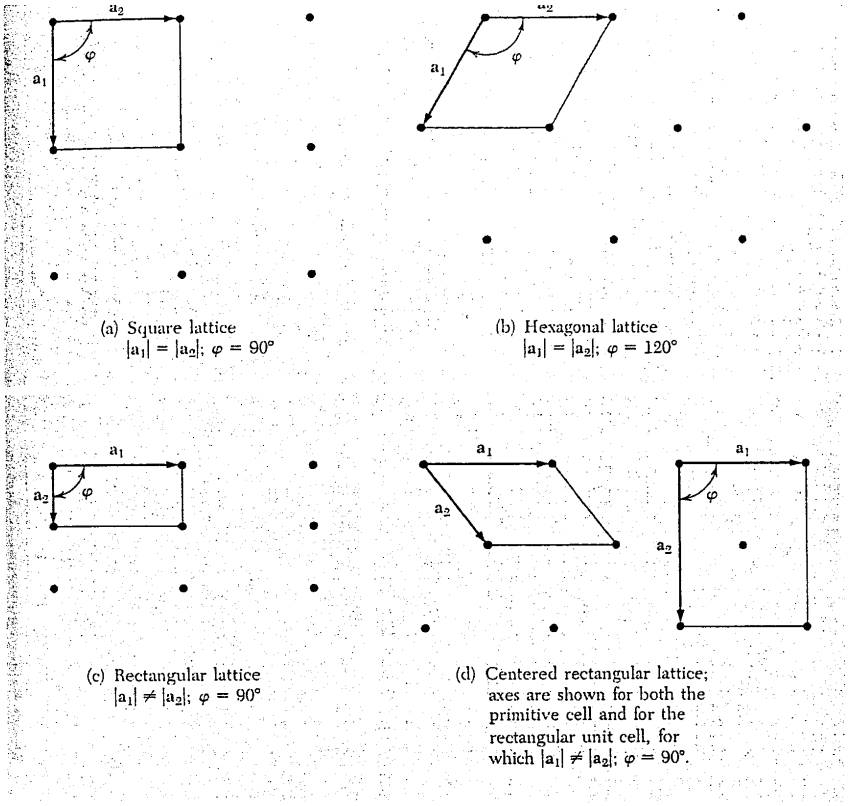
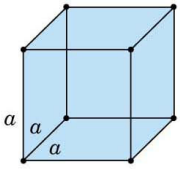


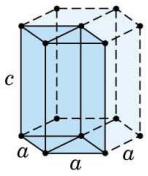
Figure 4.14
The Wigner-Seitz cell for a two-dimensional Bravais lattice. The six sides of the cell bisect the lines joining the central points to its six nearest neighboring points (shown as dashed lines). In two dimensions the Wigner-Seitz cell is always a hexagon unless the lattice is rectangular (see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



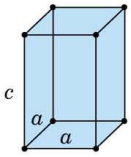
2-D lattices



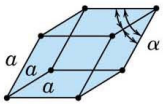
Cubic
a=b=c
α=β=γ=90°



Hexagonal
a=b≠c
α=β= 90° ; γ=120°

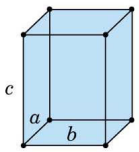


Tetragonal
a=b≠c
α=β=γ=90°

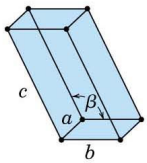


Rhombohedral
a=b=c=
α=β=γ≠90°

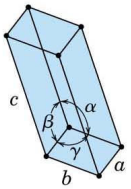
3-D lattices



Orthorhombic
a≠b≠c
a=b=g=90°



Monoclinic
a≠b≠c
α=γ=90°≠β



Triclinic
a≠b≠c
α≠β≠γ≠90°

Primitive Cell: FCC Lattice

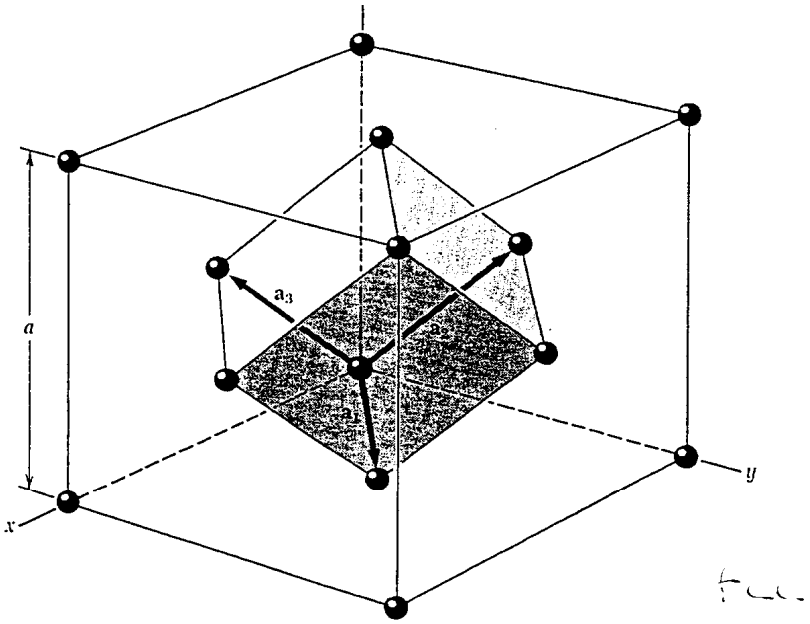


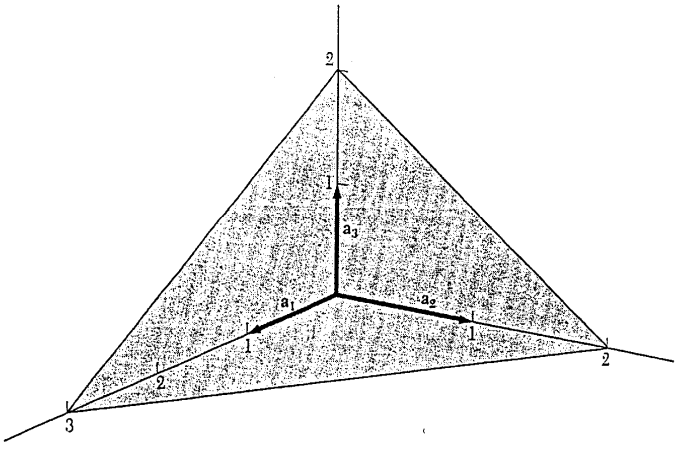
Figure 13 The rhombohedral primitive cell of the face-centered cubic crystal. The primitive translation vectors $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ connect the lattice point at the origin with lattice points at the face centers. As drawn, the primitive vectors are:

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

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

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:

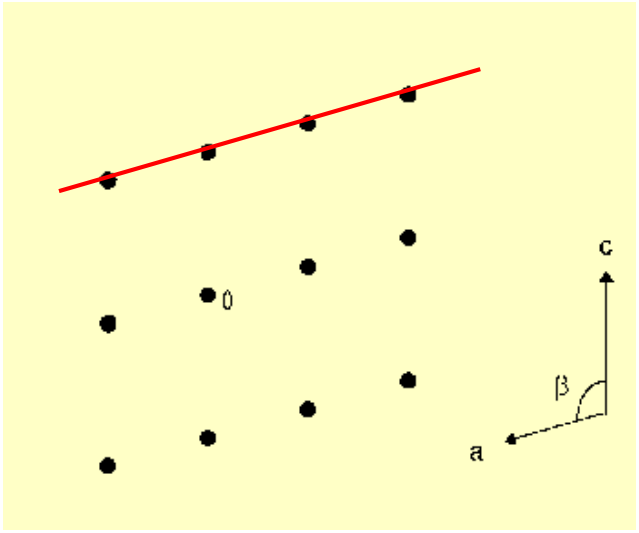


$$h:k:l = \frac{1}{x_1} : \frac{1}{x_2} : \frac{1}{x_3}$$

Figure 15 This plane intercepts the $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ axes at $3\mathbf{a}_1$, $2\mathbf{a}_2$, $2\mathbf{a}_3$. 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).

Miller indices of lattice planes

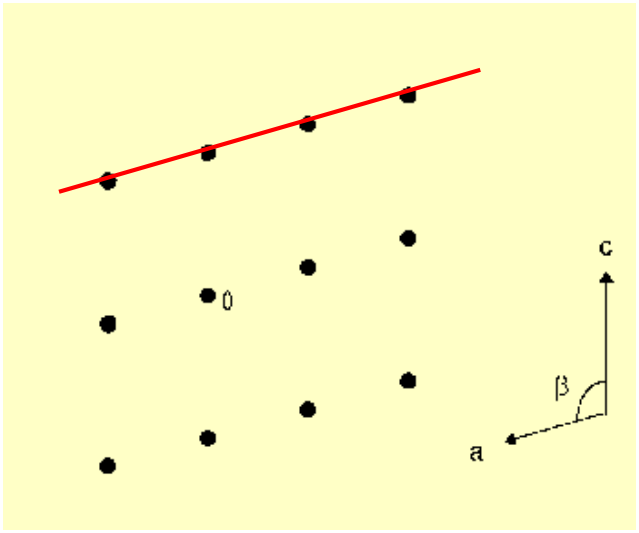
We will use a monoclinic unit cell to avoid orthogonal axes; define a plan and consider some lattice planes



Miller indices of lattice planes

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

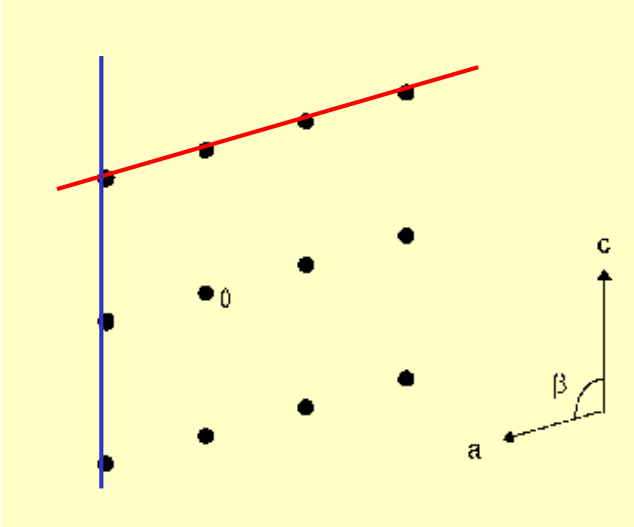
(001)



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)

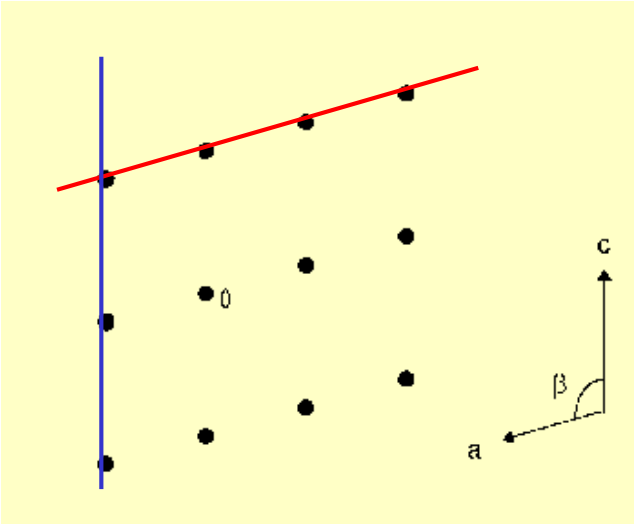


Miller indices of lattice planes

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

(001)

(100)

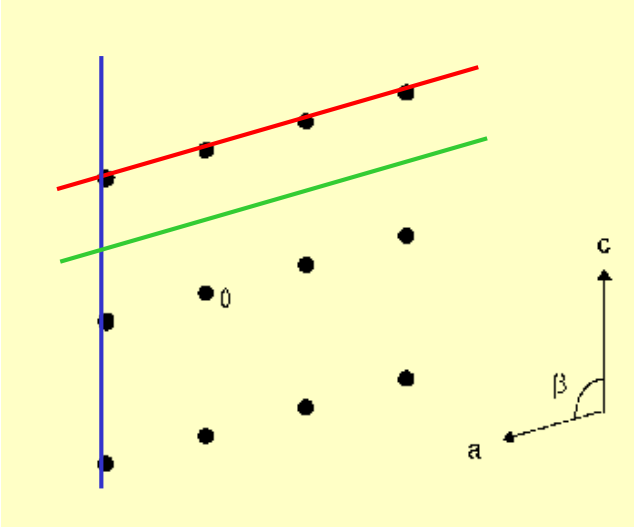


Miller indices of lattice planes

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

(001)

(100)



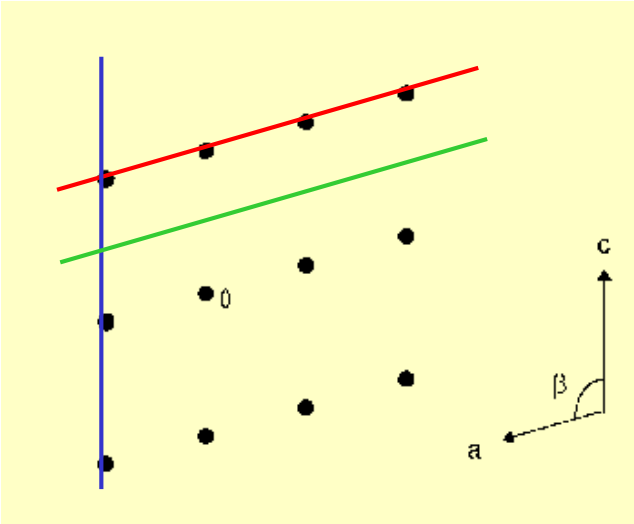
Miller indices of lattice planes

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

(001)

(100)

(002)



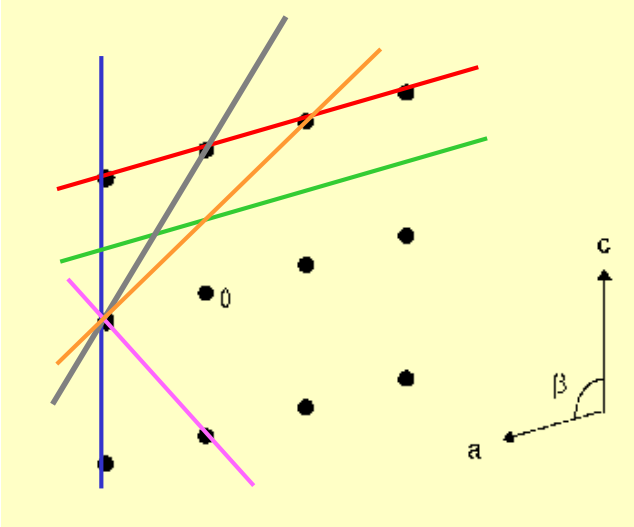
Miller indices of lattice planes

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

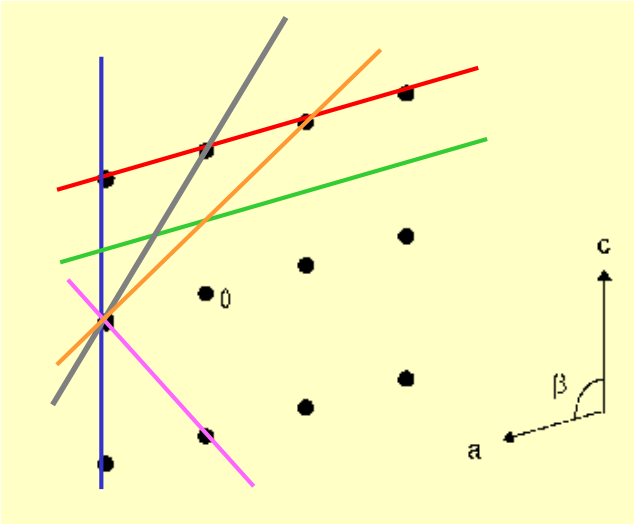
We will use a monoclinic unit cell to avoid orthogonal axes; define a plan and consider some lattice planes

(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

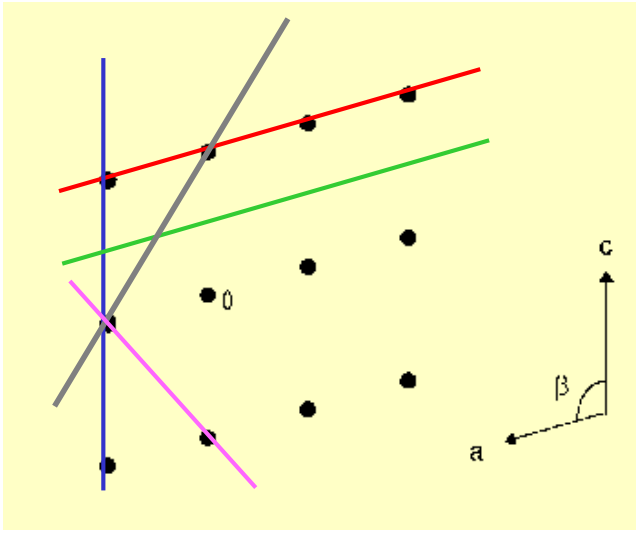
(001)

(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)

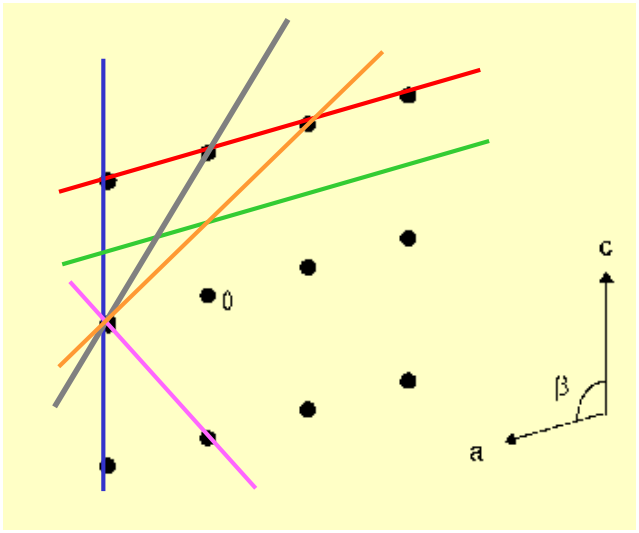
(100)

(002)

(101)

$(10\bar{1})$

(102)



Miller indices of lattice planes

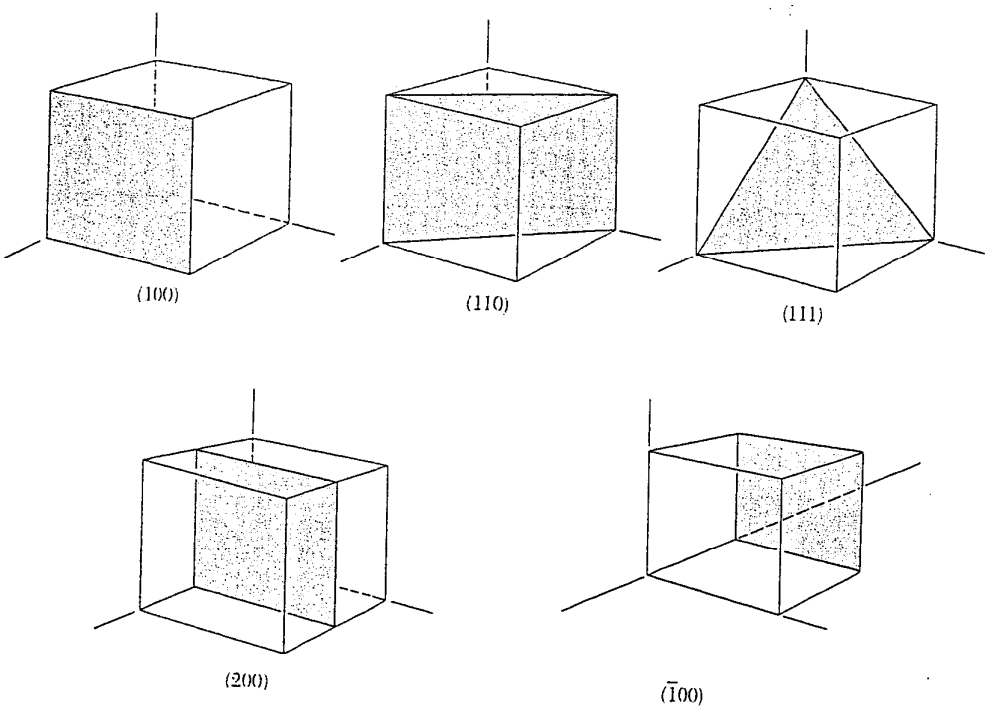
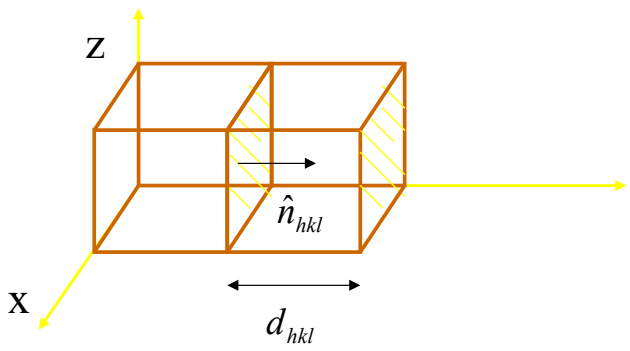


Figure 16 Indices of important planes in a cubic crystal. The plane (200) is parallel to (100) and to ($\bar{1}$00).

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} :



Miller indices were derived as the reciprocal (or inverse) of unit cell intercepts.

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

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

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. What is the payoff for defining such a reciprocal lattice? No, the reciprocal lattice simplifies the interpretation of x-ray diffraction from crystals because:

- **A diffraction pattern is not a direct representation of the crystal lattice**
- **The diffraction pattern is a representation of the *reciprocal lattice***