

Electron Microscopy I

Lecture 05

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1. From light microscopy to electron microscopy

1.1 Light and matter waves

1.2 Fundamentals of optical imaging: geometrical optics

1.3 Wave optics: Abbe's theory of imaging, Fourier optics

2. Practical aspects of transmission electron microscopy (TEM) and scanning transmission electron microscopy (STEM)

2.1 Structure and function of a transmission electron microscope

2.2 Lens aberrations in electron optics and their effect on resolving power

2.3 Sample preparation

2.4 Radiation damage

3. Electron diffraction in the solid state/kinematic diffraction theory

4. Contrast formation and practical examples of the imaging of crystalline objects in solid state and materials research

5. Dynamic electron diffraction

6. Imaging of the crystal lattice/high-resolution electron microscopy (HRTEM)

7. Scanning transmission electron microscopy

8. Electron holography

9. Transmission electron microscopy with phase plates

2.3 Radiation damage

Radiation damage

"Direct"

Radiation damage under the microscope

- Nuclear displacement damage ("knock-on damage")
- Electron excitation damage (radiolysis)

"Indirect"

Radiation damage under the microscope

- Contamination (*polymerization of hydrocarbon molecules* ($C H_{nm}$) on the sample)
- Heating (radius r_0 of the illuminated sample area proportional to the temperature increase)

2.3 Radiation damage

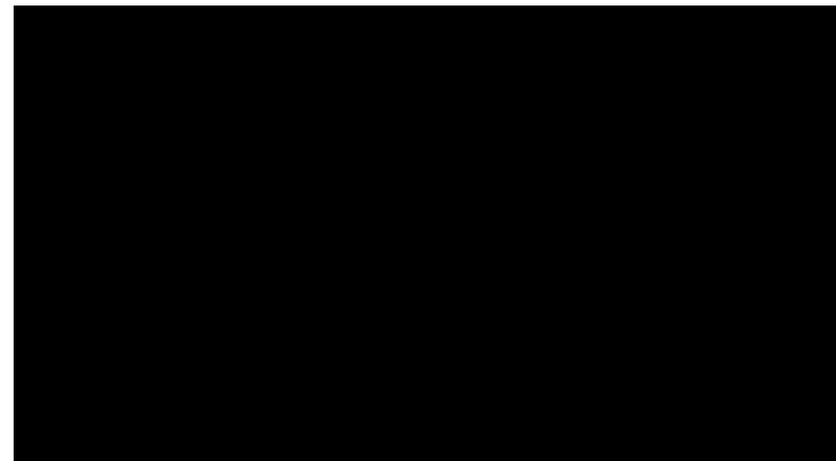
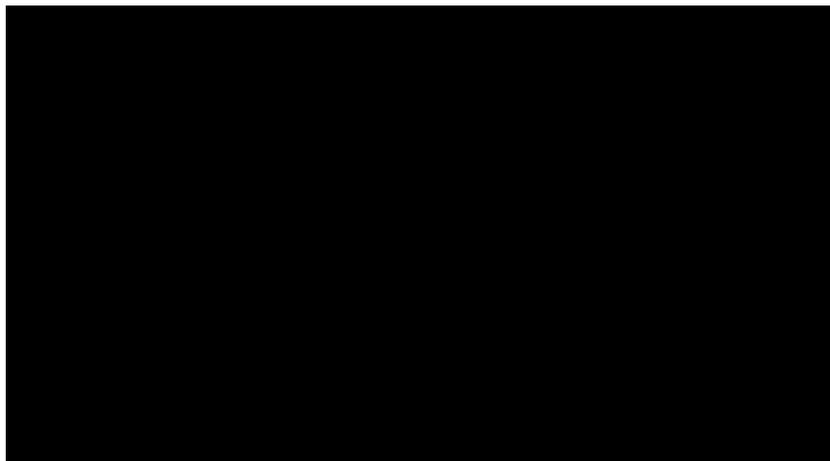
"Direct" radiation damage under the microscope



Nuclear displacement
damage ("knock-on damage")



Electron excitation damage
(radiolysis)



Electron - atomic nucleus
interaction

Electron - valence electron
interaction

Nuclear relocation
→ leads directly to a bond
dissociation

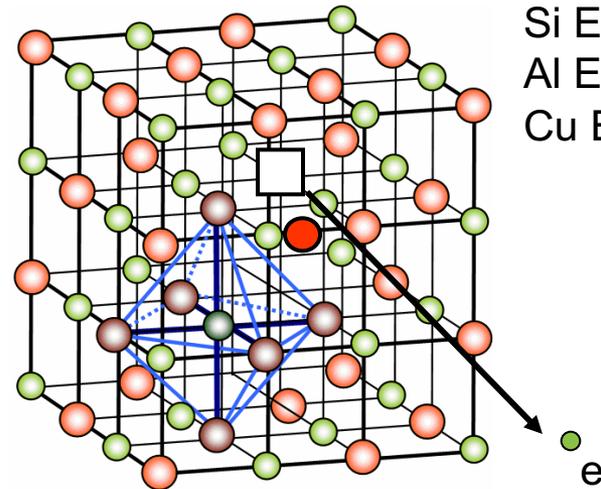
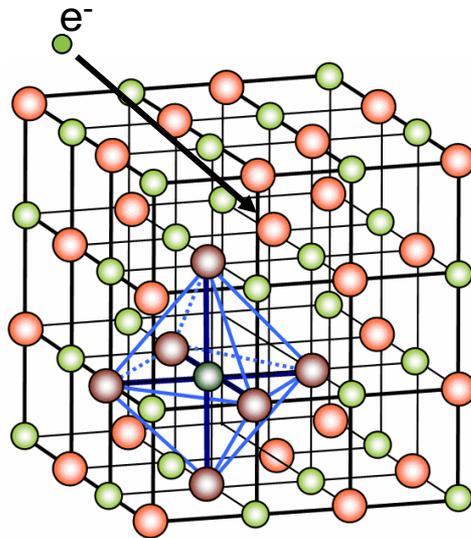
Nuclear relocation
→ Leads to ionization
→ Leads to local sample heating

2.3 Radiation damage

"Direct" radiation damage under the microscope

- Nuclear displacement damage ("knock-on damage")

Nuclear displacement damage



Minimum electron energy
"Threshold energy"

For:

Si $E_0 > 145$ keV

Al $E_0 > 170$ keV

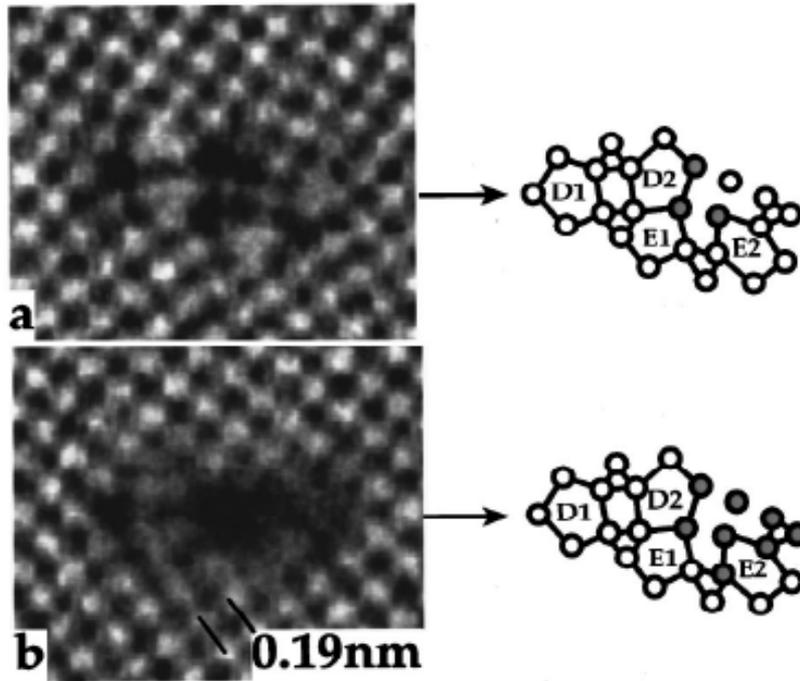
Cu $E_0 > 300$ keV

- Formation of vacancies and interstitial atoms when
Binding energy of the atom $<$ energy transferred during impact
- Formation of extensive defects (stacking faults, cavities) with high void and
Interstitial atom concentrations
→ Limitation of the irradiation time of an object, reduction of electron energy

2.3 Radiation damage

Nuclear displacement damage ("knock-on damage")

Grain boundary in Si, 300 keV electron energy



Electron beam-induced transformation of a nanopillar into a nanotube

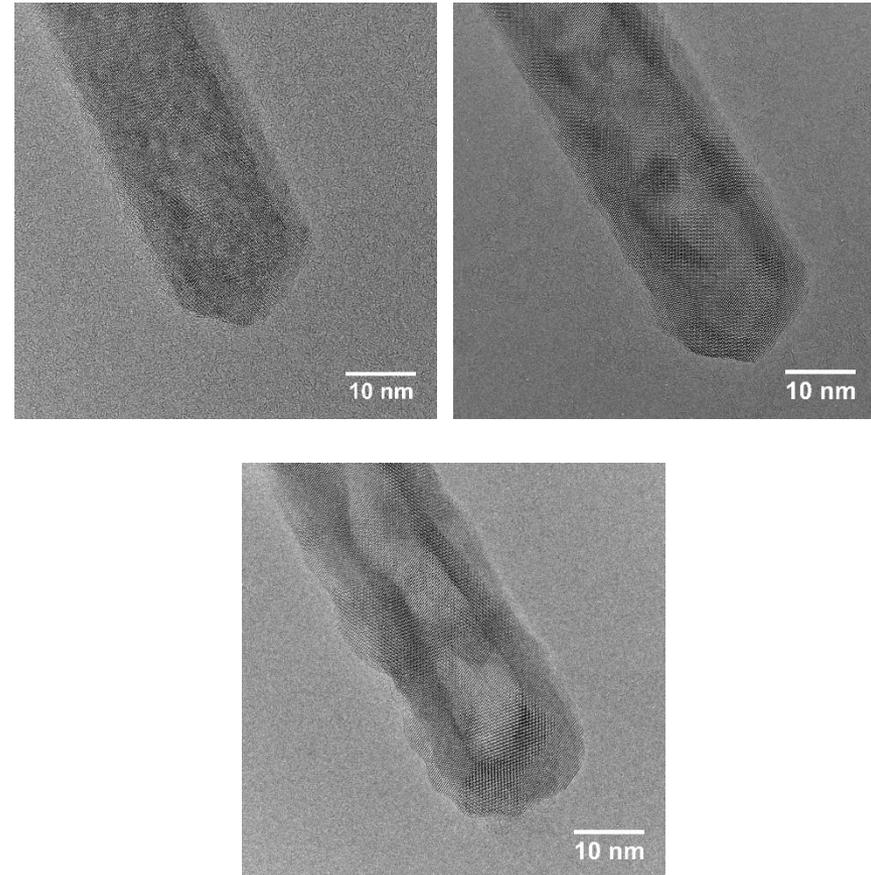


FIG. 1. Z-contrast images and derived structures of the $\Sigma = 25 \{710\} \langle 001 \rangle$ symmetric tilt boundary at two stages of exposure to electron irradiation: (a) a nearly unaffected core with all columns visible but those shaded showing reduced intensity; (b) a partially affected core with several columns appearing darker.

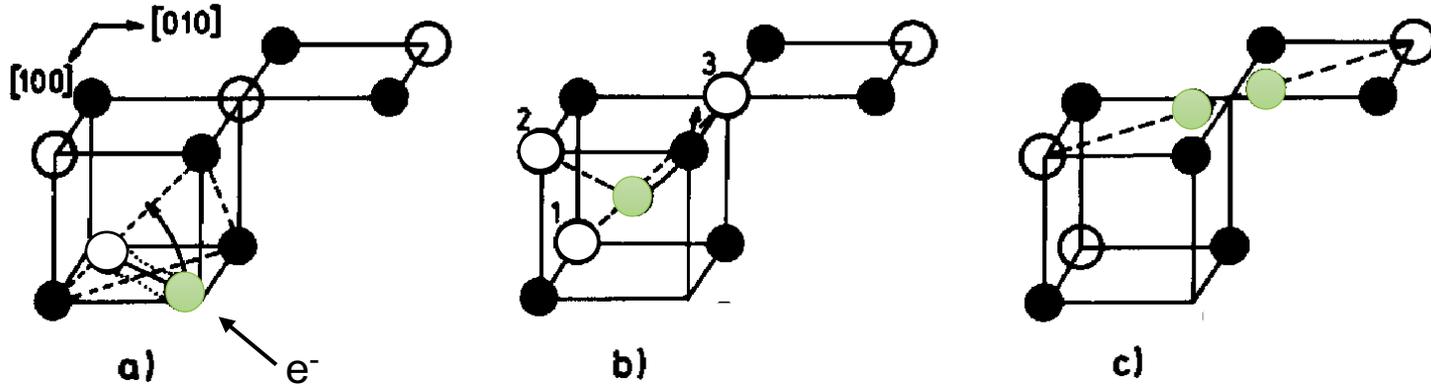
A. Maiti et al, Appl. Phys. Lett. 75, 2380 (1999)

R. Popescu (LEM)

2.3 Radiation damage

Radiolysis in electrically insulating materials

Example NaCl structure:



L. Reimer, Transmission Electron Microscopy, Fig. 11.8



- Structural rearrangement by excitation of electrons in the sample material in higher Energetic or non-binding states
 - *Reduction by cooling the sample in a sample holder cooled with liquid nitrogen*
 - *Increase in electron energy (probability of an electronic excitation process decreases)*
- Radiolysis in electrically conductive samples insignificant
- Radiolysis dominant in ionic crystals, (non-conductive) ceramic oxides, polymers and samples from the life sciences

2.3 Radiation damage

"Indirect" radiation damage

- Contamination
- Heating

Polymerization of hydrocarbon molecules (C H)_{nm}

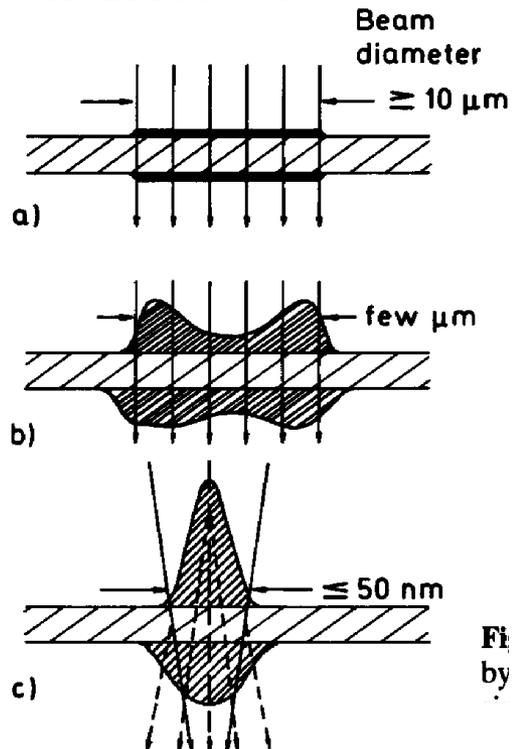
- Residual gas atmosphere (e.g. pump oils, vacuum grease from rubber seals)
- Contamination from sample preparation residues

on the sample surface due to the influence of the electron beam

Remedy:

- Extremely clean work (gloves)
- Cleaning in Ar/O plasma
- Improvement of the vacuum by cold trap to liquid nitrogen temperature (condensation of C H)_{nm}
- Liquid nitrogen cooling holder (reduction of surface diffusion)

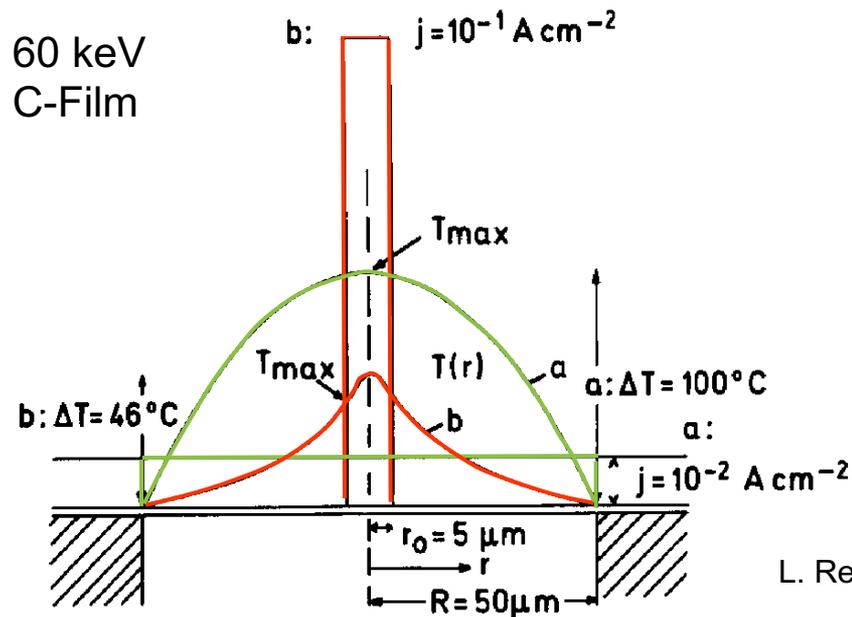
Contamination



L. Reimer, Transmission Electron Microscopy, Fig. 10.10

2.3 Radiation damage

Sample heating



- Hardly any experimental data available
- Thermal conductivity of the sample and thermal coupling to the sample holder crucial
- Melting of small particles and small excretions in the microscope observed without heating
- Calculation:
Dissipated heat by electron beam =
Dissipated heat through heat conduction

L. Reimer, Transmission Electron Microscopy, Fig. 11.2 and Tab. 11.3

Table 11.3. Rise of temperature ΔT in the center of a circular diaphragm ($R = 50 \mu\text{m}$) covered with a supporting film and irradiated with 100 keV electrons.

	Uniform illumination	Small-area illumination
Substance	$R = 50 \mu\text{m}, j = 100 \text{ A m}^{-2}$	$r_0 = 0.5 \mu\text{m}, j = 10^4 \text{ A m}^{-2}$
Formvar	62°C	6°C
Glass (SiO)	27°C	2.5°C
Metal (Cu)	0.3°C	0.03°C

Radius r_0 of the illuminated sample area is decisive for temperature rise

Summary chapter 2

- The structure of a transmission electron microscope (TEM) is comparable to that of a light microscope: "light source", condenser, large-area illumination of the sample, imaging lens system, image plane with camera
- In scanning transmission mode (STEM), illumination is achieved with a focused electron beam that is scanned across the sample. The image is generated by the locally detected electron intensity, which controls the brightness of the corresponding image pixel. An imaging lens system is not required for image generation.
- However, images in TEM and STEM mode are comparable (see Chapter 4), as the interaction of electrons with the sample determines the image.
- Images (real space) and diffraction images (reciprocal space) of the same sample area can be generated by extending the focal length of the intermediate lens.
- Diffraction images provide local crystal structure information and allow the sample to be specifically oriented in relation to the electron beam, e.g. in a 2-beam condition or zone axis orientation.
- In the rear focal plane of the objective lens there are diaphragms with different diameters that determine the imaging mode.
- "Conventional" TEM bright-field or dark-field imaging (imaging with one reflex) is created by selecting a small aperture. A large aperture must be used for high-resolution TEM images so that electrons from at least 2 reflections interfere in the image.

Summary chapter 2

- A homogeneous magnetic field focuses electrons with the exception of electrons that move parallel to the optical axis
- Real electron lenses therefore generate inhomogeneous magnetic fields
- Magnetic and electrostatic **round lenses** for electrons are subject to lens aberrations that depend on the object-side aperture angle a_0 of the beam bundle
- The resolving power of electron-optical systems is limited by lens aberrations and not by the electron wavelength
- The spherical aberration is dominant for large a_0 . The error disk diameter is given by $\frac{1}{2}c_s a_0^3$ (c_s : spherical aberration constant). Modern devices contain a corrector lens system for the spherical aberration.
- Other lens defects include chromatic aberration and astigmatism, although astigmatism can be routinely corrected under the microscope.
- Specimens for TEM must be very thin, as electrons and solids interact strongly. Maximum sample thicknesses depend on the electron energy and material density. Typical maximum thicknesses are 1 mm for "conventional" TEM and a few 10 nm for high-resolution TEM.
- There are different techniques for sample preparation - depending on the material, purely mechanical, chemical, electrochemical or with a focused ion beam for "target preparation". The aim is to prepare the sample material free of artifacts.
- The interaction of the sample with electrons can damage the sample in the microscope. A distinction is made between direct damage (displacement damage and radiolysis) and indirect damage (contamination and heating of the sample)

3. Electron diffraction in the solid state

Contrast through interaction between electrons and sample

————→ Contrast interpretation based on a detailed understanding of the
Interaction between electrons and sample

Approach

Interaction of electrons with a single atom



Interaction with crystalline solids



Kinematic diffraction theory (single scattering)



Dynamic diffraction theory (multiple scattering)

Ch. 5

General validity of the kinematic diffraction theory for
Electron, X-ray, neutron diffraction, ...

3.1 Interaction of electrons with individual atoms

Elastic and inelastic scattering processes

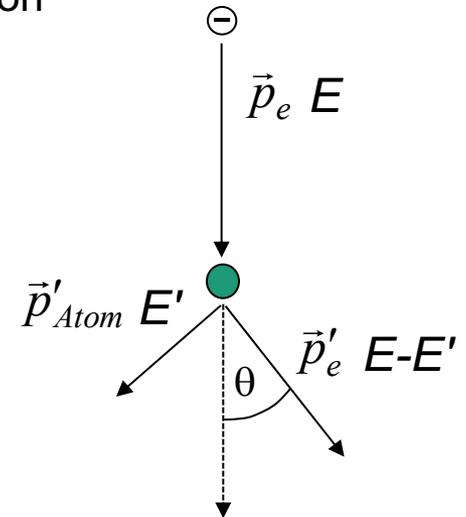
- *Elastic scattering process:*
Prerequisite: conservation of momentum and energy
- *Inelastic scattering process:*
Conservation of momentum and energy **does not apply!**
Generation of excited states or ionization of the target atom (radiolysis)
in the solid state additionally: excitation of phonons, plasmons

Elastic collision of an electron with a single atom: "billiards" physics
Collision of two particles without detailed knowledge of the interaction

Energy transferred to the target atom during elastic impact

$$E' = \frac{2E(E + 2E_R)}{Mc^2} \sin^2 \theta / 2 = \frac{E(E + 1.02)}{496A} \sin^2 \theta / 2$$

- E : kinetic energy of the electron (in 10^6 eV) before the collision
- E_R : Rest energy of the electron $0.511 \cdot 10^6$ eV
- M : Mass of the atom in $A m_p$ (m_p : atomic mass unit)
- c : Speed of light
- θ : Scattering angle
- p : Pulse (e: Electron, At



3.1 Interaction of electrons with individual atoms

Elastic scattering

Energy transferred during impact = energy loss of the primary electron

E	100 keV			1 MeV		
	C ($A = 12$)	Cu ($A = 63.5$)	Au ($A = 197$)	C	Cu	Au
θ						
0.5°	0.5 meV	0.1 meV	0.03 meV	9 meV	1.7 meV	0.54 meV
10°	0.15 eV	29 meV	9 meV	2.7 eV	0.5 eV	0.17 eV
90°	10 eV	1.9 eV	0.6 eV	179 eV	34 eV	11 eV
180°	20 eV	3.8 eV	1.2 eV	359 eV	68 eV	22 eV

L. Reimer, Transmission Electron Microscopy, Table 5.1

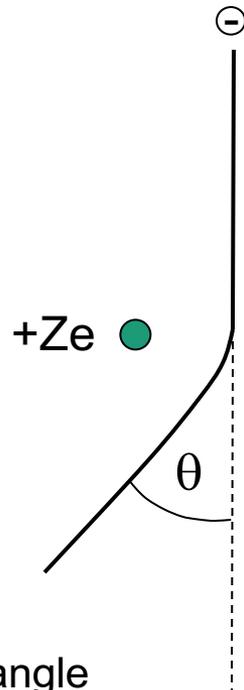
For the small scattering angles that dominate in the TEM, θ applies as a good approximation:
The energy and wavelength of the electron do not change with elastic scattering!

Displacement damage from approx. 100 keV for scattering processes with large scattering angle for typical binding energies of atoms in solids between 5 and 30 eV

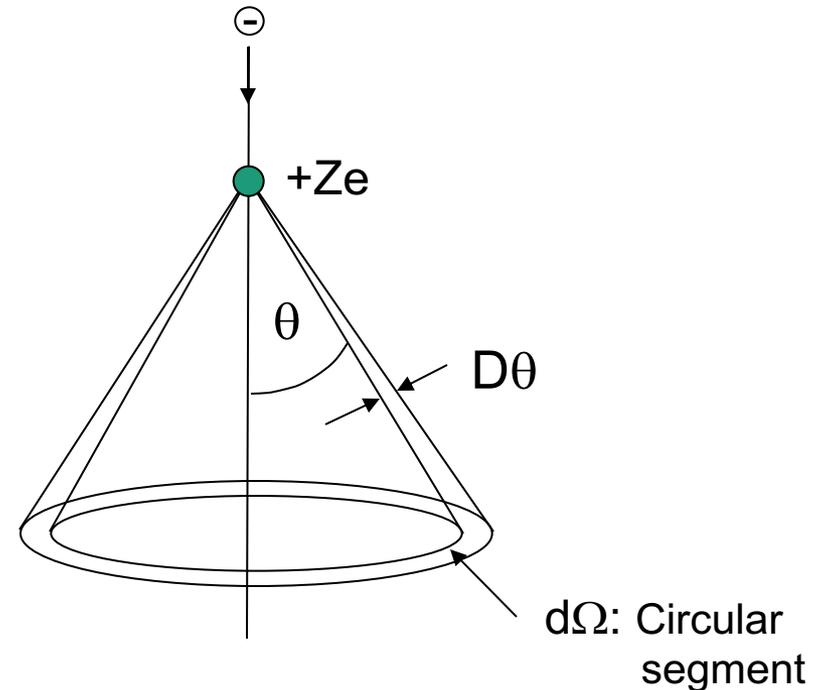
3.1 Interaction of electrons with individual atoms

Description of elastic scattering processes: Particle image

Classical by Rutherford (1911): Coulomb interaction between charged atomic nucleus and electron without taking into account the shielding effect of the electron shell



θ : Scattering angle
 Z: Atomic number of the scattering atom



Differential cross section:
 Probability for scattering process with scattering angle θ $\frac{d\sigma(\theta)}{d\Omega}$

3.1 Interaction of electrons with individual atoms

Differential Rutherford scattering cross section (not relativistic)

Scattering probability:

$$\frac{d\sigma(\theta)}{d\Omega} = \frac{e^4 Z^2}{4(4\pi\epsilon_0)^2 m^2 v^4 \sin^4 \frac{\theta}{2}}$$

Z: Atomic number of the scattering atom

v: electron velocity

m: electron mass

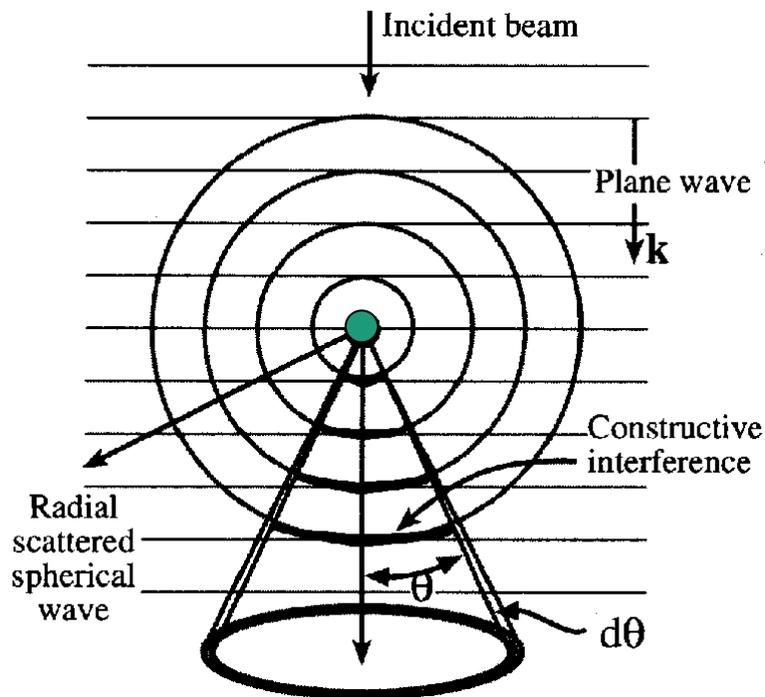
e: Elementary charge

Problem: Differential scattering cross-section diverges for $\theta \rightarrow 0$, as shielding of the atomic nucleus by the electron shell is not taken into account. *(To be solved quantum mechanically, time-independent and relativistic Schrödinger equation)*

Solution of the scattering problem taking into account the shielding by the Electron shell by quantum mechanical calculation: Solution of the time-independent relativistic Schrödinger equation

3.1 Interaction of electrons with individual atoms

Description of elastic scattering processes (*stationary*): Wave pattern



Incident plane electron wave

$$\psi = \psi_0 e^{(2\pi i \vec{k} \vec{r})}$$

Wave scattered on a point charge

$$\psi_s = \psi_0 f(\theta) \frac{e^{(2\pi i k r)}}{r}$$

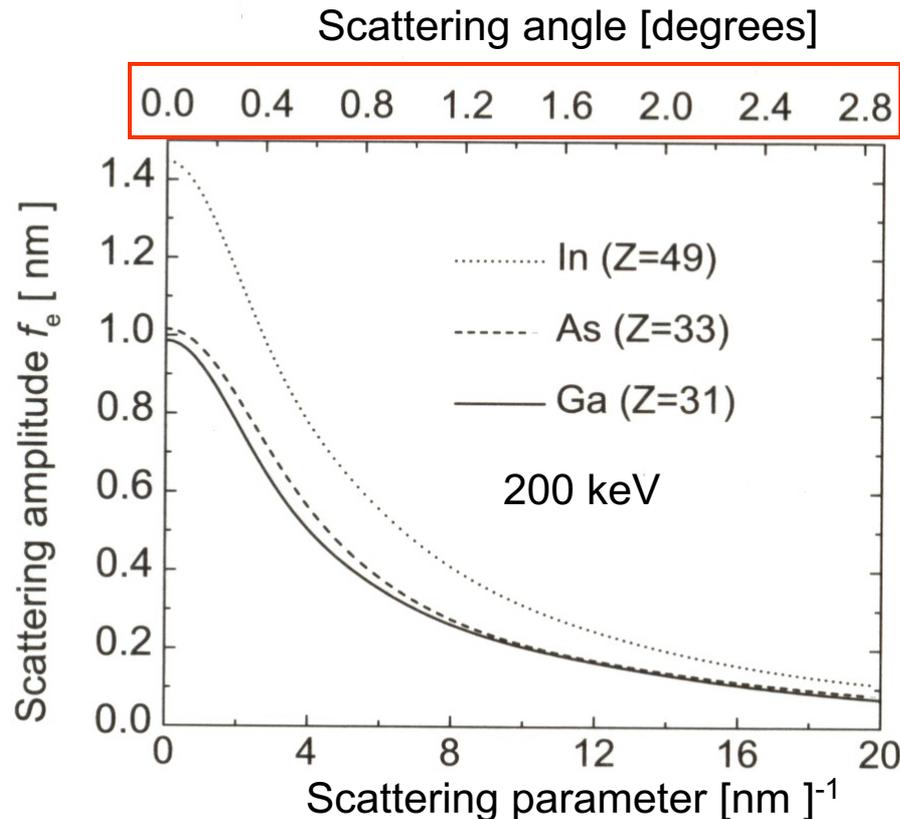
$f(\theta)$: atomic form factor, angular dependence of the Amplitude of the scattered wave

Resulting wave

$$\psi = \psi_0 \left(e^{(2\pi i \vec{k} \vec{r})} + i f(\theta) \frac{e^{(2\pi i k r)}}{r} \right)$$

D.B. Williams, C.B. Carter, Transmission Electron Microscopy, Fig.3.6, p.42

Atomic form factors for Ga, In, As



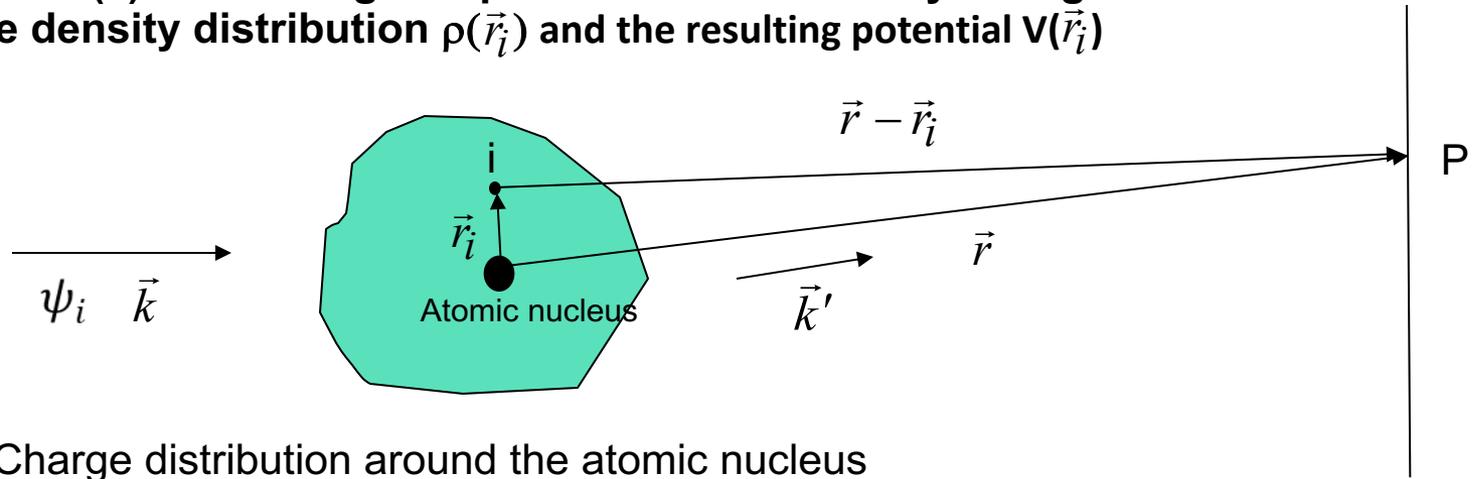
The following applies to $f(\theta)$:

- The amplitude of the scattered spherical wave decreases very quickly as the scattering angle increases
→ **Strong tendency towards forward scattering**
- The amplitude increases with the atomic number Z
- Not shown here, as $f(\theta)$ is only shown for 200 keV: the amplitude decreases with the Electron energy

A. Rosenauer, Transmission Electron Microscopy of Semiconductor Nanostructures", Fig. 2.2

3.1 Interaction of electrons with individual atoms

Calculation of $f(\theta)$: Scattering of a plane electron wave by a single atom with charge density distribution $\rho(\vec{r}_i)$ and the resulting potential $V(\vec{r}_i)$



Blue area: Charge distribution around the atomic nucleus

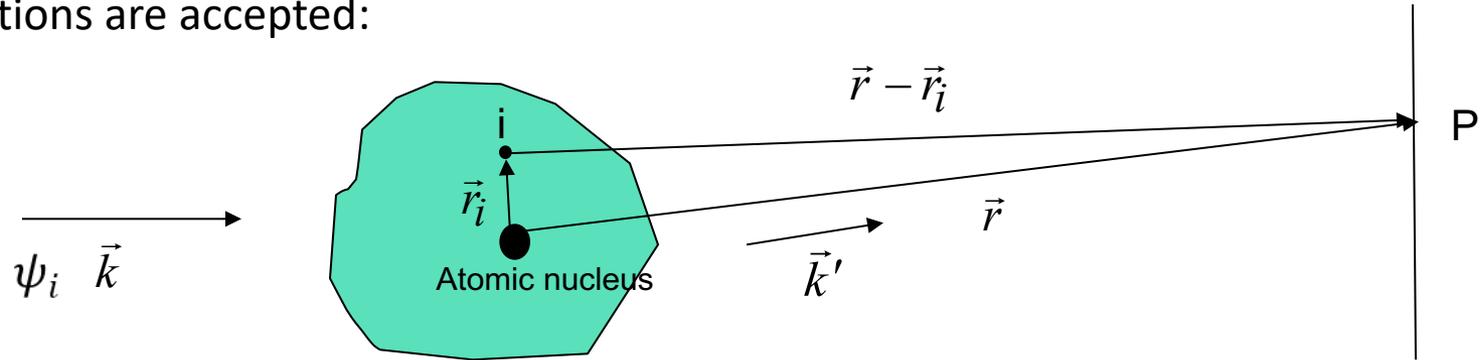
Conversion of the Schrödinger equation into an integral equation using Green's function

$$\psi(\vec{r}) = \psi_i + \psi_s = \psi_i + \frac{2\pi me}{h^2} \int_{Atom} V(\vec{r}_i) \frac{\exp(2\pi i k |\vec{r} - \vec{r}_i|)}{|\vec{r} - \vec{r}_i|} \psi(\vec{r}_i) d^3 \vec{r}_i$$

Incident plane wave ψ_i Scattered wave ψ_s Total wave function on Location \vec{r}_i $\psi(\vec{r}_i)$
 $V(\vec{r}_i)$ Potential on site \vec{r}_i Green's function

3.1 Interaction of electrons with individual atoms

Simplifications are accepted:



1st Born's approximation $V(\vec{r}_i) \ll$ Electron energy

- incident wave ψ_i is not significantly weakened when passing through V
- $\psi(\vec{r}_i) = \psi_i$ and $|\psi_s| \ll |\psi_i|$
- Single scattering, i.e. ψ_s is no longer scattered

Approximation $|\vec{r}|$ and $|\vec{r} - \vec{r}_i| \gg |\vec{r}_i|$

$$\psi_s = \frac{\exp(2\pi i k r)}{r} \frac{8\pi^2 m e}{h^2} \int_{Atom} V(\vec{r}_i) \exp(2\pi i (\vec{k} - \vec{k}') \cdot \vec{r}_i) d^3 \vec{r}_i$$

with $\vec{k} - \vec{k}' = \vec{g}$

$$\psi_s = \frac{\exp(2\pi i k r)}{r} \frac{8\pi^2 m e}{h^2} \int_{Atom} V(\vec{r}_i) \exp(2\pi i \vec{g} \cdot \vec{r}_i) d^3 \vec{r}_i$$

f(θ)

- Scattering potential from integration of the Poisson equation for the charge distribution ρ
- Atomic form factors are dependent on the charge distribution in the atom
- Amplitude of the scattered wave is proportional to the Fourier transform of the scattering potential

3.1 Interaction of electrons with individual atoms

Atomic form factor under

- Consideration of scattering at the atomic nucleus and shielding by the electron shell
- Use of Born's 1st approximation (does not apply to heavy atoms!)
- Consideration of relativistic effects

$$|f(\theta)|^2 = \frac{d\sigma(\theta)}{d\Omega} = \frac{4R^4 Z^2 (1 + E/E_0)^2}{a_H^2} \frac{1}{[1 + (\theta/\theta_o)^2]^2} \quad \theta_o = \frac{\lambda}{2\pi R}$$

Connection between
Particle and wave image

$$R = a_H Z^{-1/3}$$

Z: Atomic number of the scattering atom E: kinetic energy of the electron R: Shielding radius
 E_0 : Rest energy of the electron a_H : Bohr radius

- There are numerous different approaches for calculating differential scattering cross sections
- Calculated atomic form factors for electron scattering on individual atoms e.g. by Doyle and Turner, Acta Cryst. A24, 390 (1968), which, however, do not optimally describe the scattering behavior of atoms in ionic and covalent crystals (error a few %)!
- Charge distributions of atoms in crystals must be known as well as possible.

3.1 Interaction of electrons with individual atoms

Inelastic scattering processes: Generation of characteristic X-rays and bremsstrahlung

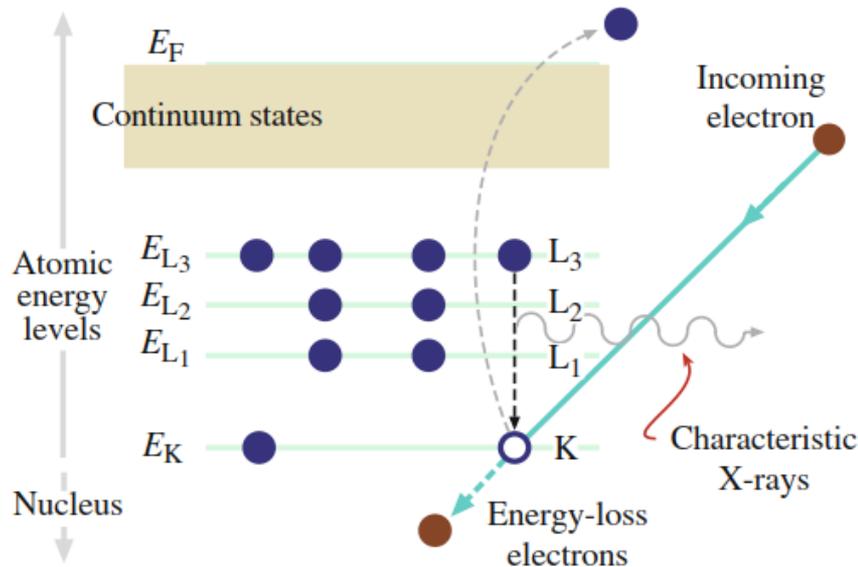


FIGURE 4.2. The ionization process. An inner (K) shell electron is ejected from the atom by a high-energy electron. When the hole in the K shell is filled by an electron from the L shell, characteristic (K_α) X-ray emission occurs. The beam electron loses energy but continues on through the specimen.

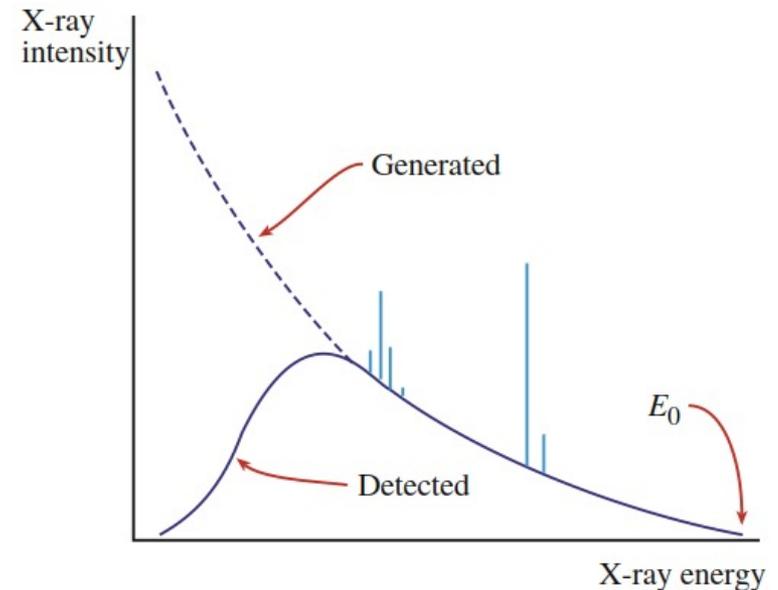


FIGURE 4.6. The bremsstrahlung X-ray intensity as a function of energy. The generated intensity increases rapidly with decreasing X-ray energy but at energies $< \sim 2$ keV the bremsstrahlung is absorbed in the specimen and in any detector being used so the observed intensity in the detected spectrum drops rapidly to zero. E_0 is the energy of the electrons that cause the X-ray emission. Two families of characteristic lines are also shown superimposed on the bremsstrahlung.

D.B. Williams, C.B. Carter, Transmission Electron Microscopy, Fig.4.2 and Fig.4.6

Scattering on collective excitations of the solid: Phonon scattering

Generation of a phonon

- small energy change of the electron in the magnitude of $k_B T \approx 25 \text{ meV}$ at 20°C
 - Heating of the sample
- Large scattering angles (order of magnitude 10 degrees)
 - Darkening of the image through suppressing electrons by the lens aperture

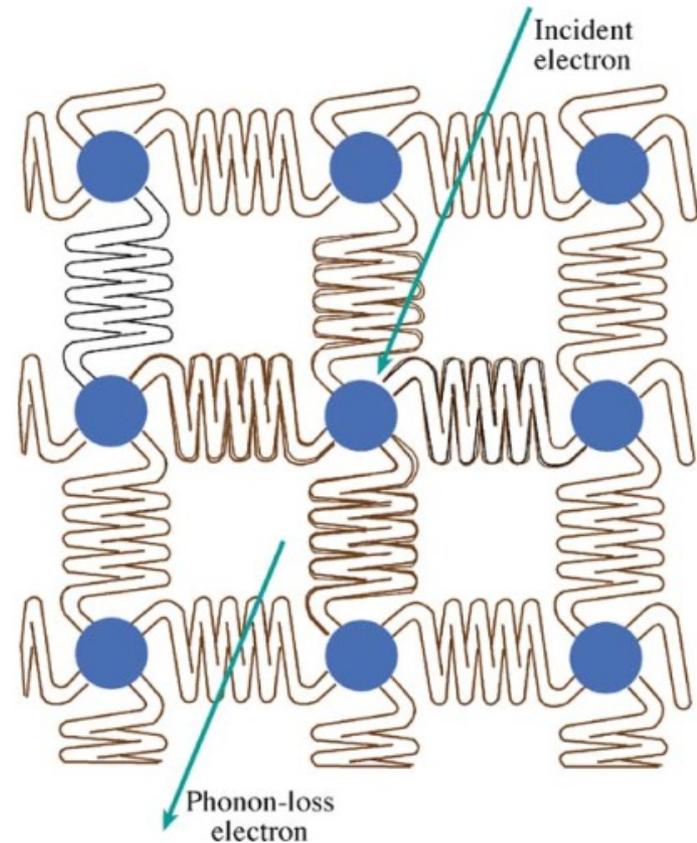
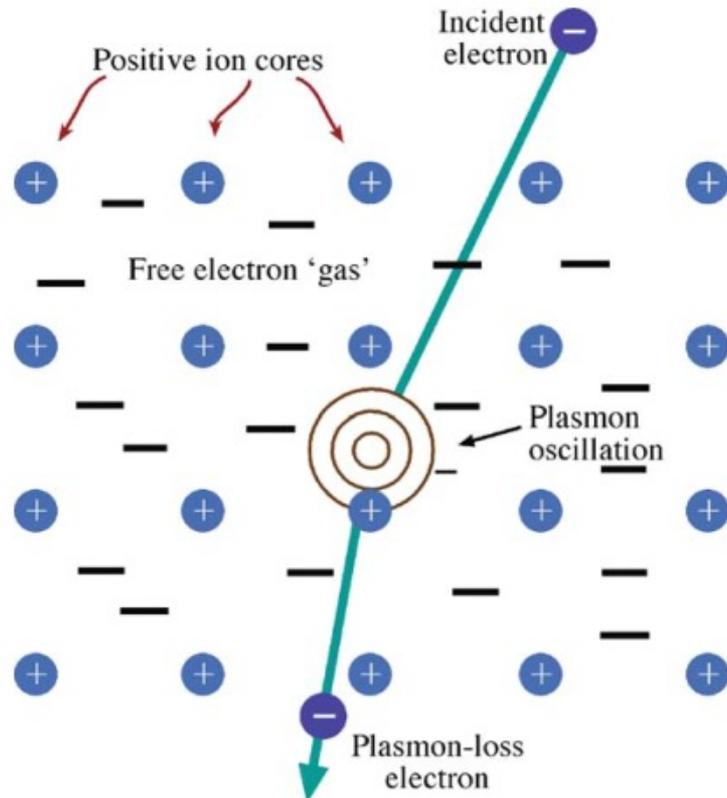


FIGURE 4.10. An illustration of the crystal lattice as a group of atoms linked elastically by springs. The bonds vibrate when struck by a high-energy electron creating lattice oscillations or phonons and these vibrations are equivalent to heating the specimen.

D.B. Williams, C.B. Carter, Transmission Electron Microscopy, Fig. 4.10

3.1 Interaction of electrons with individual atoms

Scattering on collective excitations of the solid: Plasmon scattering



- Oscillations of the free electron gas in metals and semiconductors, vibrations of valence electrons in insulators
- Energy losses of the primary electrons between a few eV and 40 eV

FIGURE 4.9. Schematic diagram of a high-energy beam electron exciting a plasmon oscillation in a free-electron gas that permeates the ion cores in a metal.

D.B. Williams, C.B. Carter, Transmission Electron Microscopy, Fig.4.9

3.2 Kinematic Diffraction Theory

Elastic scattering of electrons on a group of atoms

Prerequisite for kinematic description: single scattering

Scattering by two atoms B, C

Scattered wave at a distance $R \gg r$

Phase shift between the two scattered waves $\Delta\varphi$

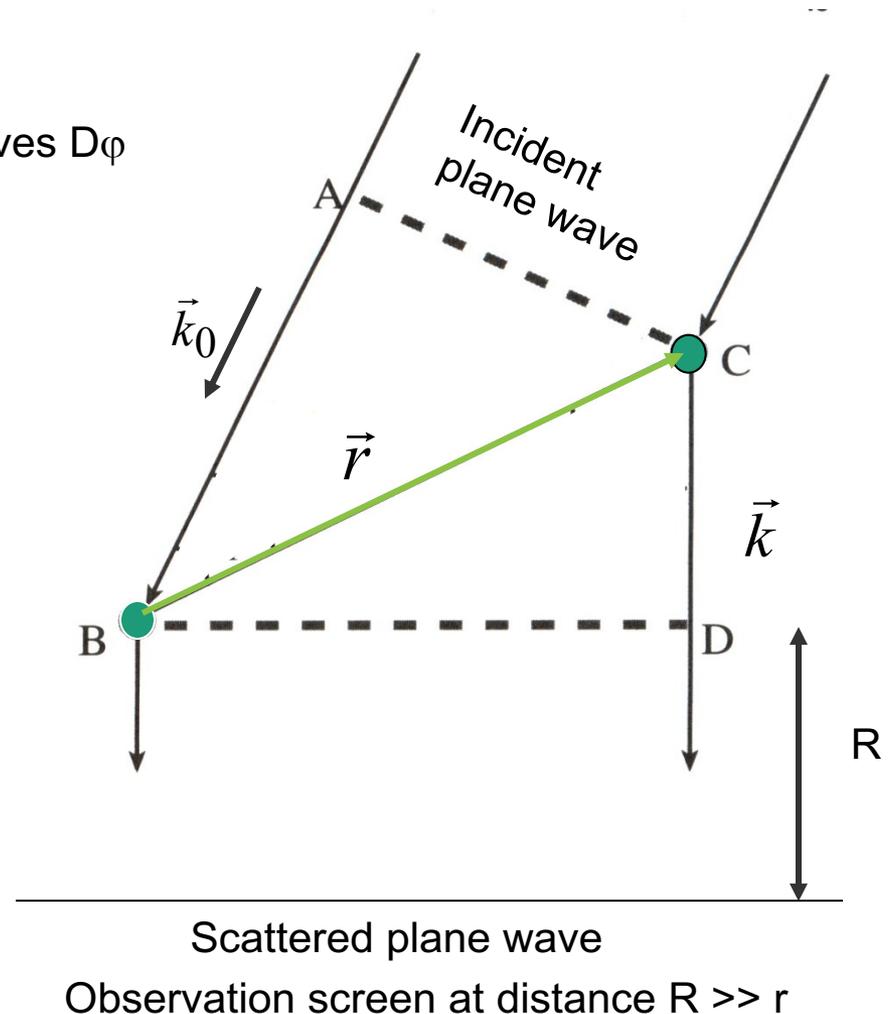
with $|\vec{k}| = |\vec{k}_0| = 1/\lambda$ for elastic scattering

$$\Delta\varphi = 2\pi \frac{\Delta l}{\lambda}$$

$$\Delta l = AB - CD$$

$$\Delta\varphi = 2\pi \vec{r} \cdot (\vec{k} - \vec{k}_0)$$

Δl : path difference



3.2 Kinematic Diffraction Theory

Scattered wave at a distance R ($R \gg r_i$) and in the direction of \vec{k}

$$\psi_s = \psi_0 \frac{\exp(2\pi i kR)}{R} \left\{ f_B(\theta) + f_C(\theta) \exp(2\pi i [\vec{k} - \vec{k}_o] \vec{r}) \right\}$$

Scattering on M arbitrarily arranged atoms

$$\psi_s = \psi_0 \underbrace{\frac{\exp(2\pi i kR)}{R}}_{\text{Is described below neglected}} \underbrace{\sum_{i=1}^M f_i(\theta) \exp(2\pi i [\vec{k} - \vec{k}_o] \vec{r}_i)}_{\text{Scattering amplitude } F_{(\theta)}}$$

\vec{r}_i : Atom positions in relation to the atom at the origin

Intensity of the scattered wave on the screen: $I \propto |F(\theta)|^2$

3.2 Kinematic Diffraction Theory

Scattering at a crystal lattice (ordered arrangement of atoms)

Scattering amplitude (general)

$$F(\theta) = \sum_i f_i(\theta) \exp(2\pi i [\vec{k} - \vec{k}_0] \cdot \vec{r}_i)$$

For crystals: $\vec{g} = \vec{k} - \vec{k}_0$

$$F(\theta) = \sum_i f_i(\theta) \exp(2\pi i \vec{g} \cdot \vec{r}_i)$$

Condition for constructive interference (maximum scattered intensity) :

$$\vec{g} \cdot \vec{r}_i = \text{integer}$$

Suitable definition of \vec{g} for maximum scattering intensity

3.2 Kinematic Diffraction Theory

Relationship between real and reciprocal lattice

lattice point in local space characterized by

$$\vec{r} = u\vec{a}_1 + v\vec{a}_2 + w\vec{a}_3$$

u,v,w

∈ integers

lattice point in the reciprocal lattice characterized by

$$\vec{g} = h\vec{a}_1^* + k\vec{a}_2^* + l\vec{a}_3^*$$

h,k,l

\vec{a}_i : basis vectors of the lattice in the spatial domain

\vec{a}_i^* : basis vectors of the lattice in reciprocal space

Construction rule for base vectors of the reciprocal lattice

$$\vec{a}_i \cdot \vec{a}_j^* = \delta_{ij} \quad \text{with} \quad \begin{aligned} \delta_{ij} &= 0 \text{ for } i \neq j \\ \delta_{ij} &= 1 \text{ for } i = j \end{aligned}$$

So that $\vec{g}\vec{r} = uh\vec{a}_1\vec{a}_1^* + uk\vec{a}_1\vec{a}_2^* + \dots\dots wl\vec{a}_3\vec{a}_3^* = \text{integer}$

3.2 Kinematic Diffraction Theory

Relationship between real and reciprocal lattice

Base vectors of the reciprocal lattice

$$\vec{a}_1^* = \frac{\vec{a}_2 \times \vec{a}_3}{V_e} \quad \vec{a}_2^* = \frac{\vec{a}_1 \times \vec{a}_3}{V_e} \quad \vec{a}_3^* = \frac{\vec{a}_1 \times \vec{a}_2}{V_e}$$

Volume of the unit cell: $V_e = \vec{a}_i (\vec{a}_j \times \vec{a}_k)$

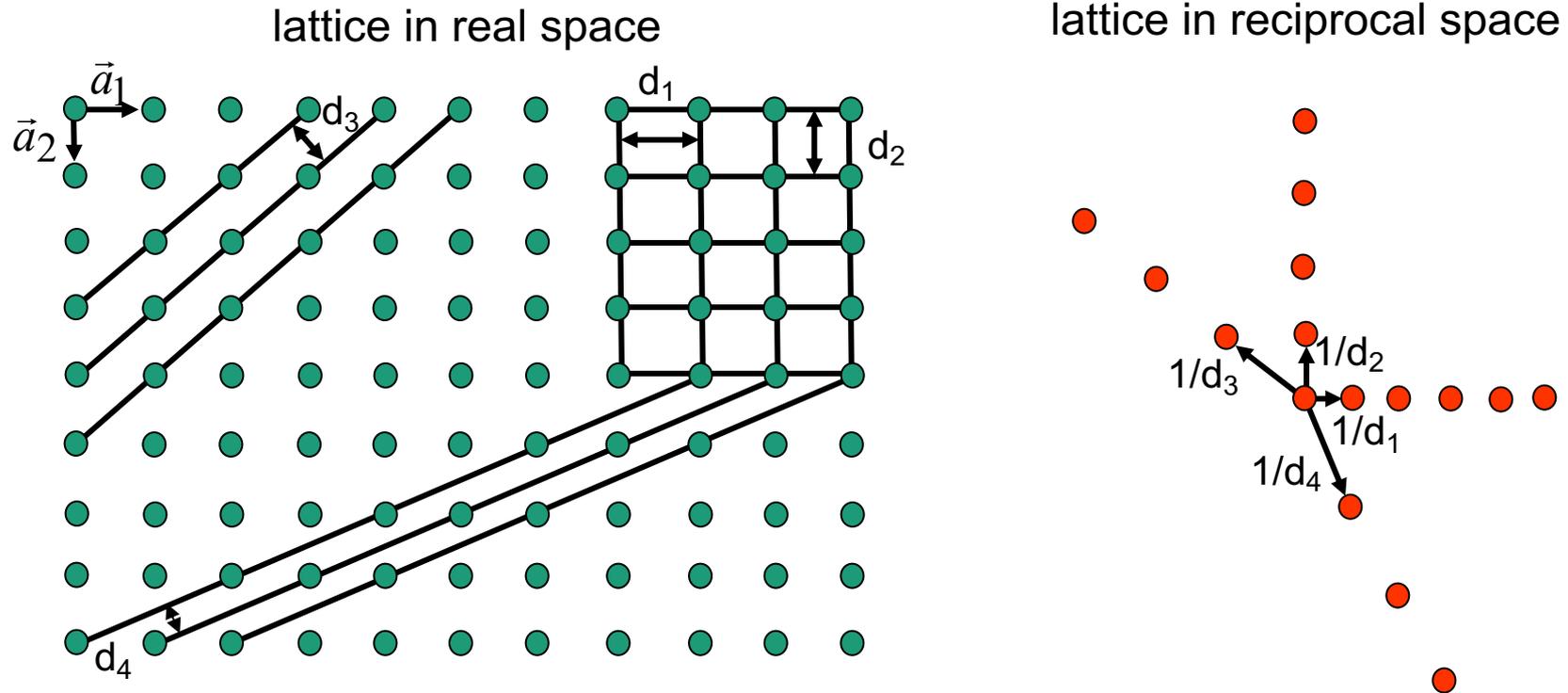
Definition for reciprocal lattice vectors also applies to lattice with non-orthogonal basis vectors in real space

$$\vec{g} = h\vec{a}_1^* + k\vec{a}_2^* + l\vec{a}_3^*$$

h, k, l: Miller's indices for the characterization of planes (sets) in the reciprocal lattice

3.2 Kinematic Diffraction Theory

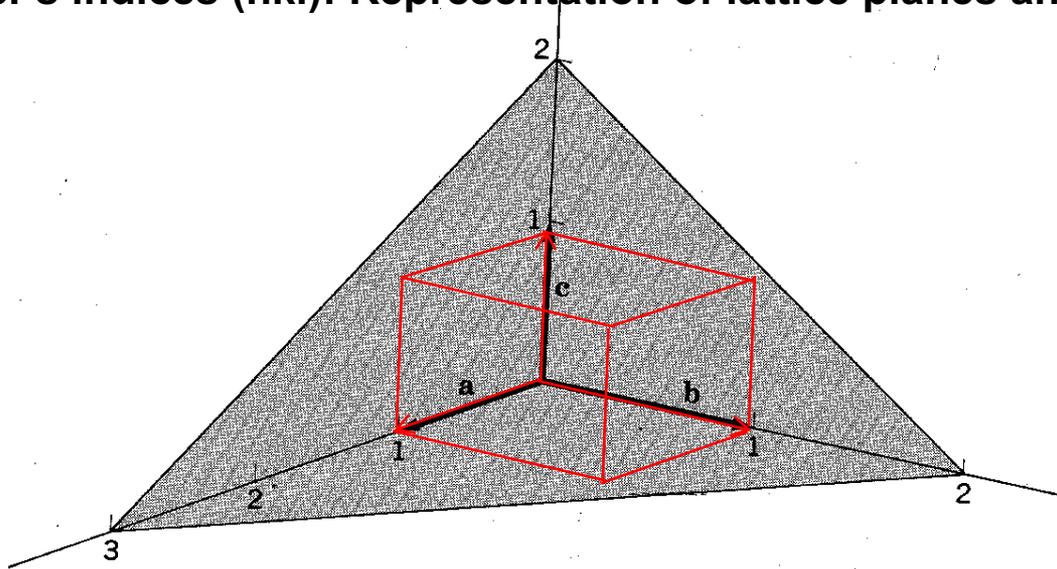
Relationship between lattice in real space and reciprocal lattice (2-dimensional)



Each lattice plane (set) in real space has a point in the reciprocal lattice

3.2 Kinematic Diffraction Theory

Miller's indices (hkl): Representation of lattice planes and their distances



Points of intersection of the plane with the axes: $3a$, $2b$, $2c$
 reciprocals $1/3$, $1/2$, $1/2$

Miller indices: smallest integers that are in the same ratio to each other (2 3 3)

lattice plane(s) characterized by reciprocal lattice vector

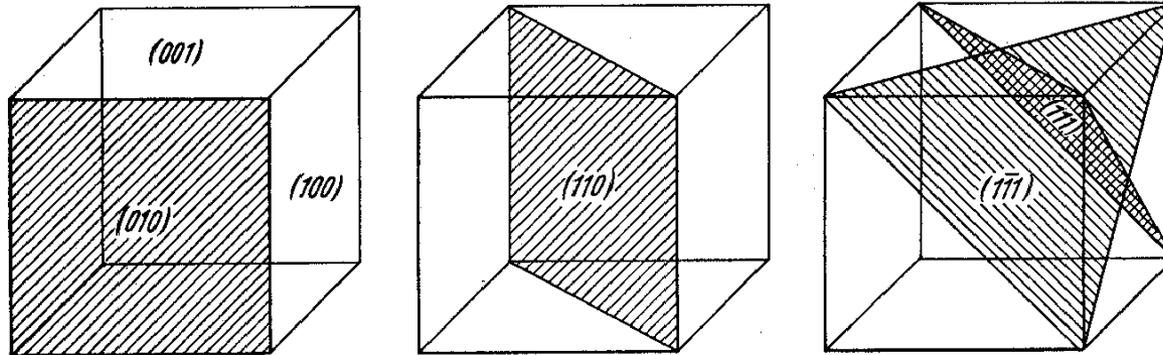
$$\vec{g} = 2\vec{a}_1^* + 3\vec{a}_2^* + 3\vec{a}_3^*$$

With the length

$$|\vec{g}_{hkl}| = \sqrt{(ha_1^*)^2 + (ka_2^*)^2 + (la_3^*)^2} = \frac{1}{d_{hkl}}$$

3.2 Kinematic Diffraction Theory

Miller indices: Representation of lattice planes



Presentation conventions:

(hkl) : certain lattice plane(s)

$\{hkl\}$: Types of plane sets with the same symmetry properties

e.g. in cubic lattices (100) , (010) , (001) , (100) , ...

$[hkl]$: certain direction

$\langle hkl \rangle$: Types of directions with the same properties

In cubic crystals the following applies: $[hkl] \perp (hkl)$

3.2 Kinematic Diffraction Theory

Miller indices: Representation of planes and plane distances

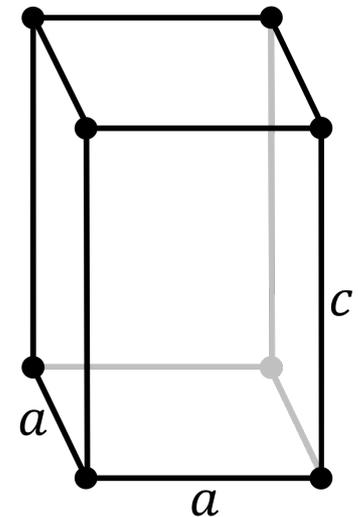
The following relation holds for **cubic** lattices: $d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$

with lattice parameter a

because of $|\vec{a}_1^*| = |\vec{a}_2^*| = |\vec{a}_3^*| = \frac{1}{a}$

In **tetragonal** lattices with valid: $|\vec{a}_1| = |\vec{a}_2| = a$ und $|\vec{a}_3| = c$

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



3.2 Kinematic Diffraction Theory

Lattice plane spacing can be calculated for all 7 crystal systems on the basis of Miller's indices (hkl)

Cubic:

$$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2}$$

Tetragonal:

$$\frac{1}{d^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2}$$

Hexagonal:

$$\frac{1}{d^2} = \frac{4}{3} \left(\frac{h^2 + hk + k^2}{a^2} \right) + \frac{l^2}{c^2}$$

Rhombohedral:

$$\frac{1}{d^2} = \frac{(h^2 + k^2 + l^2) \sin^2 \alpha + 2(hk + kl + hl)(\cos^2 \alpha - \cos \alpha)}{a^2(1 - 3 \cos^2 \alpha + 2 \cos^3 \alpha)}$$

Orthorhombic:

$$\frac{1}{d^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$$

Monoclinic:

$$\frac{1}{d^2} = \frac{1}{\sin^2 \beta} \left(\frac{h^2}{a^2} + \frac{k^2 \sin^2 \beta}{b^2} + \frac{l^2}{c^2} - \frac{2hl \cos \beta}{ac} \right)$$

$$S_{11} = b^2 c^2 \sin^2 \alpha$$

$$S_{22} = a^2 c^2 \sin^2 \beta$$

$$S_{33} = a^2 b^2 \sin^2 \gamma$$

Triclinic:

$$\frac{1}{d^2} = \frac{1}{V^2} \left(S_{11} h^2 + S_{22} k^2 + S_{33} l^2 + 2S_{12} hk + 2S_{23} kl + 2S_{13} hl \right) \text{ where}$$

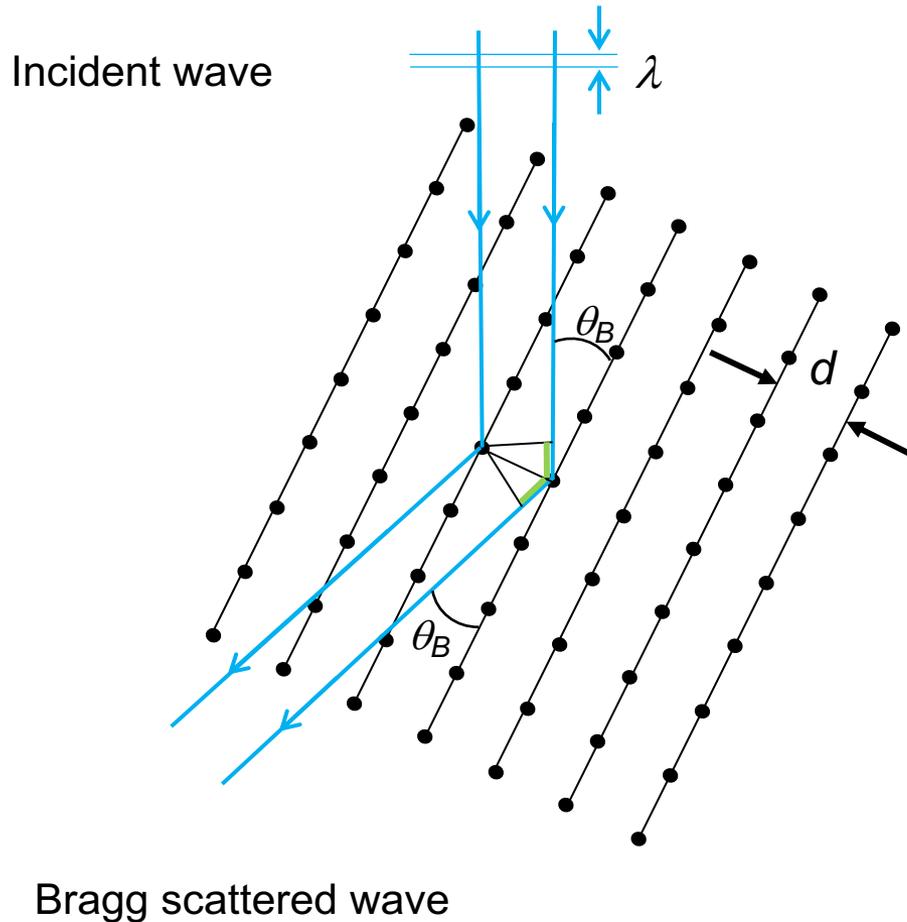
$$S_{12} = abc^2 (\cos \alpha \cos \beta - \cos \gamma)$$

$$S_{23} = a^2 bc (\cos \beta \cos \gamma - \cos \alpha)$$

$$S_{13} = ab^2 c (\cos \gamma \cos \alpha - \cos \beta)$$

3.2 Kinematic Diffraction Theory

Bragg condition: alternative condition for maximum scattering intensity



Bragg condition for constructive interference (maximum scatter intensity)

$$2d \sin \theta_B = n\lambda$$



Bragg reflex in the diffraction image

d : lattice spacing

λ : Electron wavelength

θ_B : Bragg angle

3.2 Kinematic Diffraction Theory

Ewald construction

Bragg condition

$$2d \sin \theta_B = n\lambda$$

and Laue condition

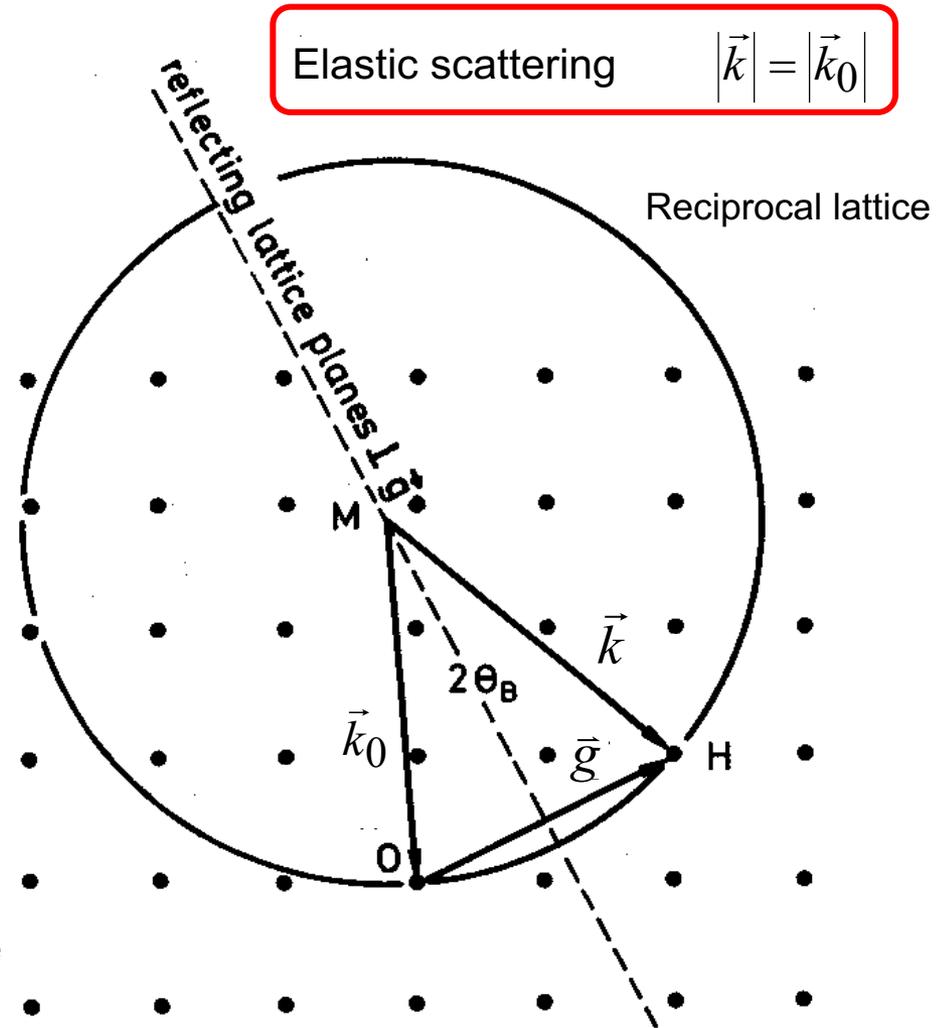
$$\vec{g} = \vec{k} - \vec{k}_0$$

are equivalent

For reciprocal lattice points of planes with (hkl), which are cut by the Ewald Kugel, the Bragg condition is fulfilled



Determination of all directions with maximum scattering intensity, which belong to a specific angle of incidence



L. Reimer; Transmission Electron Microscopy, Fig.7.8

3.2 Kinematic Diffraction Theory

Summary of the properties of the reciprocal lattice:

Definition of reciprocal lattice vectors \vec{g}_{hkl} with the condition of constructive interference

$$\vec{g}_{hkl} = \vec{k} - \vec{k}_0 \quad \text{Laue equation with } \vec{g}_{hkl} \text{ perpendicular to "reflective" lattice plane set (hkl)}$$

$$|\vec{g}_{hkl}| = \frac{n}{d_{hkl}}$$

$$2d \sin \theta_B = n \lambda \quad \text{Bragg condition equivalent to Laue equation}$$

Constructive interference is independent of the arrangement of the atoms on the lattice plane