



TU Clausthal

# Summer School: Methods in Surface Science 2025 (MSS25)

# Summer School: Methods in Surface Science 2025 (MSS25)

	Sun	Mon	Tue	Wed	Thu	Fri
09:00		Lecture: Electron Diffraction and Electron Microscopy	Lecture: Secondary- Ion Mass Spectrometr y (SIMS)	Excursion	Lab Courses	
12:00		Lunch	Lunch		Lunch	Lunch
13:30		Lecture: Electron Spectroscopy	Lab Courses		Lab Courses	Final Presentations
16:30						
19:00	Reception Get-Together					Farewell Evening

3 groups à 4 persons:

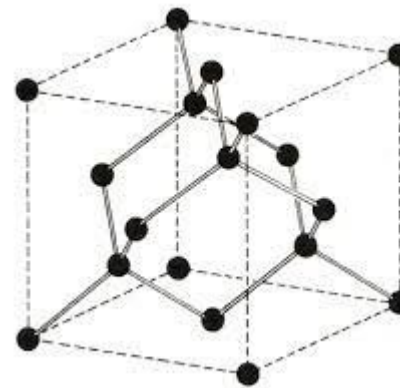
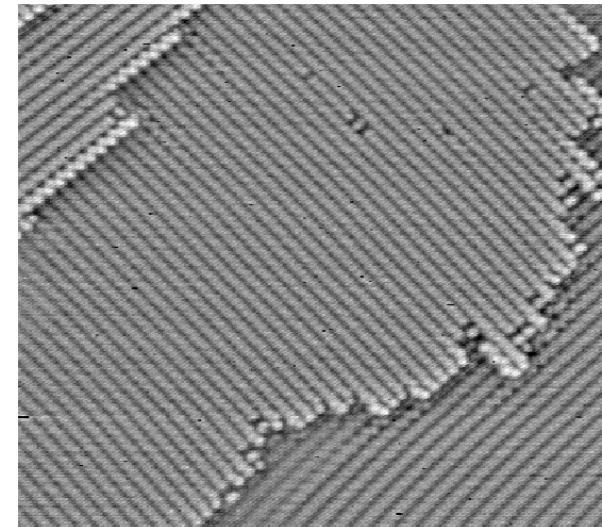
- 1 master student student from Clausthal
- max. 1 master student from Ljubljana
- 2-3 PhD students

Each group prepares a 20 min talk about one of the three experiments (drawn by lot).

## 0. Introduction – Demarcation from the extended solid

- Surface of a crystalline solid:
  - Region where the geometric and electronic structure differs noticeably from that of the extended solid
  - Usually only few atomic layers thick
  - New physical properties that differ fundamentally from those of the solid state volume

Scanning tunneling microscope (STM) image of a Si(100) surface

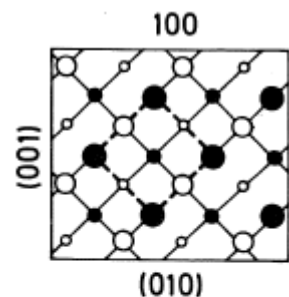


Crystal structure of silicon (diamond structure)

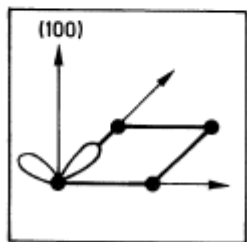
Ibach, Lüth: Solid State Physics

## 0.1 Examples

- Non-saturated (dangling) bonds of a semiconductor surface

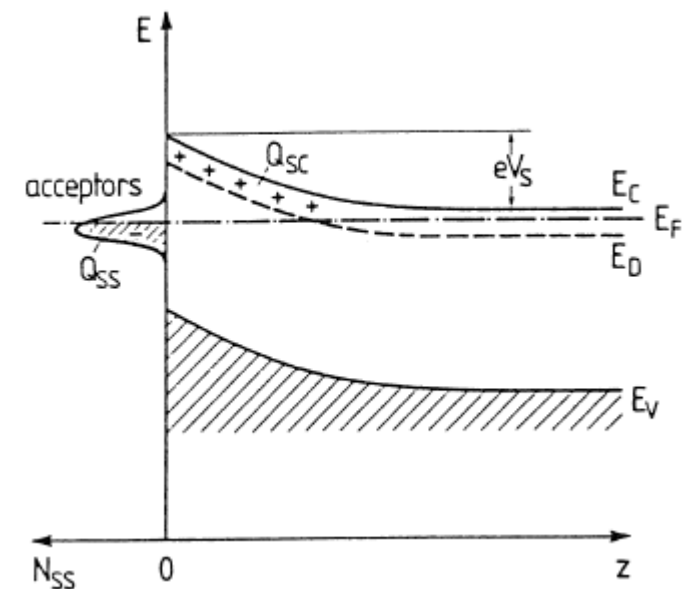


(100) surface of a semiconductor with Zincblende structure. Formation of „dangling bonds“



Reduction of energy by rearrangement of surface atoms  
→ *surface reconstruction*

Lüth: Surfaces, Interfaces and Thin Films

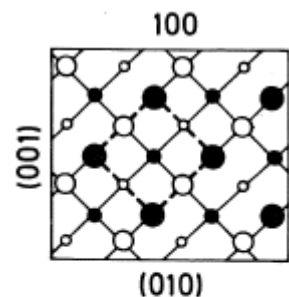


Bandstructure of a n-doped semiconductor with acceptor states at the surface

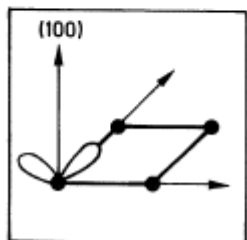
**Metallic behaviour is possible at the semiconductor surface!**

## 0.1 Examples

- Non-saturated (dangling) semiconductor surface

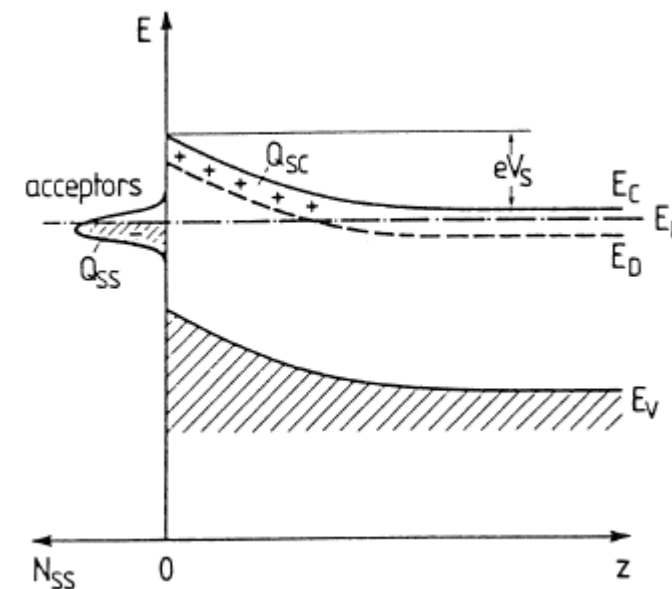


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Reduction of energy by rearrangement of surface atoms  
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Lüth: Surfaces, Interfaces and Thin Films

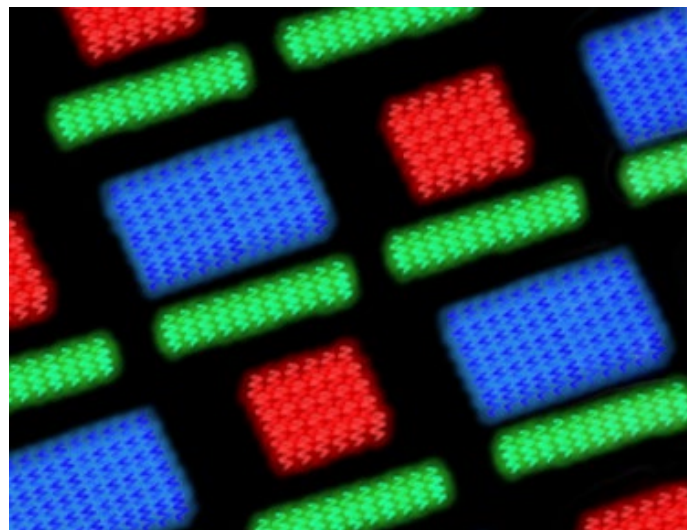
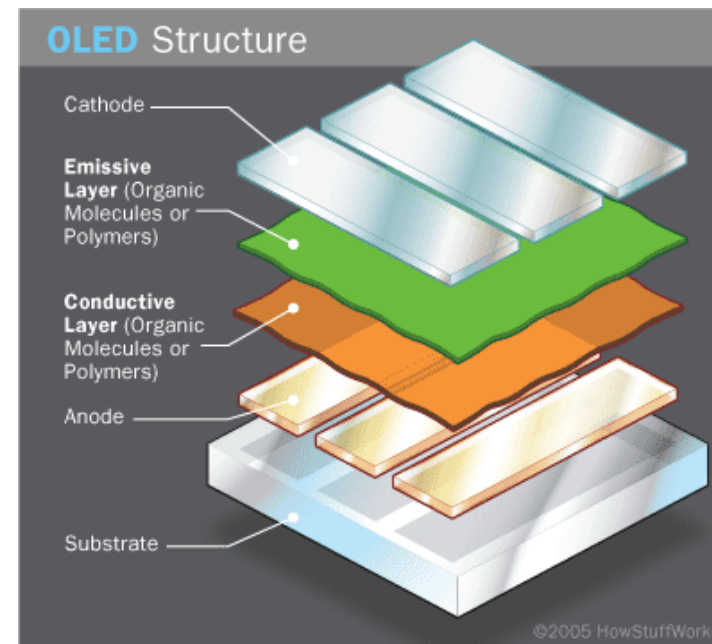
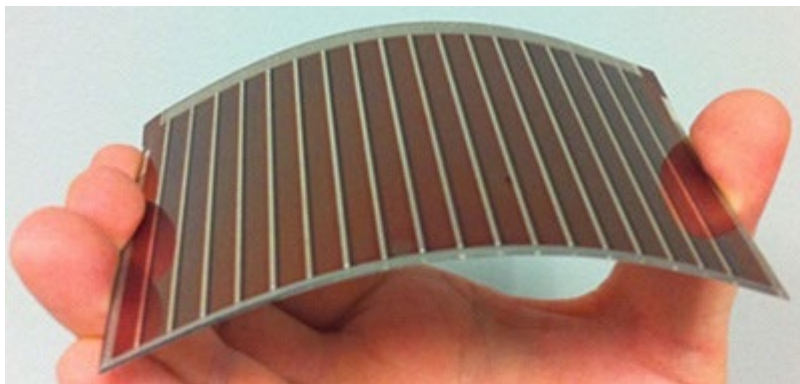


Bandstructure of a n-doped semiconductor with acceptor states at the surface

**Metallic behaviour is possible at the semiconductor surface!**

## 0.1 Examples

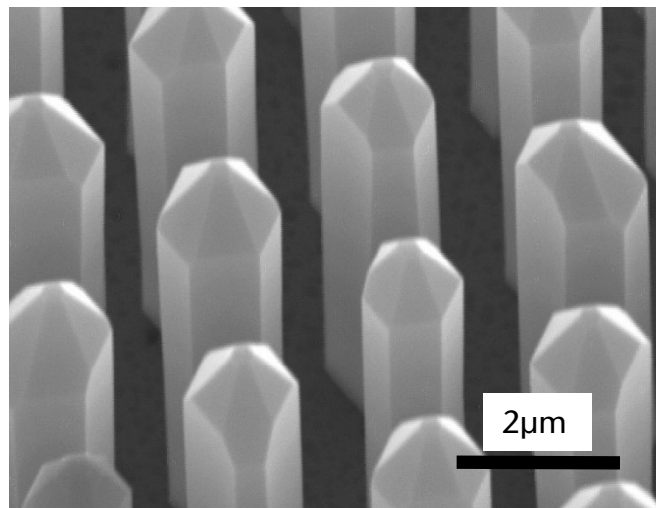
- Interfaces of organic semiconductors for light conversion



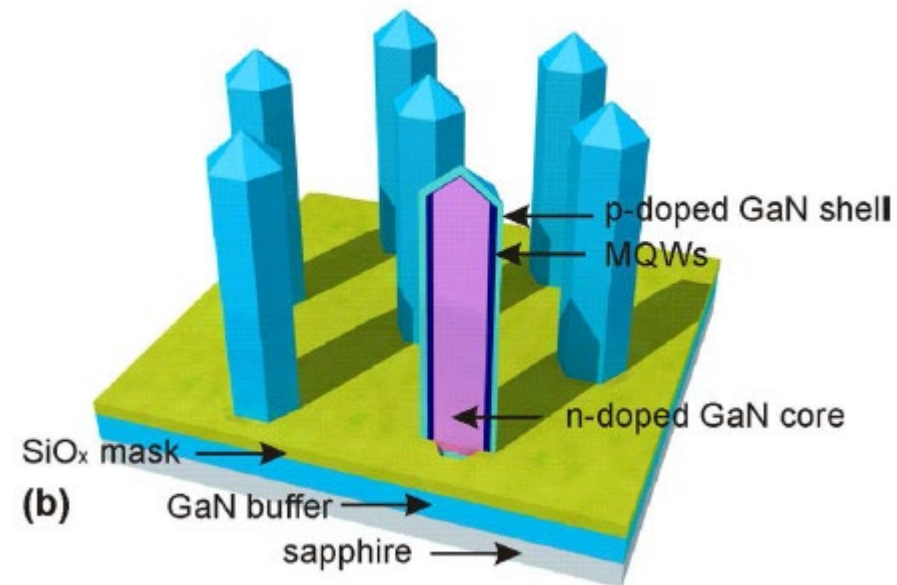


## 0.1 Examples

- GaN nanorods (for LED arrays, sensors, ....)

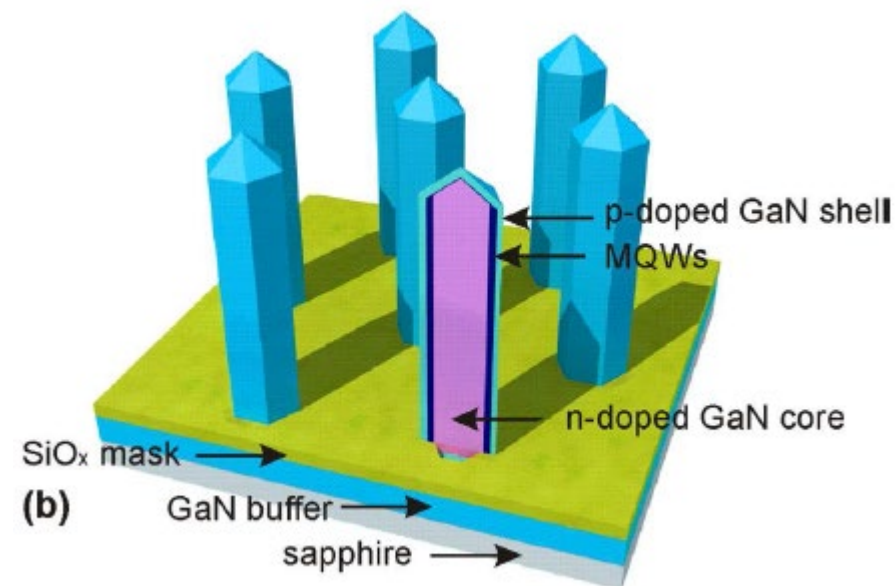
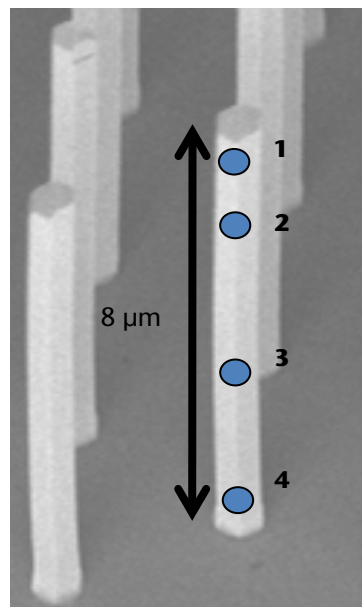
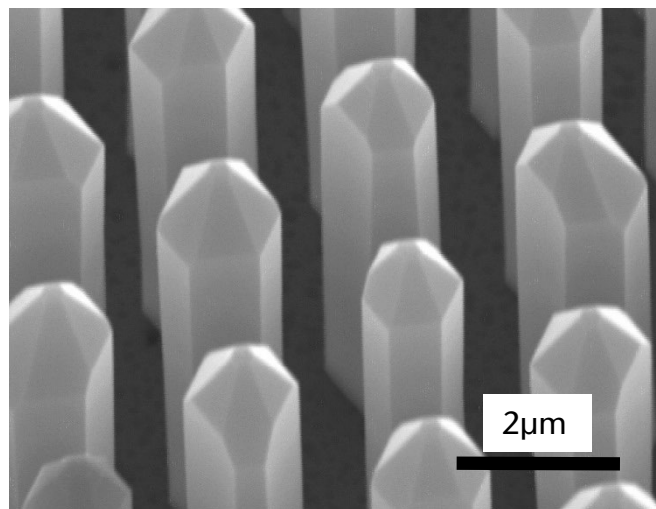


Scanning electron microscopy (SEM)



## 0.1 Examples

- GaN nanorods (for LED arrays, sensors, ....)

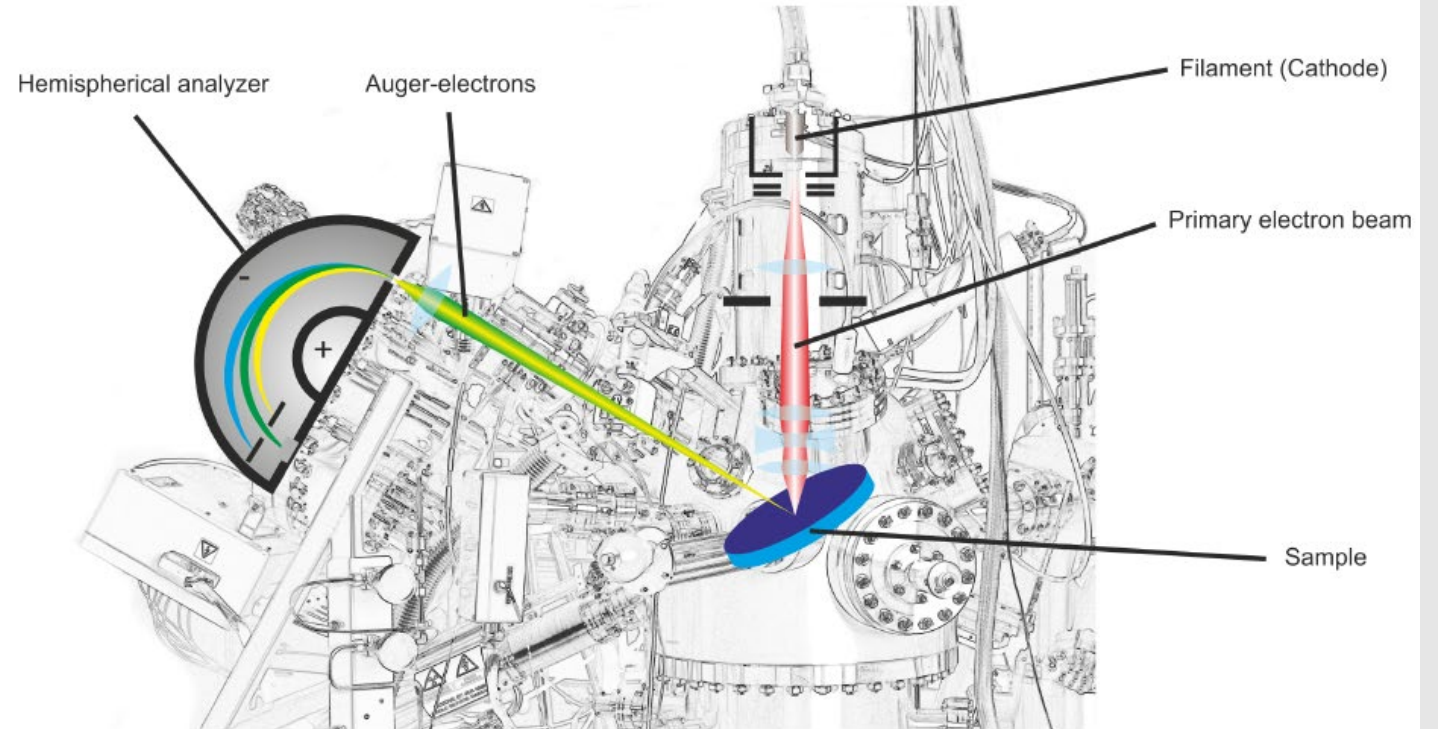


Scanning electron microscopy (SEM)

spatially resolved structural  
and chemical characterization?



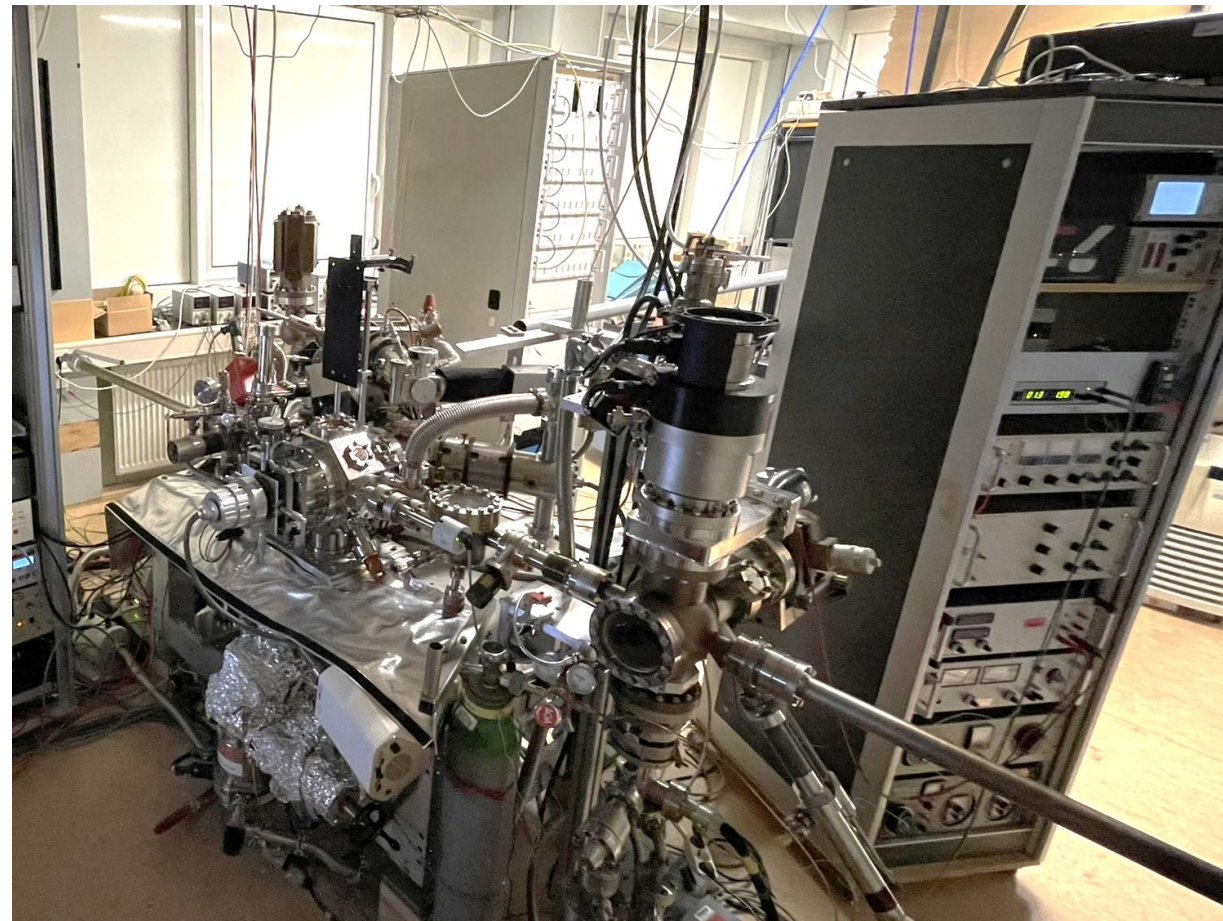
## 0.2 The NanoSAM – Scanning Auger Microscope



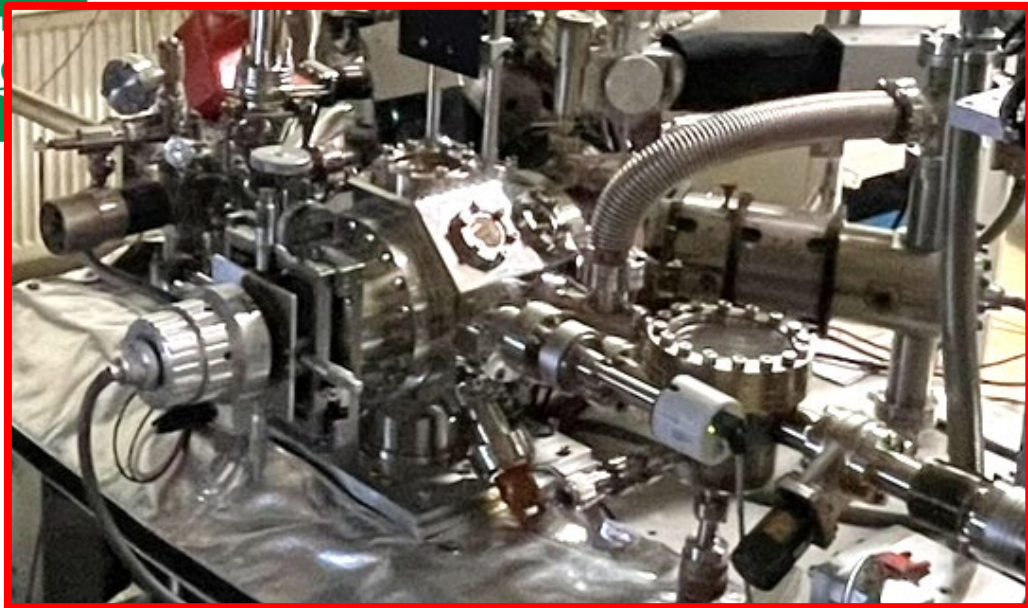
- Combination of scanning electron microscopy (SEM) and Auger electron spectroscopy (AES)
- High lateral resolution (~5 nm SEM, ~20 nm AES)
- High surface sensitivity (1 – 10 nm)

## 0.2 Low Energy Electron Microscopy (LEEM)

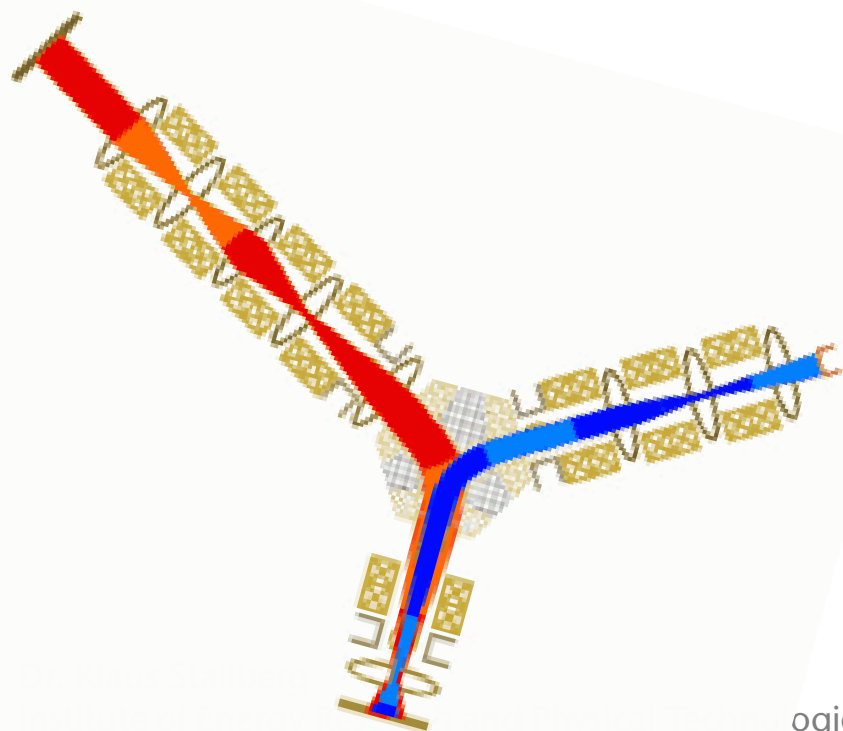
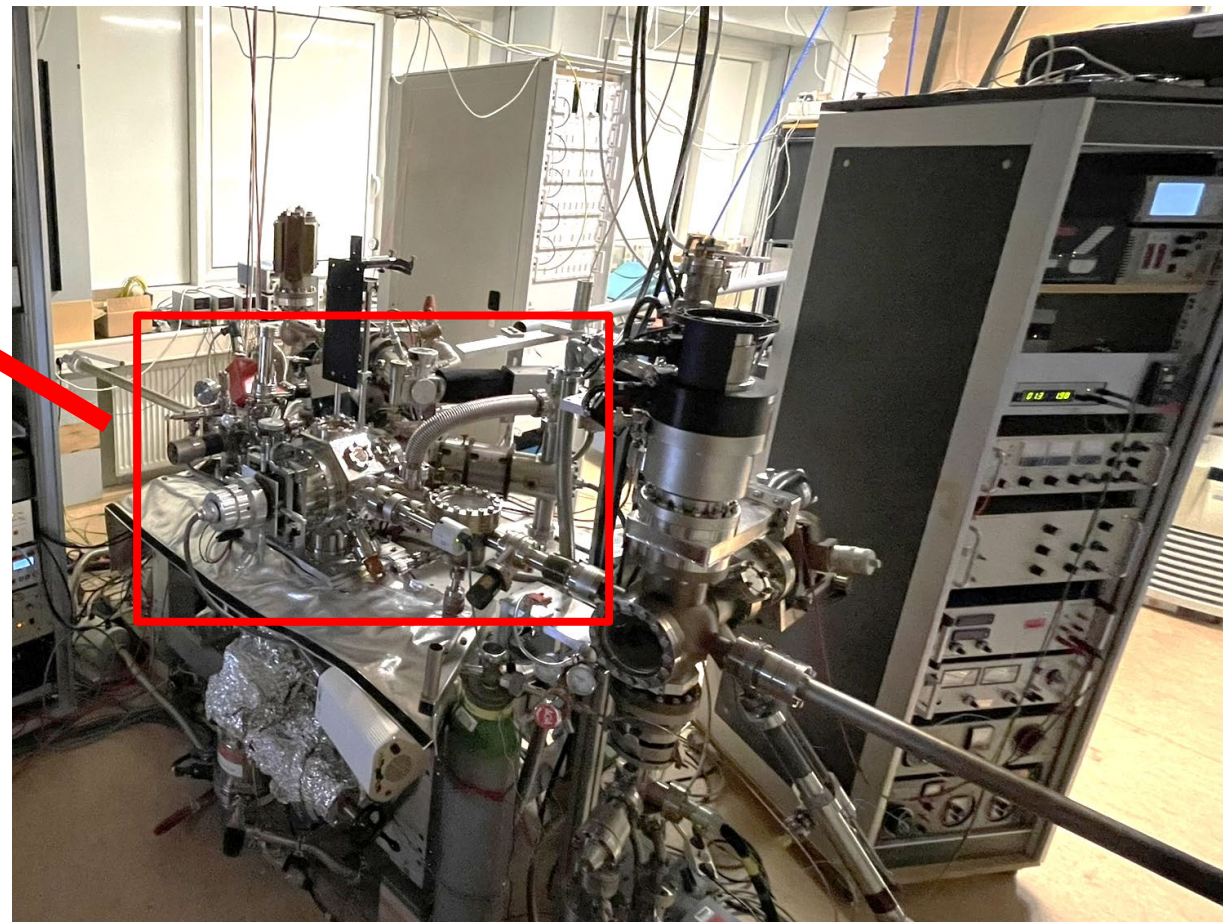
- High lateral resolution ( $\sim 12\text{nm}$ )
- High surface sensitivity ( $1 - 10\text{ nm}$ )
- Parallel imaging  
→ e.g. real-time videos of surface reactions
- Structural information from electron diffraction and dark-field imaging  
→ surface characterization on the atomic scale!





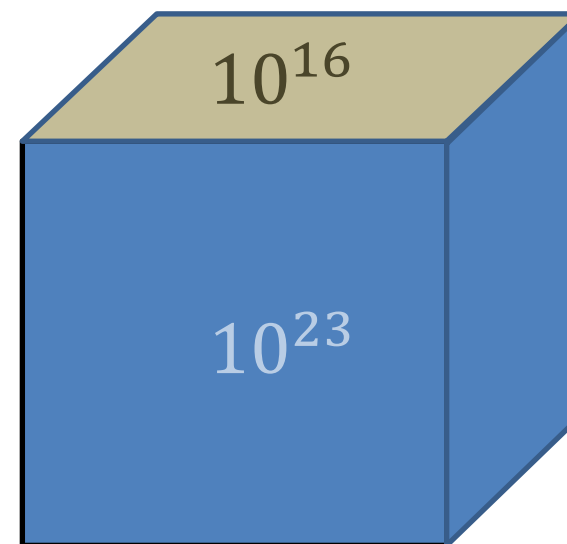


scopy (LEEM)



## 0.3 Need for surface sensitivity:

- Bulk:  $\sim 10^{23}$  atoms /  $\text{cm}^3$
- Surface atoms:  $\sim 10^{16}$  /  $\text{cm}^2$
- Bulk / surface ratio:  $10^7$   
→ bulk contribution to spectroscopic signal is **10 million times higher** than surface contribution



## 1. Electron microscopy

- Abbe's theory of image formation
  - Ernst Abbe (1873):

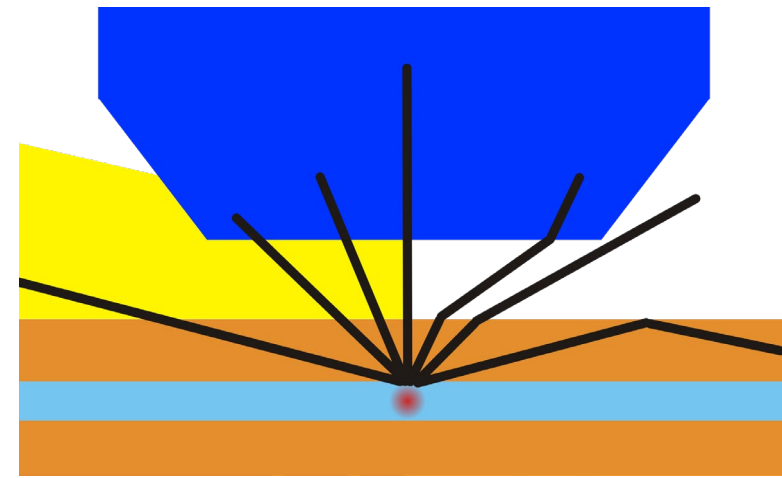
Resolution  $\delta$  is limited by objective's numerical aperture  $NA = n \cdot \sin \alpha$

$\alpha$ : half-angle of objective lense

$n$ : refractive index of working medium ( $n = 1.0$  for air,  $n \approx 1.5$  for immersion oil)

$$\delta = \frac{\lambda}{NA} = \frac{\lambda}{n \cdot \sin \alpha}$$

- $\delta_{LM} \approx 300$  nm for microscopy based on light ( $\lambda_{min} \approx 400$  nm)



wikipedia



## 1. Electron microscopy

- Image formation using electrons as a probe
  - de-Broglie-wavelength of electrons which are accelerated with  $U_a = 30$  kV (relativistic, error with classical derivation +1.45 %):

$$\lambda = \frac{hc}{\sqrt{(eU_b)^2 + 2eU_b m_e c^2}} = 6,96 \text{ pm}$$

- Length of atomic bonds:  $\sim 500$  pm
  - Theoretically, subatomic resolution is possible (however, also lens errors have to be considered)

## 1. Electron microscopy

- Scanning microscopy methods
  - Surface is scanned with a very thin electron beam ( $\sim 2$  nm diameter)
  - Sequential detection of the imaging electrons (pixel by pixel)
  - E.g. scanning / secondary electron microscopy (SEM), scanning Auger electron microscopy (SAM)
- Parallel imaging techniques
  - Investigated sample area is homogeneously irradiated with electrons (or with photons in photoemission electron microscopy – PEEM)
  - Simultaneous detection of the imaging electrons on a 2D detector
  - E.g. transmission electron microscopy (TEM), low-energy electron microscopy (LEEM), PEEM

## 1.1 Electron microscopy setup

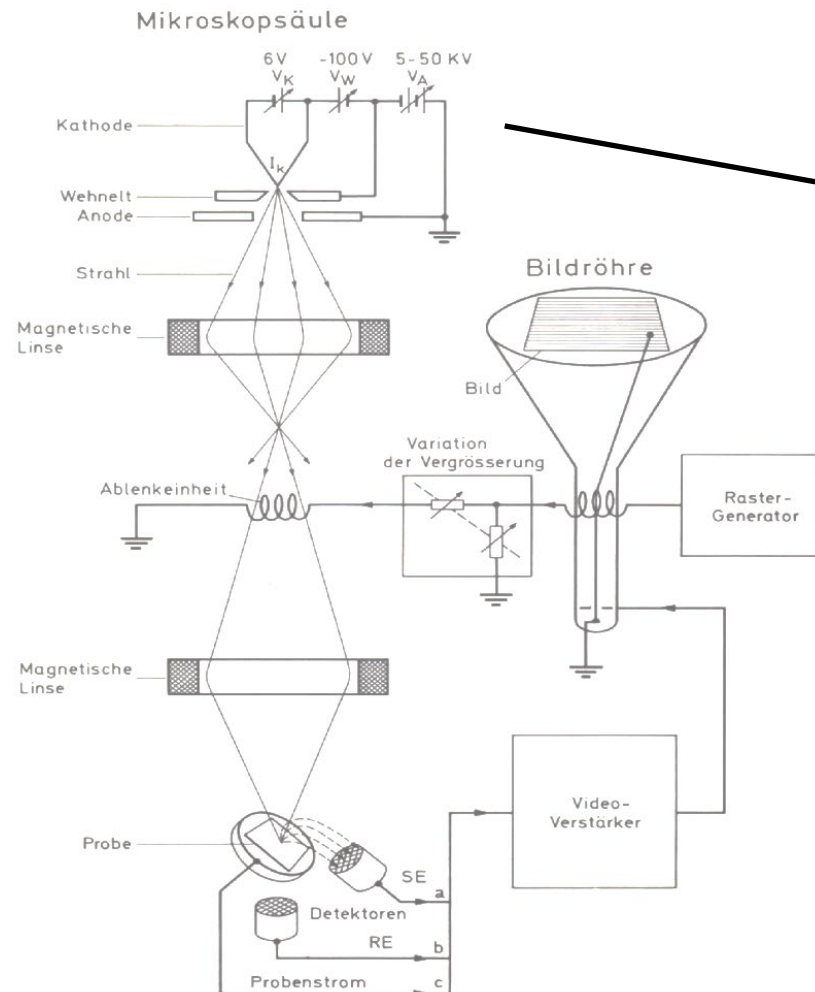


Abb. 1.1. Prinzipieller Aufbau und Wirkungsweise des Raster-Elektronenmikroskops. (SEM: scanning electron microscope)

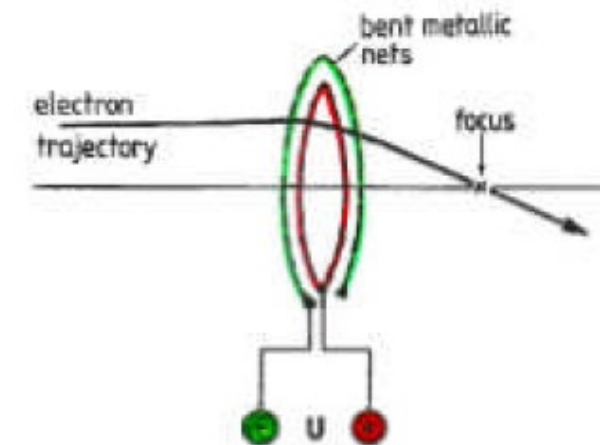
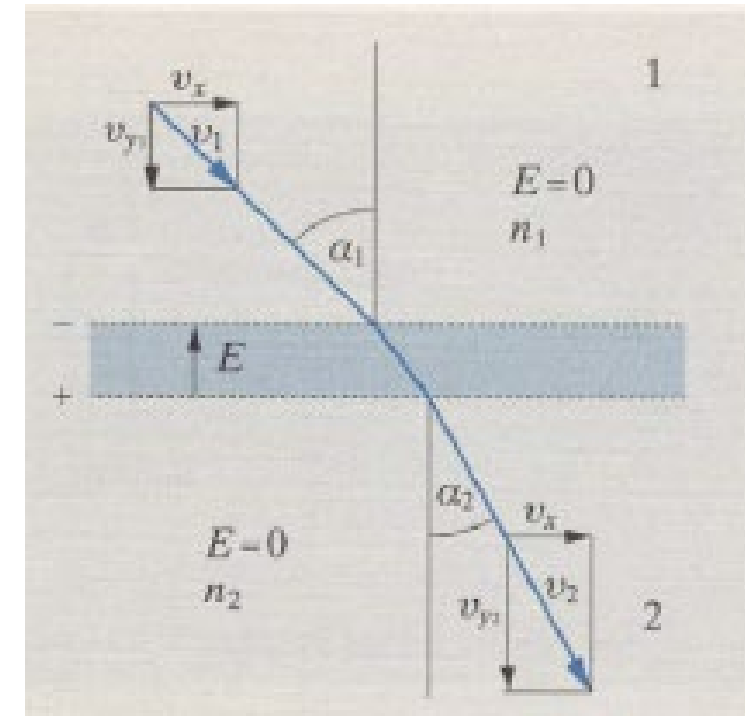


## 1.1 Principles of electron optics

- Electron lenses can be realized by inhomogeneous electric or magnetic fields
- Electrostatic electron lenses:
  - No acceleration of electrons in field free regions with potentials  $U_1$  and  $U_2$
  - In between, acceleration in y-direction
    - Snell's law for electrons at potential step  $U_1 \rightarrow U_2$ :

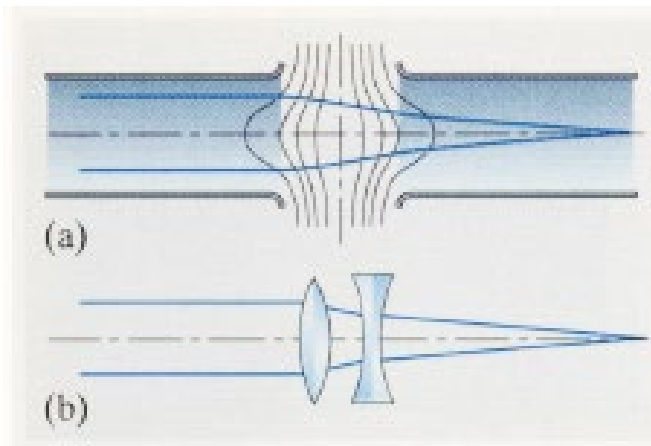
$$\frac{\sin \alpha_1}{\sin \alpha_2} = \sqrt{\frac{U_2}{U_1}}$$

- Analog to optical lens: simple model of electron lense by two bent metallic meshes with applied voltage

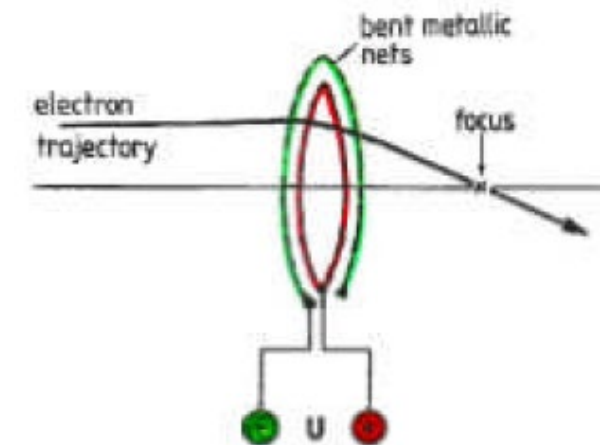
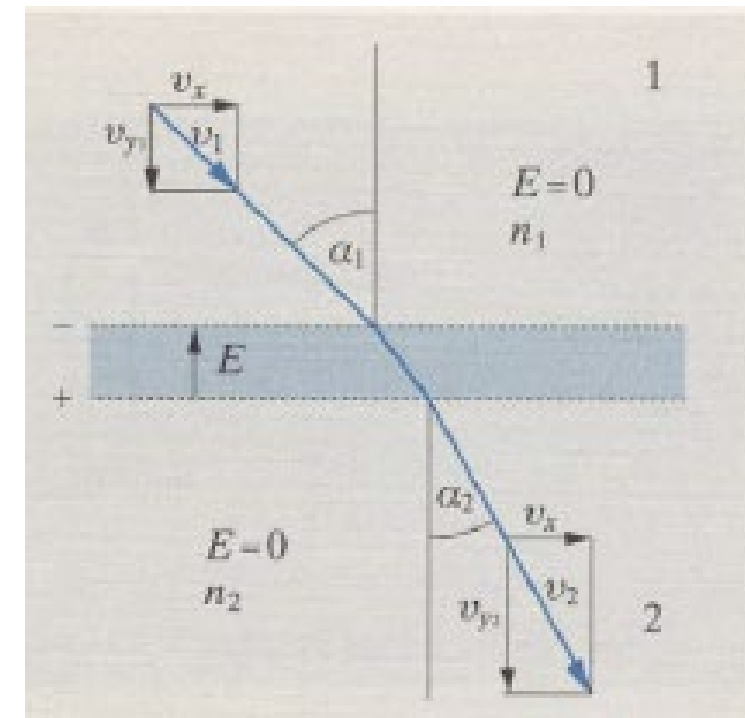


## 1.1 Principles of electron optics

- Electrostatic electron lenses
  - Metallic mesh is not even necessary, but only the curvature of the equipotential surfaces
  - Simple construction with metallic tubes or apertures



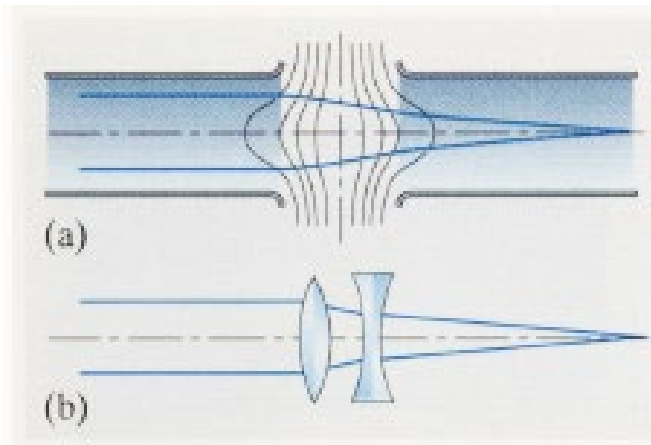
Tube lens (a) and its optical analogon (b)





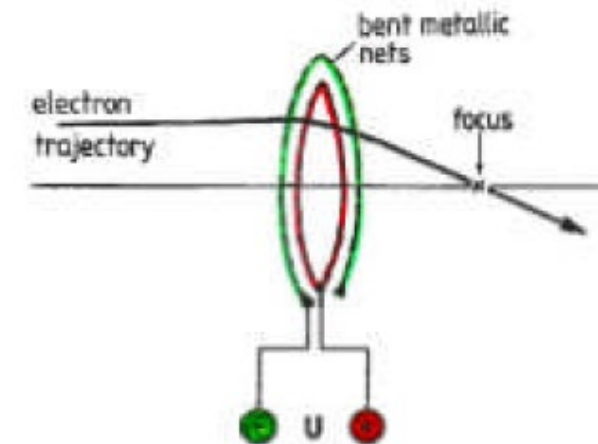
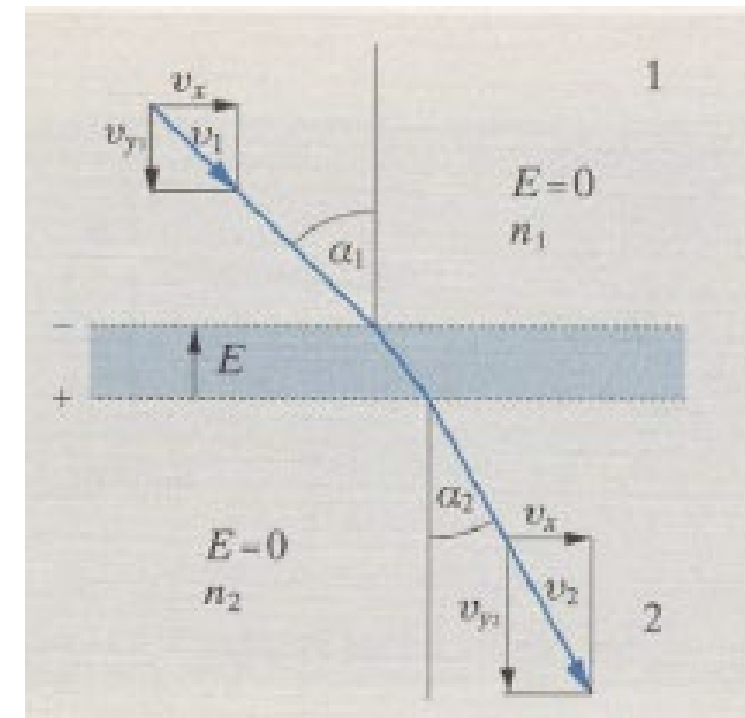
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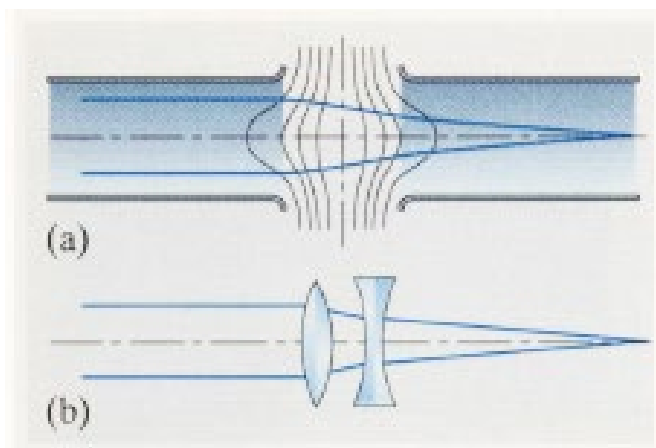
Tube lens (a) and its optical analogon (b)

Initial and final potentials are different for two-element tube lens

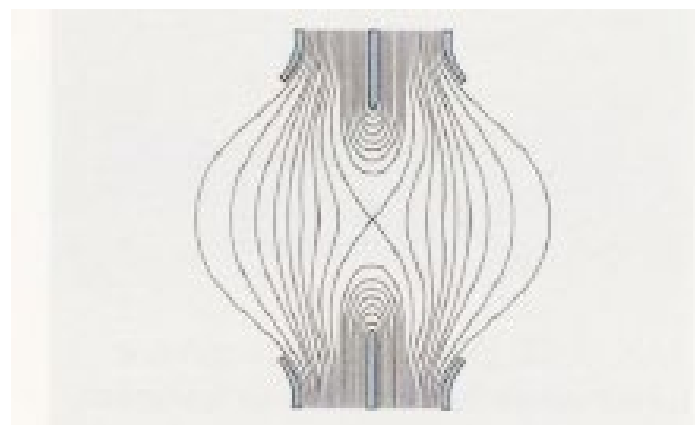


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Tube lens (a) and its optical analogon (b)



Equipotential surfaces in the electric field of an Einzel-lens

Same potential of entrance and exit for three-element Einzel-lens

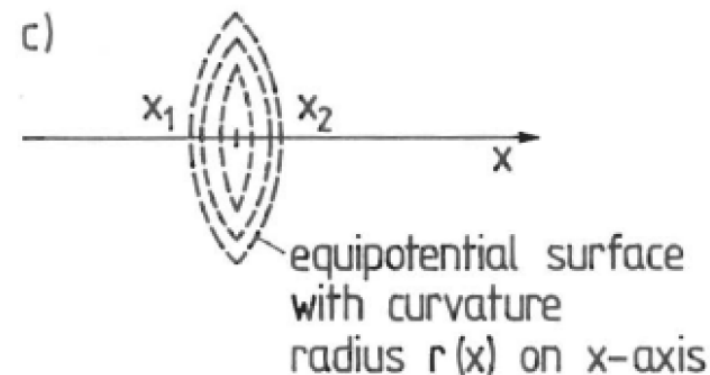
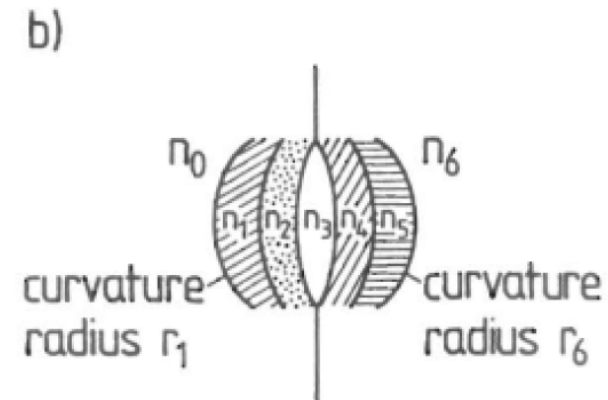
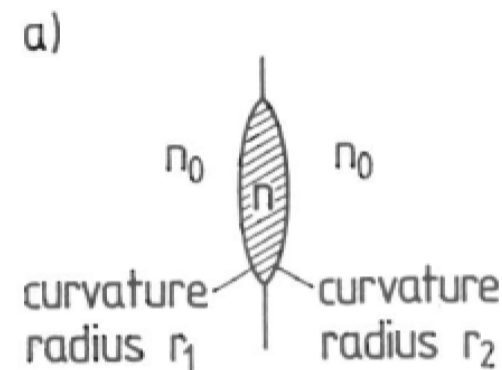
## 1.1 Principles of electron optics

- Electrostatic electron lenses:
  - Reminder: optical lenses
    - Refractive power of a single lens with two different curvatures

$$\frac{1}{f} = \frac{n - n_0}{n_0} \left( \frac{1}{|r_1|} + \frac{1}{|r_2|} \right) = \frac{\Delta n}{n_0} \left( \frac{1}{r_1} - \frac{1}{r_2} \right)$$

- Refractive power of lens system:

$$\frac{1}{f} = \frac{1}{n_0} \sum_v \frac{\Delta n_v}{r_v}$$



## 1.1 Principles of electron optics

- Electrostatic electron lenses:

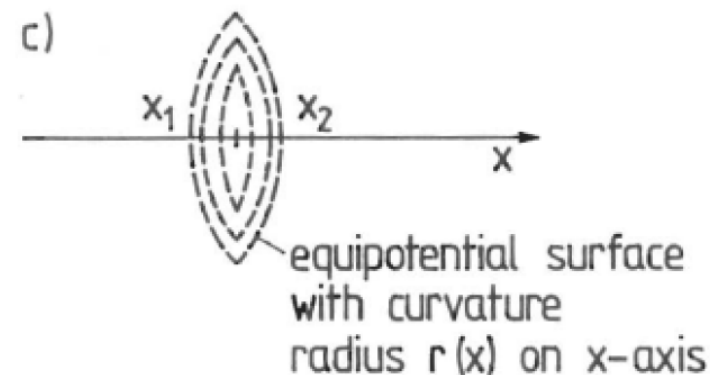
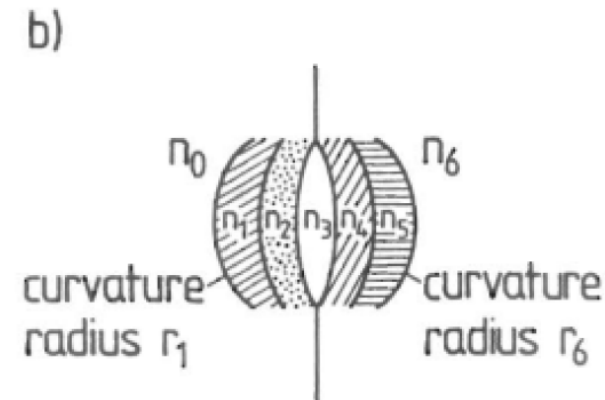
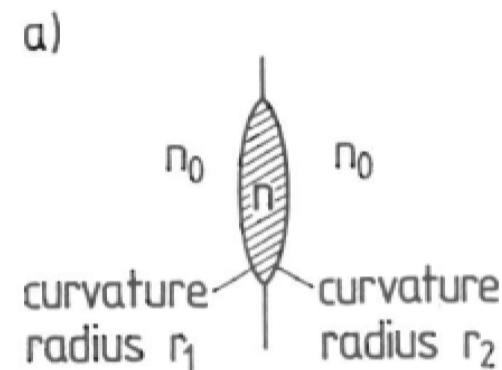
- Analog: electron lens

- Refractive power:

$$\frac{1}{f} = \frac{1}{n_2} \int_{n_1}^{n_2} \frac{dn}{r(x)} = \frac{1}{n_2} \int_{x_1}^{x_2} \frac{1}{r(x)} \frac{dn}{dx} dx$$

with refractive index for electrons:

$$n(x) = \frac{v(x)}{v_1} = \text{const} \cdot \frac{\sqrt{U(x)}}{v_1}$$



## 1.1 Principles of electron optics

- Electrostatic electron lenses:
  - For electrons travelling near the optical axis:

$$\frac{1}{f} = -\frac{q}{4} \frac{1}{\sqrt{E - qU(r)}} \int \frac{U''(x)}{\sqrt{E - qU(x)}} dx$$

$E$ : kinetic energy (far away from the lens)

$U$ : electric potential  $U = U(r) \cdot U(x)$  ( $r$ : distance to  $x$ -axis)

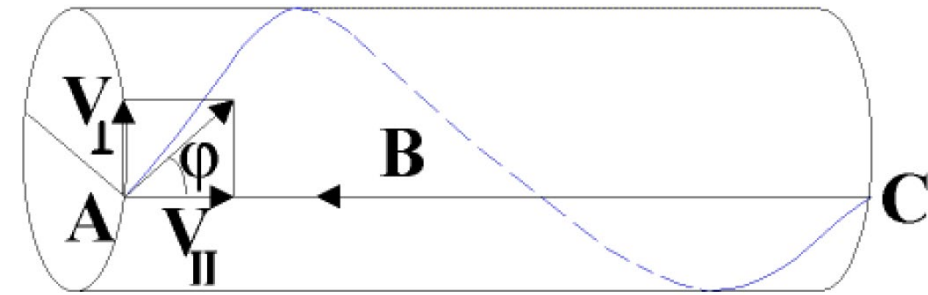
$q$ : charge of electron ( $q = -e$ )

- Electron mass  $m$  does not enter expression for refraction power

→ not only electrons but also protons, He<sup>+</sup>-ions, etc. are focussed into the same point, if they have the same primary energy (this is not the case for magnetic lenses)



## 1.1 Principles of electron optics



- Magnetic electron lenses:

- Charged particle in a homogeneous magnetic field moves on a helical trajectory
- Component  $\vec{v}_\perp$  perpendicular to the magnetic field  $\vec{B}$  rotates with cyclotron frequency

$$\omega = \frac{e}{m} \cdot B$$

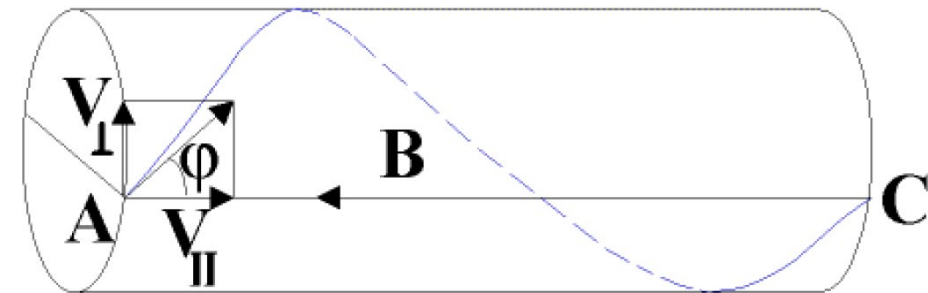
- Particles, which leave point A under different angles, arrive at a point C after the same time

$$\tau = \frac{2\pi m}{eB}$$

- Distance  $\overline{AC}$  (focal length) depends on parallel velocity component  $\vec{v}_\parallel$  and period  $\tau$

$$\overline{AC} = \vec{v}_\parallel \cdot \tau = \frac{2\pi \cdot m \cdot v \cdot \cos \varphi}{e \cdot B}$$

## 1.1 Principles of electron optics



### ■ Magnetic electron lenses:

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- Distance  $\overline{AC}$  (focal length) depends on parallel velocity component  $\vec{v}_{\parallel}$  and period  $\tau$ 
  - For small  $\varphi$ , only weak angle dependence
  - Focal length depends on particle mass

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## 1.1 Principles of electron optics

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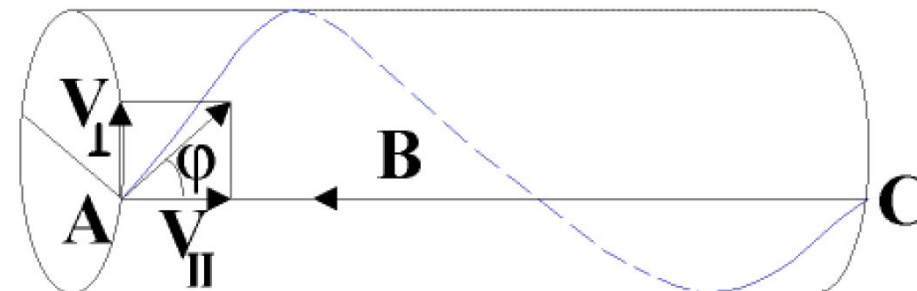
- Particles, which leave point  $A$  under different angles, arrive at a point  $C$  after the same time

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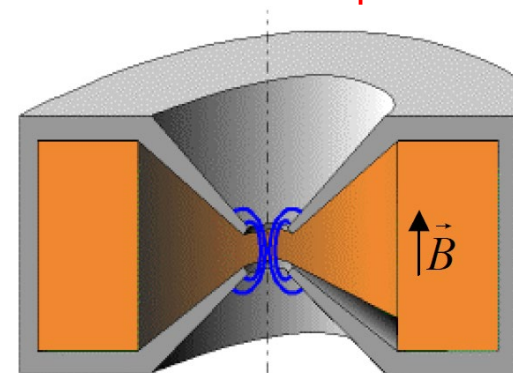
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- In practice the  $\vec{B}$ -field must be confined in a small volume



- For small  $\varphi$ , only weak angle dependence
- Focal length depends on particle mass



## 1.1 Principles of electron optics

### ■ Magnetic electron lenses:

- Magnetic field along axis can be described by Glaser's bell:

$$B = \frac{B_0}{1 + \left(\frac{z}{a}\right)^2}$$

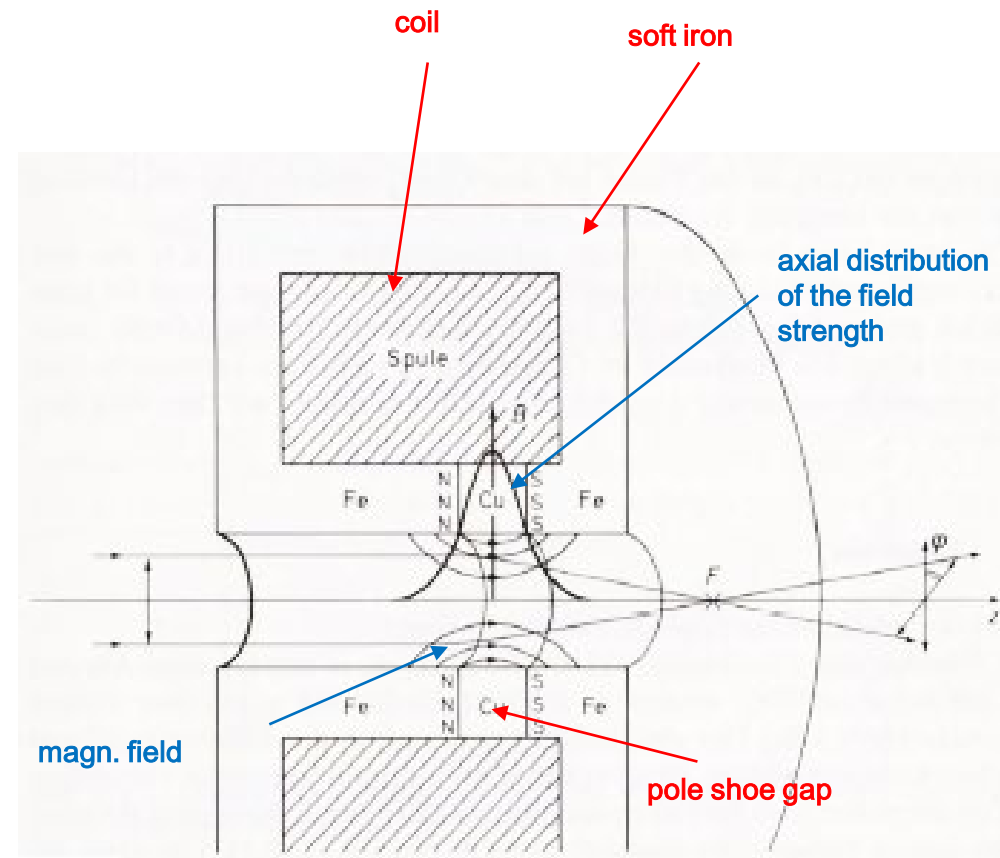
$B_0$ : amplitude of the bell-shaped field distribution

$a$ : width of the bell

- With  $k^2 = \frac{e}{8m} \frac{B_0^2 a^2}{U_0}$  follows  $f = \frac{a}{\sin\left(\frac{\pi}{\sqrt{k^2+1}}\right)}$

- Additional image rotation (helical trajectory) by

$$\varphi = \frac{\pi k}{\sqrt{k^2 + 1}}$$



Cross section through a magnetic lens

## 1.1 Principles of electron opt

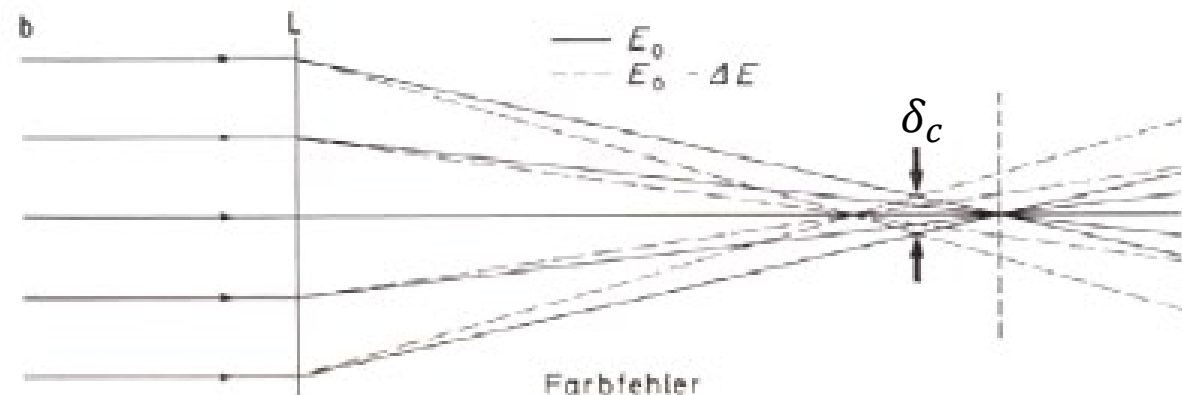
### ■ Abberations

#### ■ Chromatic abberation:

- Focal lengths of electron lenses (both electrostatic and magnetic) depends on kinetic energy
- Energy of electron beam has a certain bandwidth because of:
  - Emission process: thermal (Boltzmann-) distribution  $\Delta E = 2k_B T$
  - Boersch effect: Coulomb repulsion of electrons in foci of the electron beam
  - Imperfect high-voltage supplies: Ripples with  $\Delta U_a$  lead to energy broadening  $\Delta E = e \cdot \Delta U_a$
- Additional abberations because of imperfect lens supplies  $\Delta I_L$  ( $\Delta U_L$  for el. stat. lenses)
- Image of a point object is a disc with finite diameter  $\delta_c$  (disc of least confusion):

$$\delta_c = c_c \cdot \alpha \cdot \sqrt{\left(\frac{\Delta U_b}{U_b}\right)^2 + 2 \left(\frac{\Delta I_L}{I_L}\right)^2}$$

$\alpha$ : half beam angle, order of magnitude of the coefficient for chrom. abber.  $c_c \approx f \approx 10 \text{ mm}$





## 1.1 Principles of electron opt

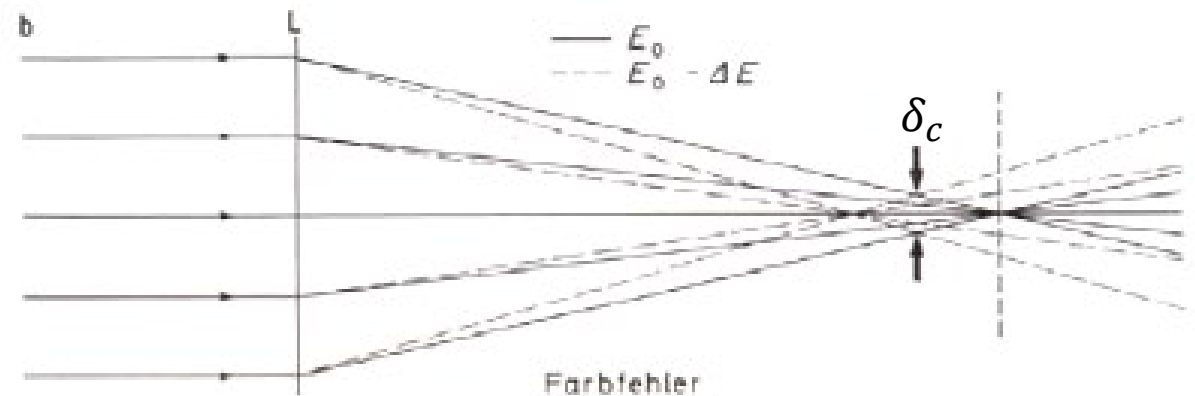
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Because of chromatic abberation voltage and current supplies for electron microscopy must be highly stabilized ( $< 10^{-6}$ )!

## 1.1 Principles of electron opt

### ■ Abberations

#### ■ Spherical abberation:

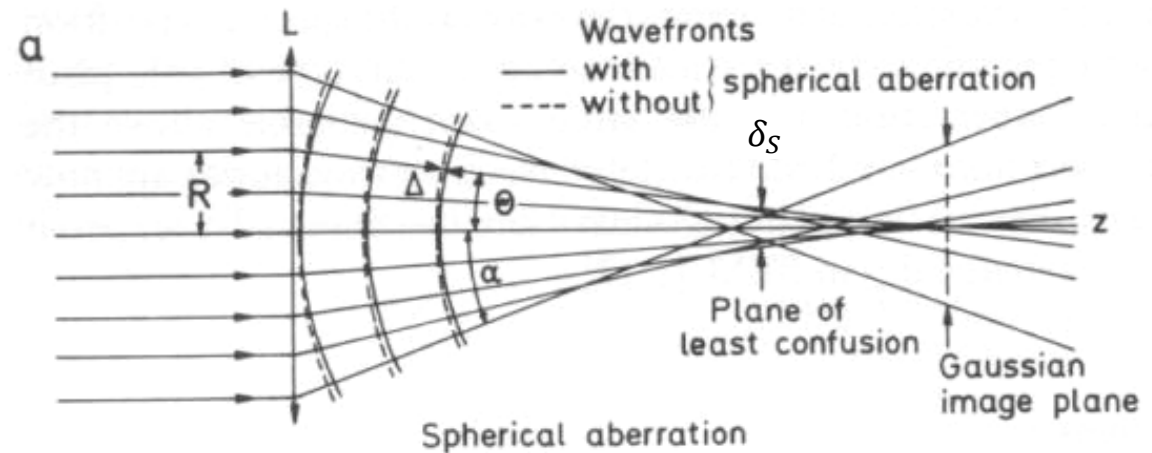
- Like for spherical lenses in light optics, stronger refractive power for beams away from the optical axis
- Point object is imaged as least confusion disc with diameter

$$\delta_s = c_s \cdot \alpha^3$$

coefficient  $c_s$  depends on lens geometrie and focal length:  $c_s \approx \frac{3f^3}{4a^2} \approx 10 \text{ mm}$  (a: width of pole shoe gap)

- Strong dependence on beam angle  $2\alpha$ .

→ Spherical abberation can be efficiently reduced by the usage of apertures



## 1.1 Principles of electron optics

### ■ Abberations

#### ■ Diffraction error:

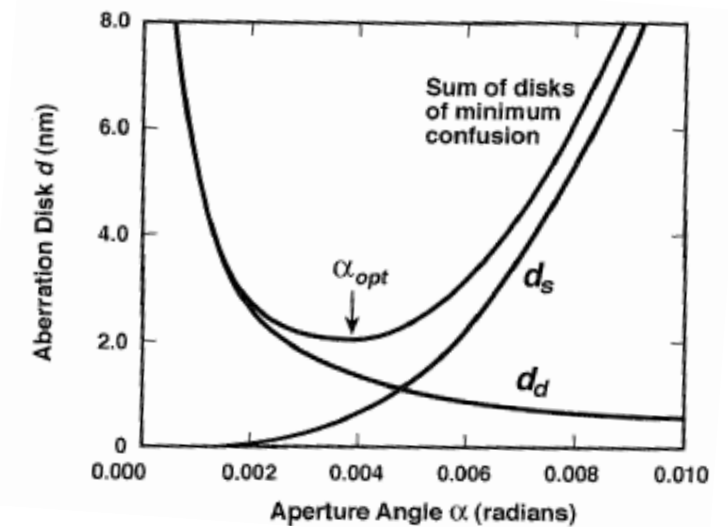
- Resolution of an ideal optical instrument is limited by diffraction at the edges of lenses and apertures (Hermann von Helmholtz 1872)
- Point of the object is imaged as a disc with diameter

$$\delta_d = 1.22 \frac{\lambda}{\sin \alpha}$$

- While reduction of the beam angle (with small apertures) reduces the spherical error, the diffraction error increases!

- Overall abberation of an electron lens:  $\delta = \sqrt{\delta_c^2 + \delta_s^2 + \delta_d^2}$

- Minimum of  $\delta$  for „optimal apertur“:  $\alpha_{opt} = \sqrt[4]{\frac{\lambda}{c_s}} \approx 0,005 \text{ rad} = 0,3^\circ$



## 1.1 Principles of electron optics

### ■ Abberations

#### ■ Diffraction error:

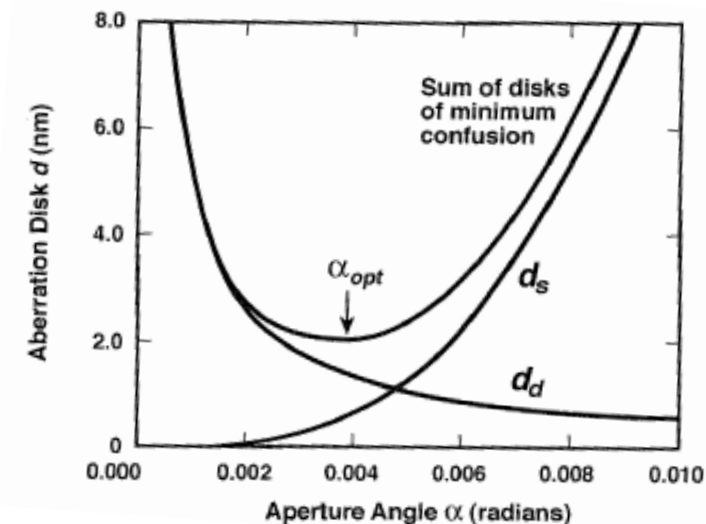
- Resolution of an ideal optical instrument is limited by diffraction at the edges of lenses and apertures (Hermann von Helmholtz 1872)
- Point of the object is imaged as a disc with diameter

$$\delta_d = 1.22 \frac{\lambda}{\sin \alpha}$$

- While reduction of the beam angle (with small apertures) reduces the spherical error, the diffraction error increases!

- Overall abberation of an electron lens:  $\delta = \sqrt{\delta_c^2 + \delta_s^2 + \delta_d^2}$

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achievable resolution without chromatic abberation (not realistic):

$$\delta_{min} = \frac{\lambda}{\alpha_{opt}} = \sqrt[4]{\lambda^3 c_s} \approx 1 \text{ nm}$$

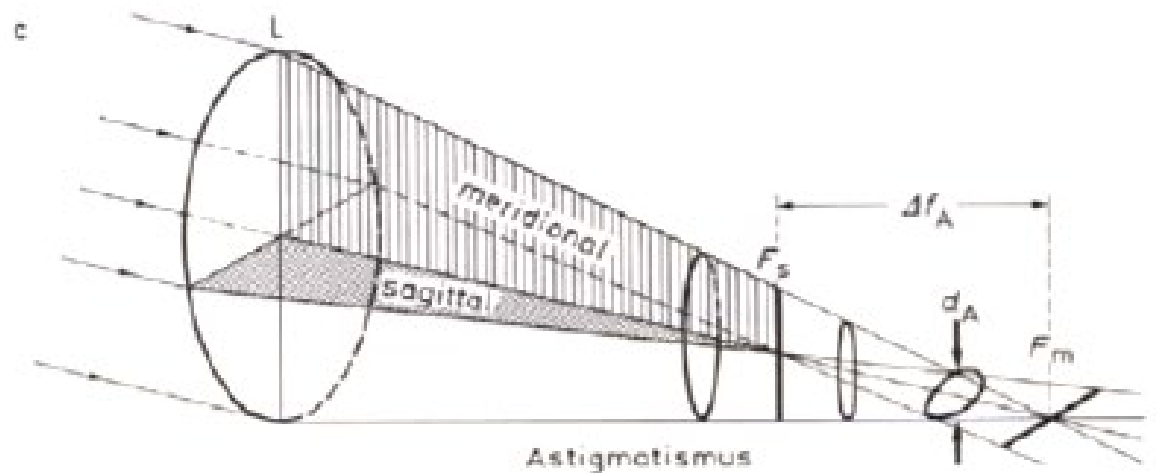
## 1.1 Principles of electron optic

### ■ Abberations

#### ■ Axial astigmatism:

- In practice always deviation from an ideal rotational symmetry of electron lenses
  - non-circular boreholes, contaminations of lenses and apertures
  - inhomogeneities in pole-shoe material
  - tilt of pole pieces
- Imperfect adjustment → off-axis beam path through electron lens
- Two by 90° rotated line foci spearated by distance  $\Delta f_A$
- In between lies the disc of least confusion with diameter

$$d_A = \Delta f_A \cdot \alpha$$



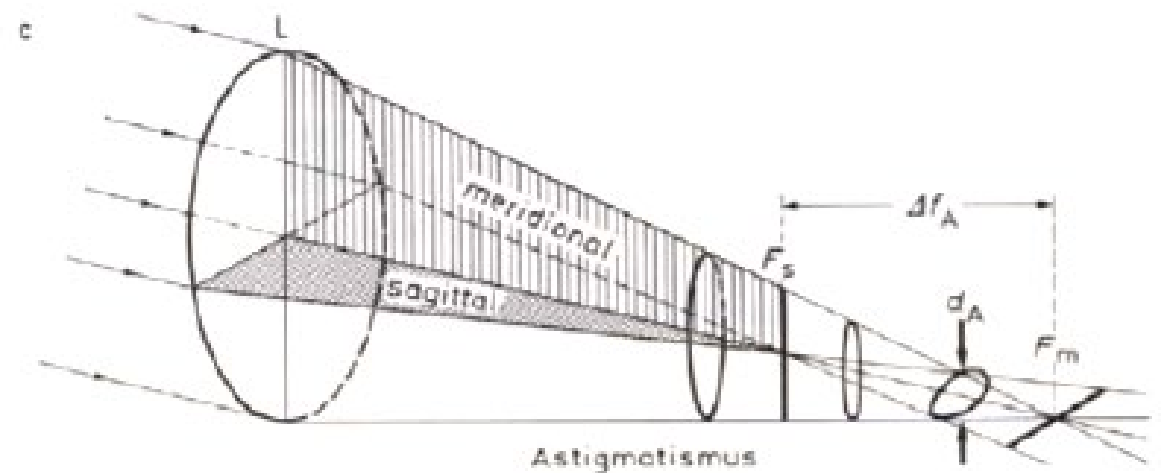
## 1.1 Principles of electron optic

### ■ Abberations

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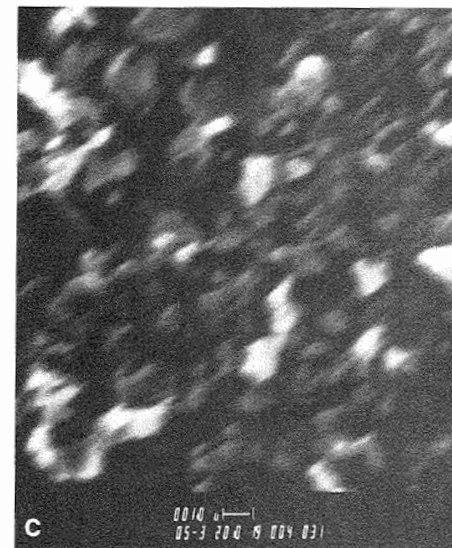
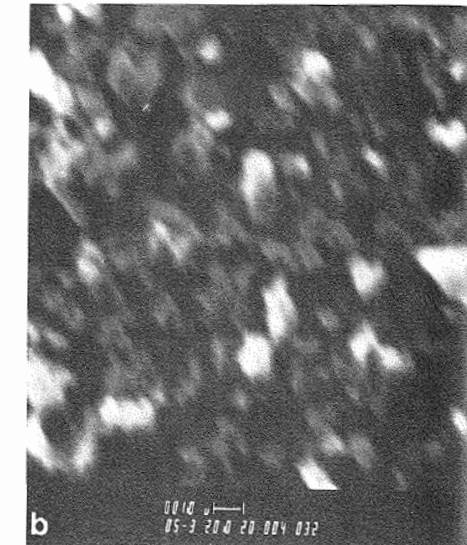
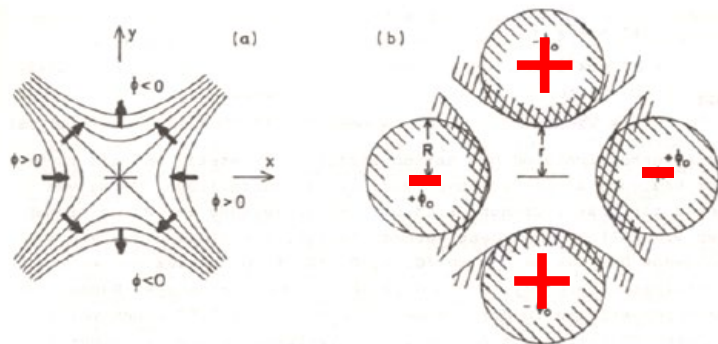


Astigmatism can be corrected!



## 1.1 Principles of electron optics

- Abberations
  - Correction of astigmatism:
    - Electrostatic or magnetic quadrupole fields act as cylindric lenses (stigmators)
    - Often, two by 45° rotated quadrupols (octupole) are used



Goldstein: Scanning Electron Microscopy and X-Ray Microanalysis

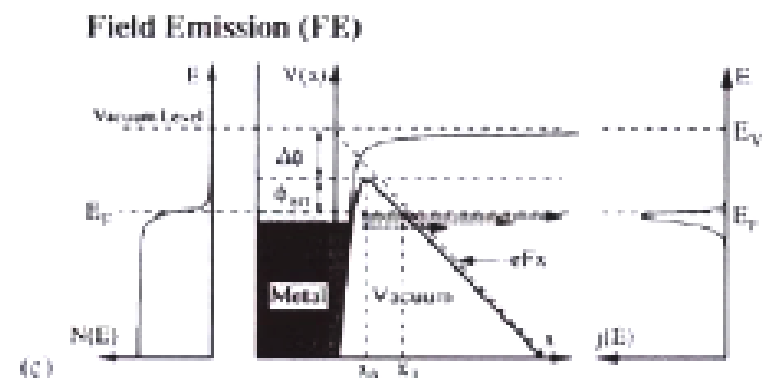
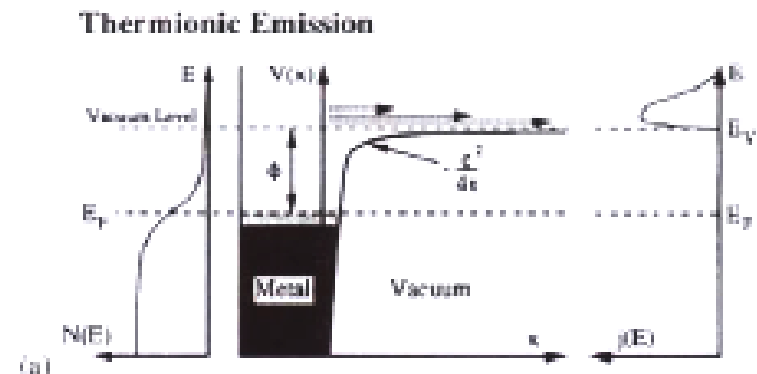


## 1.2 Electron sources

- Thermionic emitter
  - W hairpin cathode,  $\text{LaB}_6$  single crystal ( $\phi = 2.7 \text{ eV}$ )
  - Thermal emission is described by Richardson equation:  

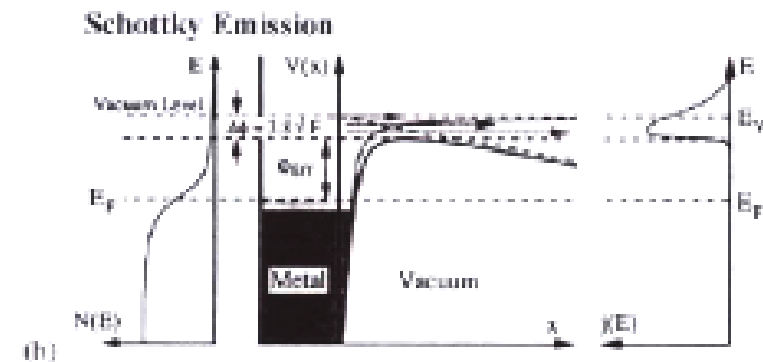
$$j = A T^2 e^{-\frac{\phi}{k_B T}} \quad (T: \text{cathode temperature, } \phi: \text{work function})$$
  - Energy width:  $\Delta E \approx 0.5 - 3 \text{ eV}$
  
- Cold field emitter
  - Single-crystalline W tip
  - Field emission described by Fowler-Nordheim equation (tunneling effect):  

$$j = \frac{k_1 E^2}{\phi} e^{-\frac{k_2 \phi^2}{|E|}} \quad (E: \text{electric field at the tip, only weak temperature dependent constants})$$
  - Emission only at the very apex, ideal point source
  - narrow thermal energy distribution  $\Delta E \lesssim 0.4 \text{ eV}$
  - Disadvantages: more easily contaminated by adsorbates, low and instable beam current



## 1.2 Electron sources

- Thermal field emission, Schottky emission
  - Single-crystalline W tip with  $\text{ZrO}_2$  layer (reduces work function)
  - Field-assisted thermionic emission
  - good point source, moderate width of energy distribution at high beam currents



## 1.2 Electron sources

- W hairpin cathode

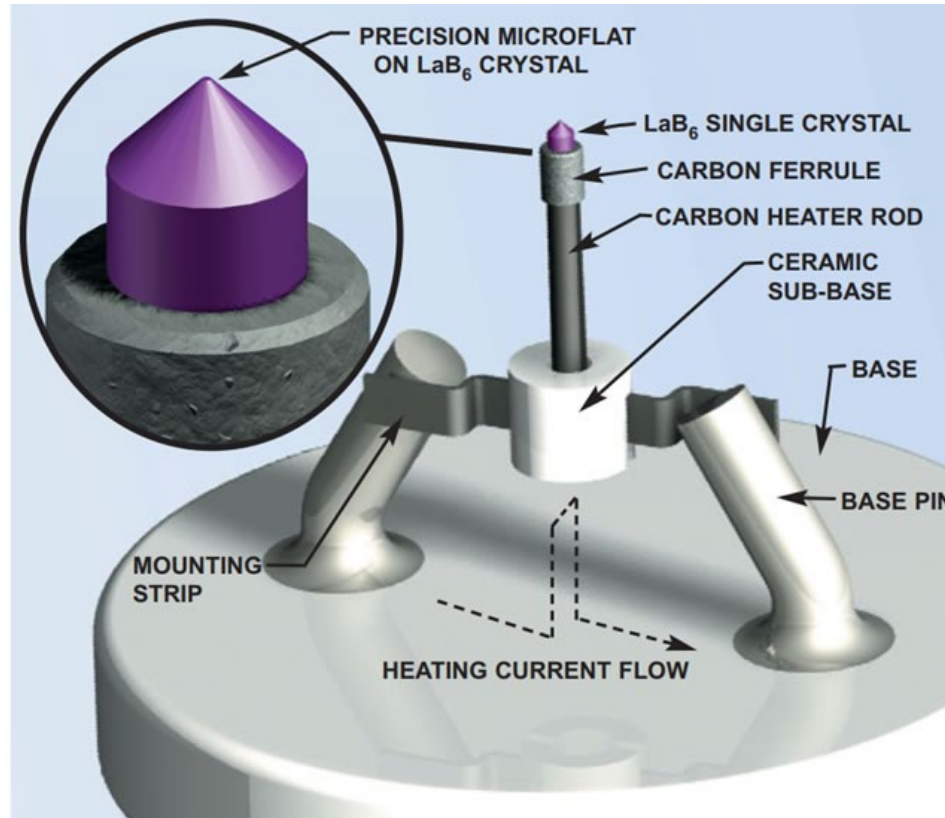


emission temperature  
~2700 K

Micro to Nano

## 1.2 Electron sources

- $\text{LaB}_6$  cathode

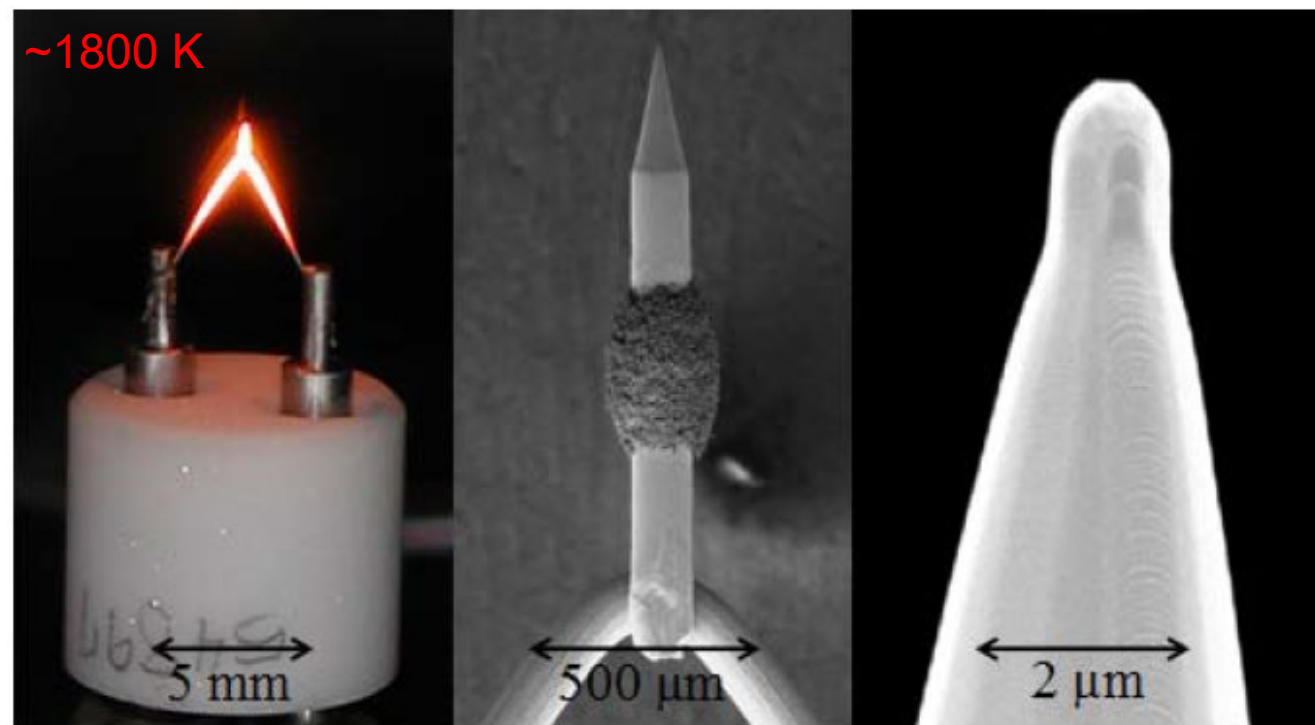


emission temperature  
~1800 K

Micro to Nano

## 1.2 Electron sources

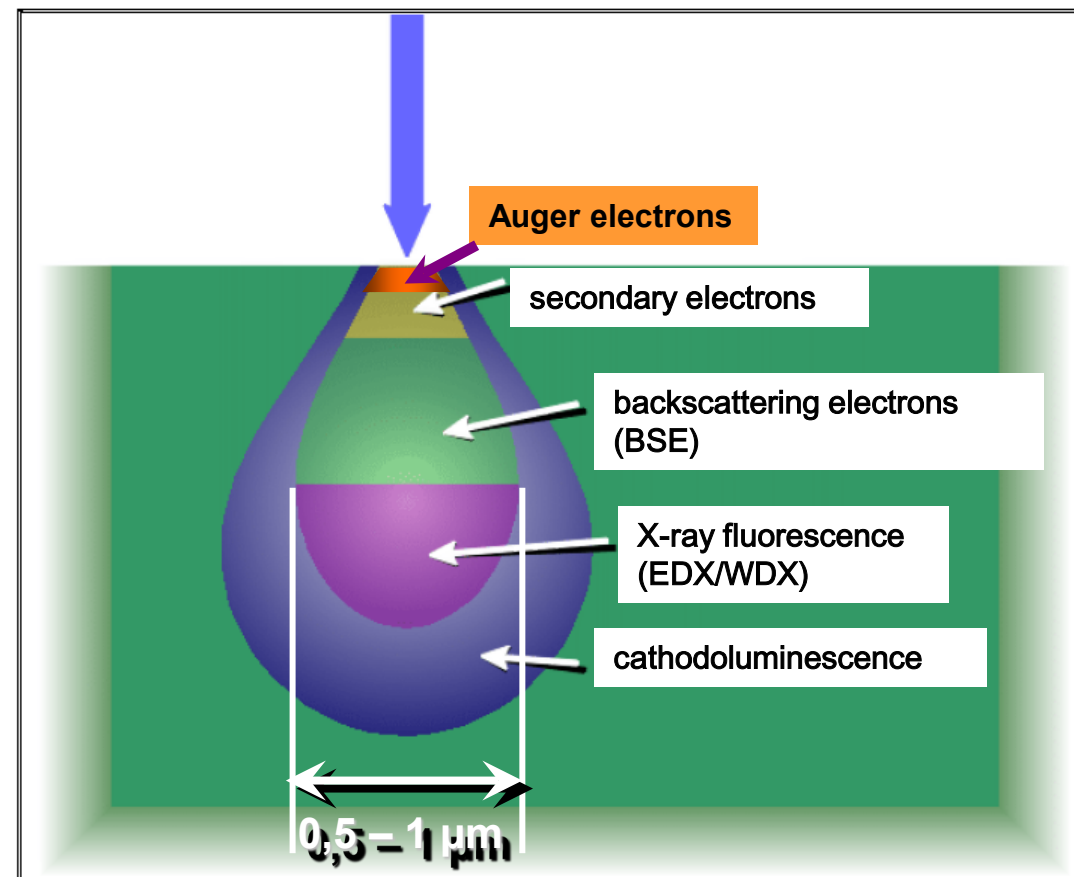
- Schottky emitter



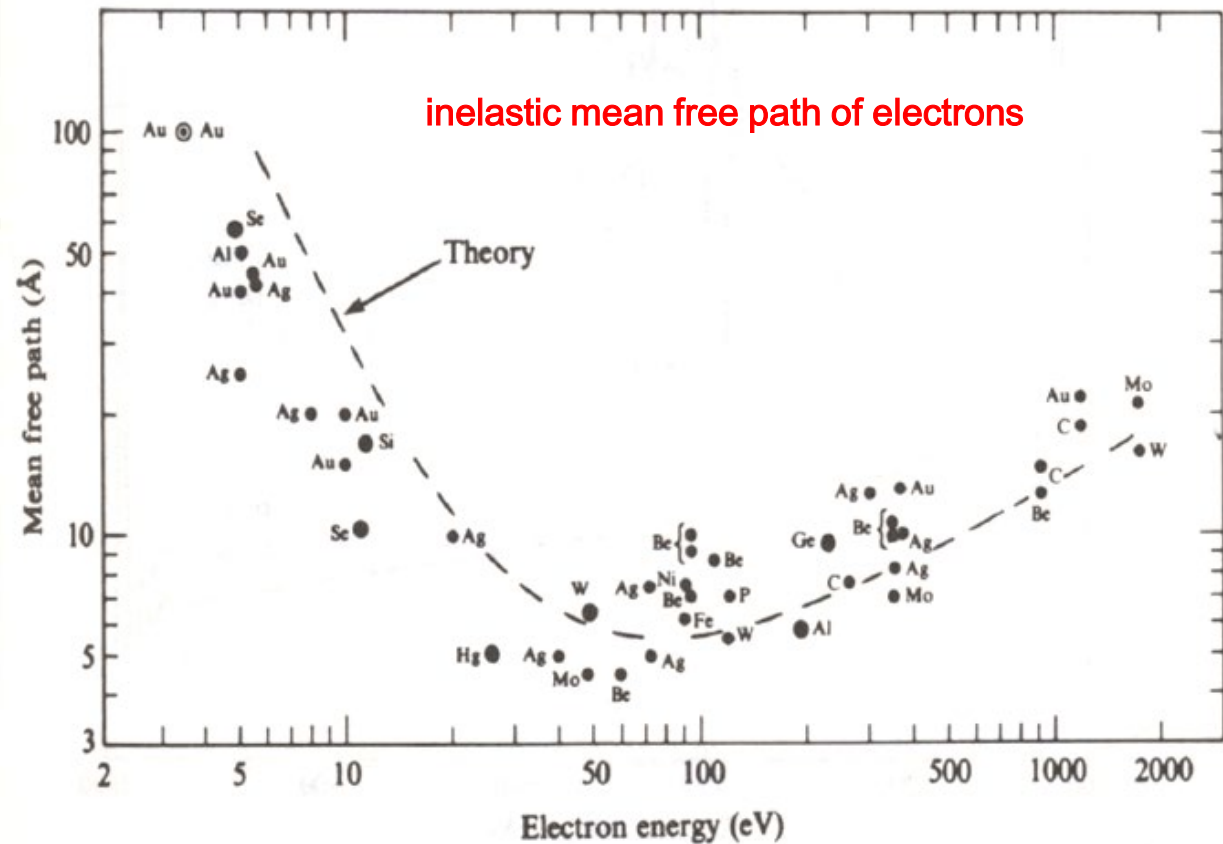
S. Bronsgeest, PhD-Thesis

## 1.3 Signal detection

- Interaction of high-energy electrons with matter
  - Backscattering electrons (BSE):
    - Incoming primary electrons are elastically scattered at the atom cores
    - Scattering cross sections increases with atomic number → **element contrast**
  - Secondary electrons (SE):
    - Inelastic scattering of primary electrons
    - SE have energy  $< 50$  eV
    - Best lateral resolution in SEM ( $\sim 1$  nm)

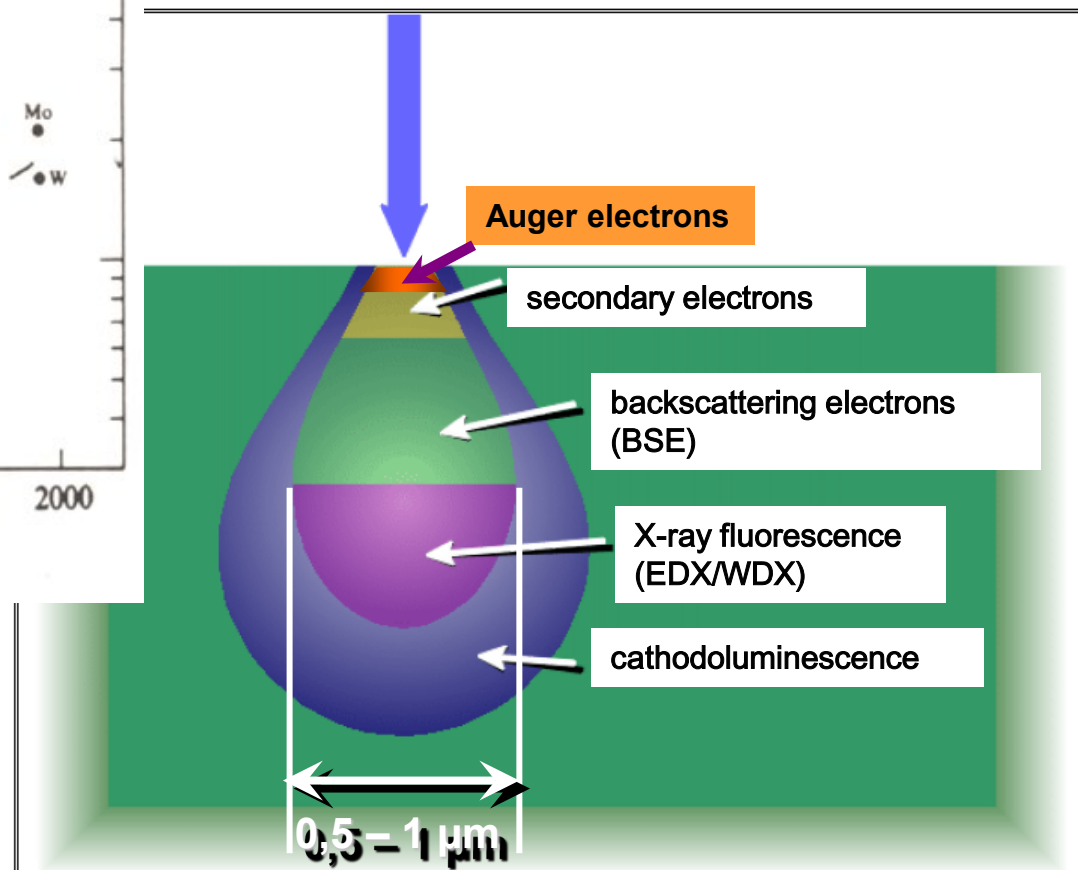


1.



secondary electrons (SE):

- Inelastic scattering of primary electrons
- SE have energy  $< 50$  eV
- Best lateral resolution in SEM ( $\sim 1$  nm)





## 1.3 Signal detection

- Simple method: measurement of the sample current (rarely used in practice )

- Sample current depends on:

- Back-scattering coefficient

$$\eta = \frac{\text{\# backscattered electrons (emitted into vacuum)}}{\text{\# primary electrons hitting the sample}}$$

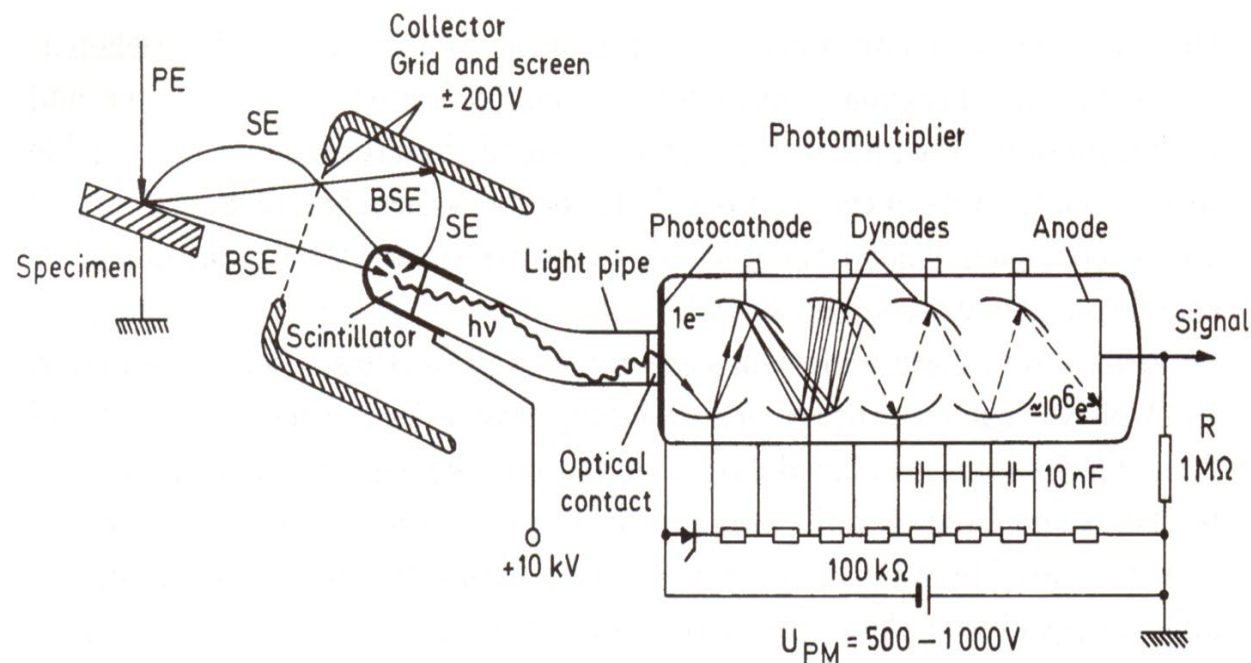
- Coefficient for secondary electron emission

$$\delta = \frac{\text{\# released secondary electrons (emitted into vacuum)}}{\text{\# primary electrons hitting the sample}}$$

- Coefficients depend on local material composition (material contrast), local surface orientation relative to primary beam, ...
- Negative sample current (net current into vacuum), if  $(\eta + \delta) > 1$

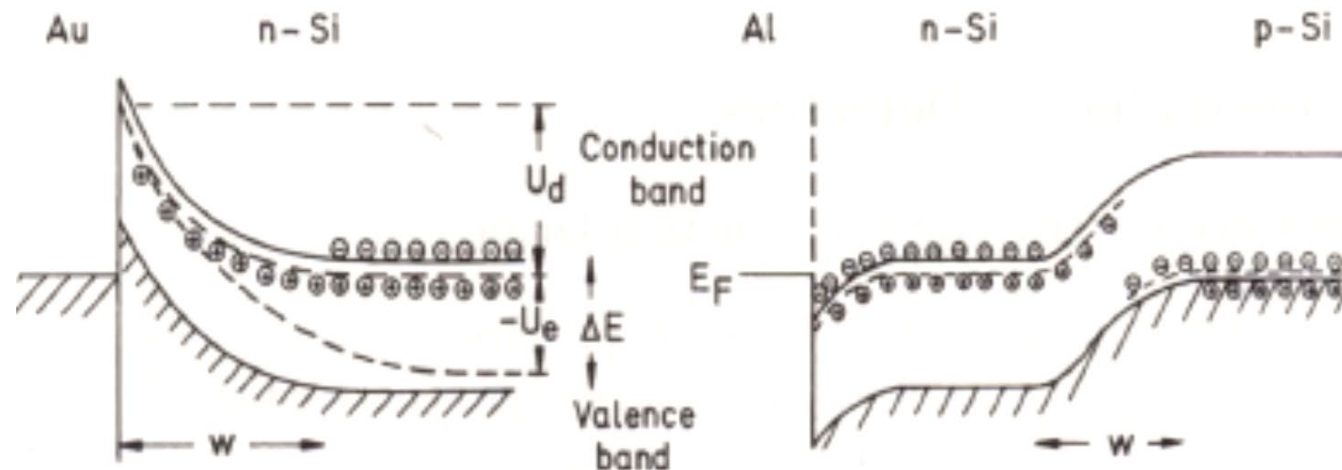
## 1.3 Signal detection

- Usually imaging with backscattered and/or secondary electrons
- Detection with scintillators (Everhart-Thornley detectors)
  - Formation of 10 – 15 photons per 10 keV electron in the scintillator material (e.g. Yttrium Aluminium Granat YAG). Amplification with photomultiplier.



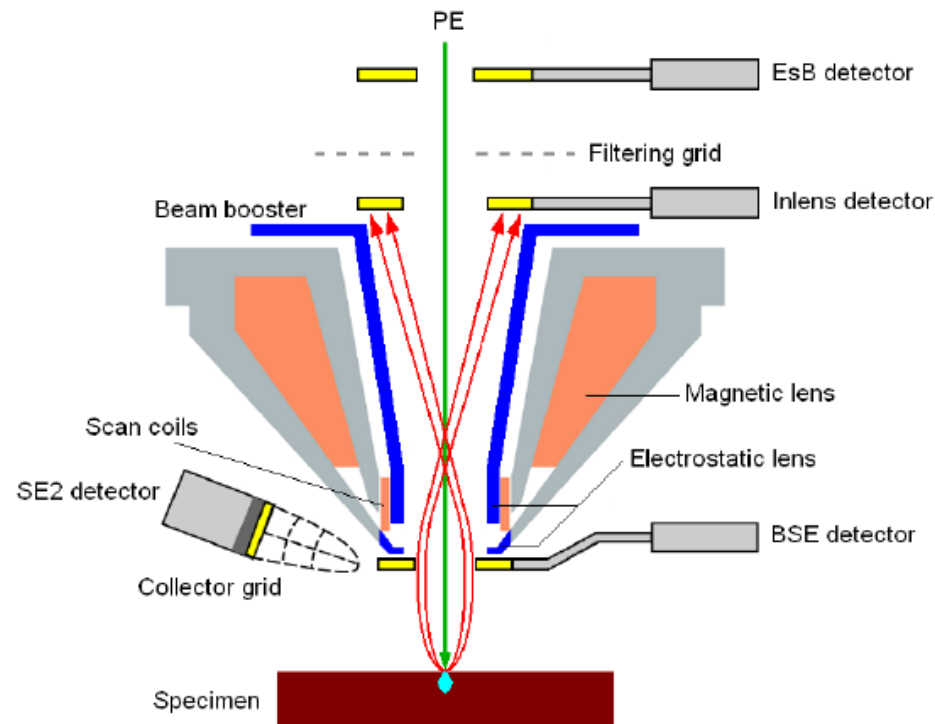
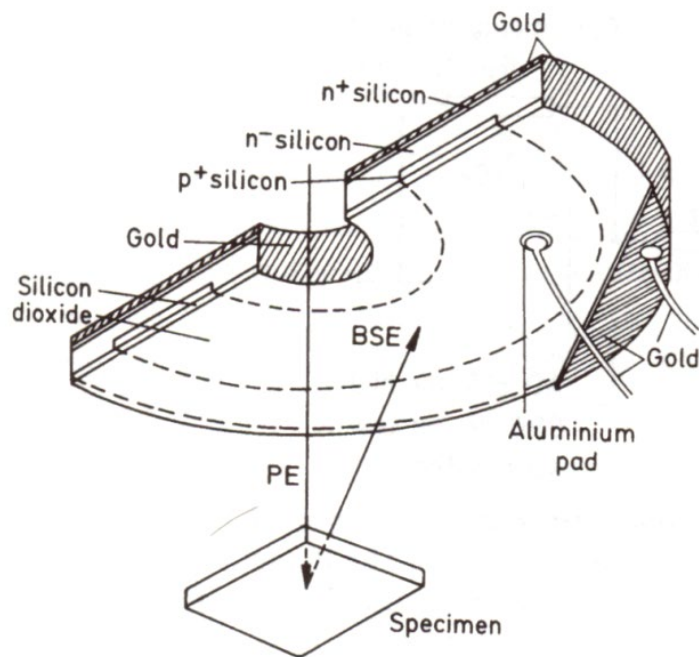
## 1.3 Signal detection

- Often also small-sized semiconductor detectors
- Principle: Creation of electron-hole pairs and charge separation at either a metal-semiconductor (Schottky) contact or a pn-junction
  - Space-charge region at the interface causes band bending
  - Electron-hole pairs dissociate at the interface and constitute the detector current



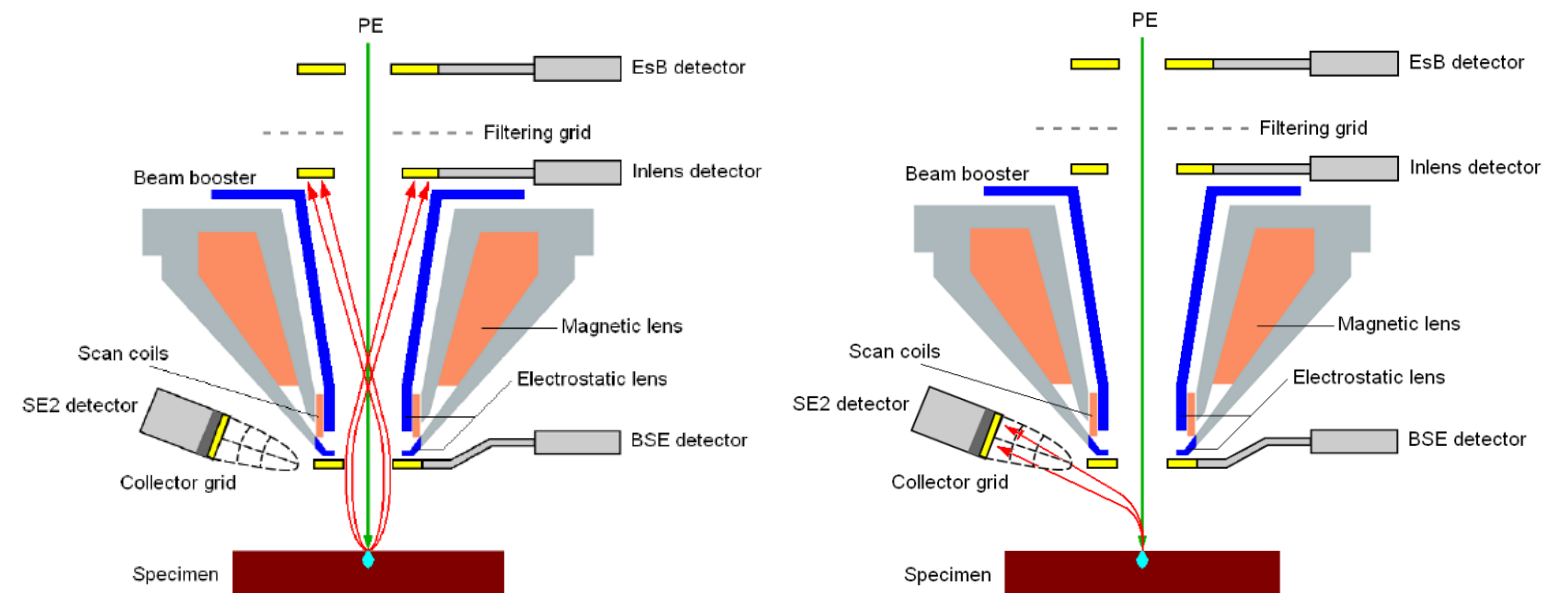
## 1.3 Signal detection

- Detectors can be fabricated ring or semi-ring shaped
- Suitable for mounting directly within the microscope column



## 1.3 Signal detection

- Different detectors allow for different contrast mechanisms:



Comparison of topographic contrast In-lens / SE 2 detector

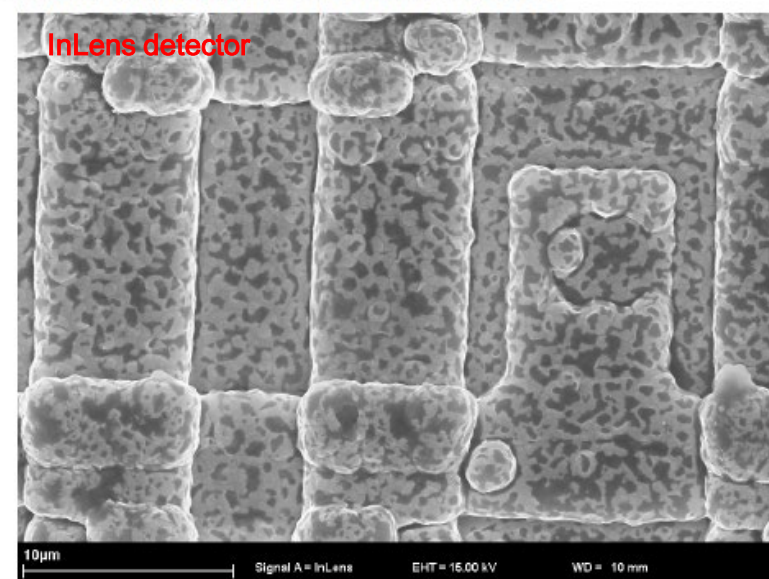


Fig. 11: good mapping of surface structures, low topographic contrast

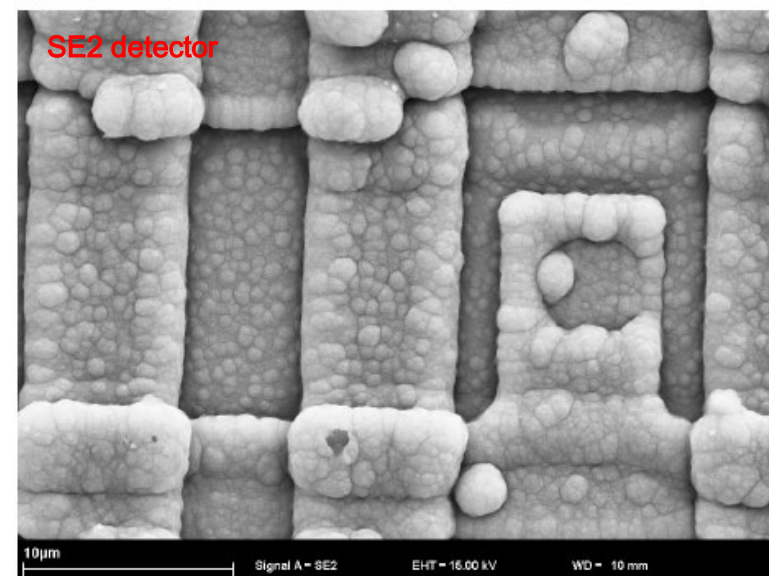
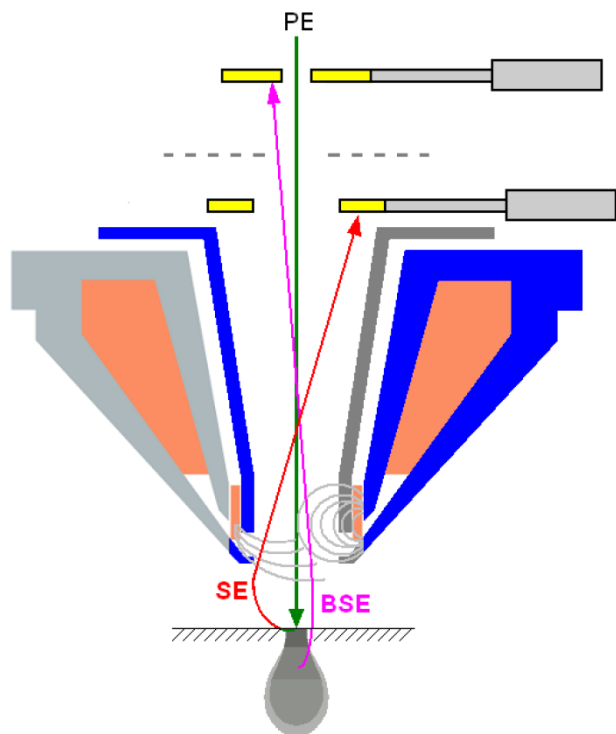


Fig. 12: good topographic mapping



## 1.3 Signal detection

- Different detectors allow for different contrast mechanisms



Comparison InLens/EsB Detector in low voltage range

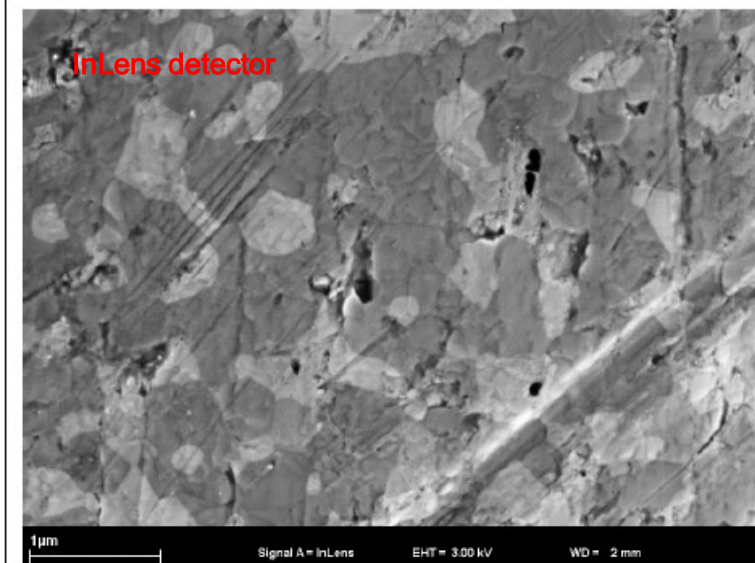


Fig. 43: Clear material and topographic contrast

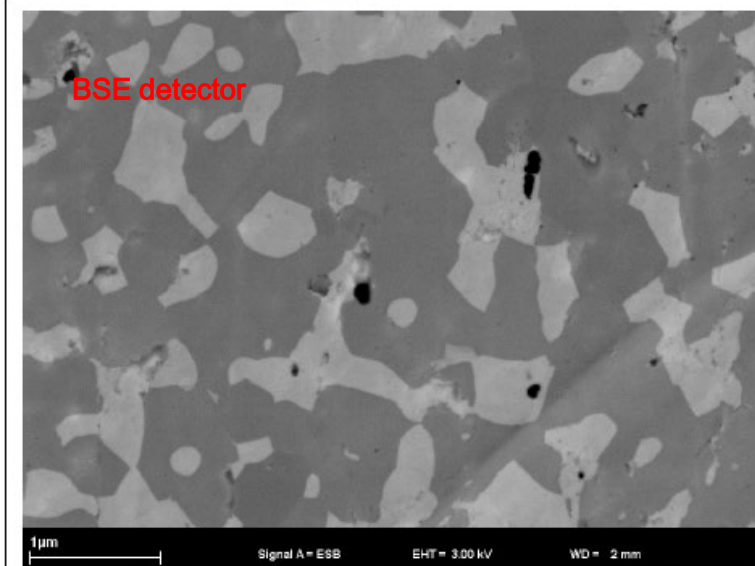
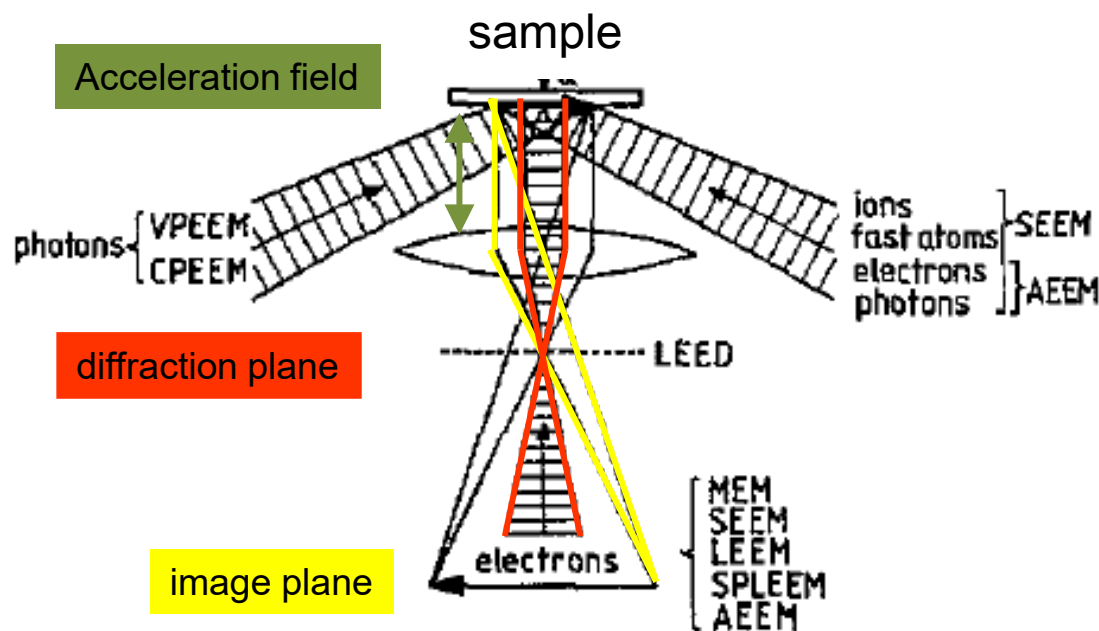


Fig. 44: Predominant material contrast, minimization of topographic contrast (ESB Grid 900V)



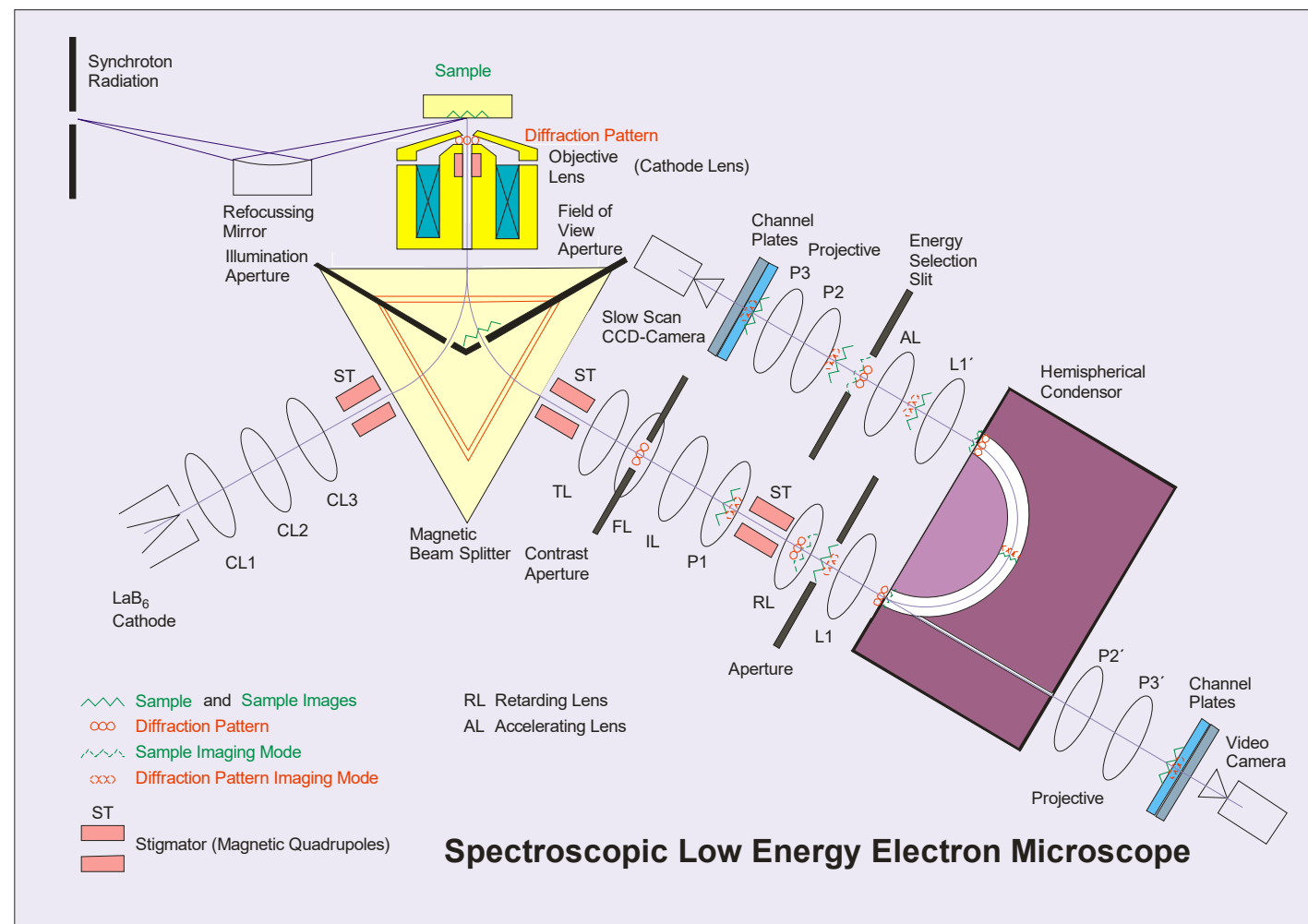
## 2.1 Principle of LEEM



- Simultaneous imaging of the whole field of view (FOV) with a cathod lens (objektive lens with an acceleration/deceleration field)
- High-energy primary electrons are decelerated to much lower energies, reflected at the sample and accelerated back to high energy
- Use of low-energy electrons possible → high surface sensitivity
- Beam path very similar to a light microscope
- Separation of incoming and outgoing electrons necessary

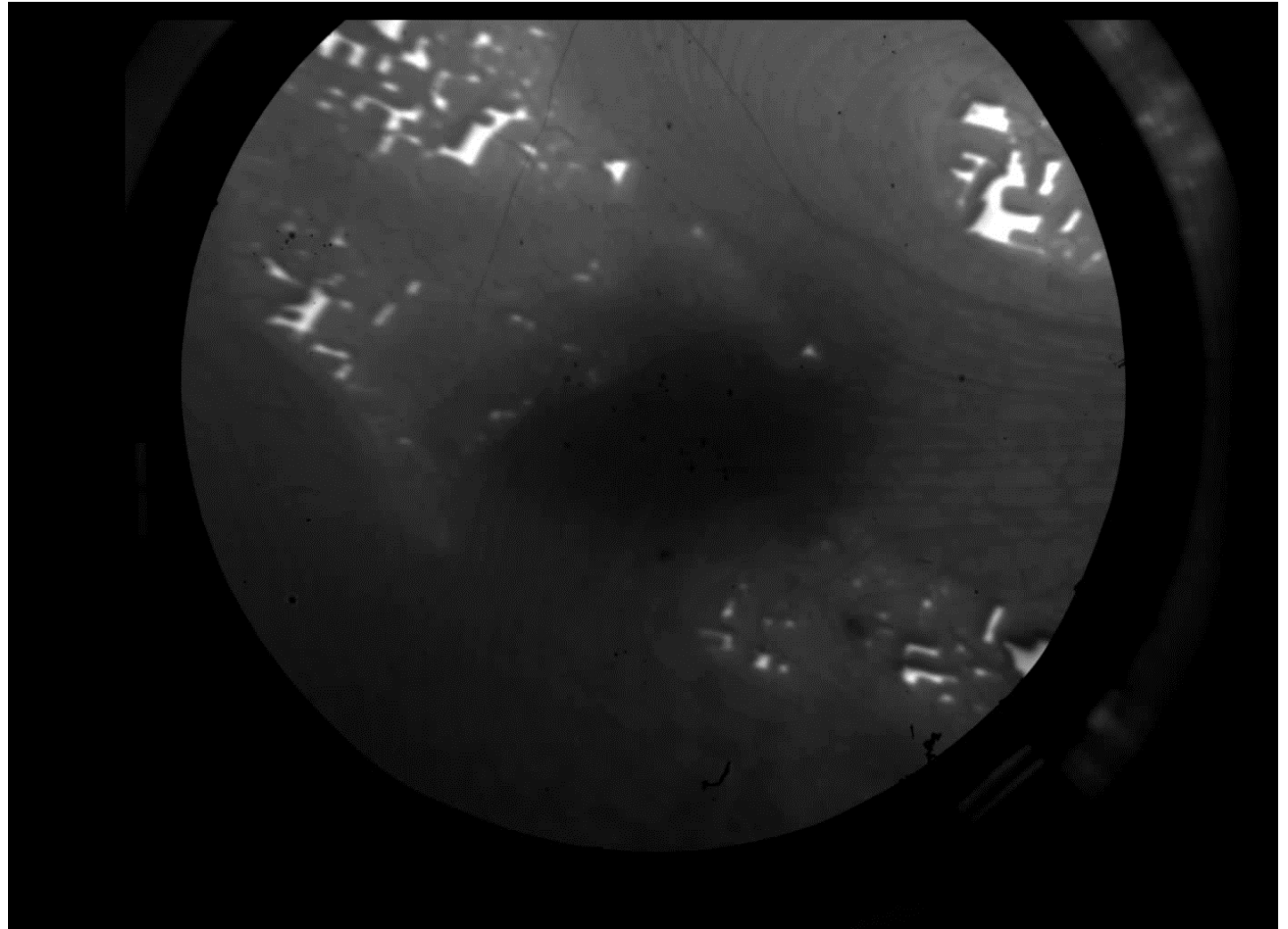
## 2.1 Principle of LEEM

Variation intermediate lens (IL) excitation enables switching between imaging the real space or the diffraction space



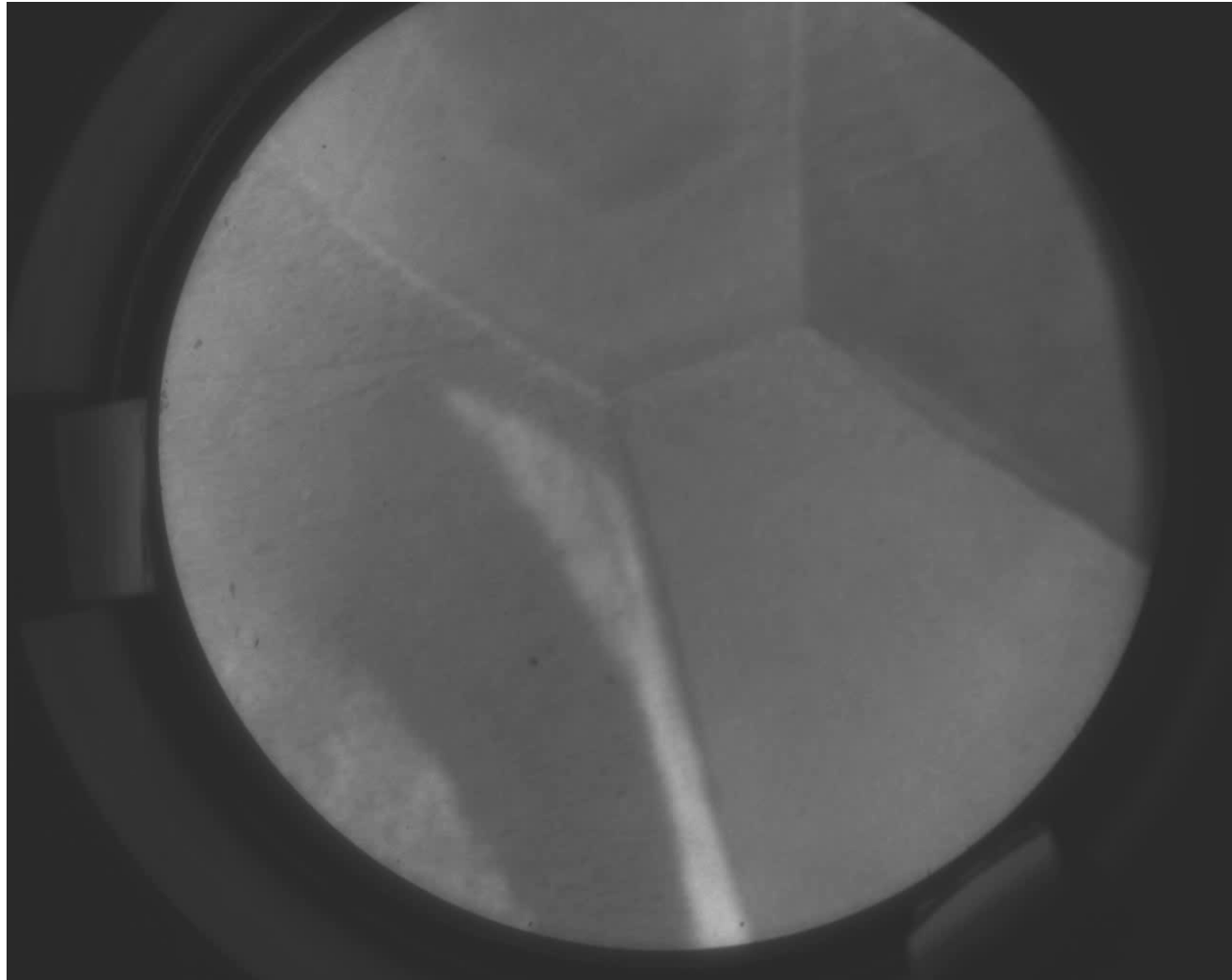
## 2.1 Principle of LEEM

- Example - oxidation of W(110)



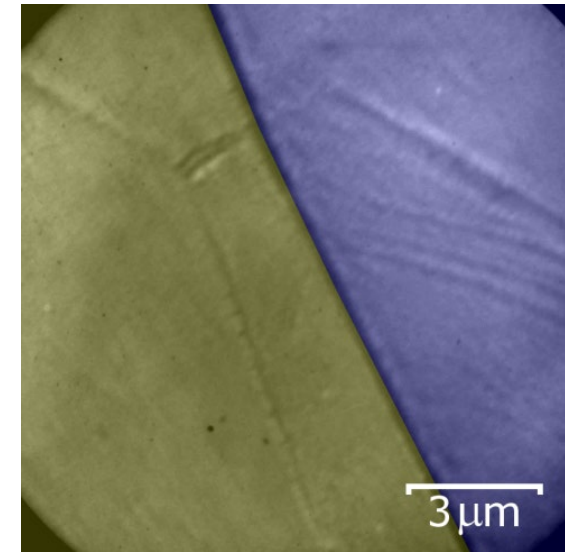
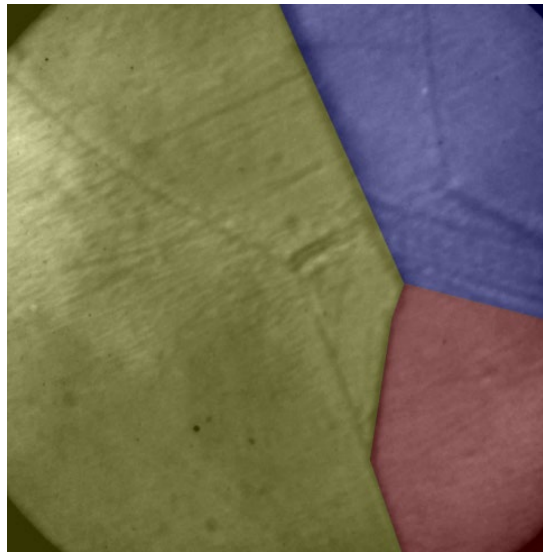
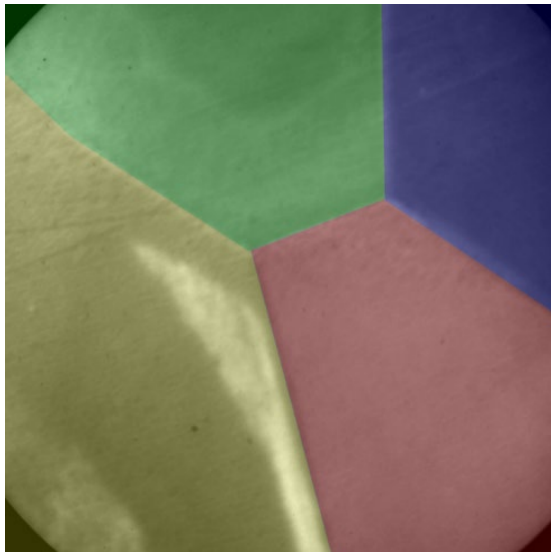
## 2.1 Principle of LEEM

- Example – grain coarsening in a Fe polycrystal ( $T \sim 500^\circ\text{C}$ )



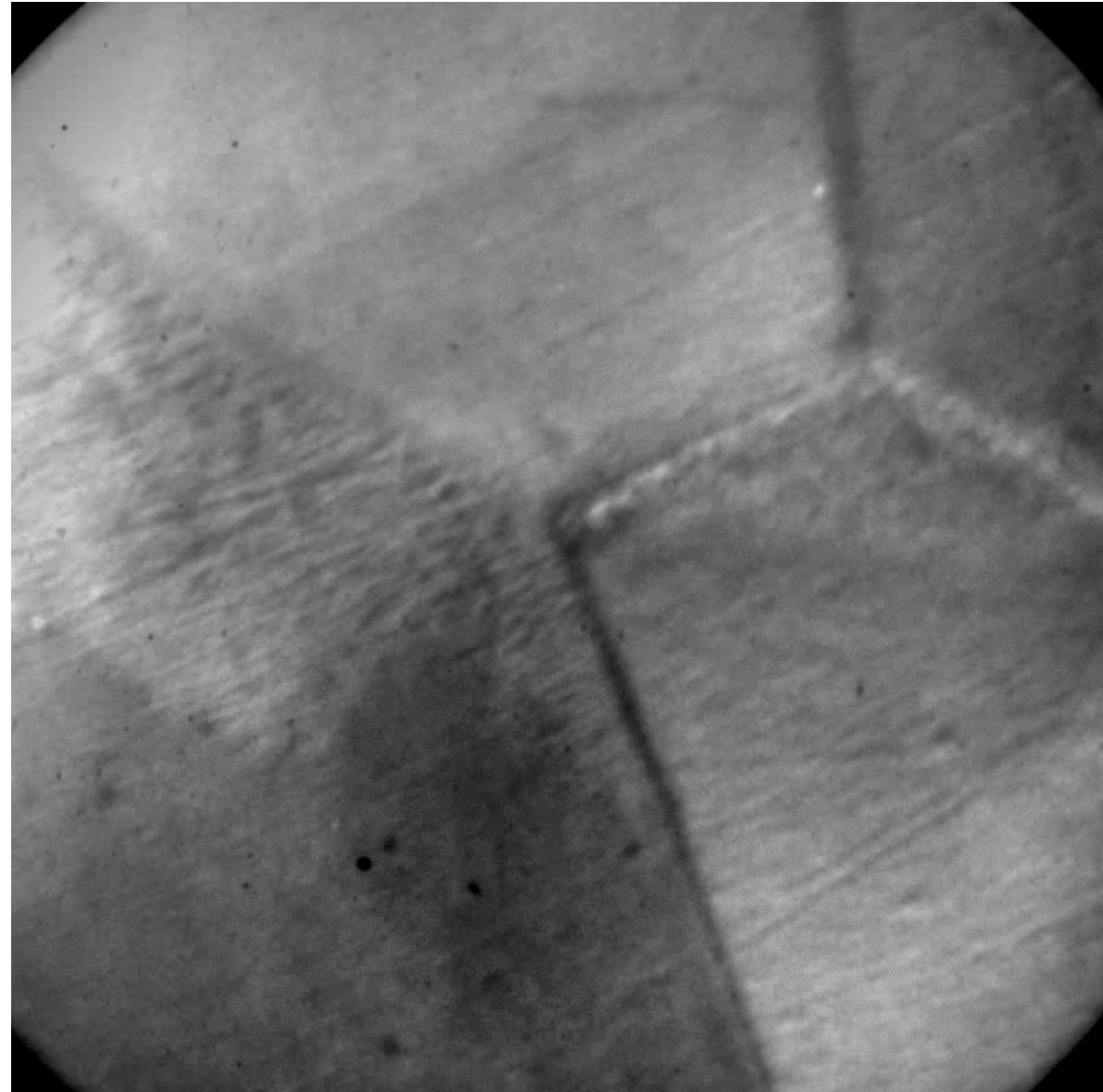
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## 2.1 Principle of LEEM

- Example – grain coarsening in a Fe polycrystal ( $T \sim 500^\circ\text{C}$ )





## 2.2 Low-energy electron diffraction (LEED)

### ■ Kinematic theory of electron diffraction

#### ■ Assumptions:

- Incoming (electron) wave stimulates emission of a spherical wave at a point  $P$  within the scattering volume
- fixed phase relation between incoming and scattered wave
- no multiple scattering events

#### ■ Amplitude $A_P$ of the incoming wave in $P$ :

- Amplitude at point  $B$  after the wave was scattered in  $P$ :

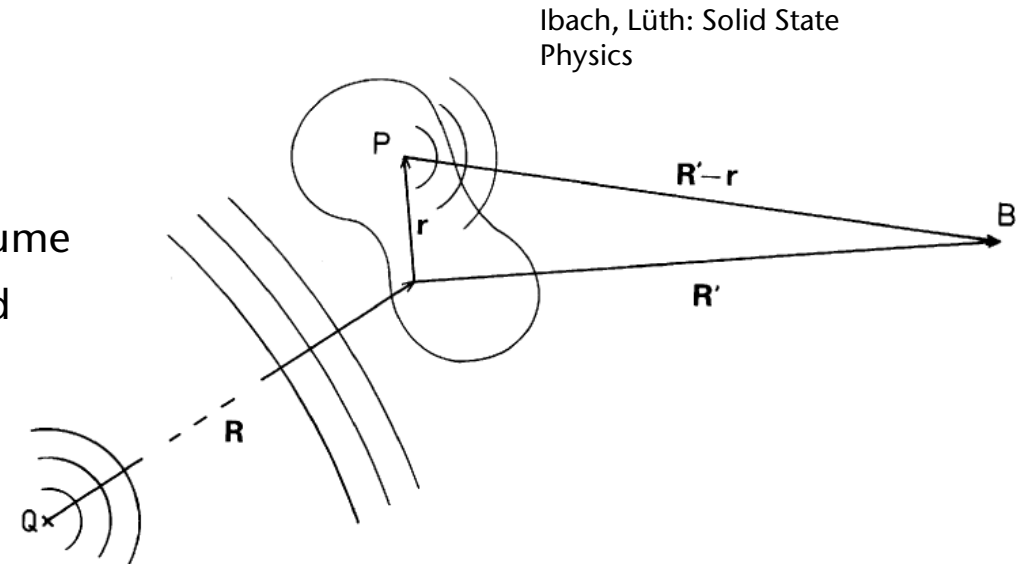
$$A_B(\vec{r}, t) = A_P(\vec{r}, t) \cdot \rho(\vec{r}) \cdot \frac{e^{ik|\vec{R}' - \vec{r}|}}{|\vec{R}' - \vec{r}|}$$

$\rho(\vec{r})$ : scattering density, describes amplitude and phase of the spherical wave starting in  $P$

- Overall amplitude in  $B$  by integration over whole scattering volume (at large distances  $R' \gg r$ ) :

$$A_B(t) \propto e^{-i\omega_0 t} \int \rho(\vec{r}) e^{i(\vec{k}_0 - \vec{k}) \cdot \vec{r}} d\vec{r}$$

gies

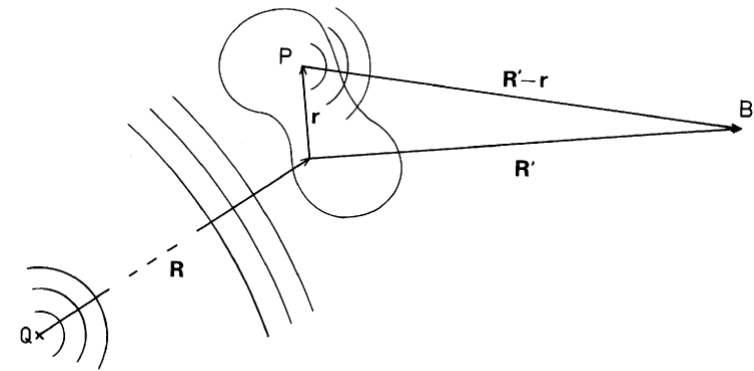


## 2.2 Low-energy electron diffraction (LEED)

- Kinematic theory of electron diffraction
  - For scattering at a crystal, the scattering density has the same spatial periodicity as the crystal structure
  - Fourier series:  $\rho(\vec{r}) = \sum_{\vec{G}} \rho_{\vec{G}} e^{i\vec{G} \cdot \vec{r}}$
  - $\rho(\vec{r})$  is lattice periodic, i.e.  $\vec{G} \cdot \vec{r}_n = m \cdot 2\pi$  for any lattice vector  $\vec{r}_n = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$  ( $\vec{a}_i$ : base vectors of the 3D lattice)
  - Can only be fulfilled if  $\vec{G} = h\vec{g}_1 + k\vec{g}_2 + l\vec{g}_3$  with  $\vec{g}_i \cdot \vec{a}_j = 2\pi\delta_{ij}$   $\left( \delta_{ij} = \begin{cases} 1, i = j \\ 0, i \neq j \end{cases} \right)$

**definition of the 3D reciprocal lattice**

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### ■ Kinematic theory of electron diffraction

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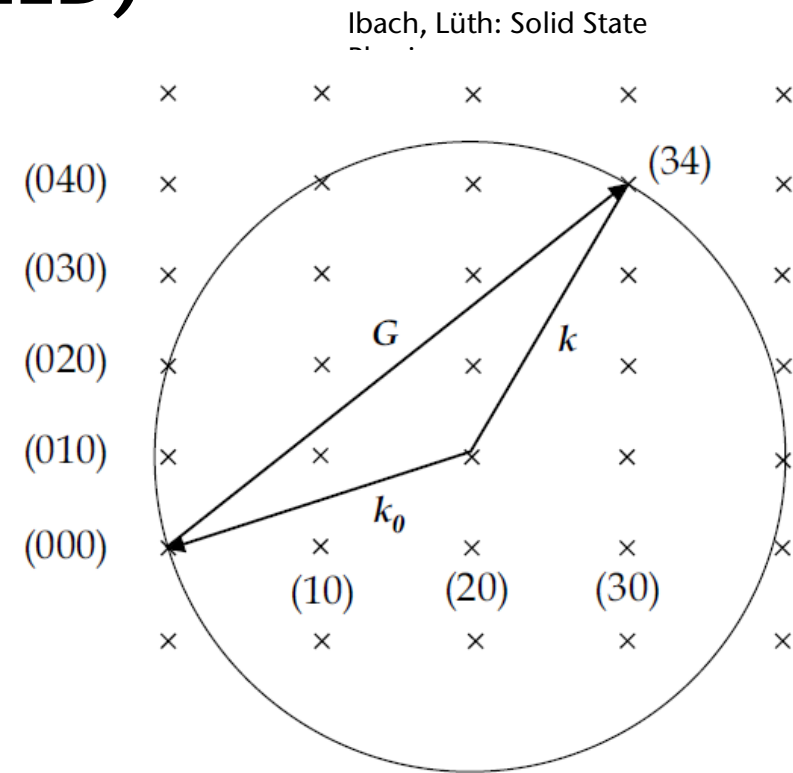
**definition of the 3D reciprocal lattice**

- Intensity of the scattered wave:  $I(\vec{K}) \propto |A_B|^2 \propto \left| \int \rho(\vec{r}) e^{-i(\vec{K} - \vec{k}_0) \cdot \vec{r}} d\vec{r} \right|^2$
- $I(\vec{K}) \neq 0$  only if  $\vec{k} - \vec{k}_0 = \vec{G}$

**Laue equation for elastic scattering at a periodic structure**

## 2.2 Low-energy electron diffraction (LEED)

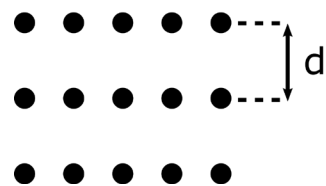
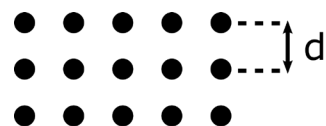
- Geometric interpretation: Ewald construction  
 $\mathbf{k}_0$ : incoming electron  
 $\mathbf{k}$ : scattered electron  
 $\mathbf{G}$ : reciprocal lattice vector
- Kinetic energy of an electron  $E = \frac{\hbar^2 k^2}{2m_e}$
- Elastic scattering: endpoints of  $\mathbf{k}$  and  $\mathbf{k}_0$  lie on the Ewald sphere
- Laue condition  $\mathbf{k} - \mathbf{k}_0 = \mathbf{G}$  is fulfilled where Ewald sphere goes through a point of the reciprocal lattice



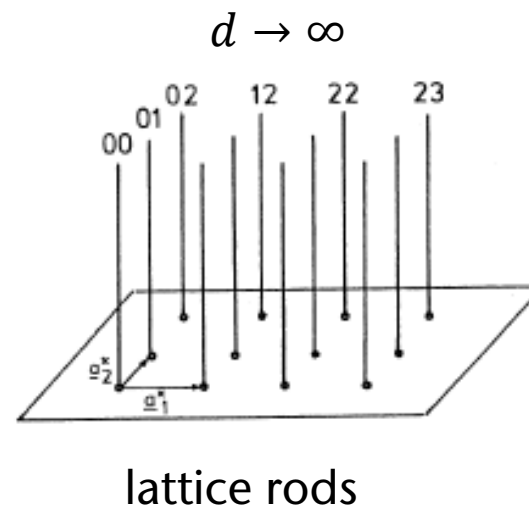
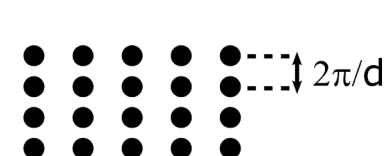
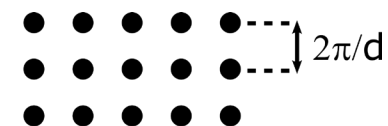
## 2.2 Low-energy electron diffraction (LEED)

- 2D Ewald construction
  - Surface can be interpreted as a „dilute“ crystal in z-direction

real space



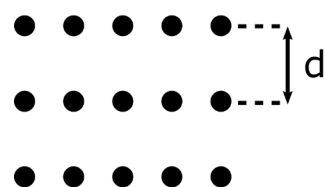
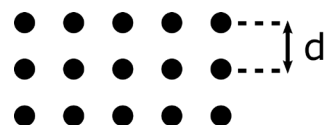
recip. space



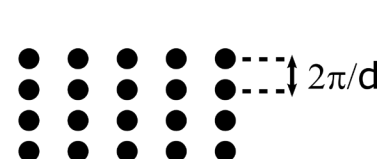
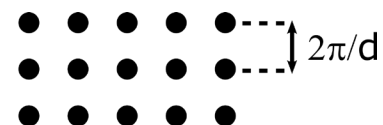
## 2.2 Low-energy electron diffraction (LEED)

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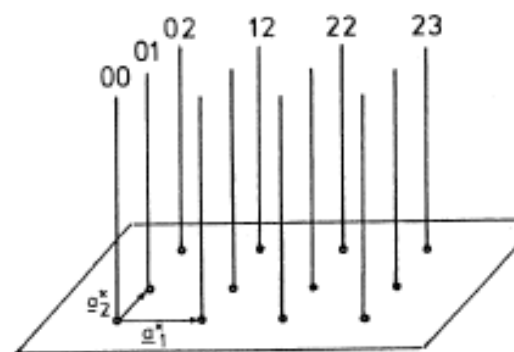
real space



recip. space

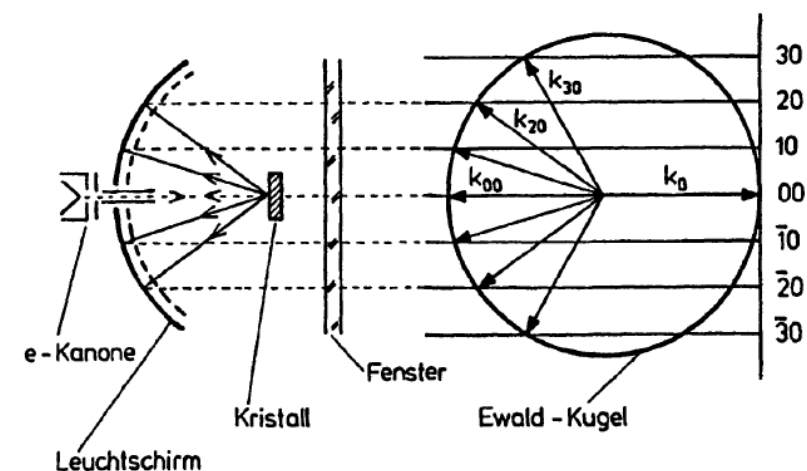


$d \rightarrow \infty$



lattice rods

LEED - System

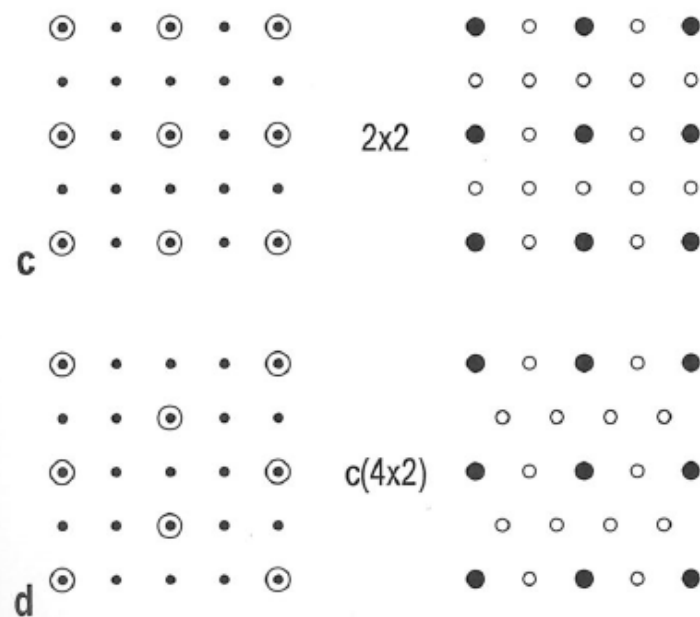
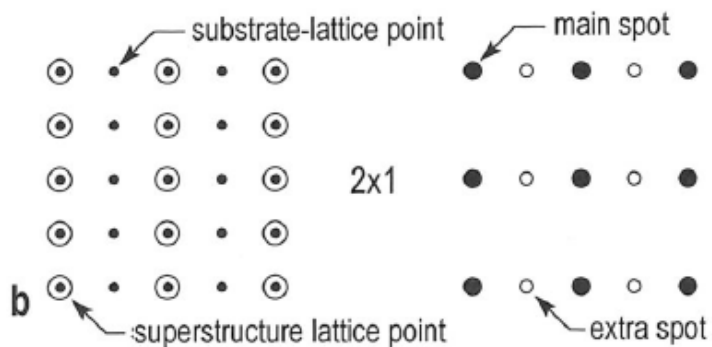
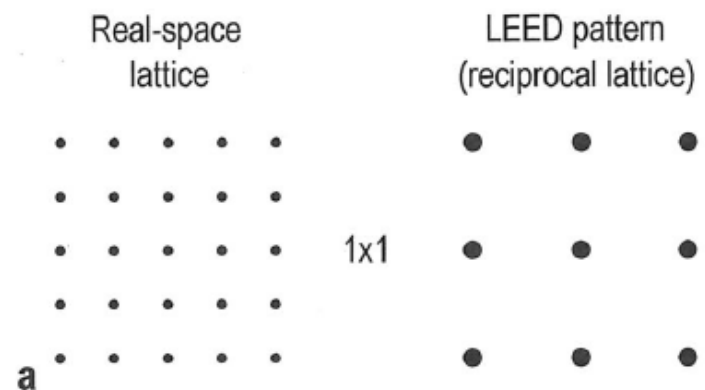


Henzler, Göpel: Oberflächenphysik des Festkörpers



## 2.2 Low-energy electron diffraction (LEED)

- LEED at adsorbate superstructures



## 2.2 Low-energy electron diffraction (LEED)

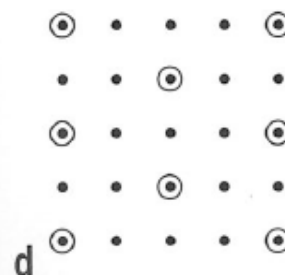
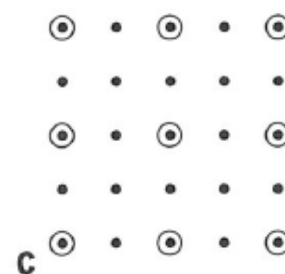
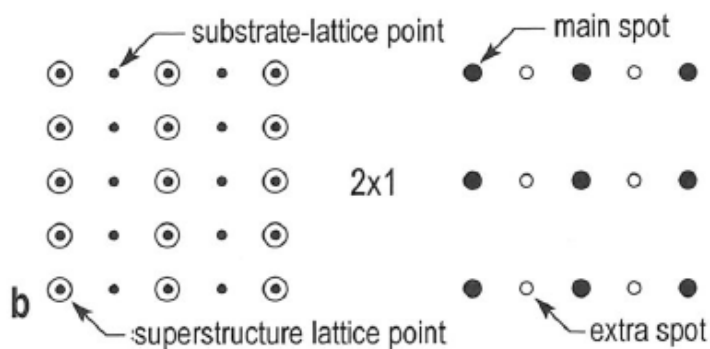
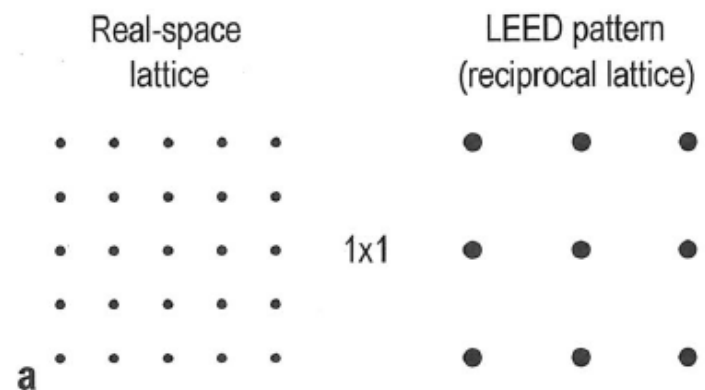
- LEED at adsorbate superstructures

definition  $\vec{g}_i \cdot \vec{a}_j = 2\pi\delta_{ij}$  leads to construction rule for 2D reciprocal lattice:

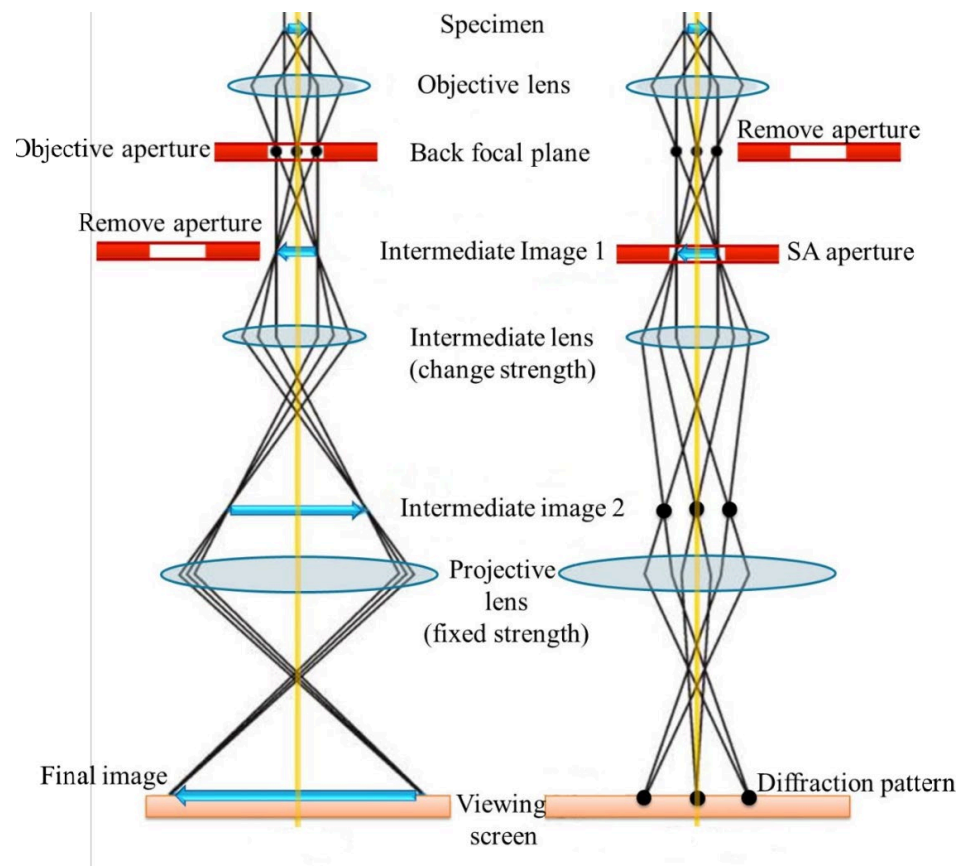
$$\vec{g}_1 = 2\pi \cdot \frac{\vec{a}_2 \times \vec{n}}{|\vec{a}_1 \times \vec{a}_2|}$$

$$\vec{g}_2 = 2\pi \cdot \frac{\vec{n} \times \vec{a}_1}{|\vec{a}_1 \times \vec{a}_2|}$$

$\vec{n}$ : surface normal vector



## 2.3 $\mu$ LEED and dark-field imaging with LEEM

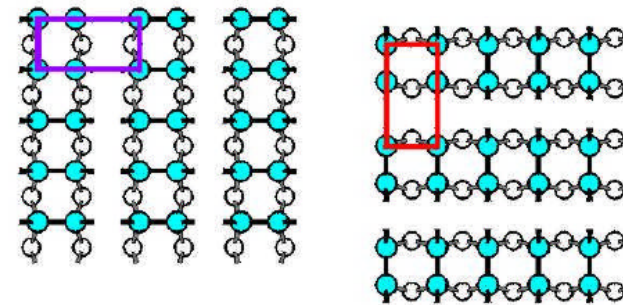
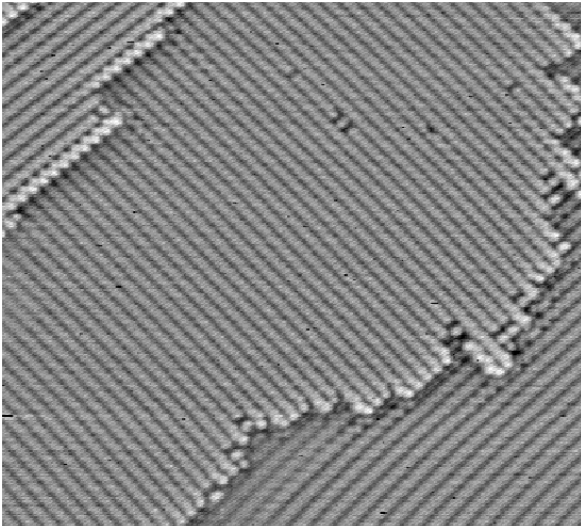


- Objective lens forms a diffraction pattern in the back focal plane and a slightly magnified intermediate image
- Focal length of intermediate lens is variable
  - Either the real image or the diffraction pattern can be imaged on the detector screen
- A selected area aperture can reduce the field of view on the sample
  - electron diffraction with lateral resolution possible ( $\mu$ LEED)

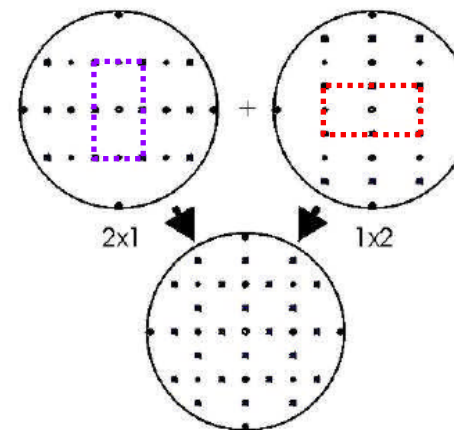
## 2.3 $\mu$ LEED and dark-field imaging with LEEM

- Dark-field imaging

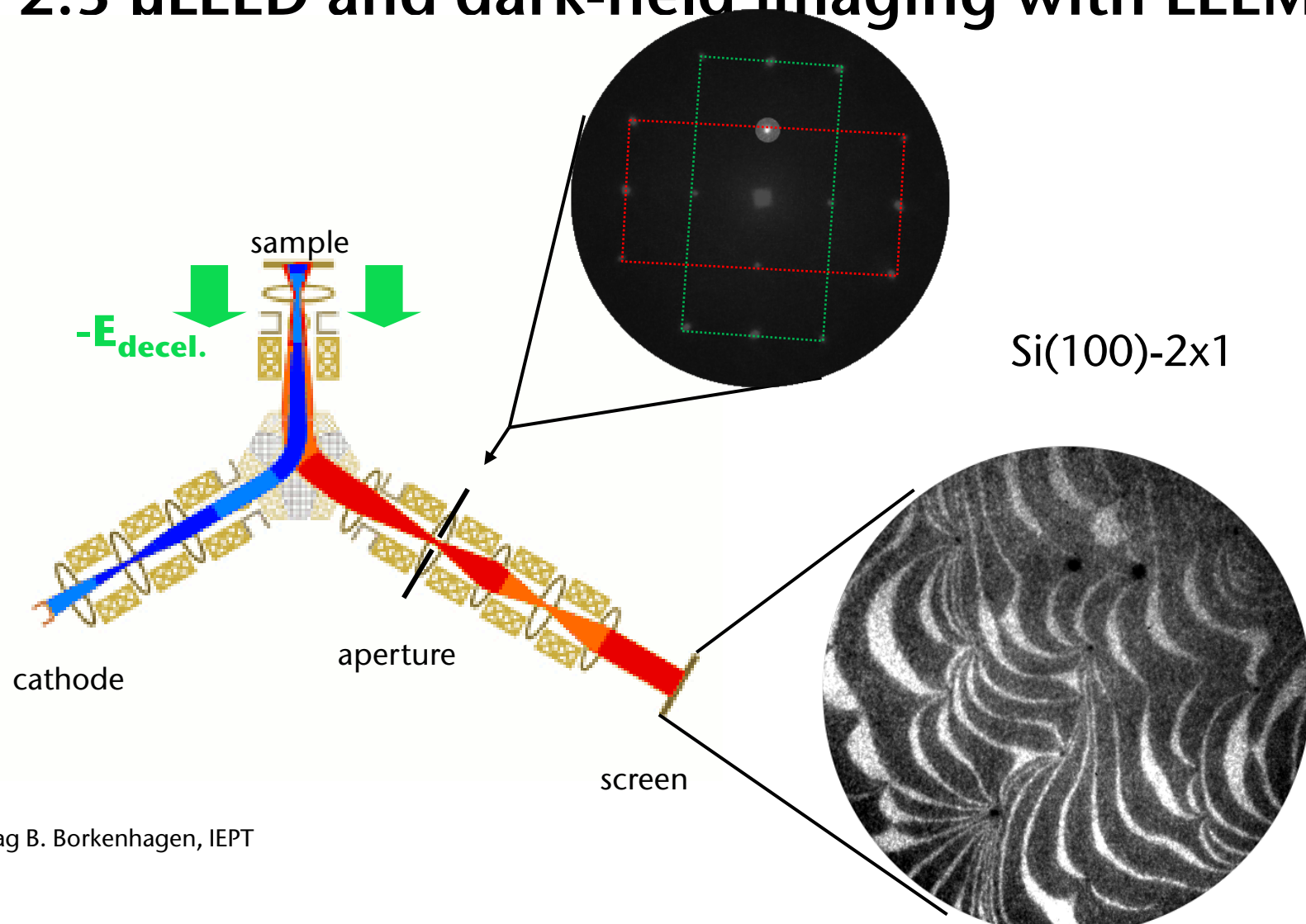
Scanning tunneling microscope (STM) image of a Si(100) surface



(2x1) and (1x2)

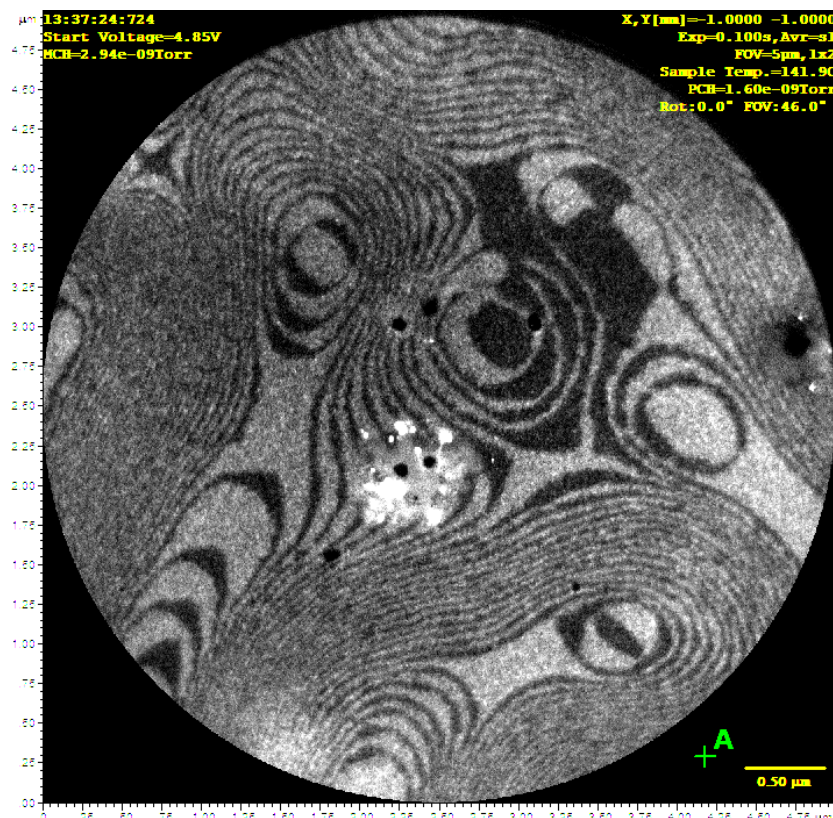


## 2.3 $\mu$ LEED and dark-field imaging with LEEM

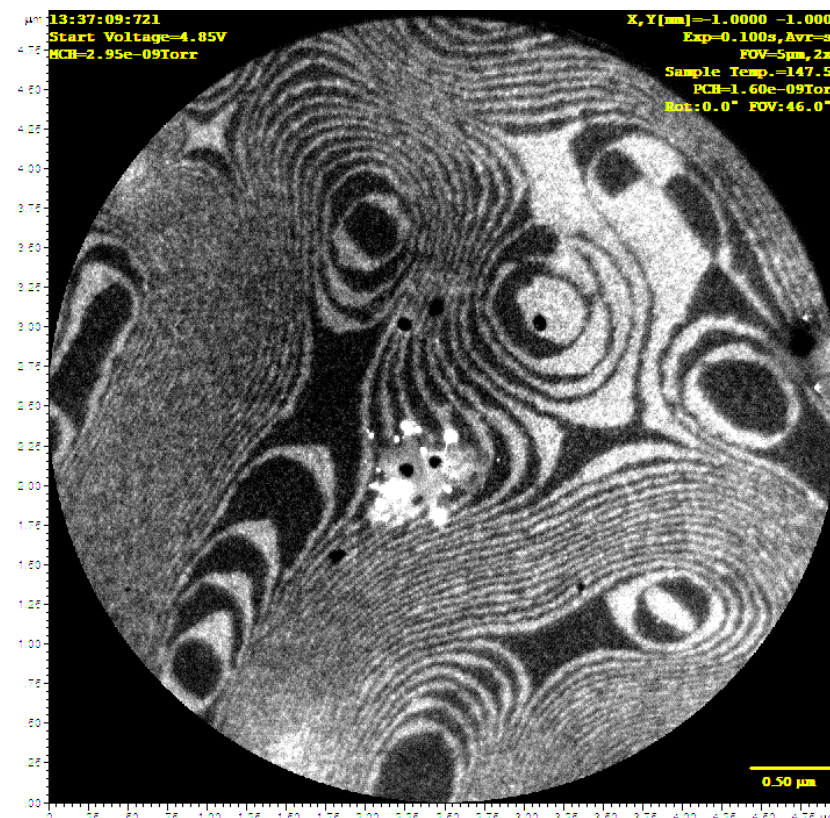




## 2.3 $\mu$ LEED and dark-field imaging with LEEM



Si(100)-2x1



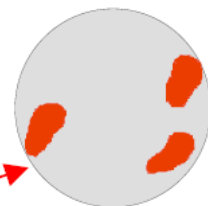
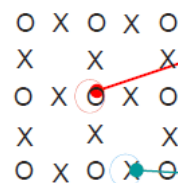
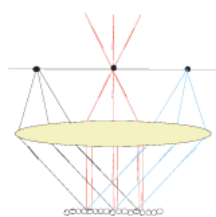
Si(100)-1x2

Dark field LEEM  
Ø Field of view: 5 µm



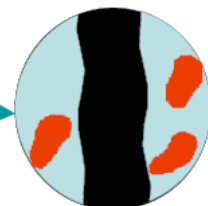
## 2.4 Contrast mechanisms in LEEM

LEED  
Diffraction  
Pattern

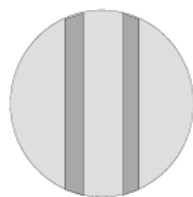
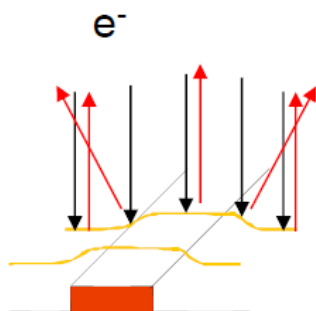


Bright Field  
Imaging

with zeroth order spot,  
contrast determined by  
reflexion coefficient



Dark Field Imaging  
with higher order spot,  
contrast by domains  
with different symmetry



Mirror Electron Microscopy (MEM)

very low energy of primary electrons,  
electrons are reflected before they reach the  
sample,  
high sensitivity to small steps at the surface