Introduction to electron microscopy

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The lecture was created for courses on Polymer Morphology.
Great majority of information in this lecture holds for non-polymeric materials as well.

Focus of the lecture:

(1) definition of basic terms: microscopy, morphology
(2) basic theory: geometrical/ray optics, wave optics, Bragg Law
(3) freeware microscopic programs for the rest of the course: ImageJ and Python/Jupyter
(4) examples: how is the theory connected with real life – throughout the lecture

Background of the slides:

blue = theory; green = examples; yellow = calculations; grey = supplements

Micrographs in this lecture:

(Almost) all micrographs in this lecture come from our laboratory + majority of samples from IMC ⇒ we can discuss/collaborate on whatever will be shown in the presentation.

Part 1

Microscopy in materials science

Contents

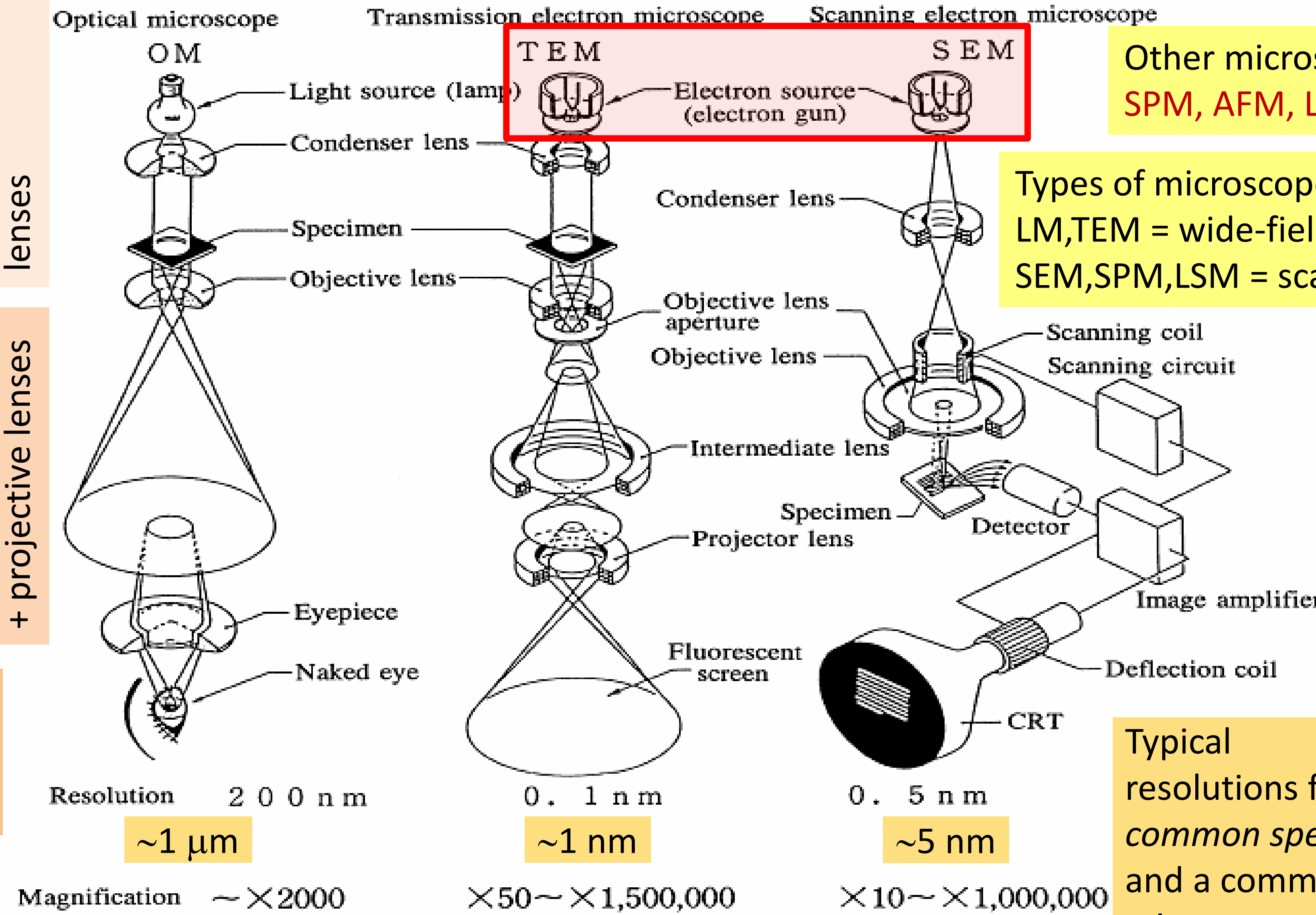
- What are the basic types of microscopes?
- What are the length scales studied by microscopic methods?
- Why do we need microscopy in materials science and engineering?
- What will you learn in this course?

Microscopy :: Types of microscopes.

source of light/e⁻ with condenser lenses

imaging part with objective + projective lenses

detector



~1 µm

~1 nm

~5 nm

Other microscopes
SPM, AFM, LSM...

Types of microscopes:
LM,TEM = wide-field
SEM,SPM,LSM = scanning

Typical resolutions for a *common specimen* and a common microscope

LM = Light Microscope TEM microscope SEM microscope

Microscopy vs. other methods :: Length scales.

Methods x dimensions, structure, microstructure, and nanostructure

Light microscopy					LSM, LS				LM
Scanning electron microscopy							FEGSEM		SEM
		Transmission electron microscopy						HRTEM,ED	TEM
		Atomic force microscopy / Scanning probe microscopy						STM	SPM
					SAXS			WAXS	XRD
10	1	0.1	0.01	0.001	0.0001	0.00001	0.000001	0.0000001	mm
10000	1000	100	10	1	0.1	0.01	0.001	0.0001	um
10000000	1000000	100000	10000	1000	100	10	1	0.1	nm
structure		microstructure			nanostructure			atoms	structure

Selected polymer structures & their typical dimensions.

polymer foams		polymer spherulites			crystalline lamellae			atomic structure	
				polymer blends		copolymers		of polymer	
(macro)composites		polymer (micro)composites			polymer nanocomposites			crystals	

- **Microscopic methods** are focused on morphology =
  = phase structure = supermolecular structure = micro/nanostructure
- **Diffraction methods** are focused mostly on crystal structure
  (although SAXS is used to investigate nanostructures)
- **Spectroscopic** are focused mostly on molecular structure (IR, UV/vis, NMR, ESR...)
- **Other methods** aim at thermal (DSC, TGA...) or mechanical properties (tensile tests...)

Note: morphology starts above 1 nm:
$\Rightarrow$ no atoms
$\Rightarrow$ no HRTEM...

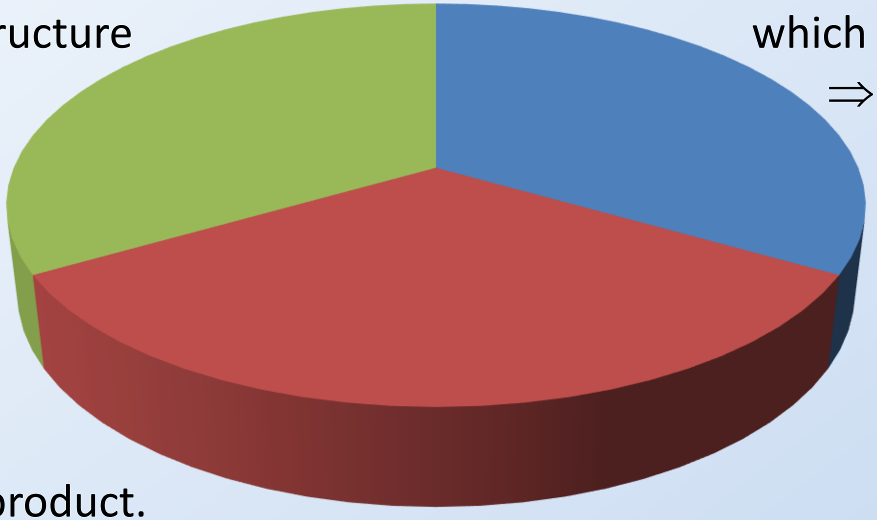
Microscopy in materials science :: Why is it used?

- Properties of a product are given by: composition, processing, and design.
- Experienced engineers claim that the above three factors have the same weight ~ 1/3.

What influences properties of a final product?

Composition:
Includes both chemical composition and micro/nanostructure = morphology.
⇒ morphology is studied by **microscopy**

Processing:
Influences micro/nanostructure, which impacts on properties.
⇒ micro/nanostructure is studied by **microscopy**



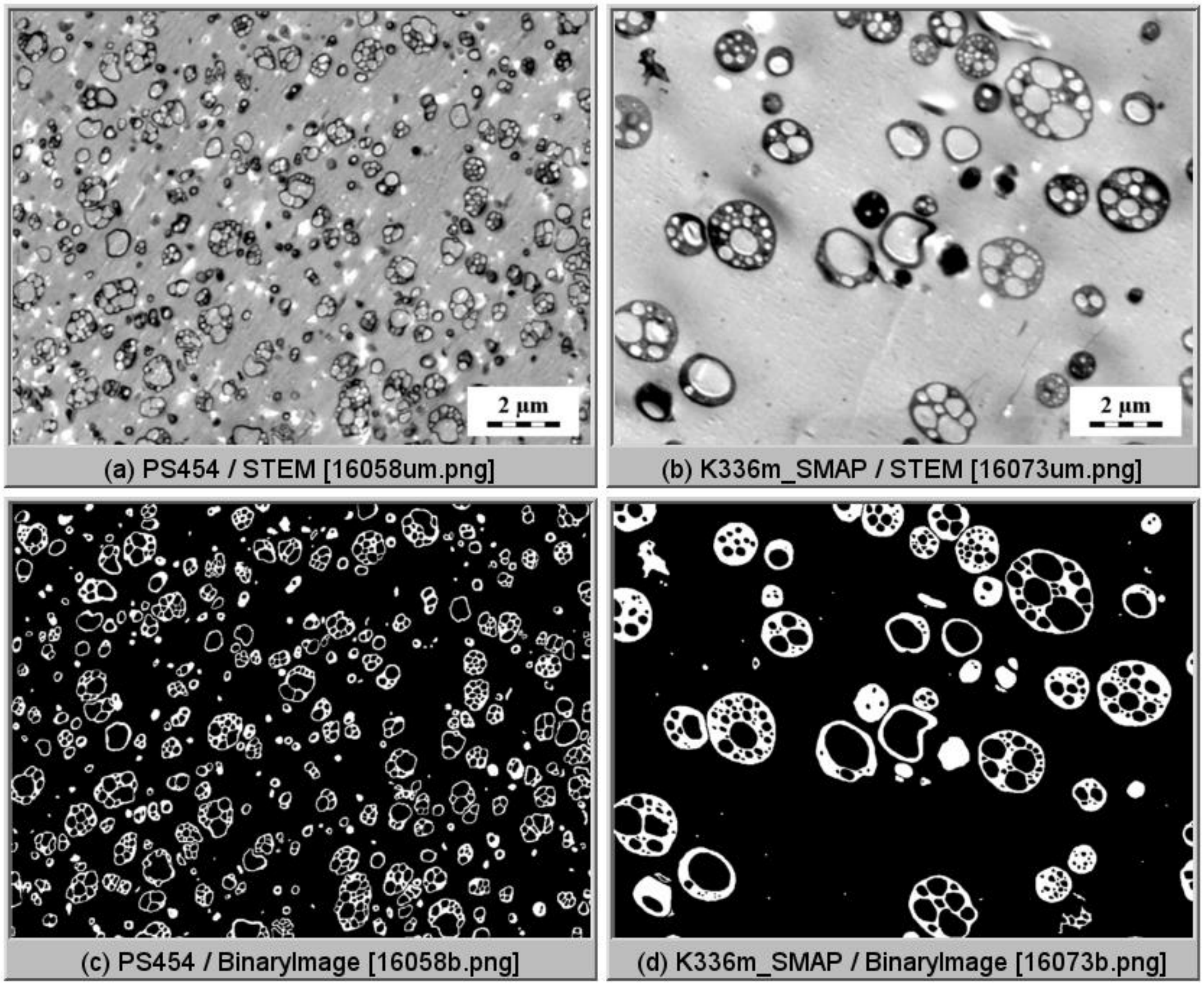
Design:
This means size and shape of the product.
Trivial example: Insufficient stiffness can be improved by preparing bigger component.
⇒ specific design may need specific processing → impact on morphology → **microscopy**

- **Conclusion**: *microscopy is used* to characterize materials and *find the correlations among composition, processing, morphology and properties of materials*.

Numerous correlations [morphology-properties] will be shown during the course.

Morphology & properties ::

Example: HIPS (part 1 - morphology)



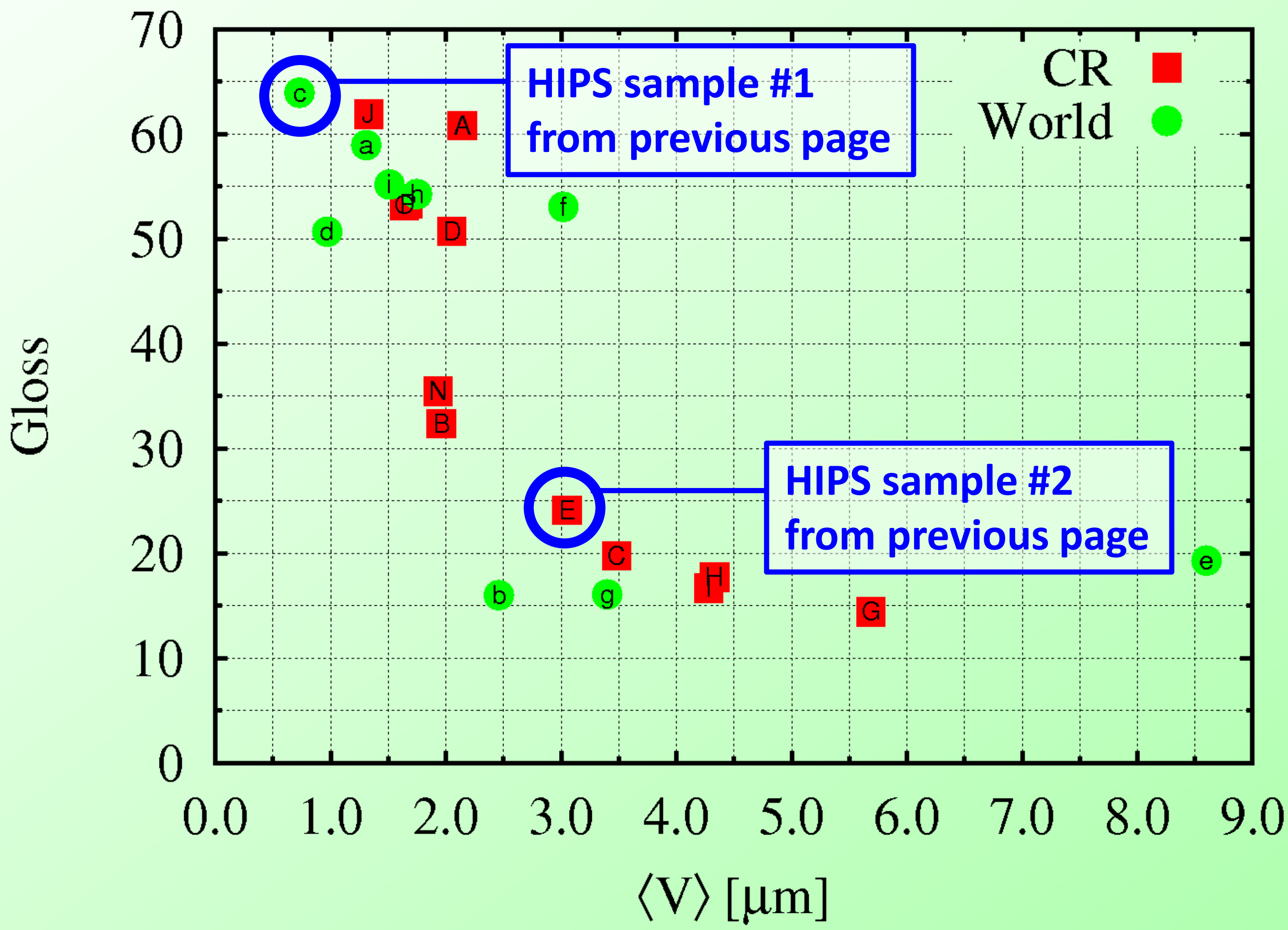
(a) PS454 / STEM [16058um.png]
(b) K336m_SMAP / STEM [16073um.png]
(c) PS454 / BinaryImage [16058b.png]
(d) K336m_SMAP / BinaryImage [16073b.png]

Notes:
1) HIPS is a common copolymer of PS and BP.
2) Year production of PS ≈ 20 megatons.
3) From 1960, more than 50% of PS is in the form of HIPS.
4) These two HIPS polymers have the same chemical composition and differ only in morphology.
5) HIPS morphology is strongly influenced by processing technology.
6) Physical properties are VERY different
⇒ see next slide.

STEM micrographs and binary images of various high-impact polystyrenes.

Morphology & properties ::

Example: HIPS (part 2 - properties)



Conclusion:

1) All points in the graph represent high-impact polystyrenes (HIPS) with more-or-less the same chemical composition.

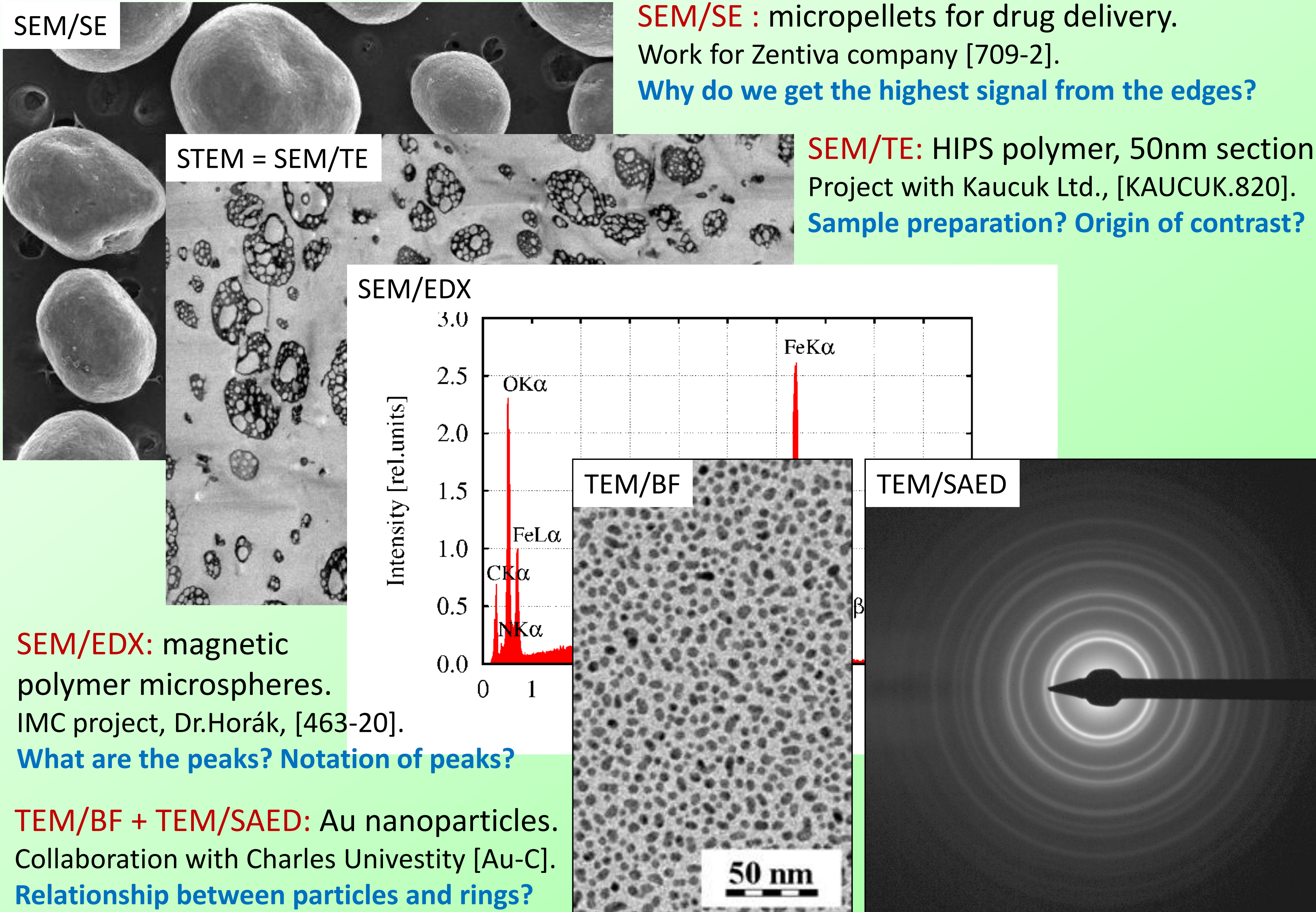
2) Although the chemical composition is the same, the morphology and properties are very different.

Gloss of high-impact polystyrenes as a function of particle size.

Source: IMC, Dept. of Polymer morphology, research report for company SYNTHOS.

The strong correlations between morphology and properties = reason for EM studies.

Sample micrographs :: What will you learn in this course?



SEM/SE : micropellets for drug delivery.
Work for Zentiva company [709-2].
Why do we get the highest signal from the edges?

SEM/TE: HIPS polymer, 50nm section.
Project with Kaucuk Ltd., [KAUCUK.820].
Sample preparation? Origin of contrast?

SEM/EDX: magnetic polymer microspheres.
IMC project, Dr.Horák, [463-20].
What are the peaks? Notation of peaks?

TEM/BF + TEM/SAED: Au nanoparticles.
Collaboration with Charles Univestity [Au-C].
Relationship between particles and rings?

Part 2

Brief revision of optics (for microscopists)

Contents

- ❖ Elements of geometrical/ray optics needed to understand EM.
- ❖ Elements of physical/wave optics needed to understand EM.
- ❖ Elements of diffraction:
  - Brief revision of diffraction as taught at secondary schools
  - Simple and important formula: Bragg's Law = BL
  - Basics of Kinematic diffraction theory = KDT
    (including justification of the basic formula of KDT)

Optics :: Main branches

Optics

Geometrical/ray optics

Approximation: photons and electrons are rays.

What can be explained: reflection, refraction, mirrors, lenses...

Note: Basics of ray optics are even in Physics at primary schools.

Physical/wave optics

Approximation: photons and electrons are waves.

What can be explained:

Secondary school: Huygens principle, simple/model experiments...

University: diffraction theory, general experiments, Fourier transform...

(the basics of geometrical and physical optics for microscopy $\rightarrow$ see next slides

(electromagnetic and quantum optics $\rightarrow$ not in this course

Electromagnetic optics

Photons and electrons are electromagnetic waves.

- Physical/wave optics: the wave described by one scalar function of space and time - $\Psi(\mathbf{r},t)$.
- Electromagnetic optics: the electromagnetic field described by two related vector fields, the electric field $\mathbf{E}(\mathbf{r},t)$ and the magnetic field $\mathbf{H}(\mathbf{r},t)$ $\rightarrow$ Maxwell's equations etc...

Quantum optics...

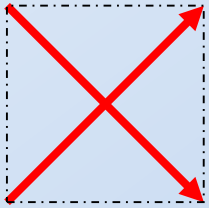
Optics :: Ray optics :: Axioms

Ray optics approximation: the photons/electrons are immaterial and non-interacting rays.

The geometrical/ray optics can be based four axioms:

[1] Rectilinear propagation of rays.
The light in homogeneous medium propagates linearly.
Real world: A beam from a torch light does not go behind the corner.

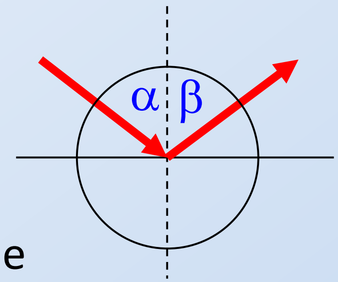
[2] Independence of rays.
Several rays can propagate through the same location independently.
Real world: Two beams from two torches do not bump into each other .



[3] Law of reflection: $\alpha = \beta$.
When a ray strikes a mirror, it is reflected:

- angle of incidence equals to angle of reflection
- incident ray, reflected ray and normal to the surface of the mirror lay in the same plane

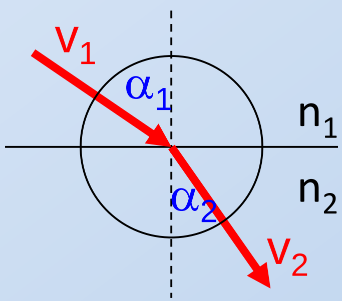
Real world: In the morning you can see your face in the mirror.



[4] Law of refraction (Snell's law = Snellius law):
$\sin(\alpha_1)/\sin(\alpha_2) = v_1/v_2 = n_2/n_1$

- (v_1, v_2) = velocities of light in media (1,2)
- (n_1, n_2) = refractive indexes in media (1,2)

Real world: A pencil partially submerged in the glass of water looks as if it was broken.




A bending pencil experiment

Optics :: Ray optics :: Lenses

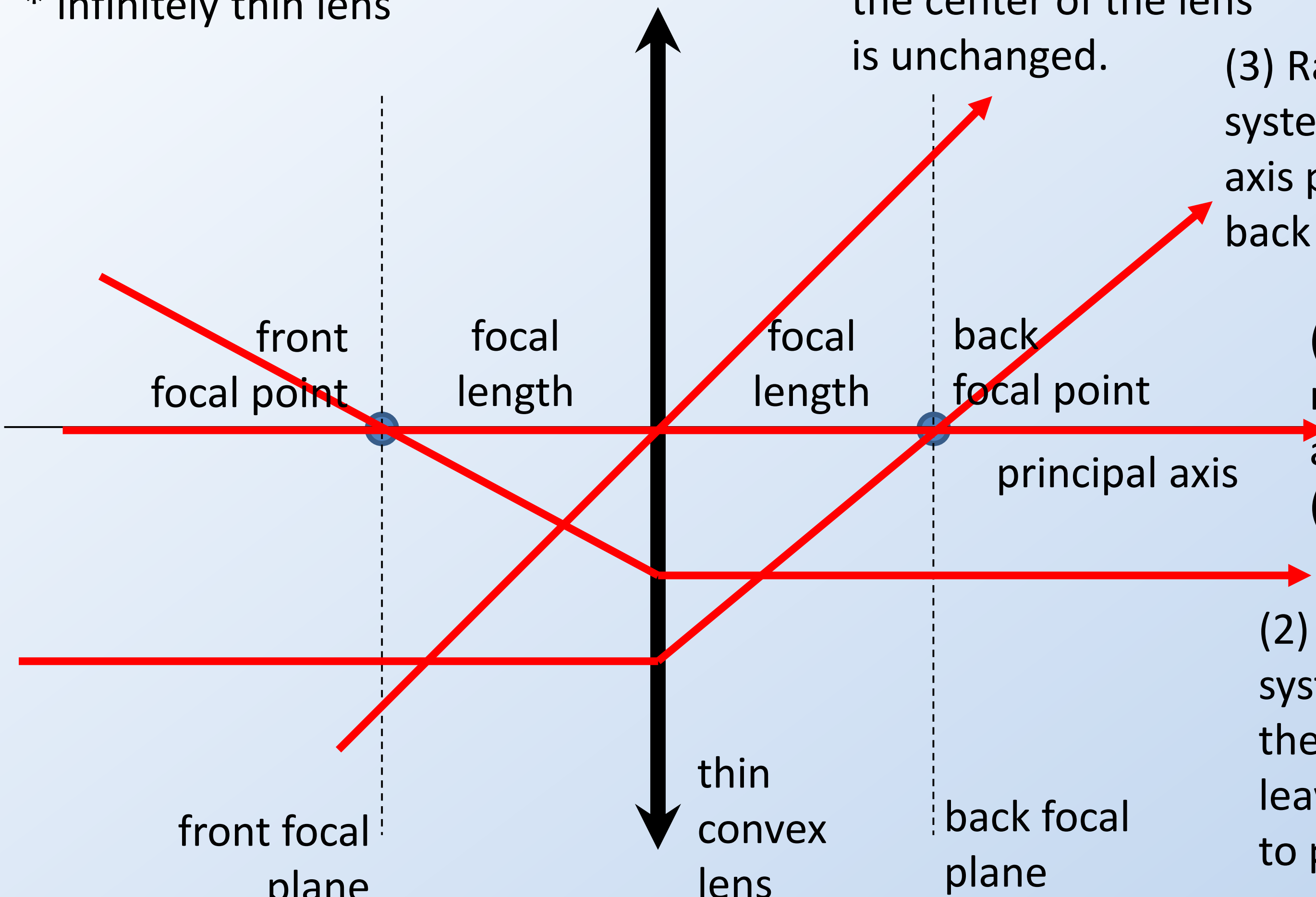
In the following slides just one case important for microscopy:
convex lens + object outside the focal length.

Note: rays (1,2,3) = principal rays.

* paraxial approximation
* infinitely thin lens

(1) The ray passing through the center of the lens is unchanged.

(3) Ray that enters the system parallel to principal axis passes through the back focal point.

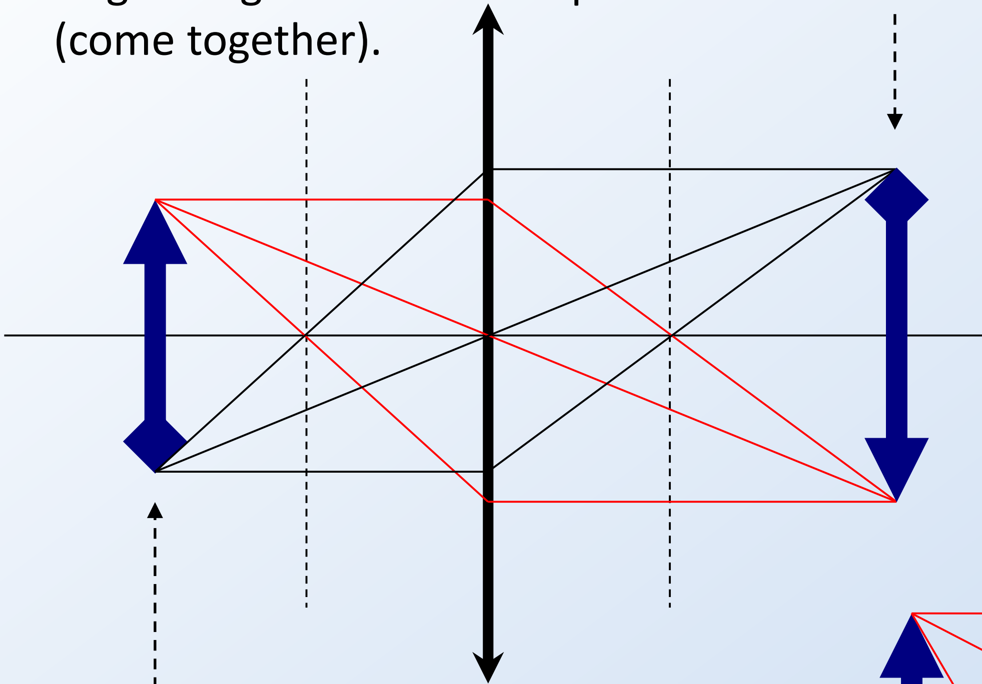


(0) Special case: ray in the principal axis passes unchanged (straight through).

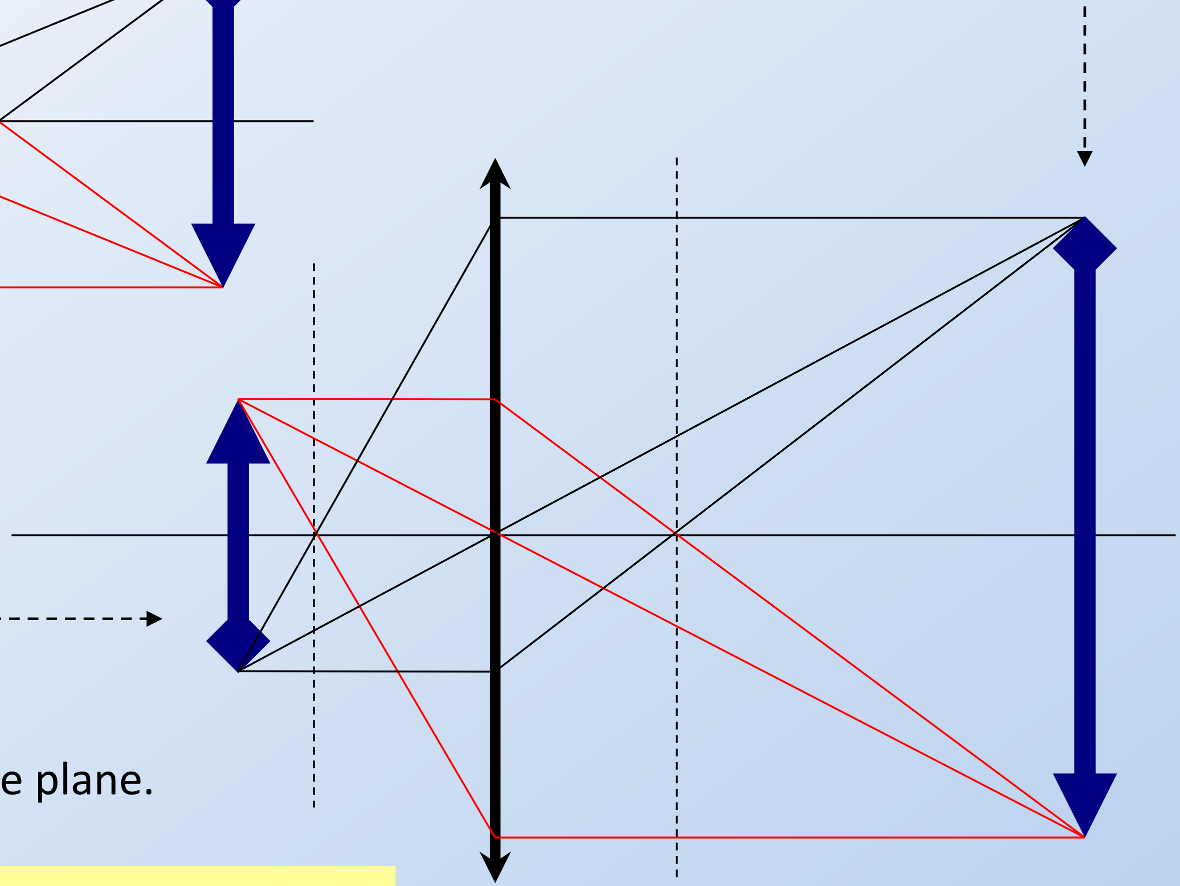
(2) Ray that enters the system passing through the front focal point leaves the lens parallel to principal axis.

Optics :: Ray optics :: Lenses and real images

Real image is formed at location, where the (principal) rays originating from the same point are focused (come together).



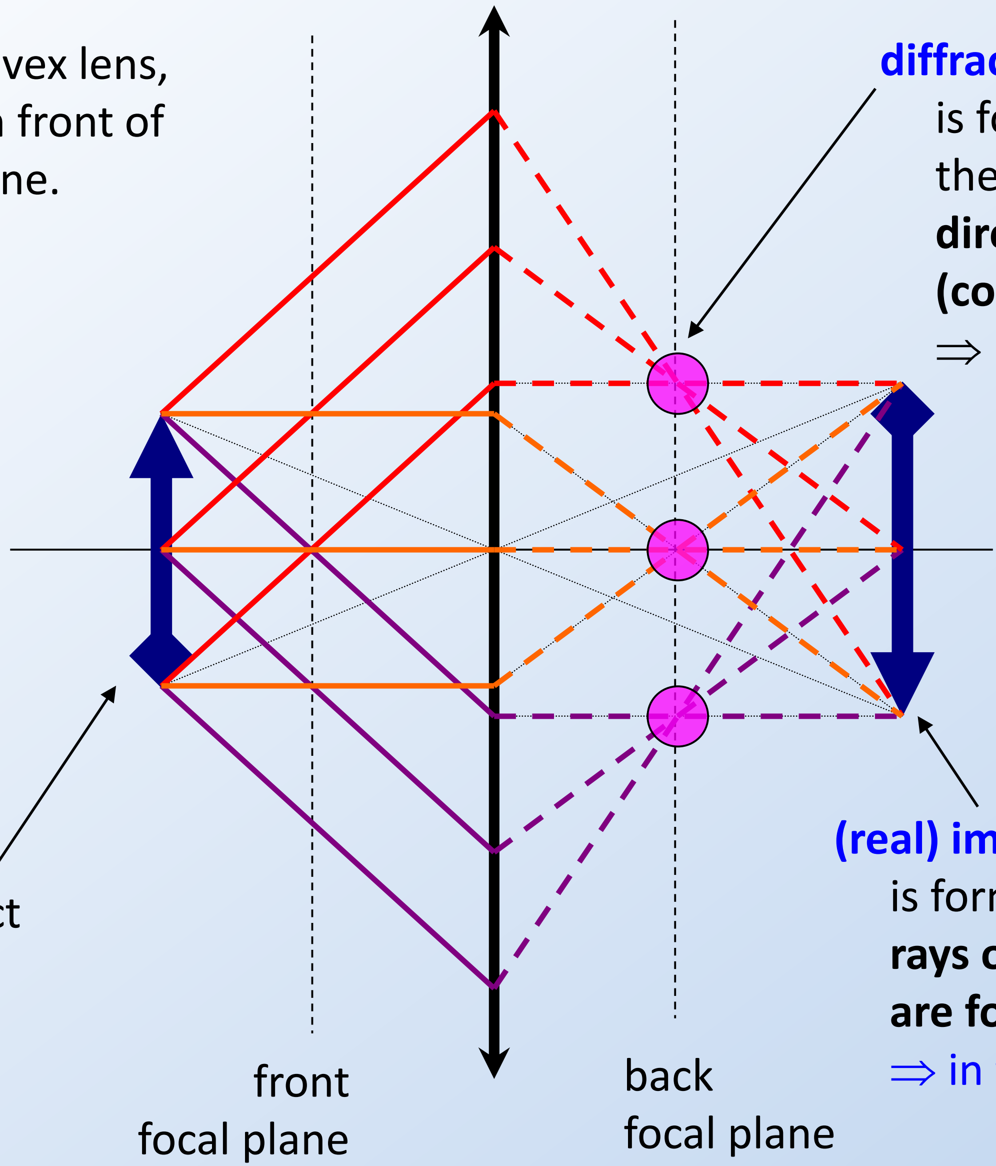
If the object is outside the focal length (= in front of the focal point/plane) the image is behind the back focal point/plane = in the image plane.



The closer the object is to the front focal plane, the more distant and larger is the image formed in the image plane.

Note: these procedures/diagrams are called ray-tracing.

Thin convex lens, object in front of focal plane.

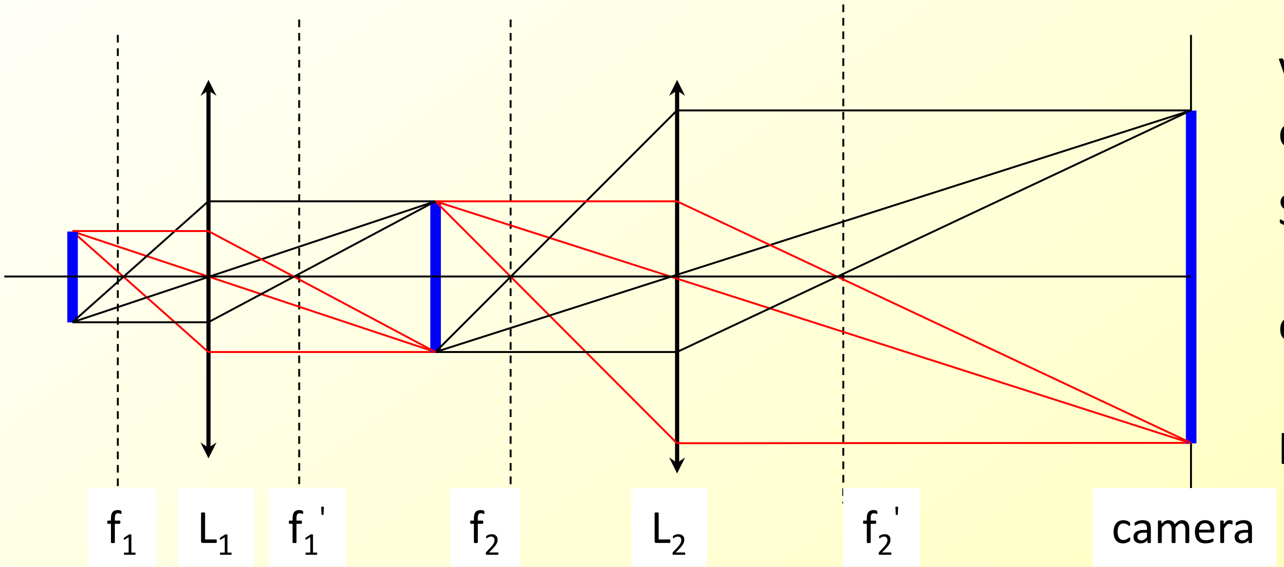


diffraction image (or pattern)
is formed at the location where the **rays passing in the same direction are focused (come together)**
⇒ in back focal plane

(real) image
is formed at the location where the **rays originating in the same place are focused (come together)**
⇒ in the image plane

Example 1 :: Ray optics :: Formation of an image in TEM (and LM).

Demo that we can draw the scheme of a TEM/LM microscope based only on ray optics.



Very simplified scheme of a TEM/LM microscope:

Sample is illuminated by parallel rays (elns/light)
objective lens L_1 makes a real image ,
projective lens L_2 makes the final image.

Thick black line = sample and its images.
L_1 = the 1st lens = objective lens (both in LM and TEM)
f_1 = front focal plane of L_1
f_1' = back focal plane of L_1
L_2 = the 2nd lens = projective lens (in LM also eyepiece)
f_2 = front focal plane of L_2
f_2' = back focal plane of L_2

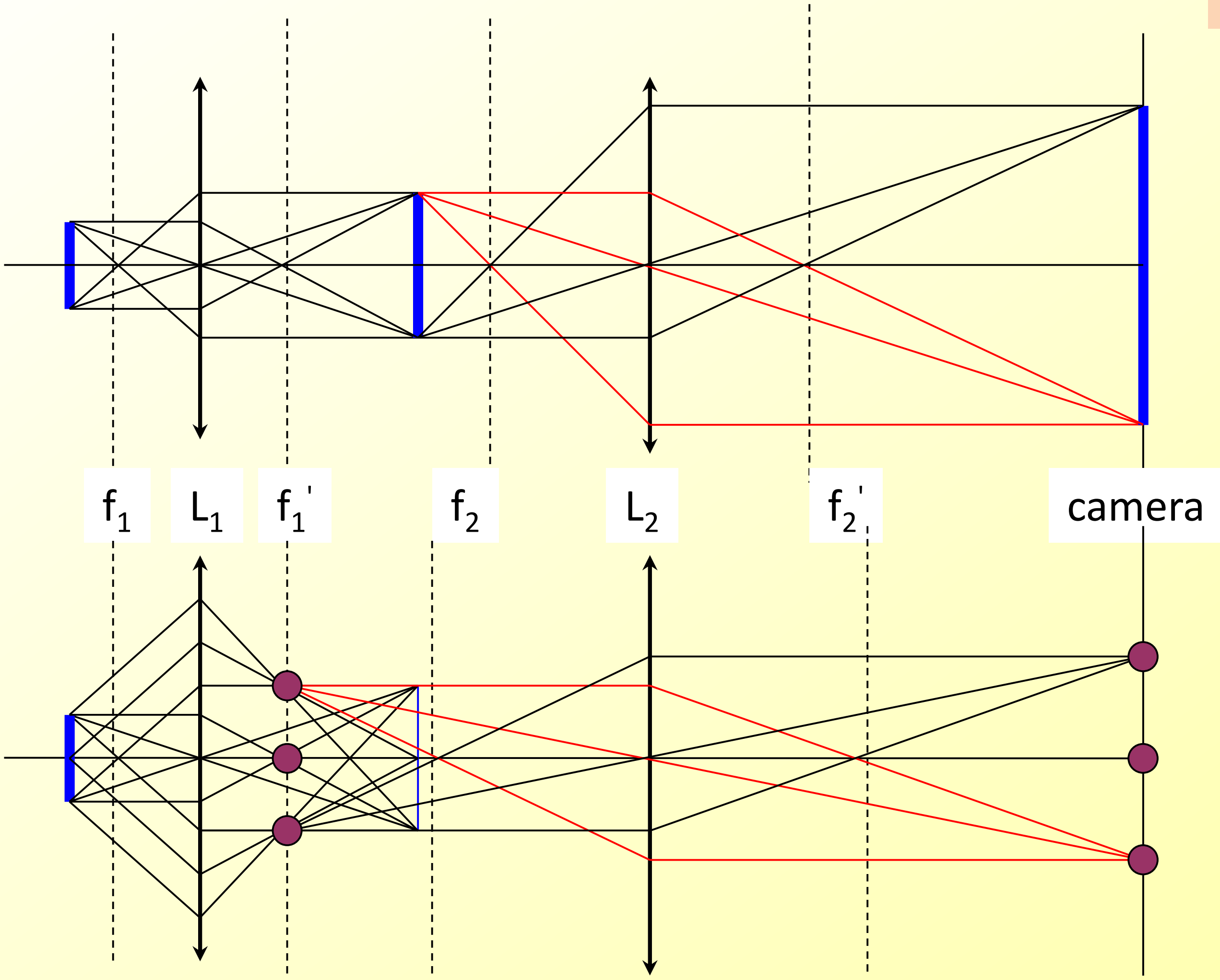
Warning:
this scheme is correct
in principle,
but the real microscopes
use more lenses,
which compensate for
optical aberrations.

Note1: the plane, in which the real image from L_1 is formed is usually called *image plane*.
Note2: the second lens L_2 is, in this case, focused at *image plane*.
Note3: the diagram ↑ is valid for both TEM and LM.

Example 2 :: Ray optics :: Formation of a diffraction pattern in TEM.

Demo that TEM can work in both imaging and diffraction mode.

* LM is rarely used in diffraction mode, but it is possible as well.



A two-lens microscope (from previous slide) in imaging mode. The 2nd lens (L_2) is focused on (real) image.

* lens L_2 is stronger than in diffraction mode (Power = $1/f_2$)

A two-lens microscope (the same as above) in diffraction mode. The 2nd lens (L_2) is focused on diffraction pattern.

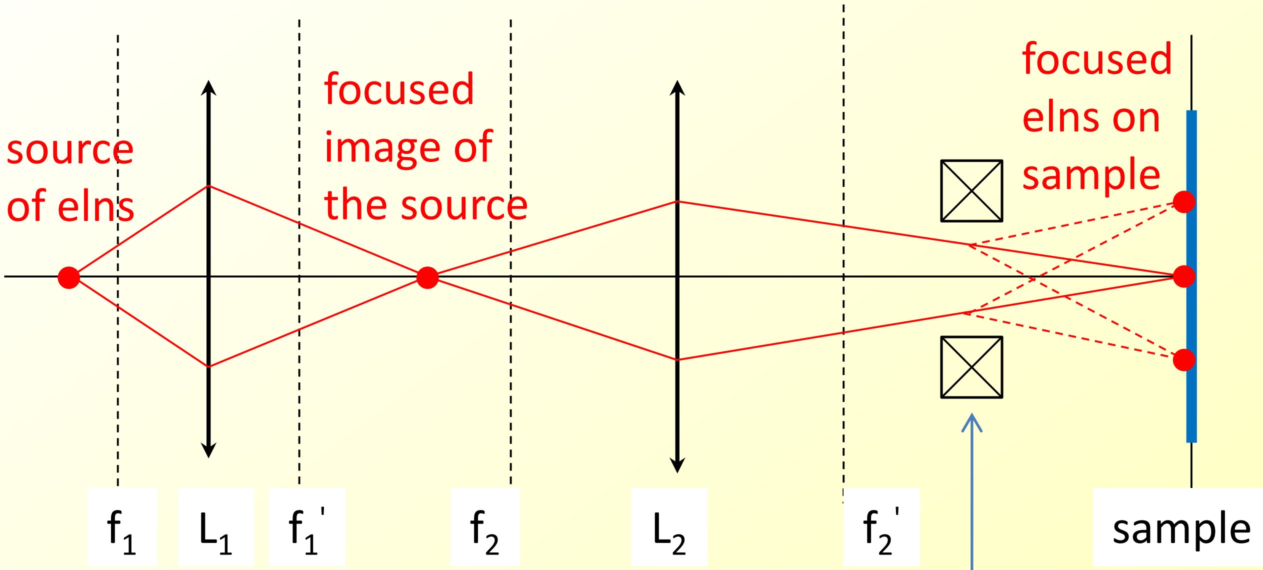
* lens L_2 is weaker than in imaging mode (Power = $1/f_2$)

- sample and its images
- diffraction pattern

Note: power of the lens ~ 1/[focal length] in EM can be altered by changing the strength of the current.

Example 3 :: Ray optics :: Formation of an image in SEM.

Demo that the ray optics can explain, in simple terms, also the principle of SEM microscope.



Very simplified scheme of a SEM microscope:

Condenser lens L_1 focuses the beam, which is further focused on the sample/specimen by objective lens L_2; the image is formed point-by-point using the final scanning lenses/coils.

Thick blue line = sample/specimen.
L_1 = condenser lens (it condensates the beam)
f_1,f_1' = front/back focal plane of lens L_1
L_2 = objective lens (it is close to the object/sample)
f_2,f_2' = front/back focal plane of lens L_2
Note: *close to the objective lens are also* ***scanning coils****, which cause movement of the beam across the specimen.*

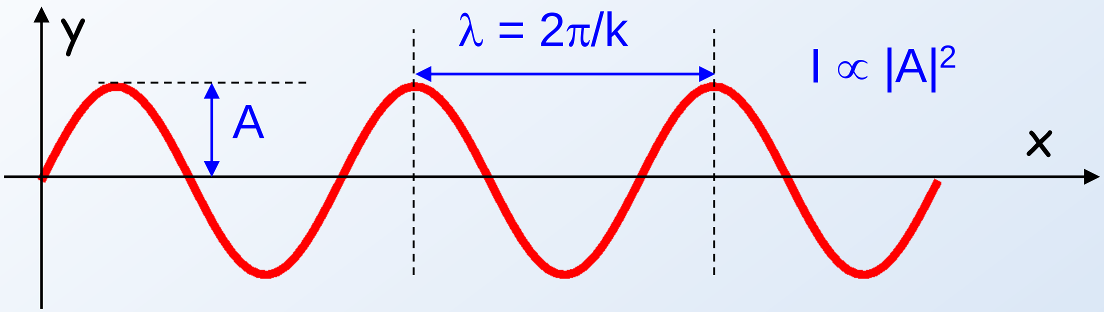
Ray-tracing technical note:
The focused image of a source has to be made by a trick. Just imagine that there is a line object instead of point source ⇒ you need the principal rays.

SEM microscope is different from LM and TEM.
SEM lenses do not form the image, they just focus the beam on the sample.
SEM image is formed point-by-point - the beam scans sample surface - emitted signal is detected.

Wave optics approximation: photons and electrons are waves.

(0) Wave-particle duality → de Broglie matter waves: $\lambda = h/p \approx h/mv$

(1) Wave = an oscillation which travels through space



$\Psi(x,t) = A\cos[\omega t - \mathbf{k}x + \Phi]$ = wave

I = intensity of wave

A = amplitude

λ = wavelength

v = velocity of (of the wave)

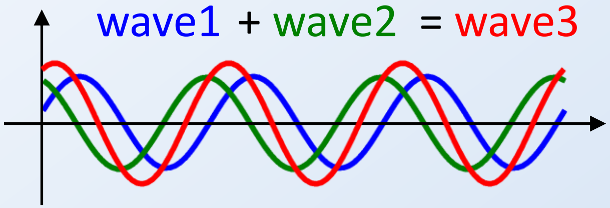
ω = angular frequency (of oscillations)

$\mathbf{k} = \omega/\mathbf{v}$ = wave number

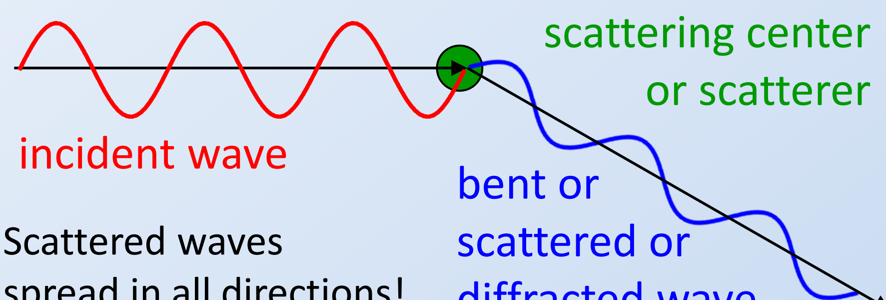
Φ = initial phase

(2) Interference = wave addition.

wave1 + wave2 = wave3

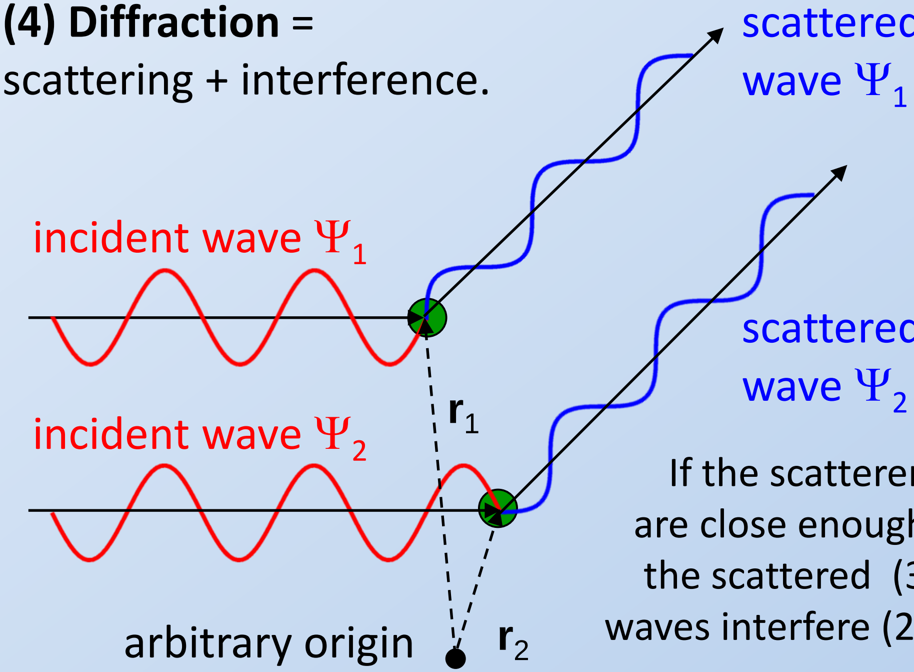


(3) Scattering = wave deflection.



Scattered waves spread in all directions!

(4) Diffraction = scattering + interference.



If the scatterers are close enough, the scattered (3) waves interfere (2).

Optics :: Wave optics :: Diffraction

Within the wave optics, we focus our attention on diffraction, because of two reasons:

(1) Diffraction is connected with the resolution limit of LM and TEM.

(2) Elements of diffraction are necessary to understand TEM/SAED.

Diffraction →

Secondary school level

- ❖ Diffraction basics
- ❖ Huygens-Fresnel principle
- ❖ Diffraction for simple/model geometries

Diffraction →

University level

- ❖ Bragg's Law
- ❖ Reciprocal lattice, Laue diffraction condition, Ewald sphere (option)
- ❖ Kinematic diffraction theory (option = not required at final exam)
- ❖ Structure analysis, dynamic diffraction theory...

In this course, we will use:

- ❖ Bragg's Law (compulsory) $\Rightarrow$ to understand the principle + calculate TEM/SAED distances
- ❖ Reciprocal lattice, LDP, EwC (option) $\Rightarrow$ to calculate TEM/SAED distances + positions
- ❖ Key results of kinematic diffraction theory (option)

  $\Rightarrow$ to calculate TEM/SAED distances + positions + intensities

  (we will show the *ab initio* calculation with a program Python/Jupyter)

Optics :: Wave optics :: Diffraction :: Bragg Law

Bragg's Law is the simplest possible description of diffraction on crystals.
It cannot explain all aspects of diffraction, but represents very useful approximation.

Bragg's law in words:

Maximum interference (= diffraction on a crystal) occurs only at the angles ($2d\sin\theta = n\lambda$).

Bragg's law assumptions:

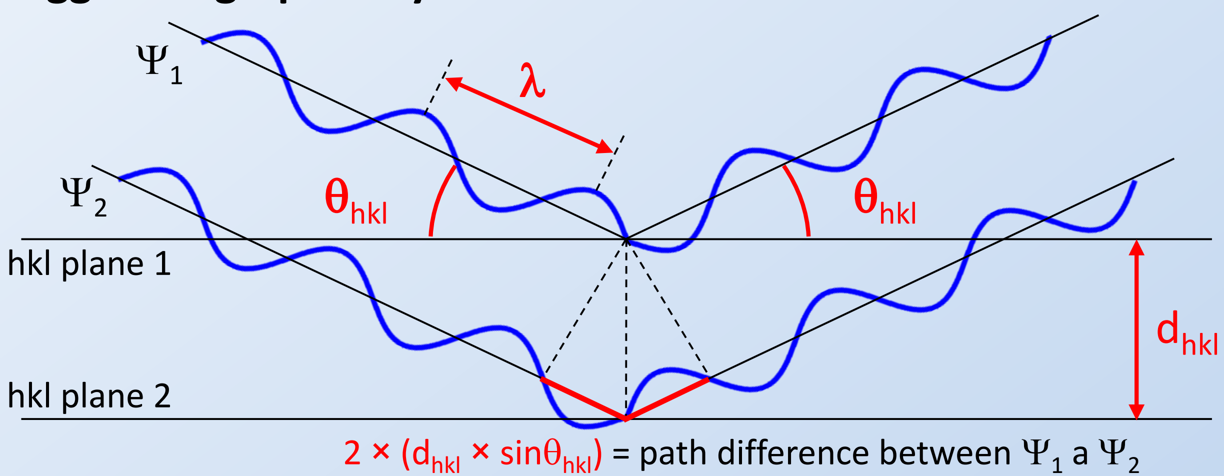
[1] Crystallographic planes are semitransparent mirrors.
Wrong: the planes are just geometrical constructions representing the periodicity of the crystal.

[2] Waves are reflected by these crystallographic planes.
Wrong: in fact the waves are scattered by atoms and then they interfere – i.e. they are diffracted.

[3] Maximum interference (= diffraction peak) occurs, if phase difference of reflected waves is 0, 2π, 4π.. = $2n\times\pi$ (n = integer), i.e. if the path length difference is 0, λ, 2λ, 3λ, .. = $n\times\lambda$.
This is true: diffraction peaks are really observed under these conditions.

[Conclusion] Although the assumptions are not completely true, the results are correct!

Bragg's law graphically:



Mathematically:

$$2d_{hkl}\sin\theta_{hkl} = n\times\lambda$$

$2d_{hkl}\sin\theta_{hkl}$: path difference between waves Ψ_1 a Ψ_2

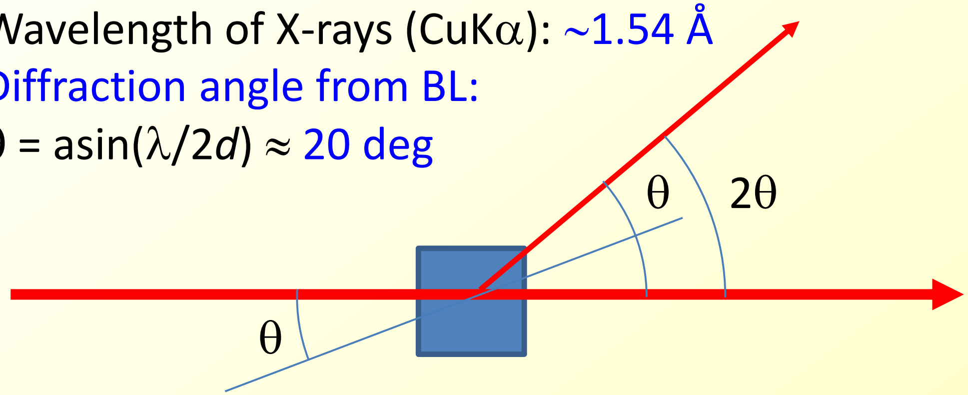
$n\times\lambda$: integer multiplication of the wavelength

Make sure that you know and understand BL.

Example 4 :: Bragg's Law in X-ray and electron diffraction

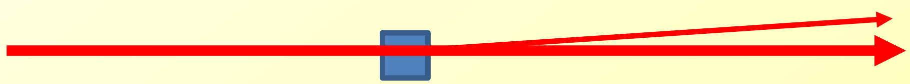
X-ray diffraction (Au **micro**crystal, $d_{hkl} = d_{111} = 2.36$ Å)

- Wavelength of X-rays (CuKα): ~1.54 Å
- Diffraction angle from BL:
  $\theta = \text{asin}(\lambda/2d) \approx$ 20 deg



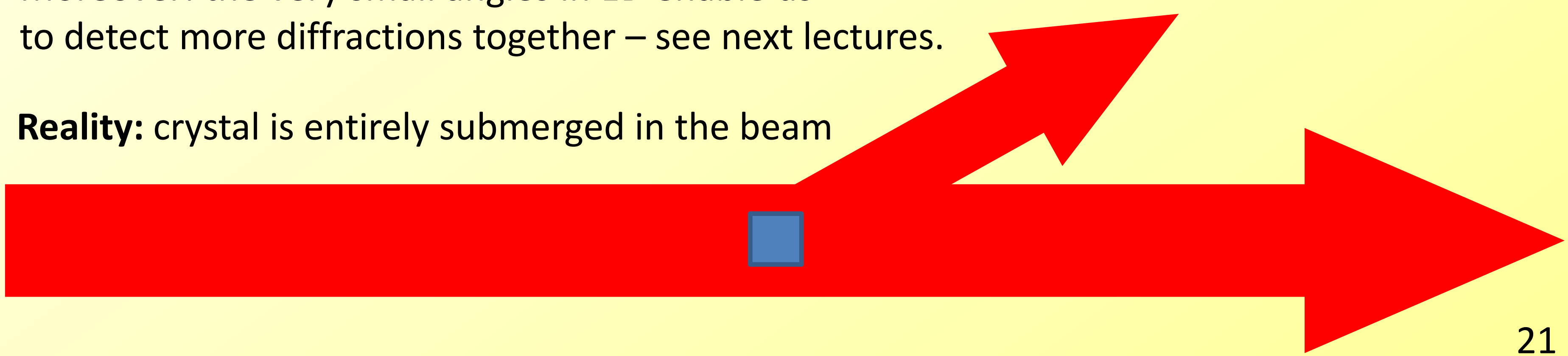
Electron diffraction (Au **nano**crystal, $d_{hkl} = d_{111} = 2.36$ Å)

- Wavelength of electrons (100 keV): ~0.04 Å
- Diffraction angle from BL:
  $\theta = \text{asin}(\lambda/2d) \approx$ 0.5 deg



Moreover: the very small angles in ED enable us to detect more diffractions together – see next lectures.

Reality: crystal is entirely submerged in the beam



Summary for XRD:

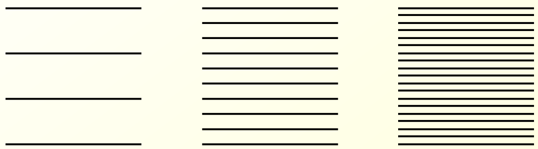
- interactions with X-rays weak
  $\Rightarrow$ crystals are big (μm)
  $\Rightarrow$ no multiple scattering
  $\Rightarrow$ kinematic diffraction theory
- X-ray wavelengths high
  $\Rightarrow$ diffraction angles are high

Summary for ED:

- interactions with elns strong
  $\Rightarrow$ crystals are small (nm)
  $\Rightarrow$ multiple scattering
  $\Rightarrow$ dynamic diffraction theory
- electron wavelengths low
  $\Rightarrow$ diffraction angles are low

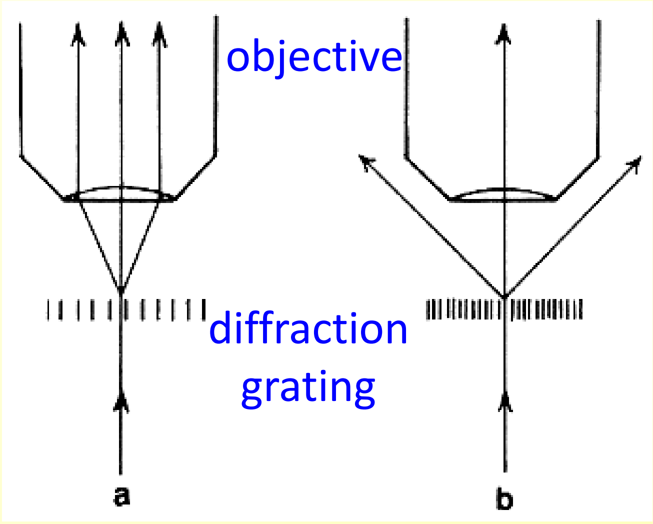
Example 5 :: Bragg's law and the best resolution of TEM/LM.

What is resolution?

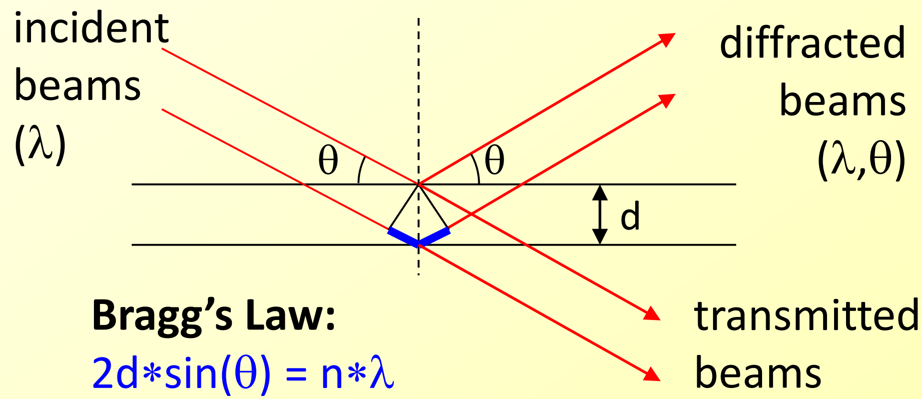


Resolution can be defined as an ability to differentiate lines with periodic distance **d** in a diffraction grating.

How in a microscope?



Connection [resolution - diffraction]?



Bragg's Law:
$2d*\sin(\theta) = n*\lambda$

Conclusion:
low distances **d** → high diffraction angles **θ**.

In a microscope:
[1] To distinguish lines at distance **d**,
we have to catch diffracted beam ad angle **θ**.
[2] At very low **d** the beam goes out of objective, and so it cannot be detected.
[3] With an infinitely large objective we would catch beam at θ=90°: $2d*\sin(90^o) = 1*\lambda$

Max.resolution ≈ diffraction limit: $d \approx \lambda/2$

For LM, this is a good approximation → see slide 3.
There are just small corrections for numerical aperture etc.

For TEM, this is not the whole story → see lecture on TEM microscopy.
The resolution decreases due to low quality of electromagnetic lenses → spherical aberration.

Part 3

Freeware microscopic programs for the rest of the course

Contents

❖ ImageJ → processing & analysis of micrographs (+ IrfanView for viewing)

❖ Python/Jupyter → CAS software, used in this course for calculations
(also for advanced/high-quality graphs – alternative to Excel, Origin…

❖ Optional, but useful for every microscopist:
IrfanView – very useful program for viewing and basic processing of images
CASINO – monte CArlo SImulation of electroN trajectory in sOlids

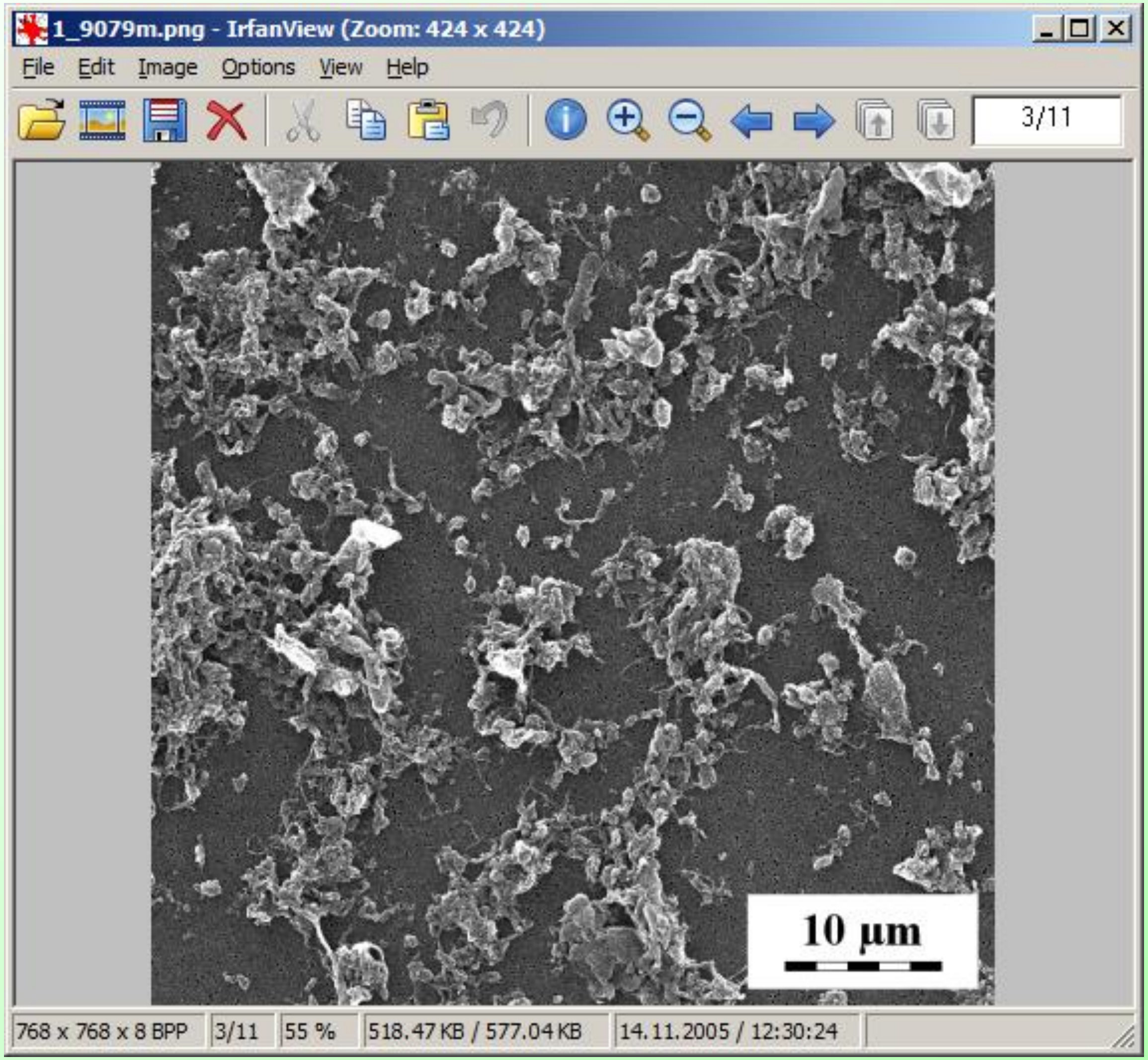
❖ Optional, but necessary if you want to process TEM/SAED:
ProcessDiffraction – converts 2D-patterns to 1D-diffractograms
PowderCell – calculates 1D-diffractograms from known structures

Alternatives to the above programs:

- ImageJ alternatives (mostly commercial) = NIS-Elements, Olympus Stream...
- Python/Jupyter alternatives = MATLAB, Mathematica, Octave, Maxima...
- CASINO = no alternatives that I would know – perhaps some commercial programs...
- ProcessDiffracton, PowderCell = various (mostly commercial) software...

Program IrfanView :: viewing and basic processing of micrographs

Obligatory for any real microscopist (but not necessary for this course).



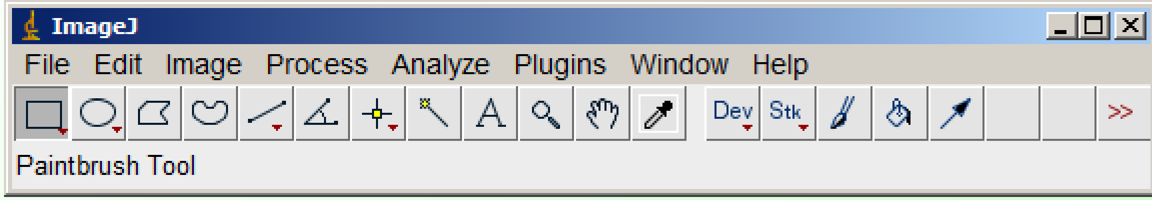
IrfanView

- freeware
  www.irfanview.com
- comfortable viewing
  of large series of micrographs
- reads (almost) all
  existing image formats
- (basic) processing of images/micrographs:
  - selections, cutting…
  - changes of size and dpi
  - conversion of formats
  - conversion to grayscale
  - and some other things..
- (basic) corrections of brightness, contrast, colors..
- (basic) image editor,
  after pressing function key F12

* there are many other similar programs – IrfanView is one of the best according to www

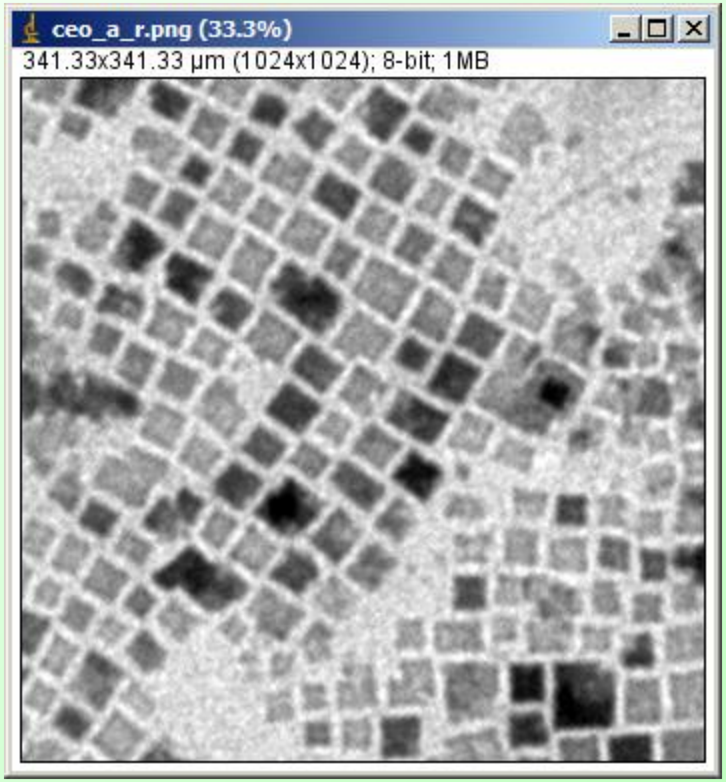
Program ImageJ :: Advanced image processing and analysis.

Obligatory for every real microscopist: adjust B/C/G, cut images, measure, insert scale...



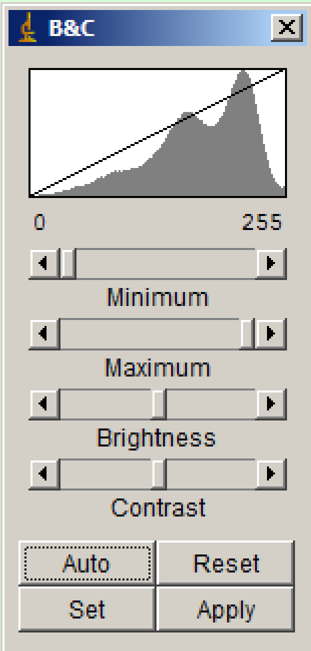
Main window of ImageJ.
http://imagej.nih.gov/ij/

HW #1 Install imageJ.



A micrograph opened in ImageJ.

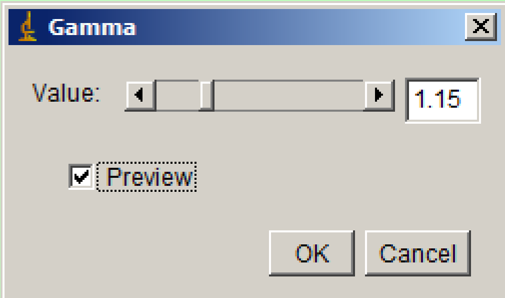
For viewing also: **IrfanView**
Light-weight and fast image viewer.



Adjustment of B&C.
B&C = Brightness & Contrast).

HW #2

Take any image, open in ImageJ, cut rectangle 300x300 pixel, suppose that the real width of image is 100 μm and insert a scale bar of length 30 μm (help on www).



Adjustment of gamma. (emphasizing of brighter or darker areas of the image).

Program Python/Jupyter :: Part 1 :: Calculations

Optional for a microscopist, but obligatory for this course – it will be used for our calculations.

- Python = modern programming language (we will use just the very basic syntax).
- Jupyter = interactive interface to Python (this is also called interactive Python = iPython).
- Install Python/Jupyter according to www-pages of the course.

HW #3

```
In [1]: import sympy as sp
        sp.init_printing()
        (x,y) = sp.symbols('x y')

In [2]: x+x
```

Out[2]: $2x$

```
In [3]: sp.diff(sp.sin(x**2 + y**2), x)
```

Out[3]: $2x\cos\left(x^2 + y^2\right)$

```
In [4]: sp.integrate(x**5 * sp.exp(x), x)
```

Out[4]: $\left(x^5 - 5x^4 + 20x^3 - 60x^2 + 120x - 120\right)e^x$

After you install Jupyter, reproduce the calculations shown in this slide.

HW #4

Note/hint to HW's #3 and #4::
Use the brief introduction to Python in the www-pages of the course

Python/Jupyter can do not only standard calculations (1+1=2) like most languages,
but also symbolic calculations (x+x=2x) including derivations, integrals (as shown above).

We will use Python/Jupyter for microscopy-related calculations, graphs and homework.

Python/Jupyter :: Part 2 :: Further possibilities

Do not reinvent the wheel! → https://scipy-lectures.org/intro/intro.html

Python+Jupyter can be employed as a freeware alternative of CAS programs such as MATLAB, Mathematica, Maxima...

More information = www-pages of the course

SciPy = Scientific Python → see www

1.1.1. Why Python?

1.1.1.1. The scientist's needs

- Get data (simulation, experiment control),
- Manipulate and process data,
- Visualize results, quickly to understand, but also with high quality figures, for reports or publications.

1.1.1.2. Python's strengths

- **Batteries included** Rich collection of already existing **bricks** of classic numerical methods, plotting or data processing tools. We don't want to re-program the plotting of a curve, a Fourier transform or a fitting algorithm. Don't reinvent the wheel!
- **Easy to learn** Most scientists are not payed as programmers, neither have they been trained so. They need to be able to draw a curve, smooth a signal, do a Fourier transform in a few minutes.
- **Easy communication** To keep code alive within a lab or a company it should be as readable as a book by collaborators, students, or maybe customers. Python syntax is simple, avoiding strange symbols or lengthy routine specifications that would divert the reader from mathematical or scientific understanding of the code.
- **Efficient code** Python numerical modules are computationally efficient. But needless to say that a very fast code becomes useless if too much time is spent writing it. Python aims for quick development times and quick execution times.
- **Universal** Python is a language used for many different problems. Learning Python avoids learning a new software for each new problem.

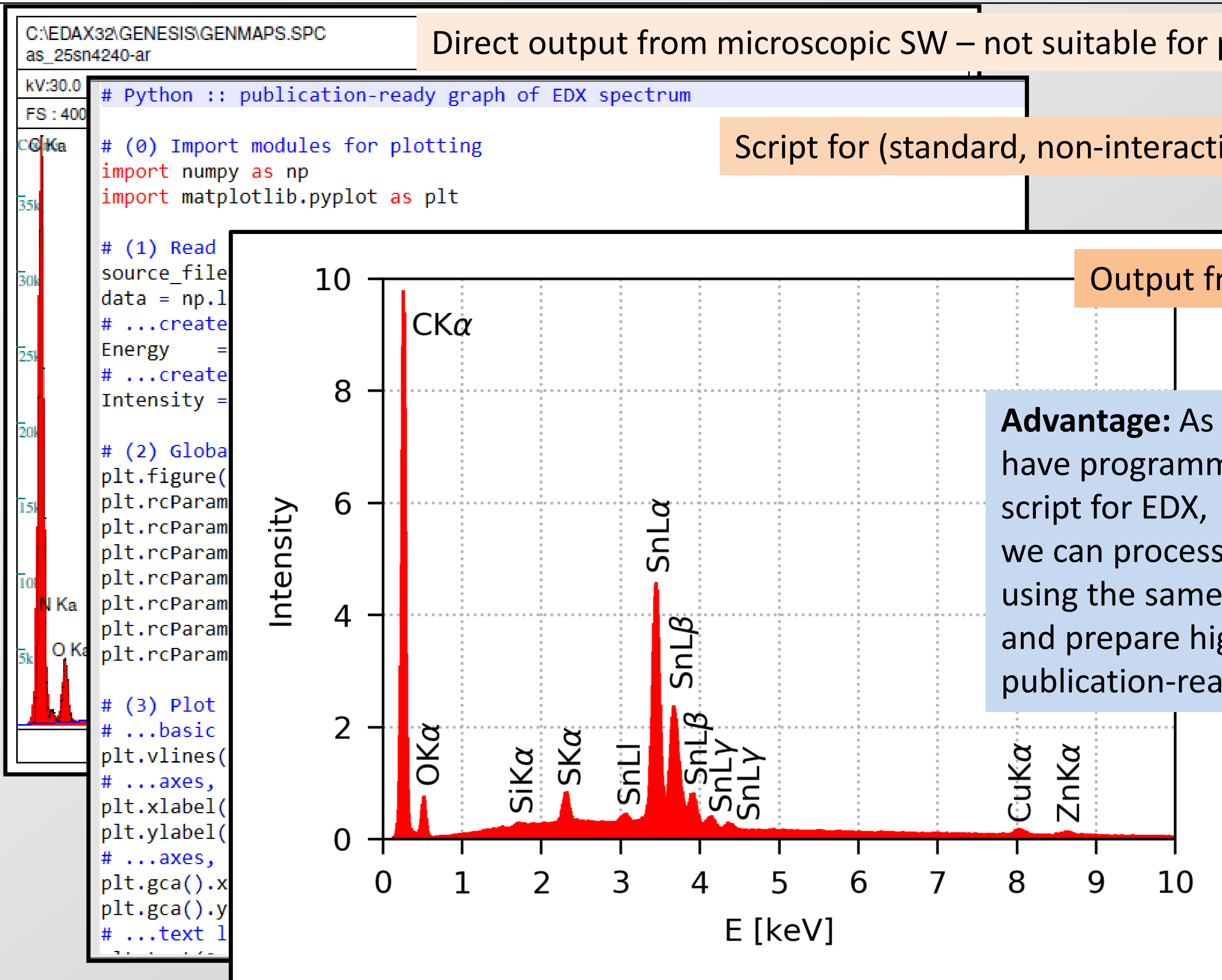
Python/Jupyter :: Part 3 :: High-quality graphs

Optional – but advantageous for advanced, repeated and/or batch processing...

Direct output from microscopic SW – not suitable for publication.

Script for (standard, non-interactive) Python.

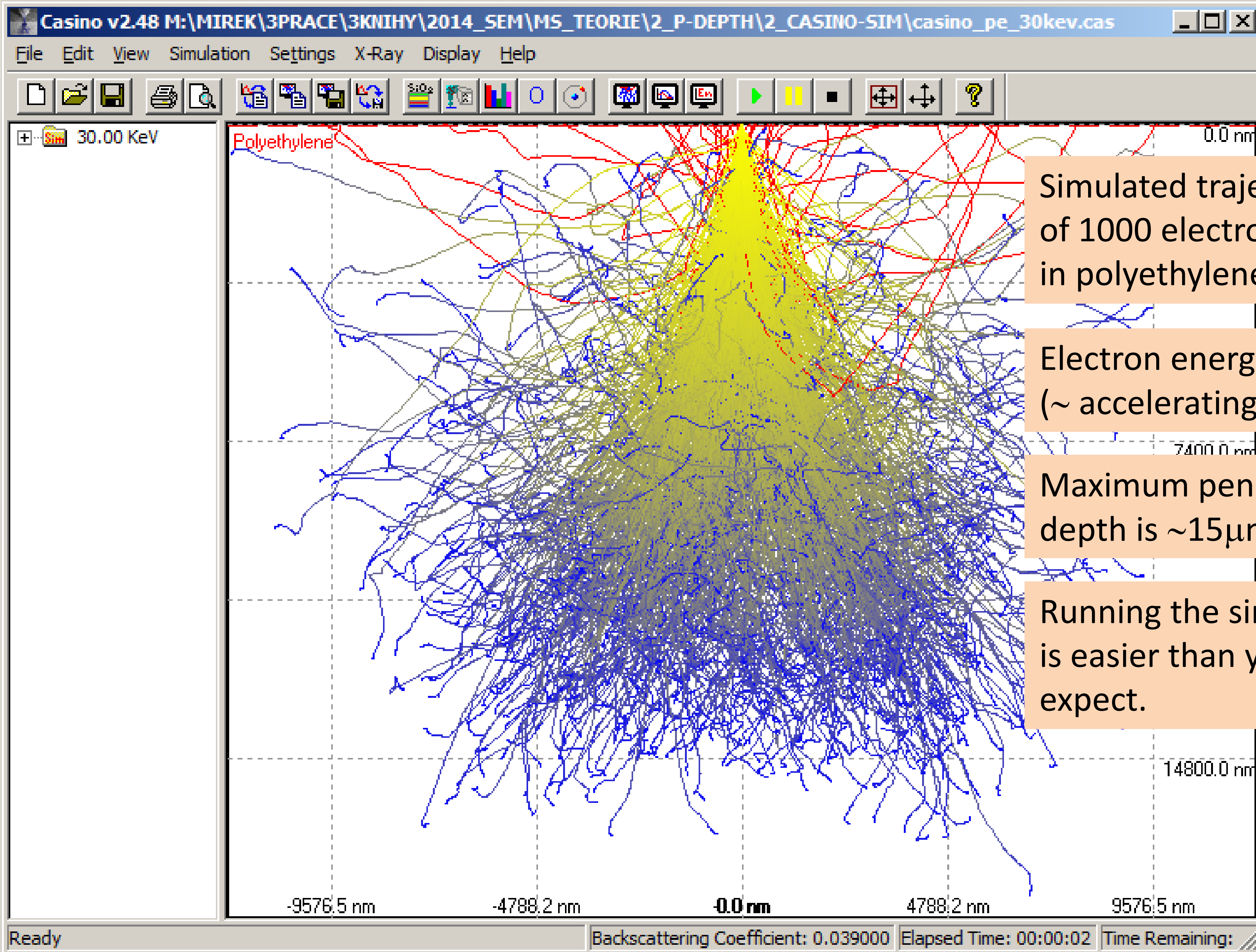
Output from Python.



Advantage: As soon as we have programmed the script for EDX,
we can process all spectra using the same way
and prepare high-quality, publication-ready outputs.

CASINO :: monte CArlo SImulation of electroN trajectory in sOlids

For a microscopist optional, but very useful for various predictions and interpretations...



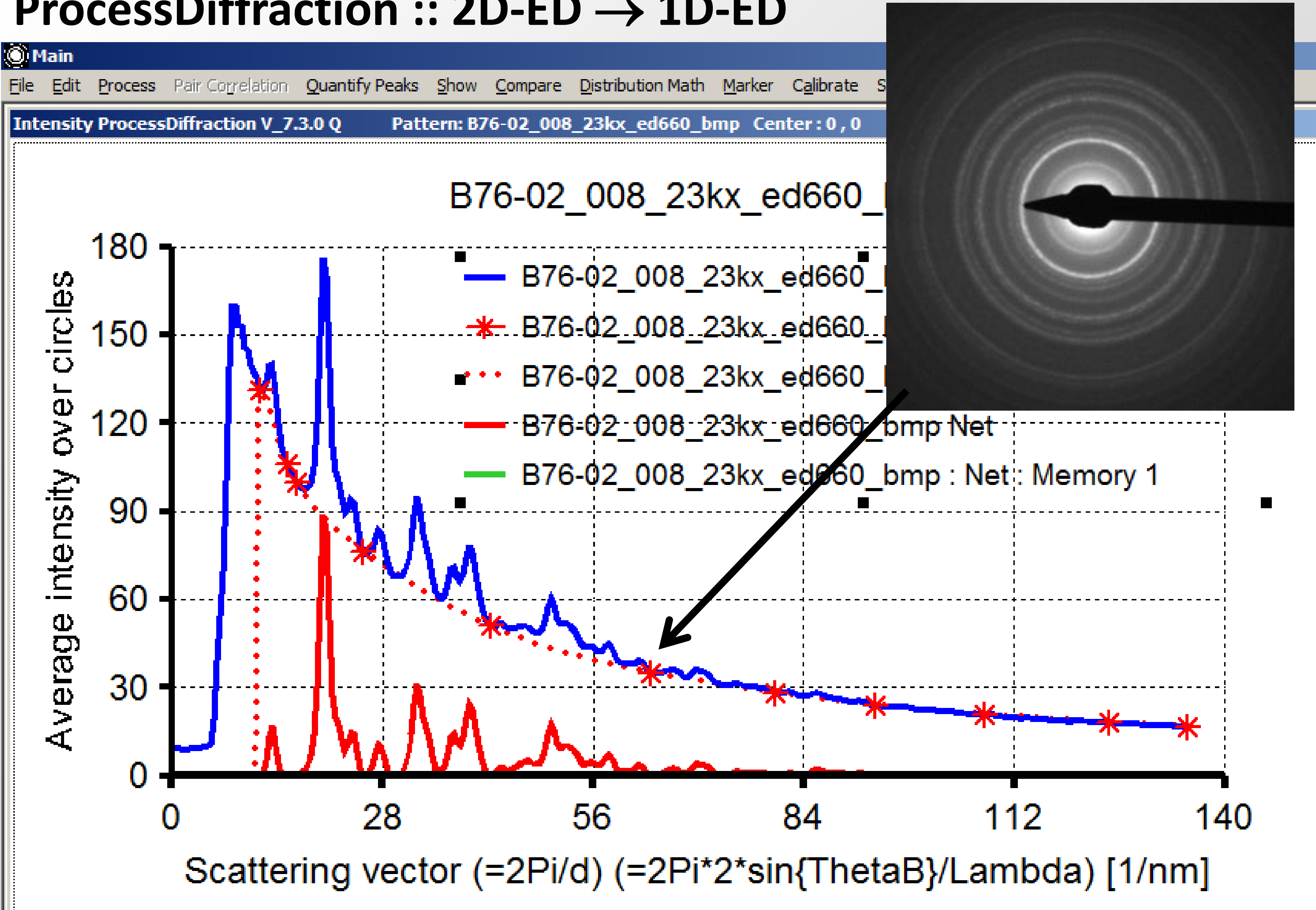
Simulated trajectories of 1000 electrons in polyethylene.

Electron energy = 30keV. (~ accelerating voltage)

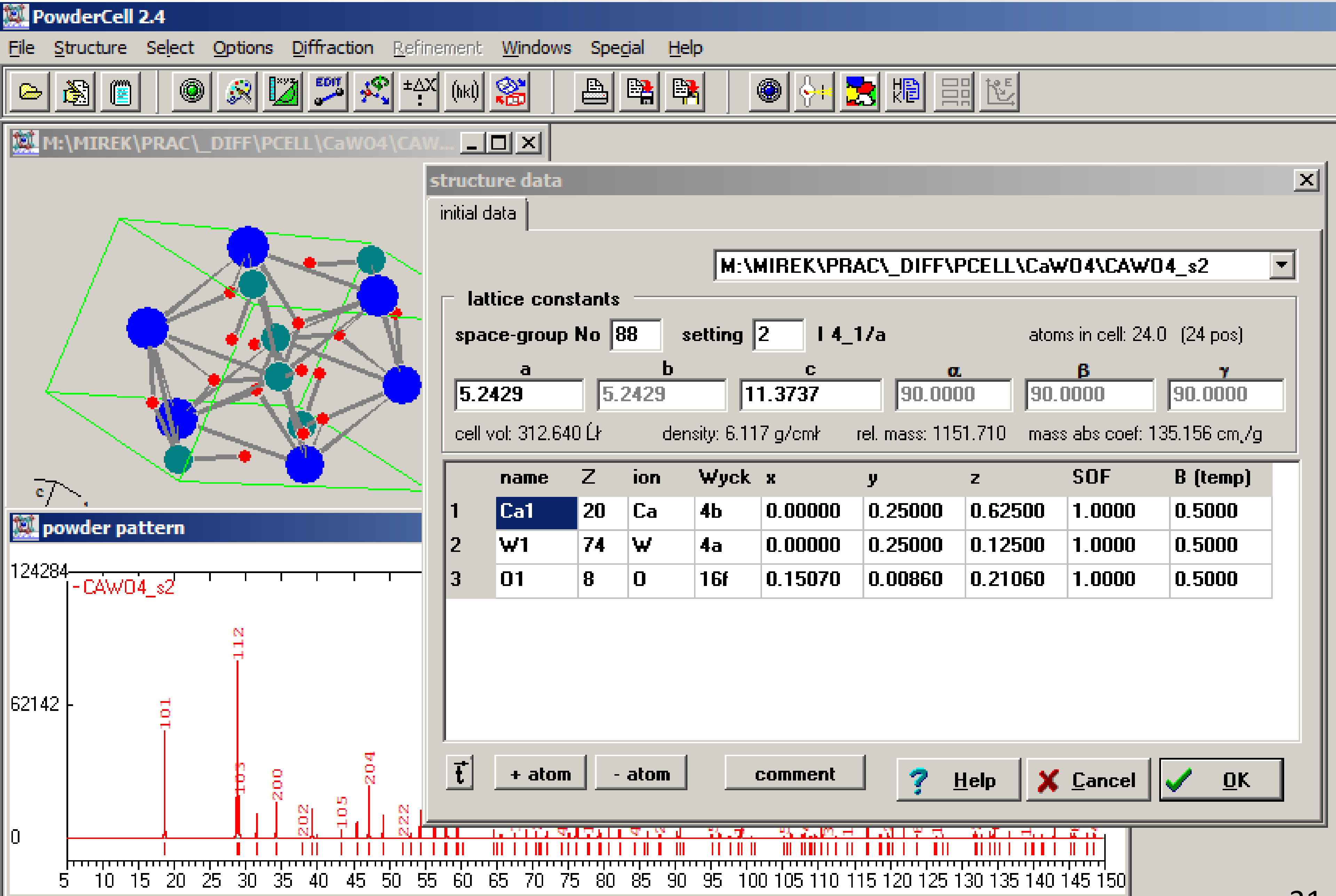
Maximum penetration depth is ~15μm.

Running the simulations is easier than you might expect.

ProcessDiffraction :: 2D-ED → 1D-ED



PowderCell :: Calculation of 1D-diffractograms



Conclusions

What have we learnt in this lecture?

- **Part 1**
  Types of microscopes, length scales in microscopy...

- **Part 2**
  Selected pieces of theory for understanding microscopic methods:
  * Ray optics → imaging/diffraction mode in LM/TEM, imaging in SEM
  * Wave optics → resolution in LM/TEM, diffraction in TEM, Bragg's Law

- **Part 3**
  Freeware programs for microscopy and the rest of this lecture:
  * ImageJ = obligatory program for each real microscopist
  * Jupyter/Python = obligatory for this course, useful in any case
  * Brief info about other useful programs: IrfanView, CASINO...

Note: optional supplements = more details about diffraction.

Thank you for your attention!

Appendix A

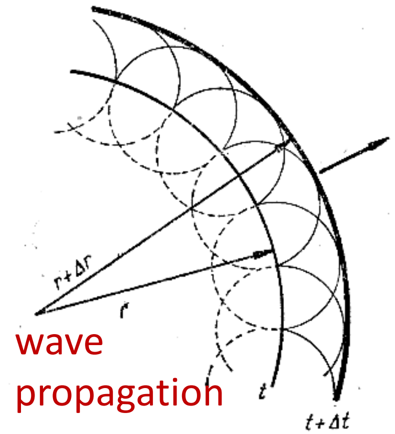
Ultra-brief revision of diffraction theory from secondary school

- ❖ This part is optional (not at exams).
- ❖ It is a reminder, what we might have learnt in secondary school. ☺

Supplement :: Wave optics :: Diffraction at secondary school

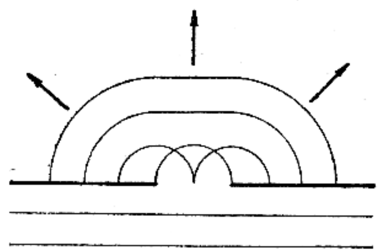
(Just for revision, completeness and understanding the background...)

Huygens-Fresnel principle



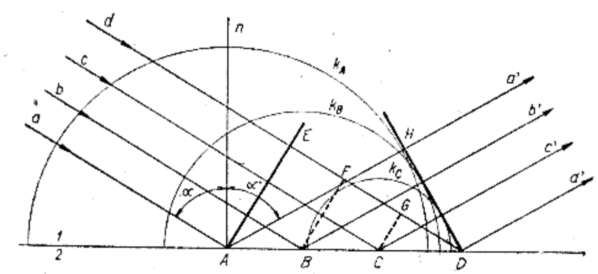
wave propagation

Obr. 119. Konstrukce vlnoplochy podle Huygensova principu



Obr. 120. Ohyb vlnění za otvorem v pevné přepážce

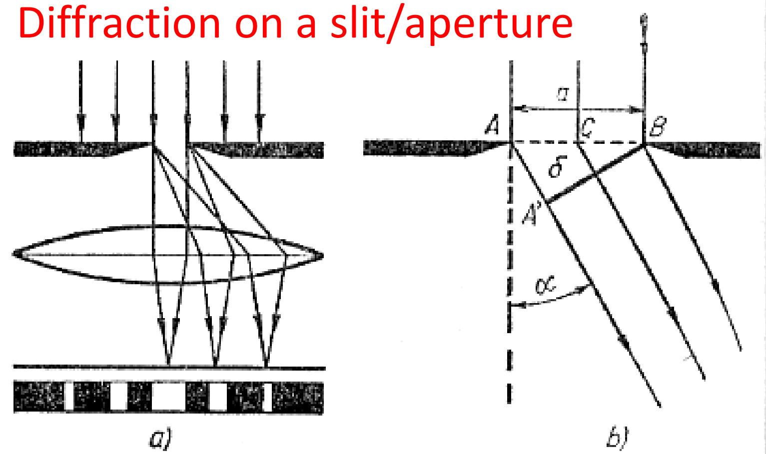
scattering



reflection

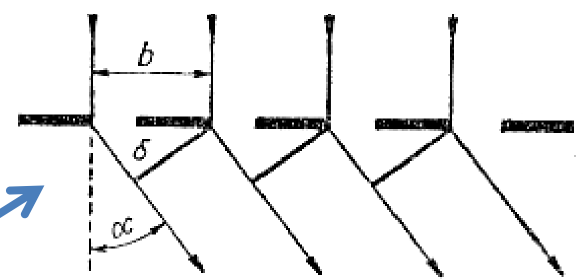
Obr. 121. Odraz rovinné vlny

Diffraction on a slit/aperture



Obr. 229. Ohyb světla na štěrbině: a) metoda pozorování; b) k výkladu jevu

Diffraction on a grating/grid



Obr. 230. Ohyb světla na difrakční mřížce

- ❖ This is the brief revision of secondary school explanation of diffraction.
- ❖ Interesting result from diffraction on a grid:
  - ⇒ the maximum interference is achieved at $\delta = k\lambda$
  - ⇒ diffraction maxima will be found at angles α according to the equation: $b*\sin(\alpha) = k\lambda$
  - ⇒ this is a general principle of reciprocity (small distances ≈ high diffraction angles)

Appendix B

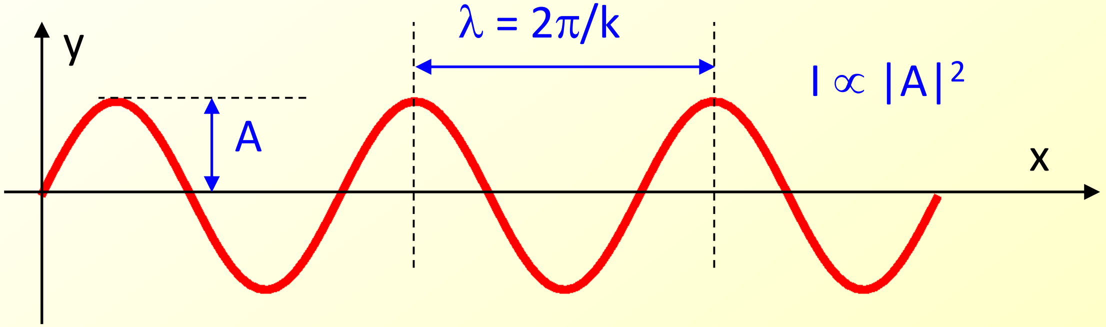
Descriptions of waves by means of cos and exp functions

- This part is optional (not at exams).
- It is a useful introduction to diffraction theory (TEM/SAED).
- Moreover, it is an interesting math that may help you in the future.

Part 1 :: Description of waves :: [cos-waves] vs. [exp-waves]

In words: wave is a move of oscillations through space.
(always connected with some energy transfer)

Graphically:



$\Psi(x,t)$ = wave
I = intensity of the wave
A = amplitude
λ = wavelength
v = velocity (of wave propagation)
ω = angular speed (of oscillations)
k = ω/v = wave vector
Φ = initial phase

Mathematically:

(1) $\Psi(\mathbf{x},t)=A\cos[\omega t-\mathbf{kx}+\Phi]$ ..cos-wave: plane wave propagating in direction **x**

(2) $\Psi(\mathbf{x},t)=A\exp[i(\omega t-\mathbf{kx}+\Phi)]$ ..exp-wave: equation (1) in exponential form

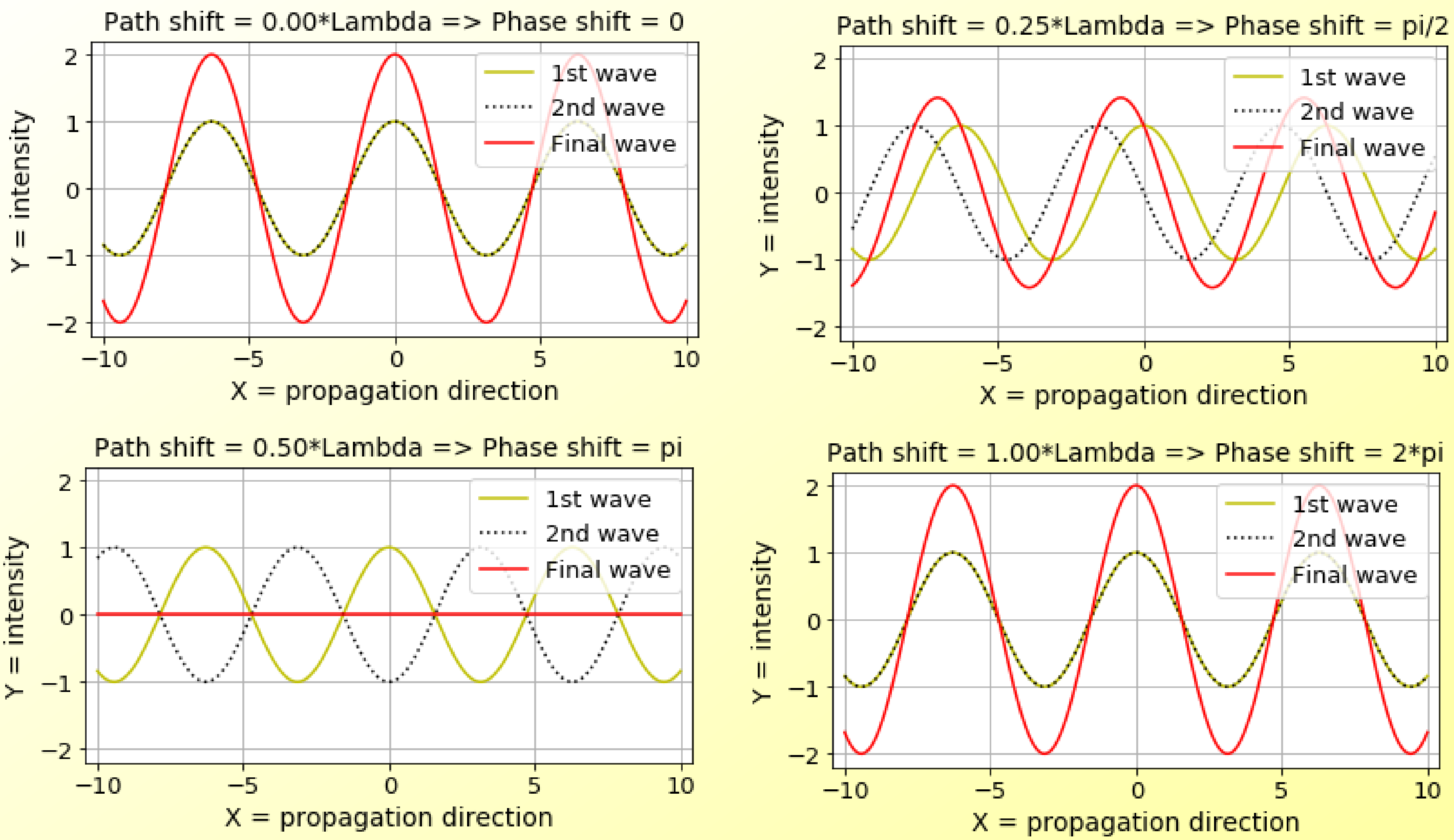
(3) $\Psi(x,t)=A\exp[i(\omega t-kx+\Phi)]$ ..exp-wave propagating along axis x (just for clarity)

(4) $\Psi(x,t)=A\exp[i\Phi]\exp[i(\omega t-kx)]$ ..exp-wave re-written
with the complex amplitude: $\mathbf{A} = A\exp[i\Phi]$

(5) $I \approx |\mathbf{A}|^2$ ..intensity of waves is what we see (eyes) or detect (films, cameras, detectors).
⇒ in theoretical derivations we calculate **A**, which is related to experimental intensities I.

Why complex amplitudes? ⇒ much easier calculations – see next slides.
Why we can exchange cos for exp? ⇒ it is a mathematical description that works.

Part 2 :: Interference of [cos-waves] graphically



- ❖ Maximum interference of waves occurs at *path shift* = nλ $\leftrightarrow$ *phase shift* = 2nπ. (n = integer)
- ❖ Minimum interference of waves occurs at *path shift* = (2n+1) λ/2 $\leftrightarrow$ phase shift = (2n+1)π.

This is a sample output from program Python/Jupyter.

Part 3 :: Interference of [cos-waves] mathematically

Two cosine waves (Ψ_1, Ψ_2)
with the same amlitudes $(A = A_1 = A_2)$ and different phases $(\phi_1 \neq \phi_2)$.

Input waves $(X = (\omega t - kx) =$ constant for given experiment):

$$\Psi_1 = A\cos(\omega t - kx + \phi_1) = A\cos(X + \phi_1)$$
$$\Psi_2 = A\cos(\omega t - kx + \phi_2) = A\cos(X + \phi_2)$$

$$\Psi_1 + \Psi_2 = A\cos(X + \phi_1) + A\cos(X + \phi_2) = A[\cos(X + \phi_1) + \cos(X + \phi_2)]$$

Trick (not universal, possible only on condition that $A_1 = A_2 = A$):

$$\cos(a) + \cos(b) = 2\cos((a+b)/2)\cos(a-b)/2)$$
$$\cos(X + \phi_1) + \cos(X + \phi_2) = 2 \times \cos\left(X + \frac{\phi_1 + \phi_2}{2}\right) \times \cos\left(\frac{\phi_1 - \phi_2}{2}\right)$$

Result (amplitudes separated, phases just partially):

$$\Psi_1 + \Psi_2 = \left[2A\cos\left(\frac{\phi_1 - \phi_2}{2}\right)\right] \times \left[\cos\left(X + \frac{\phi_1 + \phi_2}{2}\right)\right]$$

$$\sum_{j=1}^{N} \Psi_j = ???$$

`...generalization is impossible`

Orange rectangle: amplitude of the resulting wave.

Part 4 :: Interference of [exp-waves] mathematically

Two exponential waves (Ψ_1, Ψ_2)
with the same amlitudes $(A = A_1 = A_2)$ and different phases $(\phi_1 \neq \phi_2)$.

Input waves $(X = (\omega t - kx)$ = constant for given experiment):

$$\Psi_1 = A\exp(i(\omega t - kx + \phi_1)) = A\exp(i(X + \phi_1))$$
$$\Psi_2 = A\exp(i(\omega t - kx + \phi_2)) = A\exp(i(X + \phi_2))$$

$$\Psi_1 + \Psi_2 = A\exp(i(X + \phi_1)) + A\exp(i(X + \phi_2))$$

No tricks (standard treatment, universal, not only for $A_1 = A_2 = A$):

$$\begin{aligned} \exp(a+b) &= \exp(a) \times \exp(b) \\ A\exp(i(X+\phi_1)) + A\exp(i(X+\phi_2)) &= (A\exp(i\phi_1) + A\exp(i\phi_2)) \times \exp(iX) \end{aligned}$$

Result (amplitudes-and-phases completely separated):

$$\begin{aligned} \Psi_1 + \Psi_2 &= [A\exp(i\phi_1) + A\exp(i\phi_2)] \times [\exp(iX)] \\ \sum_{j=1}^{N} \Psi_j &= \left[\sum_{j=1}^{N} [A_j \exp(i\phi_j)]\right] \times [\exp(iX)] \end{aligned}$$

Orange rectangle: (complex) amplitude of the resulting wave.

...generalization is Ok

Conclusion: as for calculations, exp-waves are better than cos-waves.

This is why we use exp-waves.

Part 5 :: Equivalence of cos-waves and exp-waves in Python/Jupyter

Example of Python/Jupyter calculation

Demo, how we can test/verify/exemplify various problems with Jupyter

In [8]:
```
# Input parameters = amplitudes and phases of two waves
A1 = A2 = 1
Phi1 = pi/6
Phi2 = 2*pi/3
```

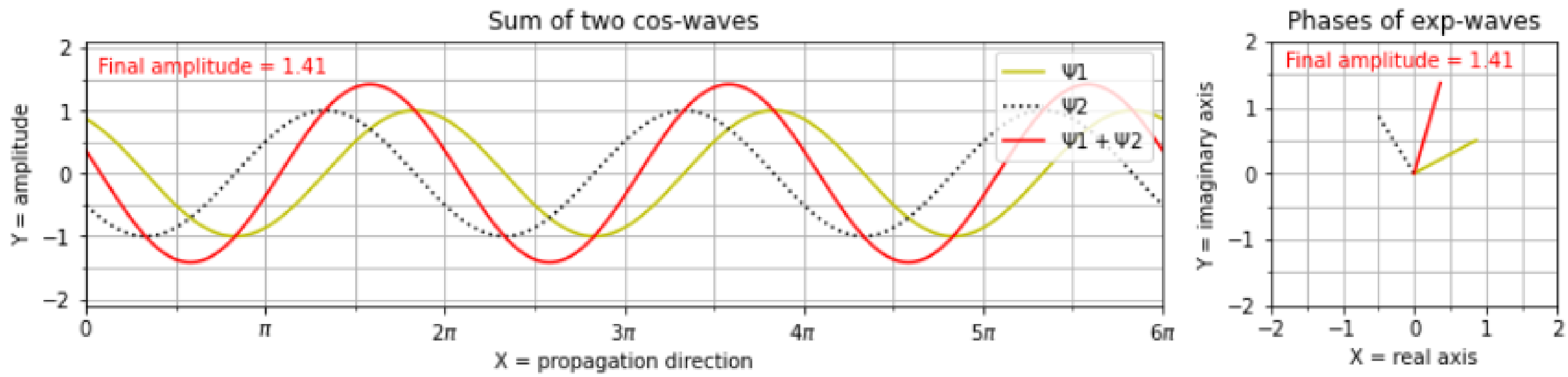
(1) Numerical verification

In [9]:
```
# Numerical summation (calculate the final amplitudes analytically)
print('Final amplitude (sum of cos-waves): %.5f' % A_of_two_cos_waves(A1,A2,Phi1,Phi2))
print('Final amplitude (sum of exp-waves): %.5f' % A_of_two_exp_waves(A1,A2,Phi1,Phi2))
```

```
Final amplitude (sum of cos-waves): 1.41421
Final amplitude (sum of exp-waves): 1.41421
```

(2) Graphical verification

In [10]:
```
# Graphical summation (determine the final amplitudes from graphs)
graphical_sum_of_two_waves(A1,A2,Phi1,Phi2)
```



(3) Conclusions (calculations + descriptions = reproducible documents)

In [11]:
```
# CONCLUSION:
# 0) We have demonstrated that waves can be described by both cos and exp functions.
# 1) In Mathematics: Strictly speaking, it is not correct, as the functions are not the same.
# 2) In Physics: Quite Ok, as the interference of cos- and exp-waves yield the same results.
# 3) Here: Numerical and graphical verification that it works (verification in not the proof!).
# 4) What is it good for? Diffraction theory -> summation of exp-waves is a key part of derivation.
```

Link to complete notebook →