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Practical Electron Optics of EEL Spectrometers & Imaging Energy Filters

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Imaging Energy Filters today are versatile tools for:

- Electron Energy Loss Spectroscopy in (S)TEM mode
- Zero-Loss Filtering in life science
- Energy-Filtered Imaging (Electron Spectroscopic Imaging)
- Energy-Filtered Diffraction
- STEM Spectrum Imaging (EELS Data Cube)
- Momentum-Resolved Spectroscopy (ωq-EELS)
- Energy-Filtered 4D STEM (STEM Data Tesseract)
- Event-based and correlated data acquisition techniques

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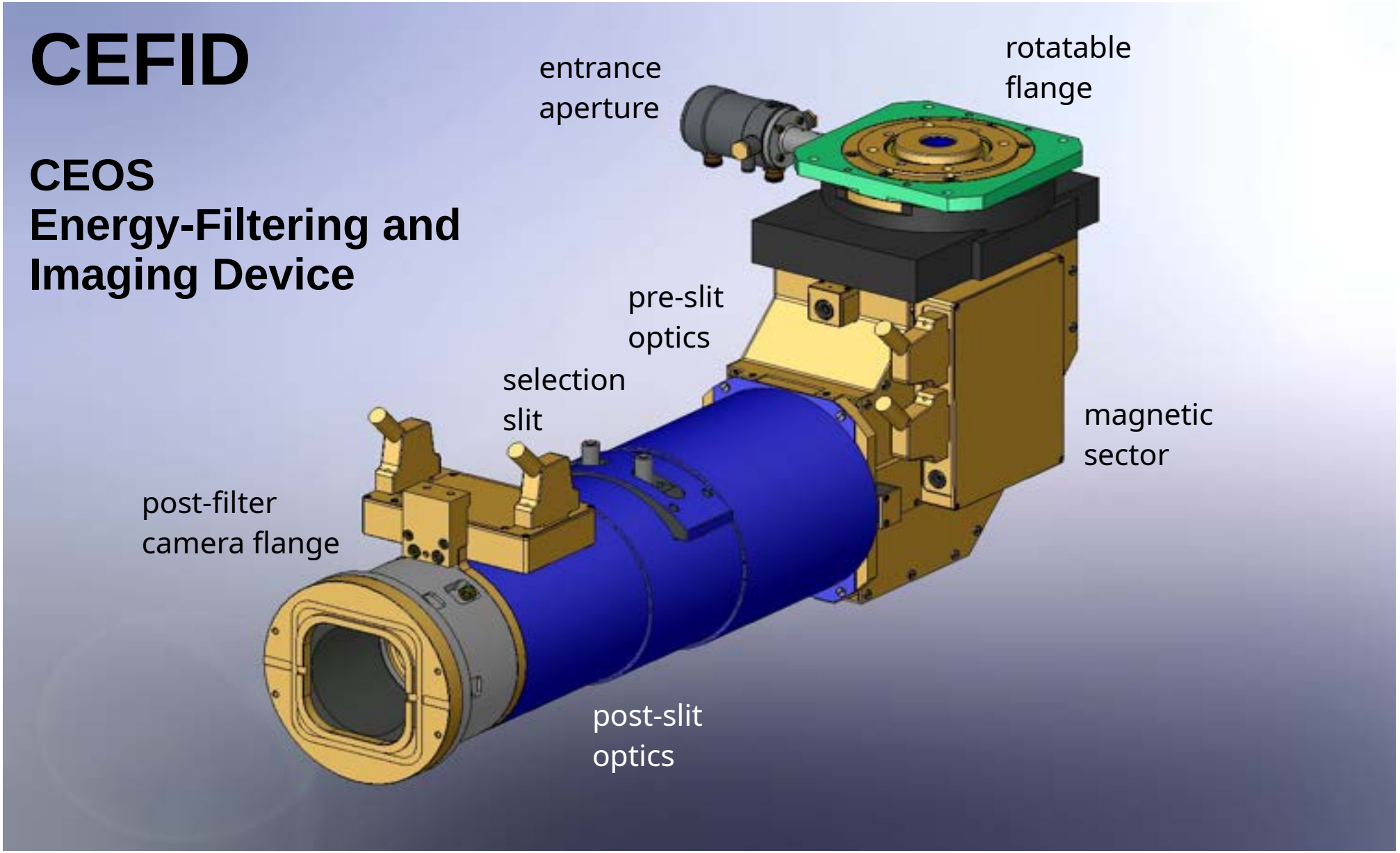
CEFID

CEOS Energy-Filtering and Imaging Device



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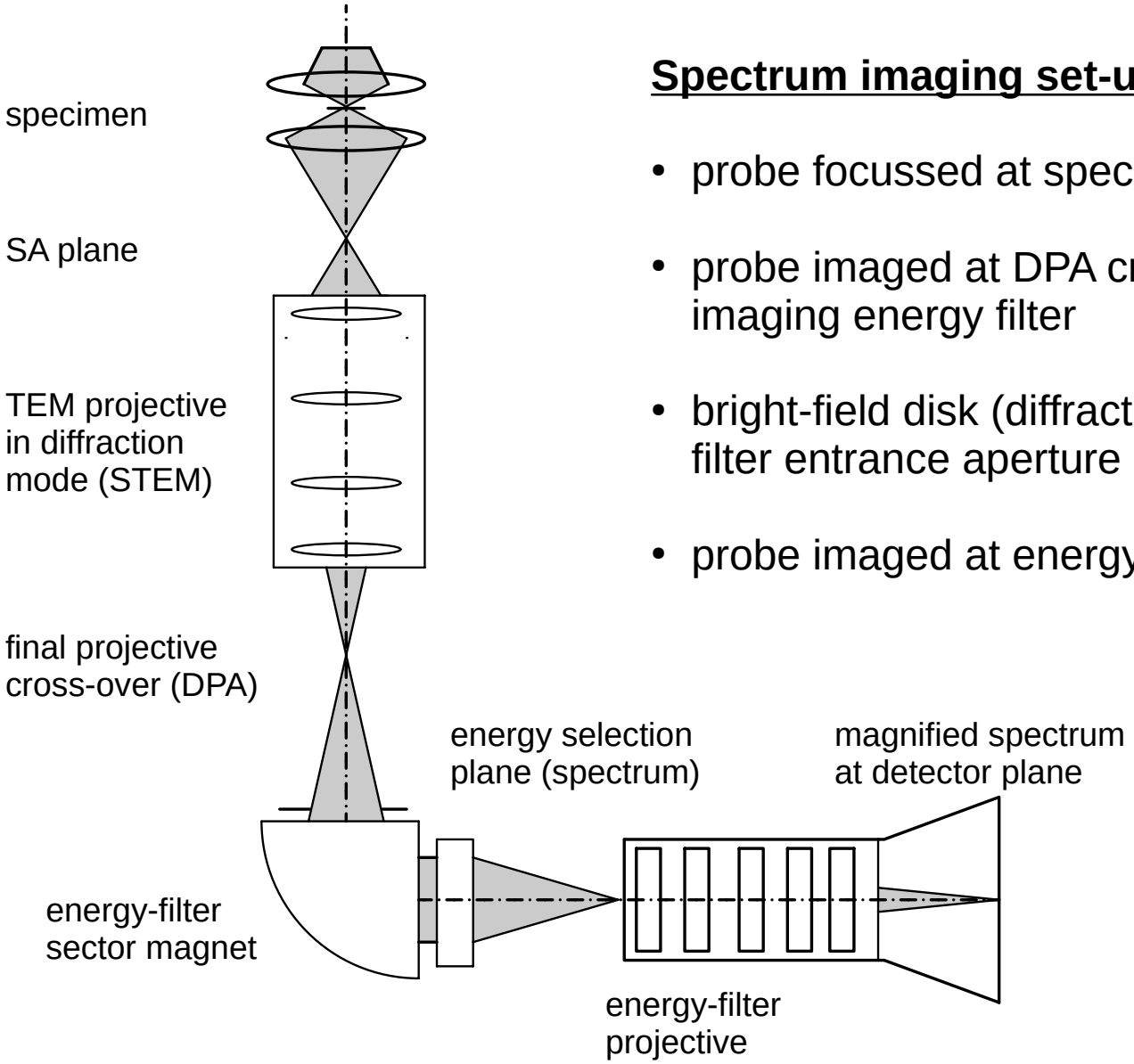

Spectrum imaging set-up (image coupled):

- probe focussed at specimen (STEM mode)
- probe imaged at DPA cross-over in front of imaging energy filter
- bright-field disk (diffraction pattern) at filter entrance aperture
- probe imaged at energy-selection plane

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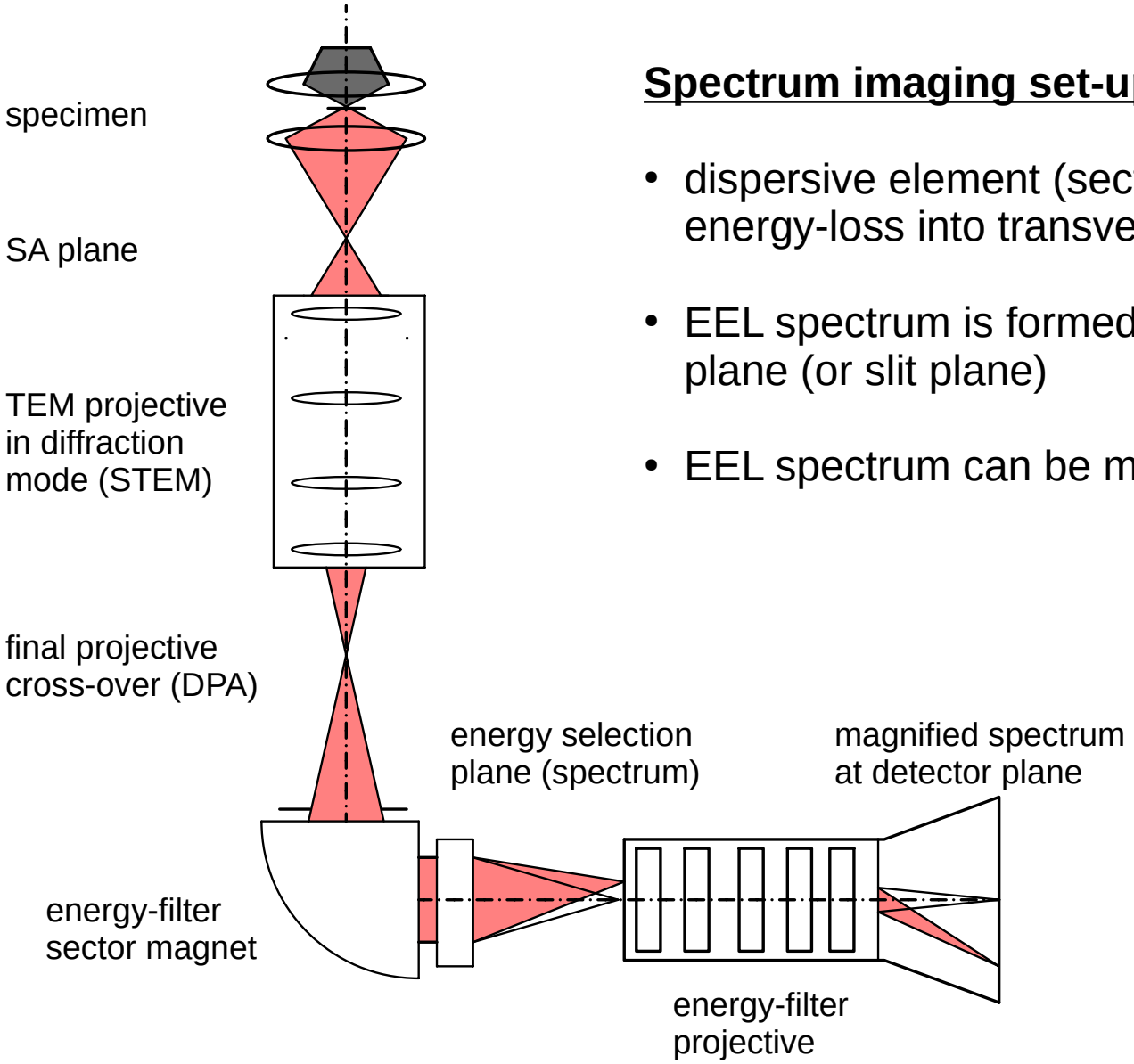

Spectrum imaging set-up (image coupled):

- dispersive element (sector magnet) translates energy-loss into transversal displacement
- EEL spectrum is formed at the energy selection plane (or slit plane)
- EEL spectrum can be magnified onto the detector

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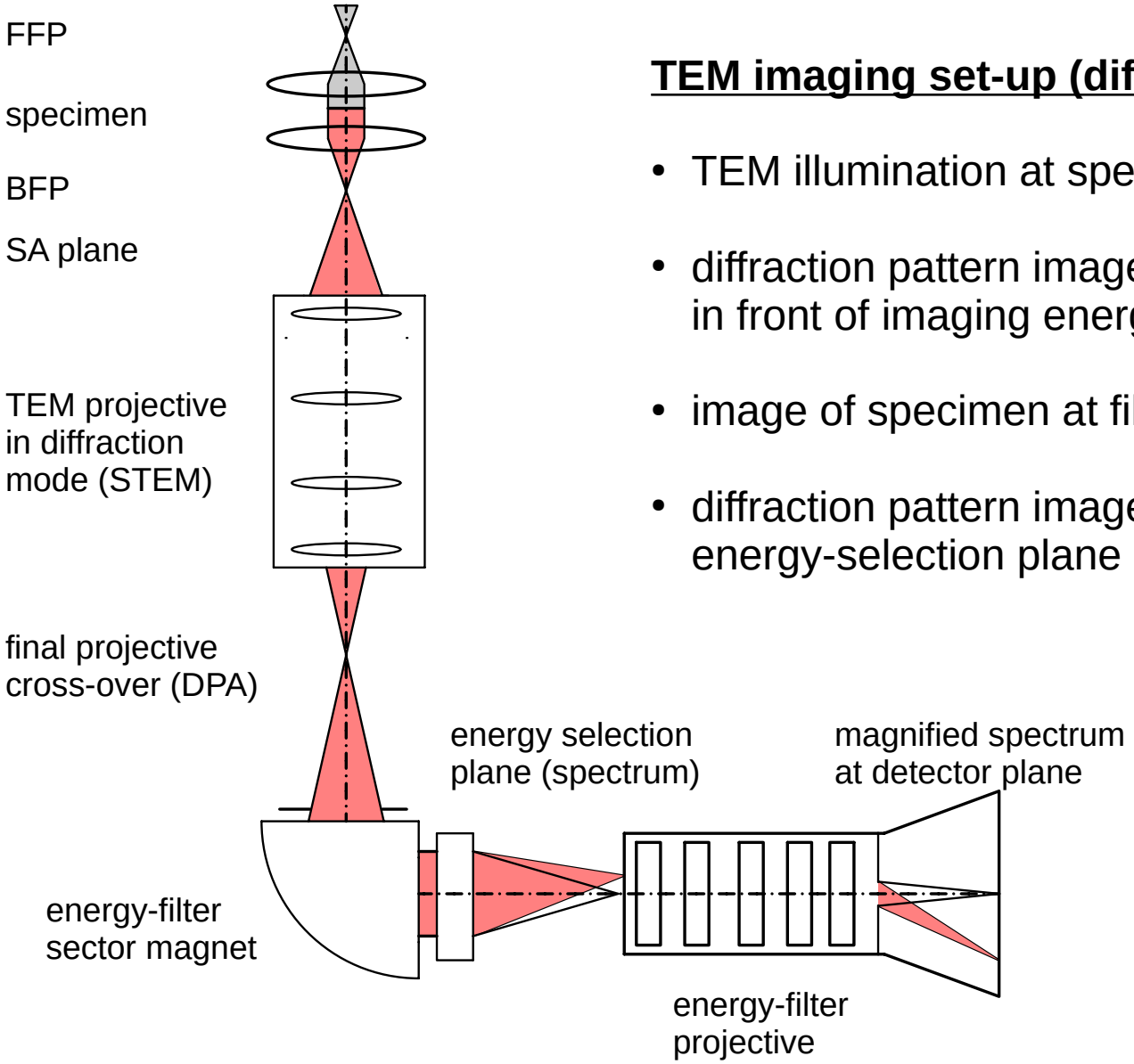

TEM imaging set-up (diffraction coupled):

- TEM illumination at specimen
- diffraction pattern imaged at DPA cross-over in front of imaging energy filter
- image of specimen at filter entrance aperture
- diffraction pattern imaged at energy-selection plane

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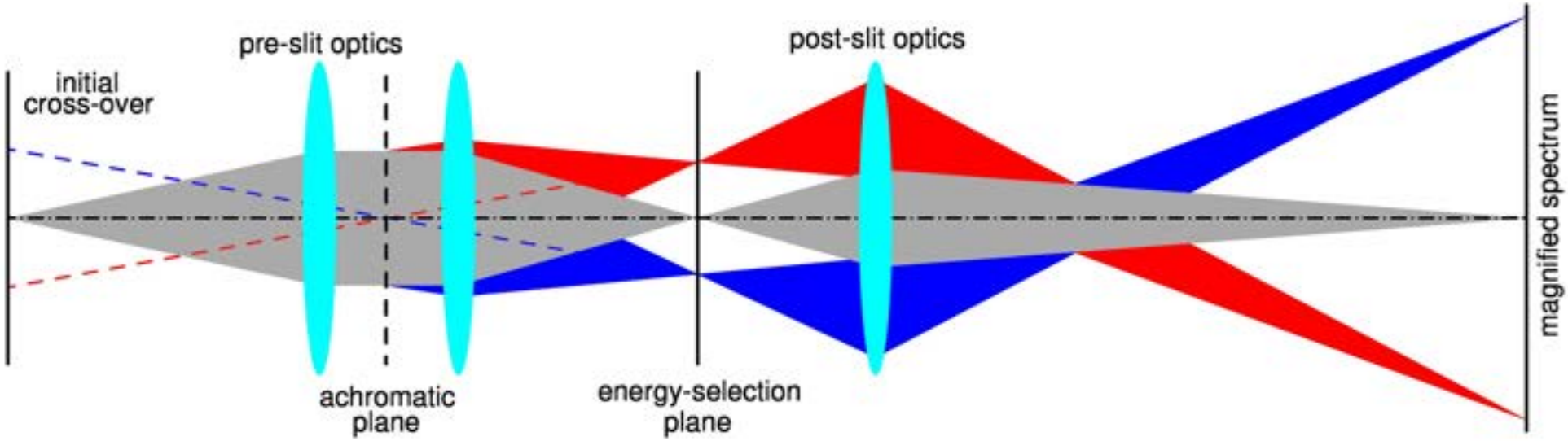
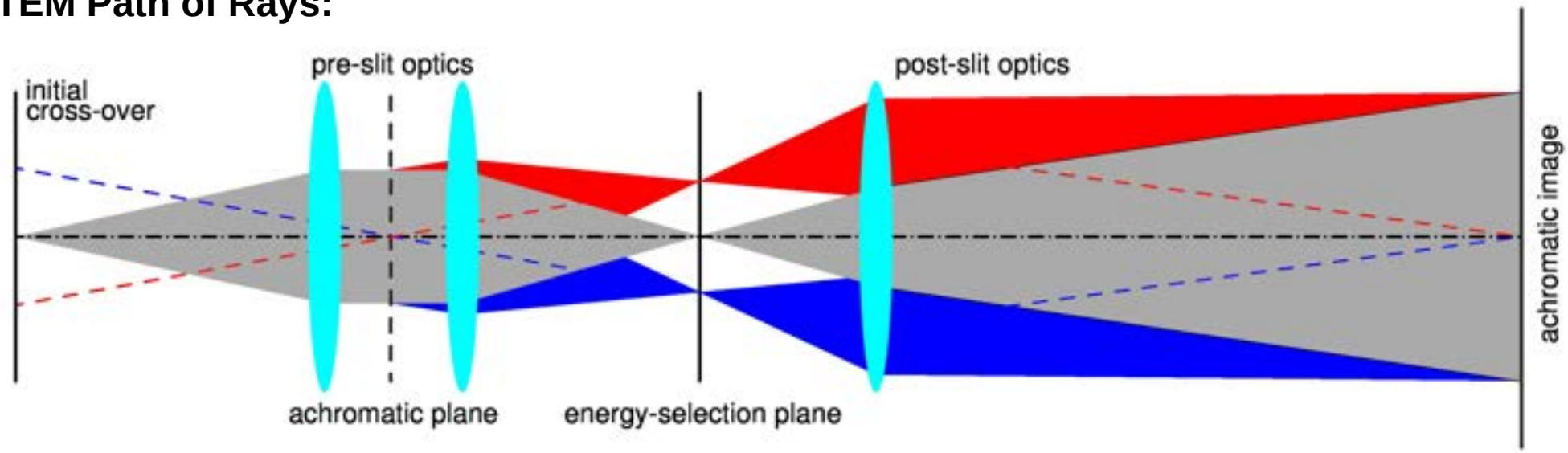
EELS Path of Rays:



EFTEM Path of Rays:



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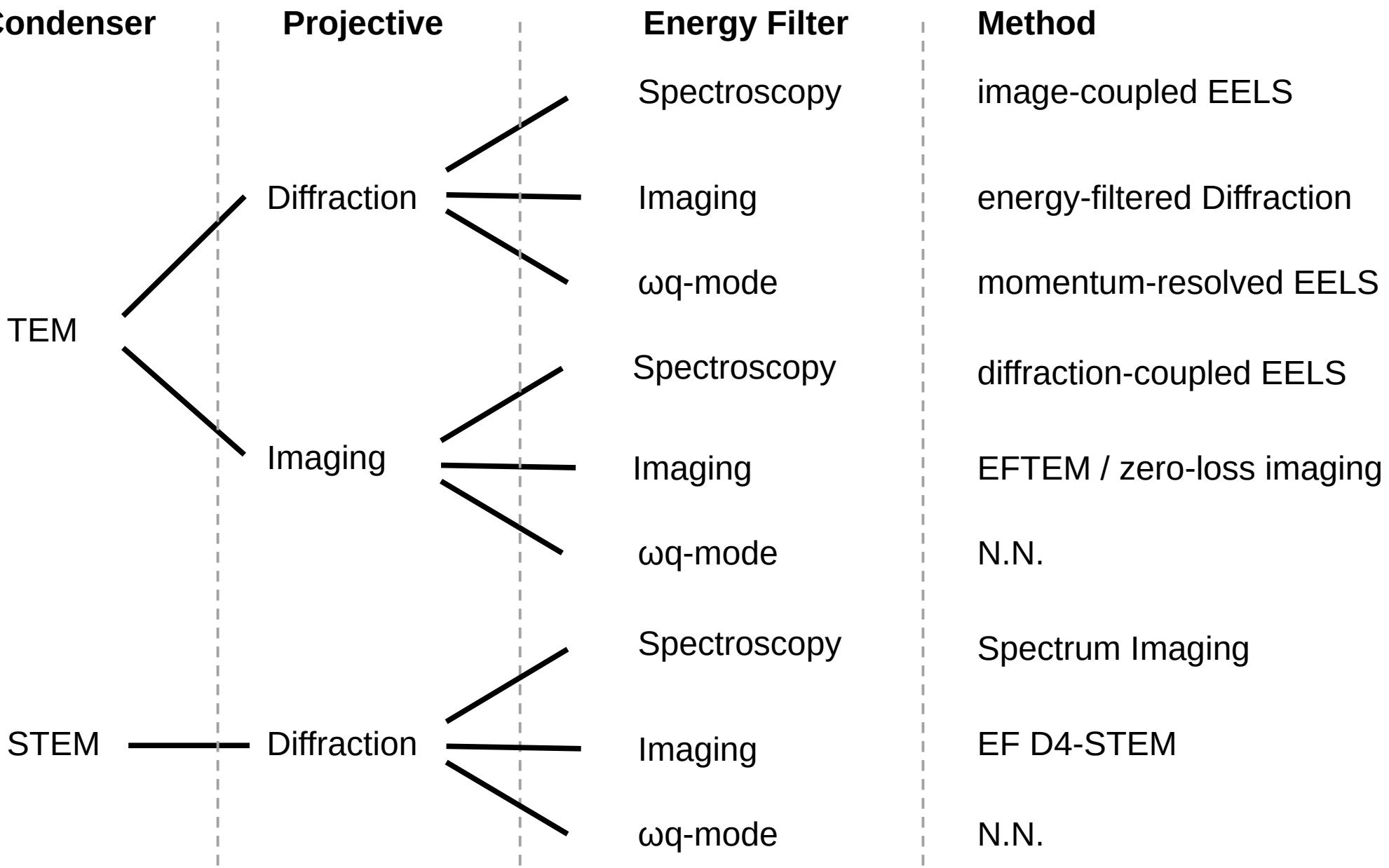

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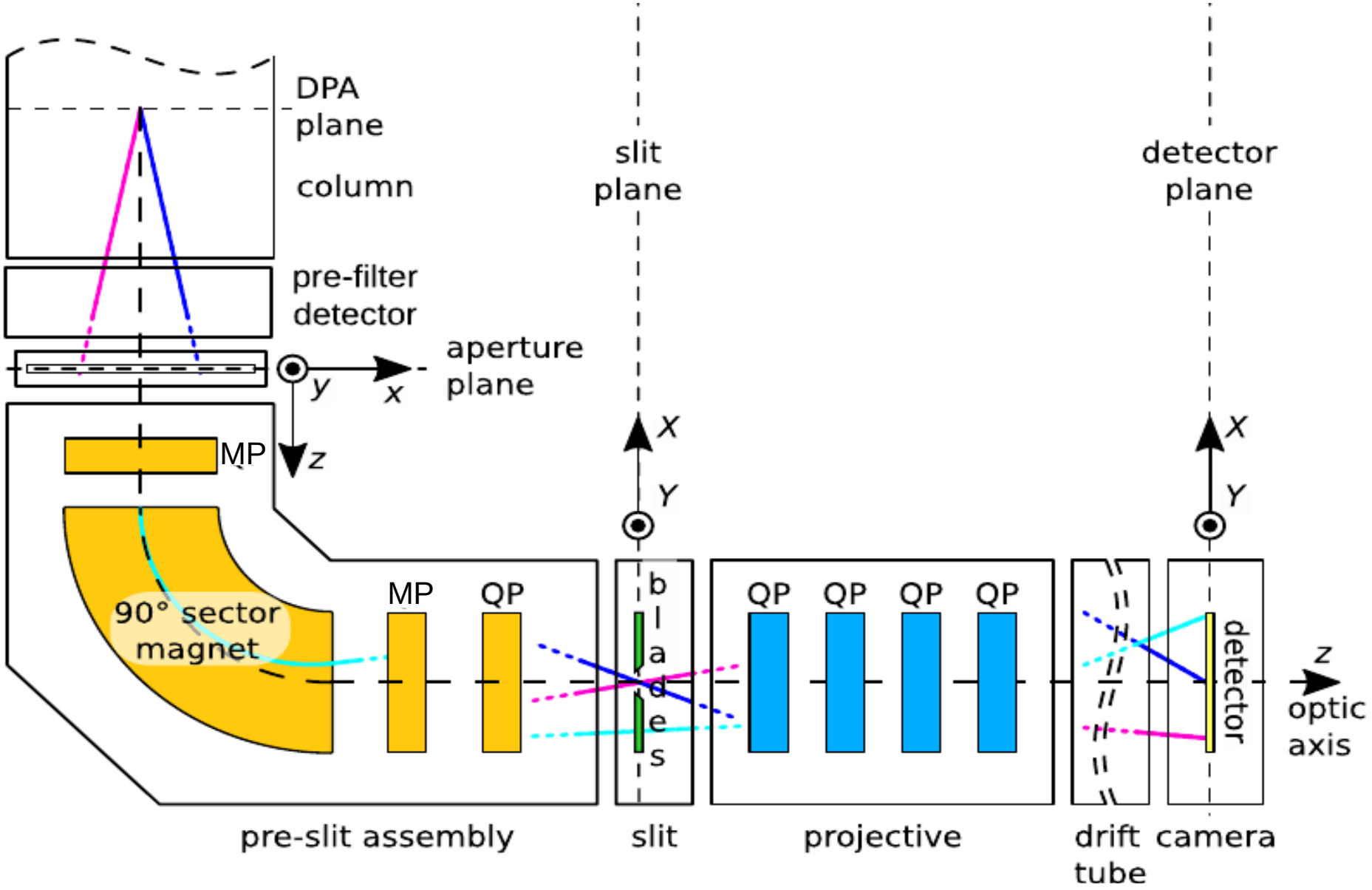

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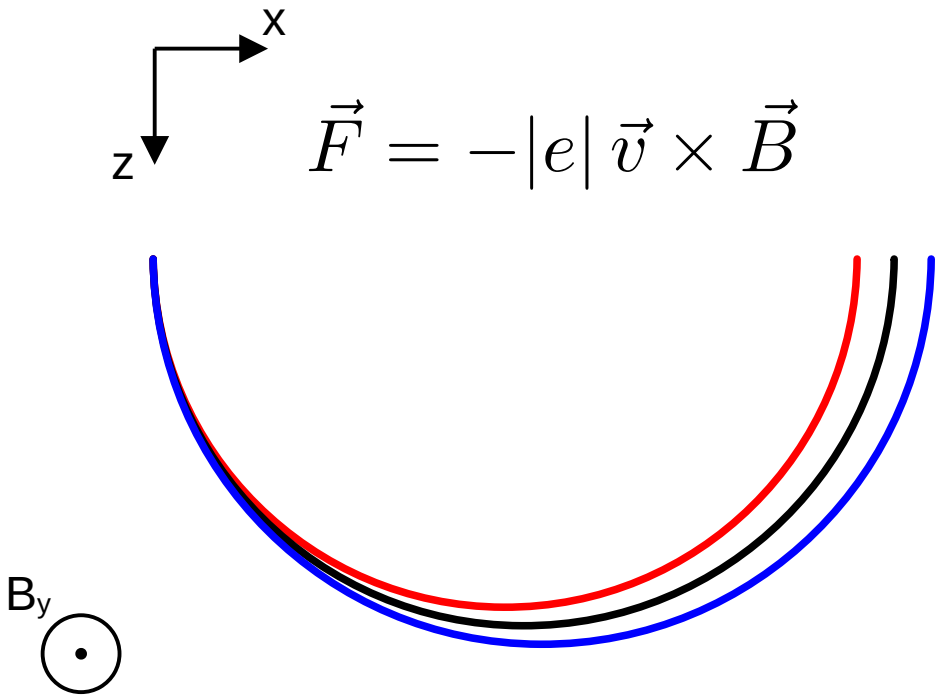
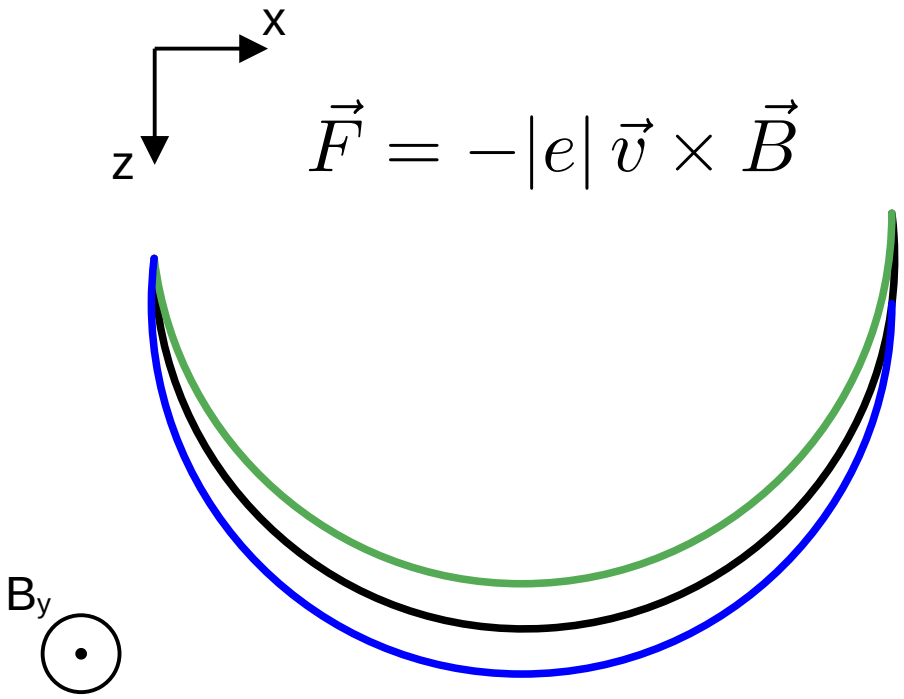
Electrons traveling in homogenious magnetic field:



- electrons travel on circles
- different energies travel on different radii
- deflection cause energy dispersion

Electrons traveling in homogenious magnetic field:



- electrons travel on circles
- different energies travel on different radii
- deflection causes energy dispersion

- electrons in xz-section are focussed toward optic axis
- focussing in ±x is asymmetric => second-order aberrations

Optics of a homogeneous sector magnet:

α, β : coordinates in filter entrace aperture $\kappa = \dfrac{\Delta E}{E_0}$: chromatic parameter

$$\begin{aligned} x(\alpha, \beta, \kappa) &= \alpha x_\alpha + \kappa x_\kappa \\ y(\alpha, \beta, \kappa) &= \beta y_\beta \end{aligned}$$

$$U^\star = U(1 + \varepsilon U) \qquad \varepsilon = \frac{|e|}{2 m_e c^2} \qquad \Lambda = \frac{1 + 2\varepsilon U}{1 + \varepsilon U}$$

$$x'' + \frac{1}{R^2} x = -\frac{\Lambda}{2R} \frac{\Delta E}{E_0} \qquad \frac{1}{R} = -\sqrt{\frac{|e|}{2 m_e U^\star}}\, \Psi_{1s}$$

Optics of a homogeneous sector magnet:

$$x'' + \frac{1}{R^2}\, x = -\frac{\Lambda}{2R}\,\frac{\Delta E}{E_0}$$

$$\frac{1}{R} = -\sqrt{\frac{|e|}{2 m_e U^\star}}\,\Psi_{1s}$$

Dispersion ray:

$$x_\kappa = -\frac{\Lambda R}{2}\left(1 - \cos\left(\frac{z}{R}\right)\right)$$

$$x'_\kappa = -\frac{\Lambda}{2}\,\sin\left(\frac{z}{R}\right)$$

for 300kV:

$$\frac{d\vartheta}{dE} = -\frac{\Lambda}{2E} \approx 2.0\,\frac{\mu rad}{eV}$$

for 60kV:

$$\frac{d\vartheta}{dE} = -\frac{\Lambda}{2E} \approx 8.8\,\frac{\mu rad}{eV}$$

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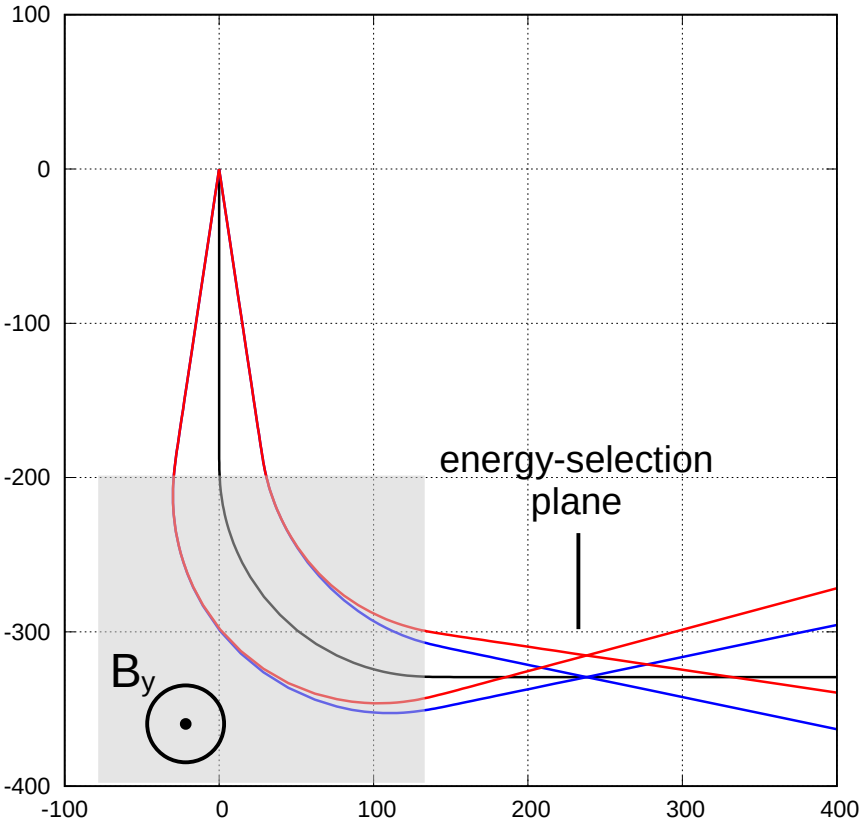
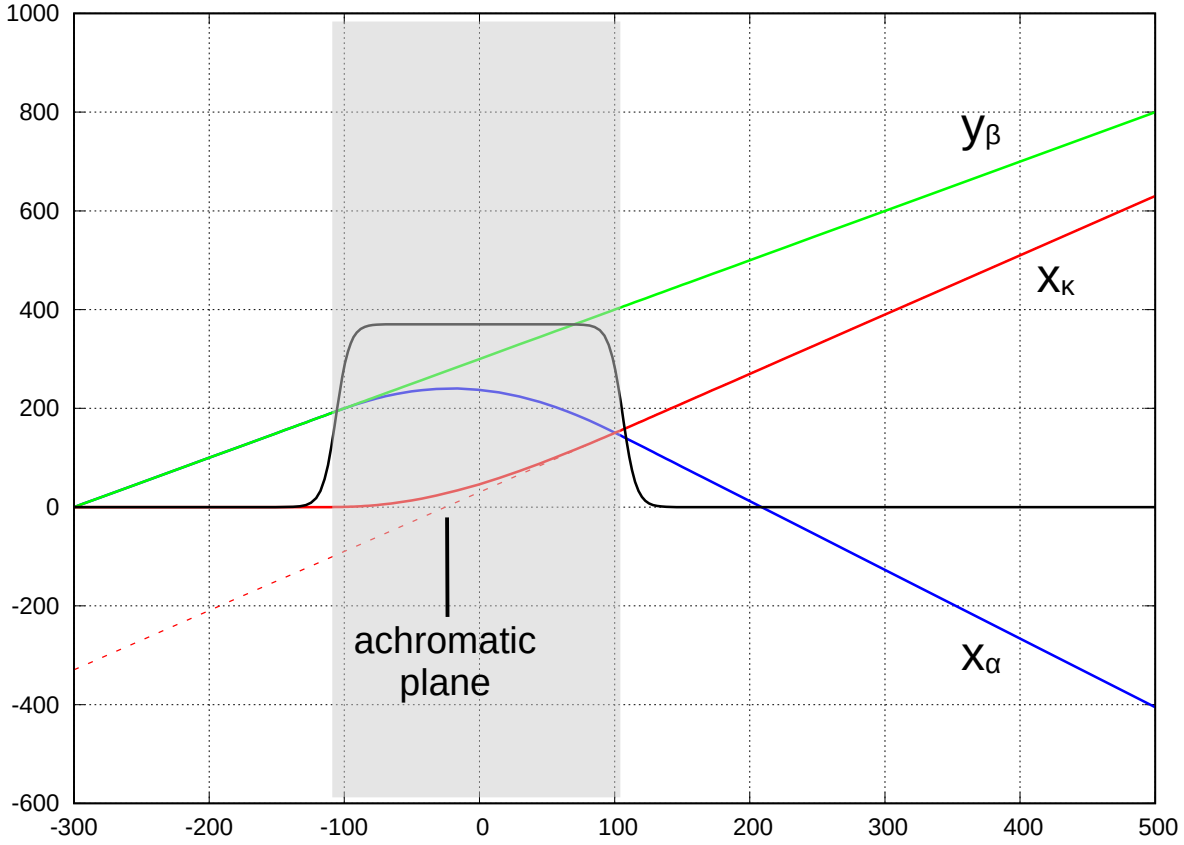
Pre-slit raypath of simple 90° sector magnet:

Course of optic axis and homocentric bundle.



Straightened optic axis and axial rays.



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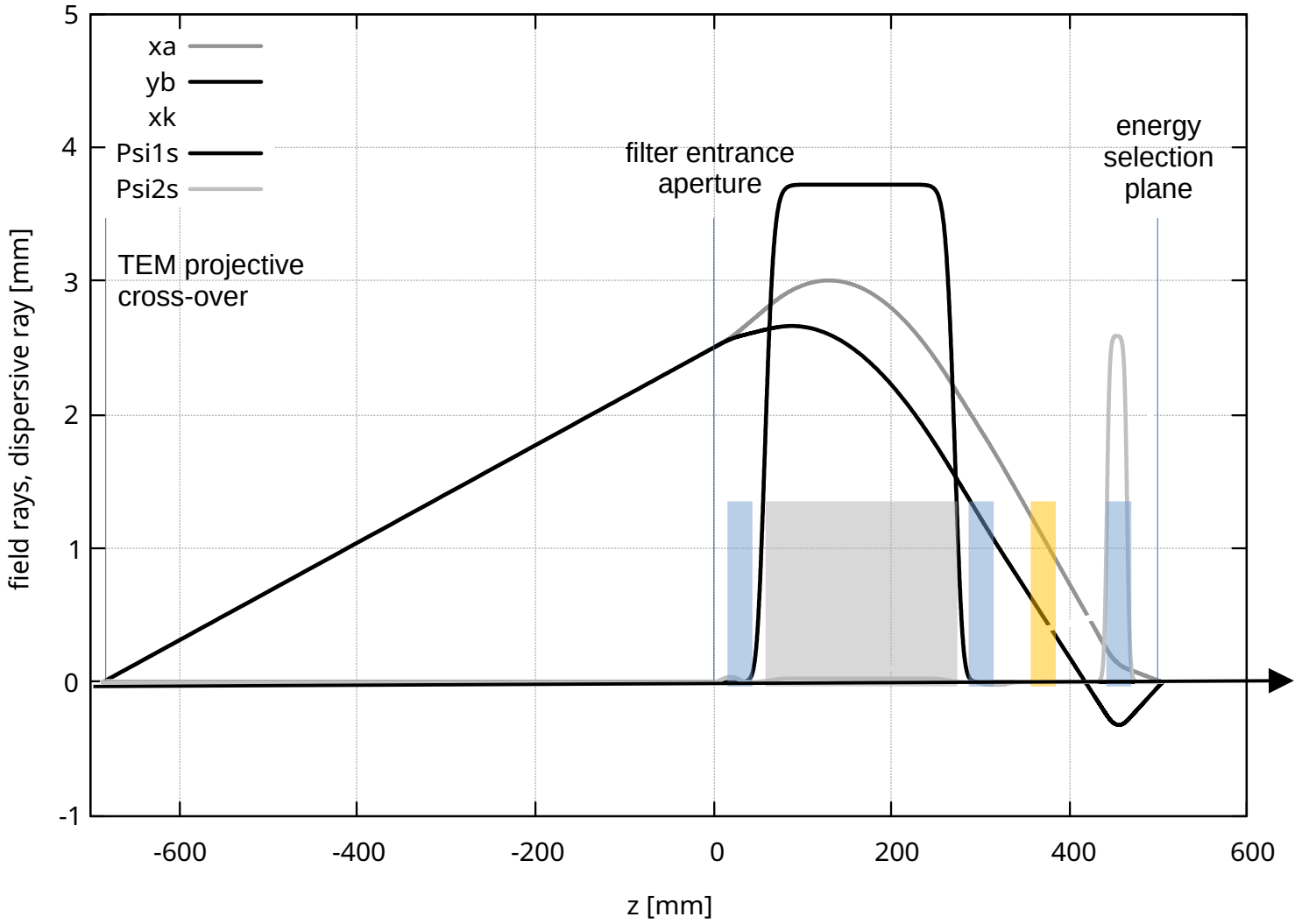
Pre-slit raypath of real spectrometer:



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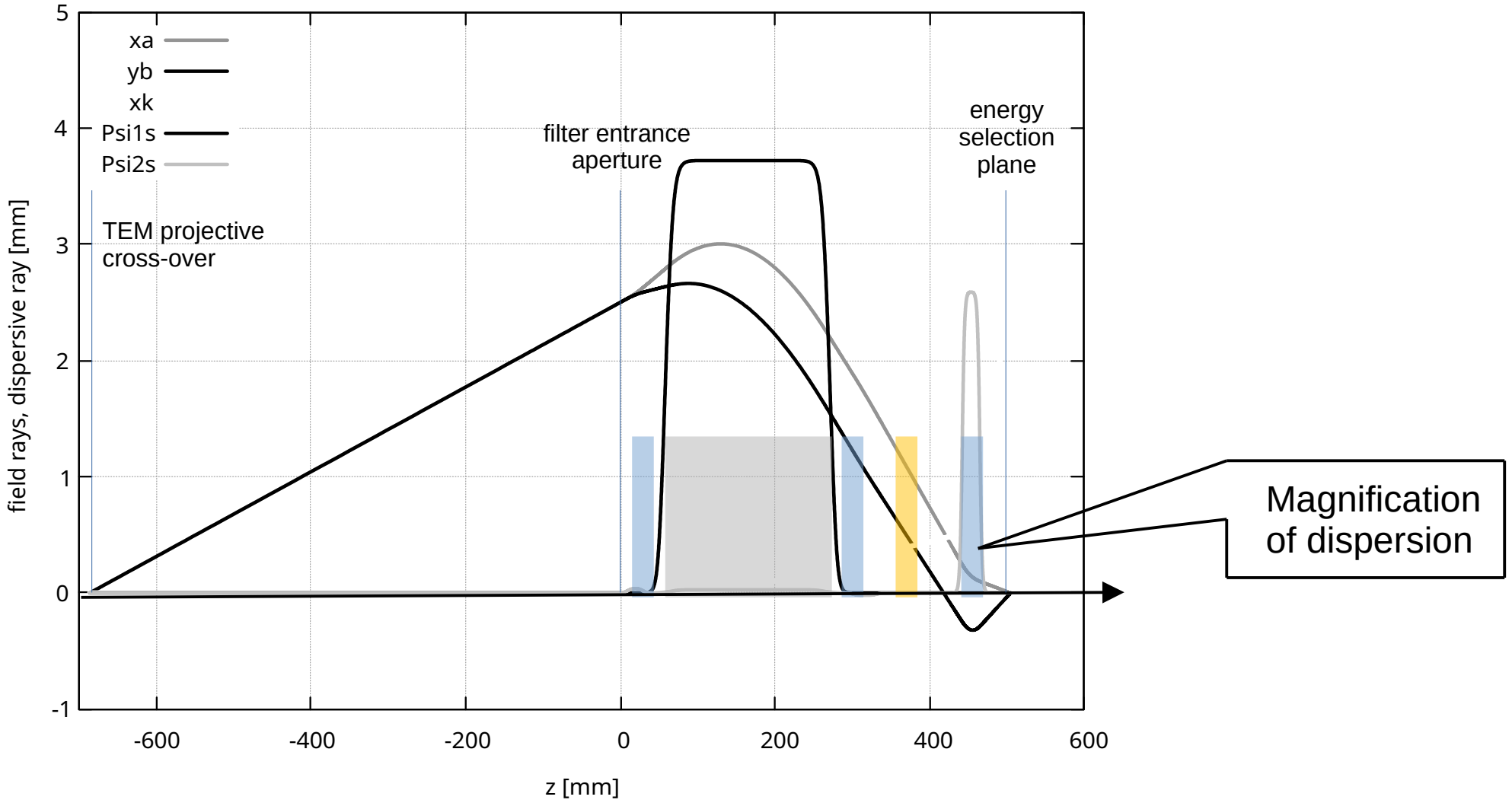
Pre-slit raypath of real spectrometer:



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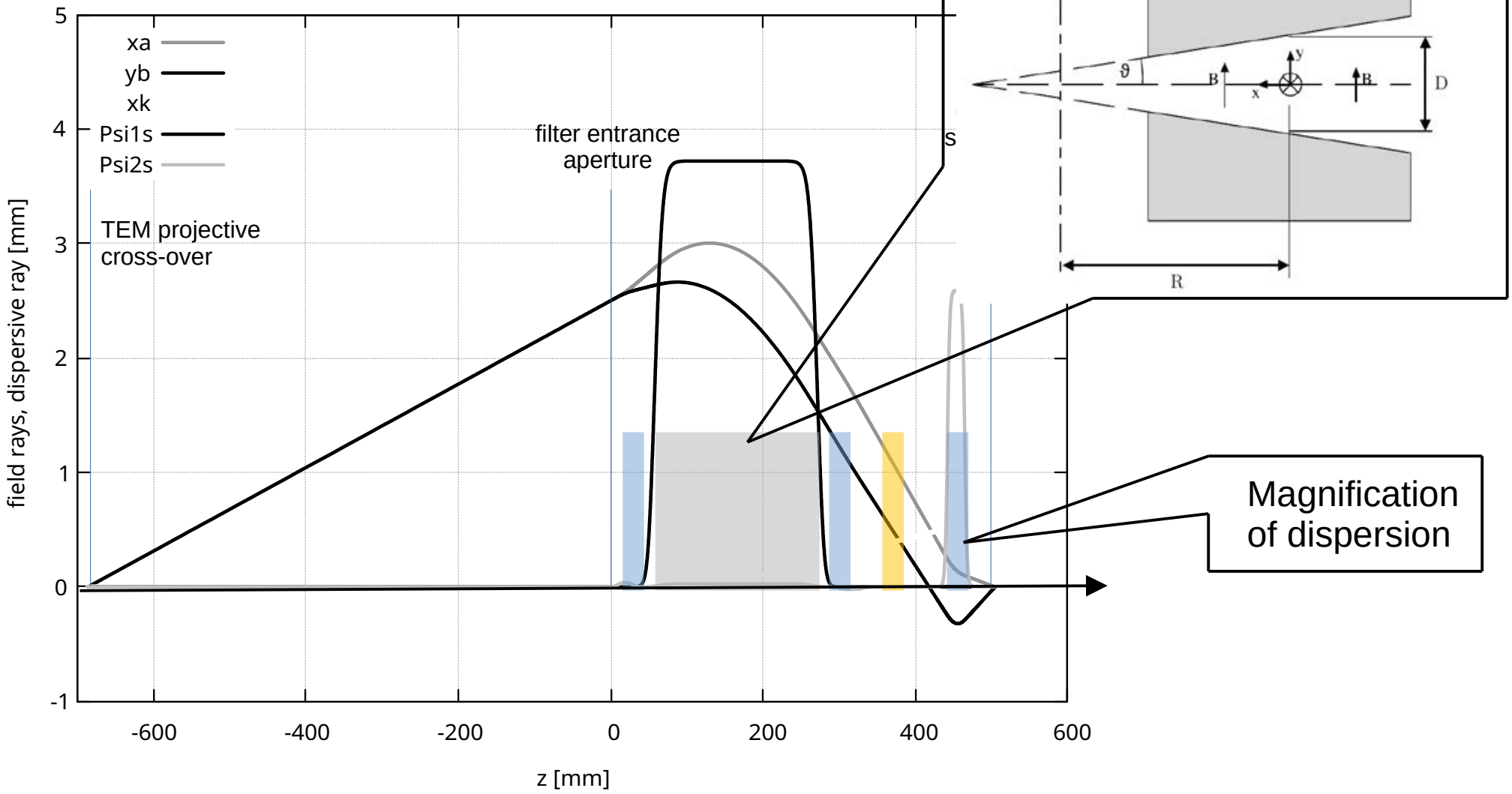
Pre-slit raypath of real spectrometer:



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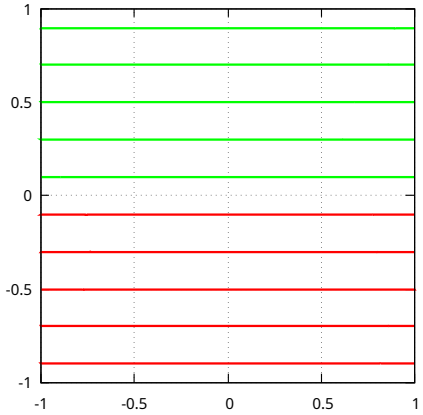
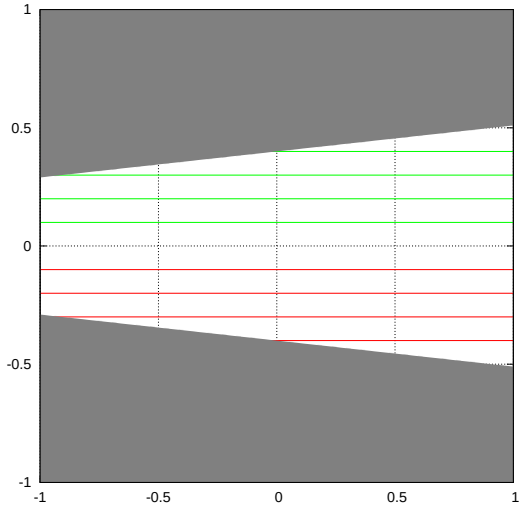
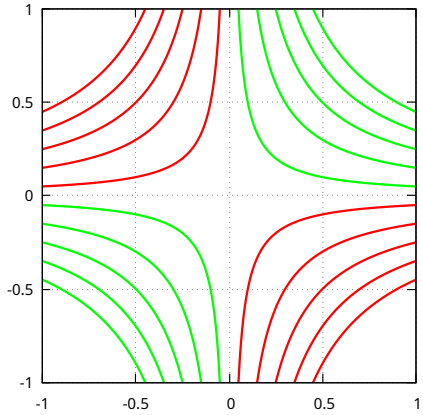
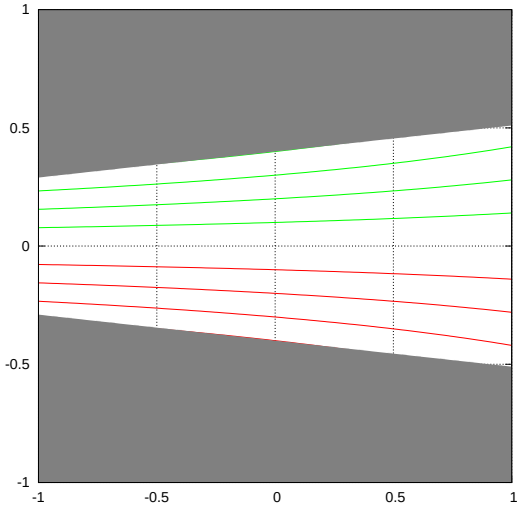
Dipole



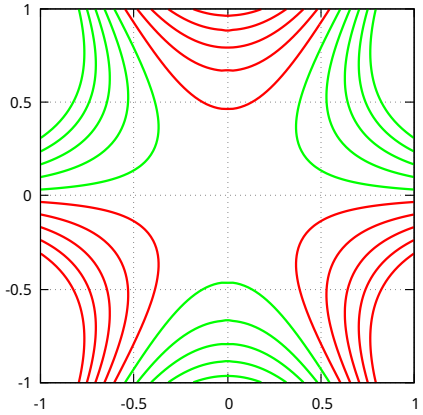


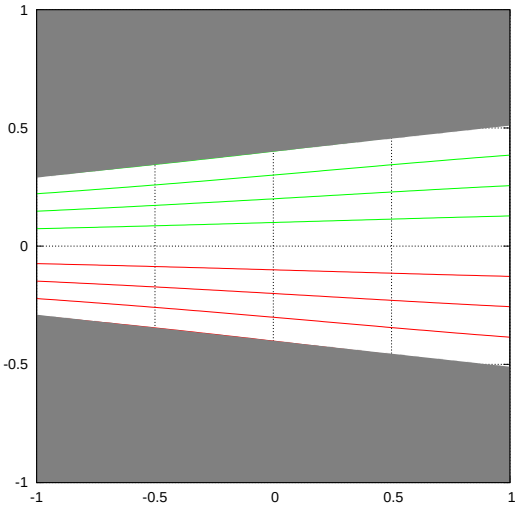
Quadrupole





Hexapole





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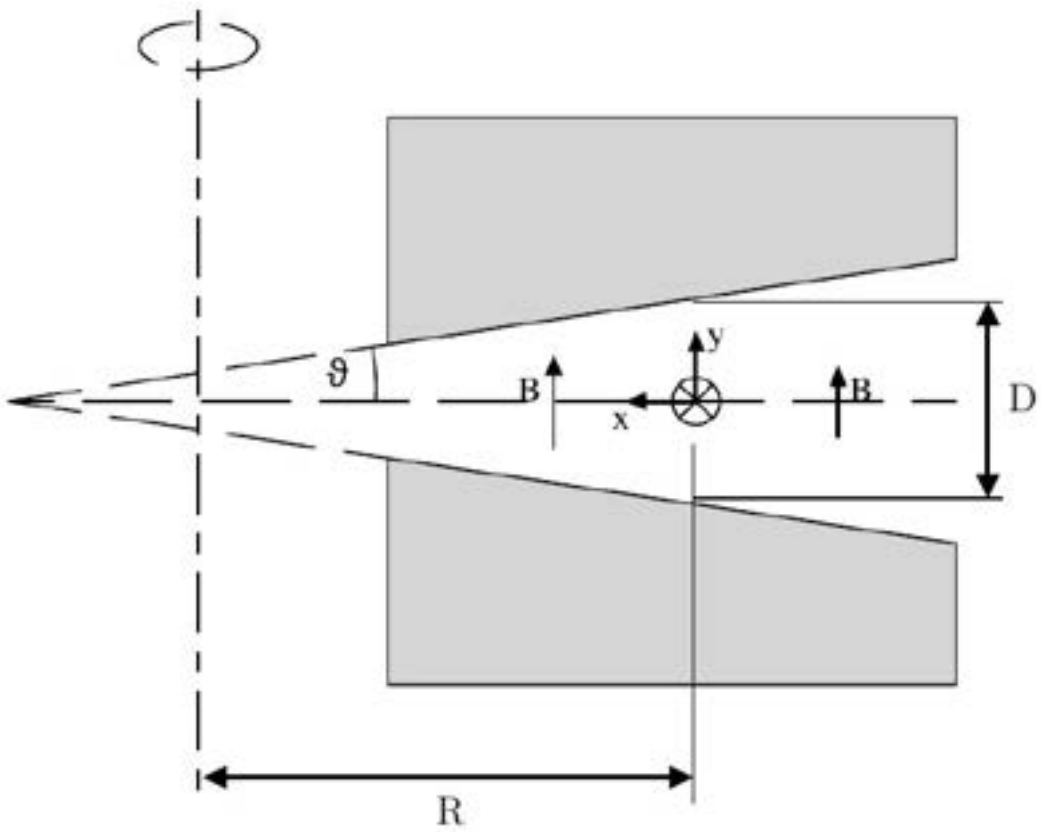

Magn. Field (Dipole Strength):

$$\mathrm{B} \quad = -\Psi_{1s} = \frac{1}{\eta\, R}$$

Quadrupole Strength:

$$\Psi_{2s} \quad = \quad \frac{1}{R}\,\xi\,\Psi_{1s}\,, \quad \xi = \frac{R}{D}\tan(\vartheta)$$

Hexapole Strength:

$$\Psi_{3s} \quad = \quad \frac{1}{12R^2}\left(16\,\xi^2 - \xi\right)\,\Psi_{1s}$$

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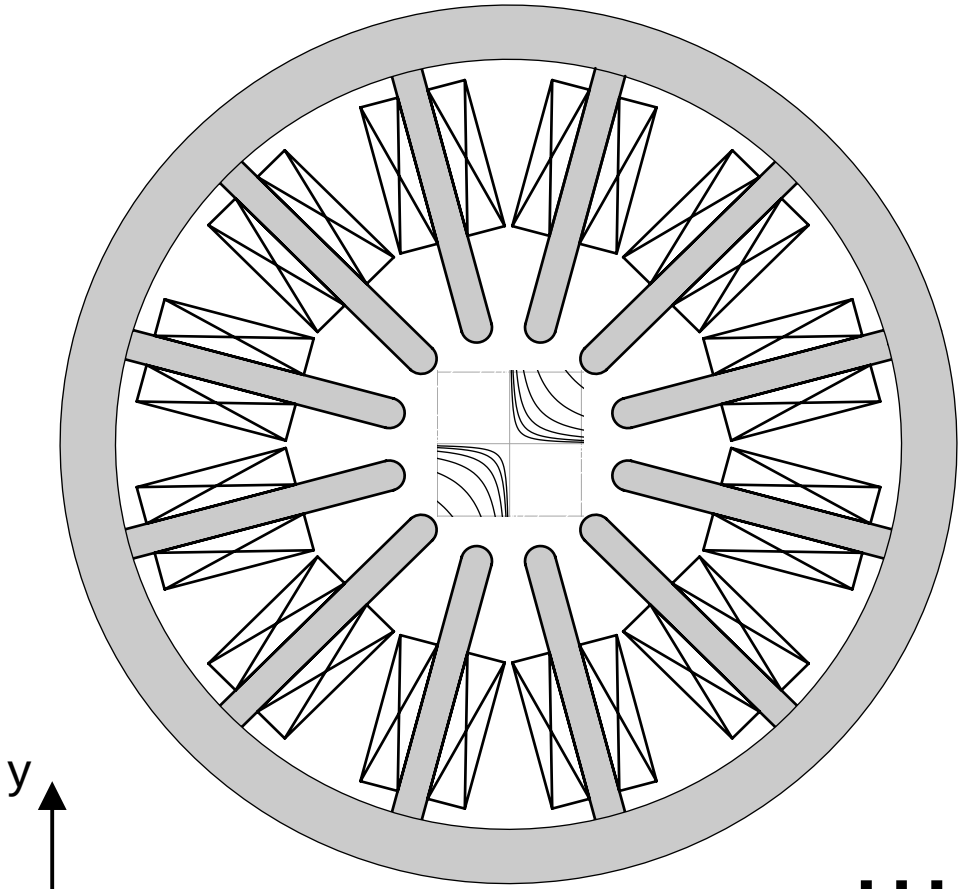
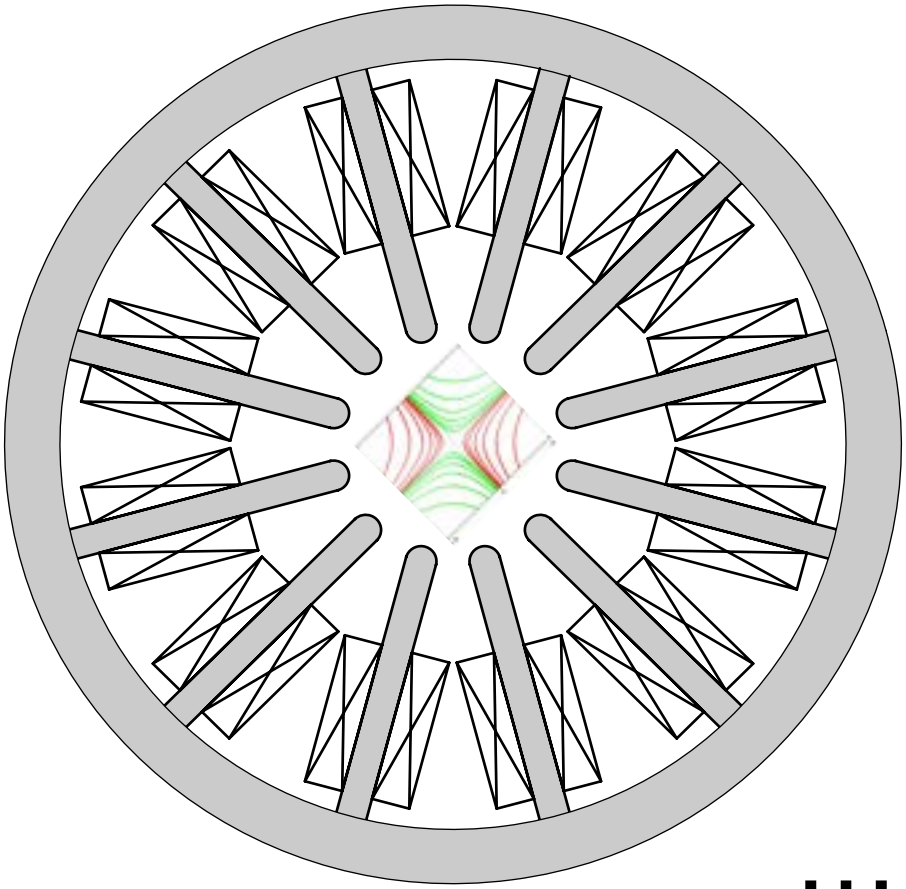
Dodecapole for correction of spectrum aberrations (NI):



Ψ_{2s}



Ψ_{2c}

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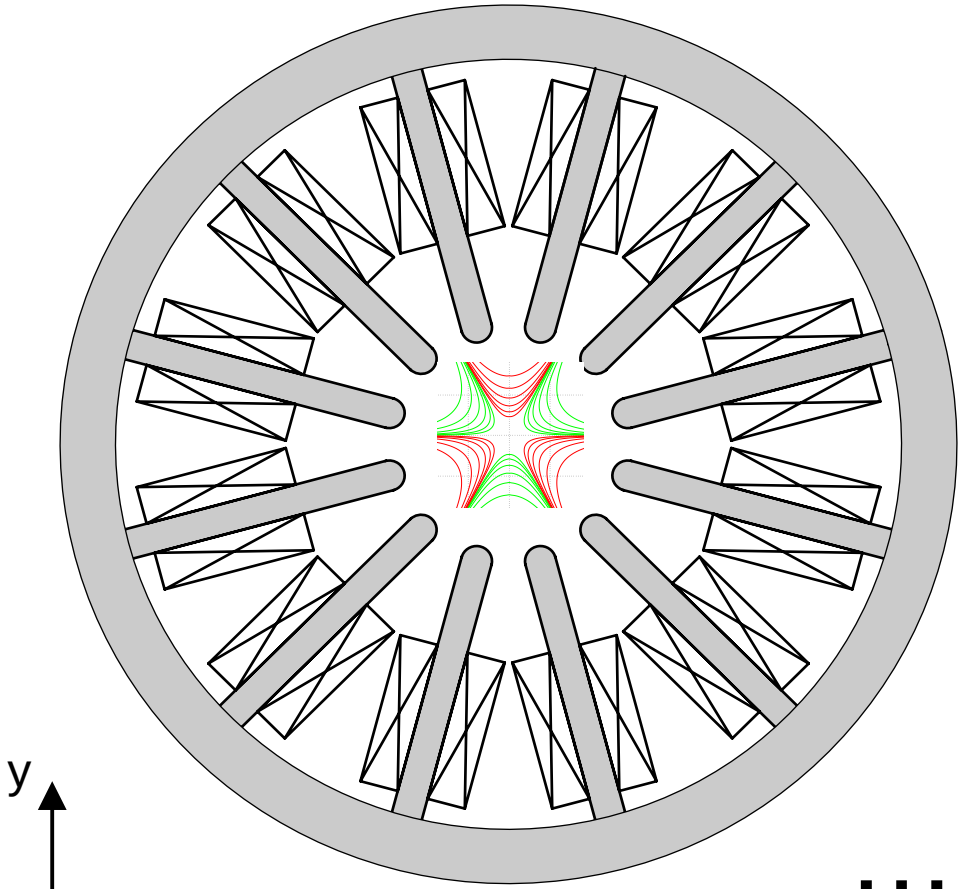
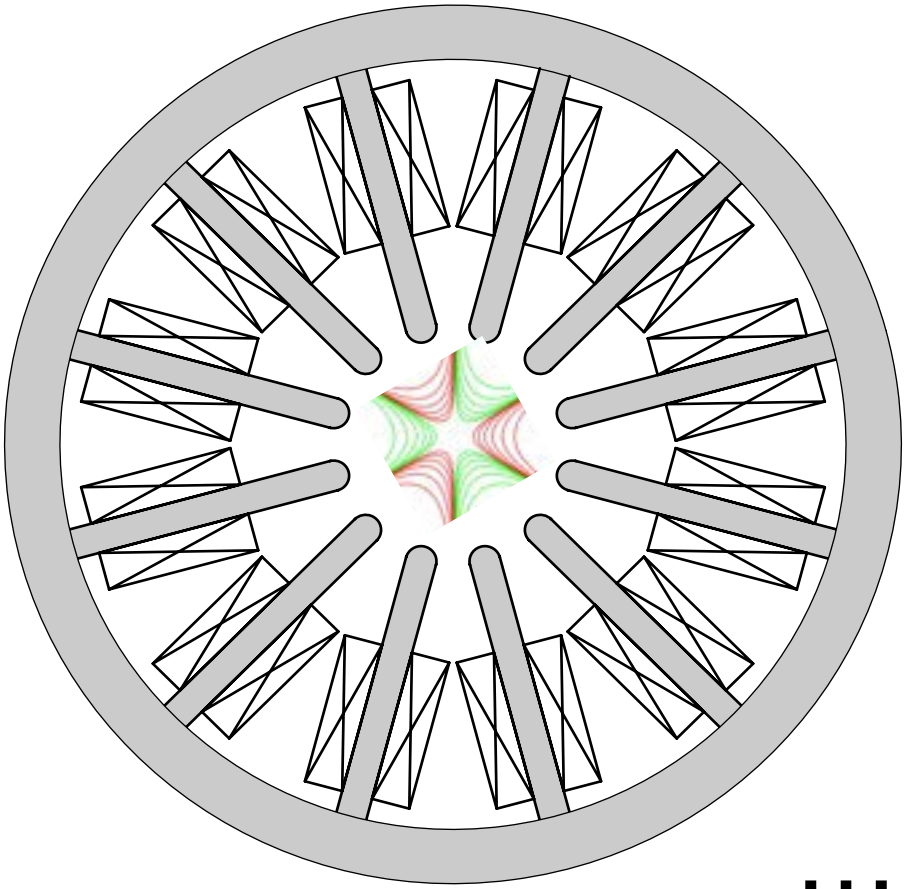
Dodecapole for correction of spectrum aberrations (NI):



Ψ_{3s}



Ψ_{3c}

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Aberrations a energy-selection plane:

α, β : coordinates in filter entrace aperture $\kappa = \frac{\Delta E}{E_0}$: chromatic parameter

Rank 1:

$$x^{(1)}(\alpha, \beta, \kappa) = \alpha x_\alpha + \beta x_\beta + \kappa x_\kappa$$
$$y^{(1)}(\alpha, \beta, \kappa) = \beta y_\beta$$

mirror symmetry: y <-> -y

Rank 2:

$$x^{(2)}(\alpha, \beta, \kappa) = \alpha^2 x_{\alpha\alpha} + \beta^2 x_{\beta\beta} + \alpha\beta x_{\alpha\beta} + \alpha\kappa x_{\alpha\kappa}$$

Rank 3:

$$x^{(3)}(\alpha, \beta, \kappa) = \alpha^3 x_{\alpha\alpha\alpha} + \alpha\beta^2 x_{\alpha\beta\beta} + \alpha^2\beta x_{\alpha\alpha\beta} + \beta^3 x_{\beta\beta\beta}$$

Aberrations a energy-selection plane:

α, β : coordinates in filter entrace aperture $\quad \kappa = \dfrac{\Delta E}{E_0}$: chromatic parameter

Rank 1: (3 x Ψ_{2s}, 1 x Ψ_{2c})

$$x^{(1)}(\alpha, \beta, \kappa) = \alpha x_\alpha + \beta x_\beta + \kappa x_\kappa$$
$$y^{(1)}(\alpha, \beta, \kappa) = \beta y_\beta$$

mirror symmetry: y <-> -y

Rank 2: (2 x Ψ_{3s}, 1 x Ψ_{3c}, ??)

$$x^{(2)}(\alpha, \beta, \kappa) = \alpha^2 x_{\alpha\alpha} + \beta^2 x_{\beta\beta} + \alpha\beta x_{\alpha\beta} + \alpha\kappa x_{\alpha\kappa}$$

Rank 3: (2 x Ψ_{4s}, 2 x Ψ_{4c})

$$x^{(3)}(\alpha, \beta, \kappa) = \alpha^3 x_{\alpha\alpha\alpha} + \alpha\beta^2 x_{\alpha\beta\beta} + \alpha^2\beta x_{\alpha\alpha\beta} + \beta^3 x_{\beta\beta\beta}$$

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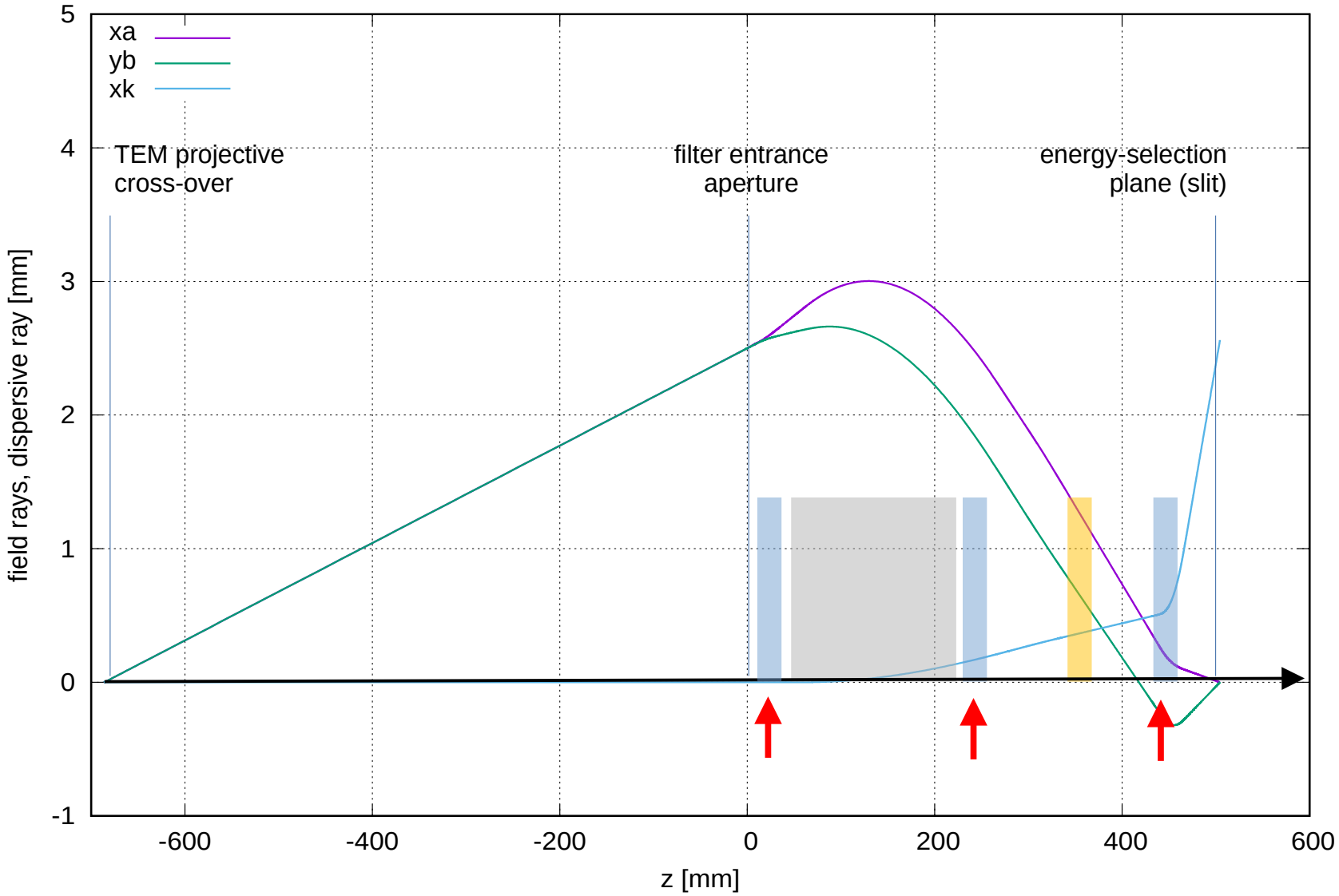

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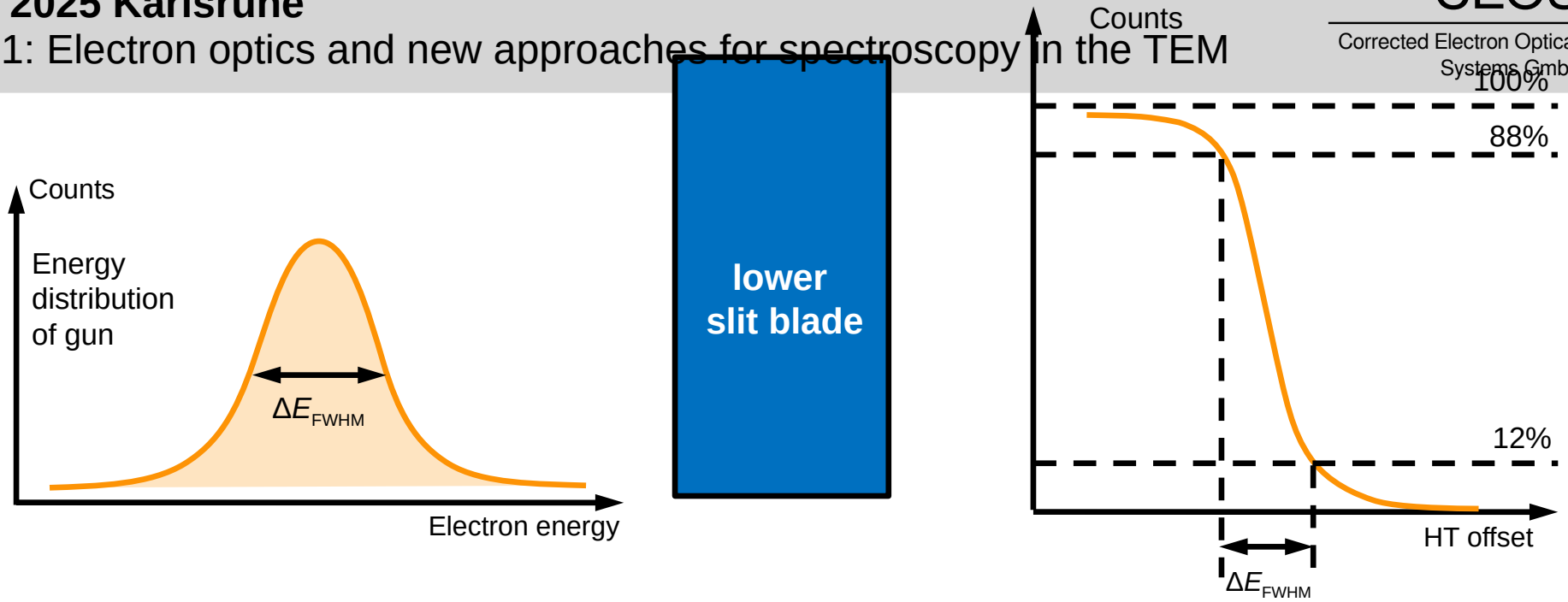

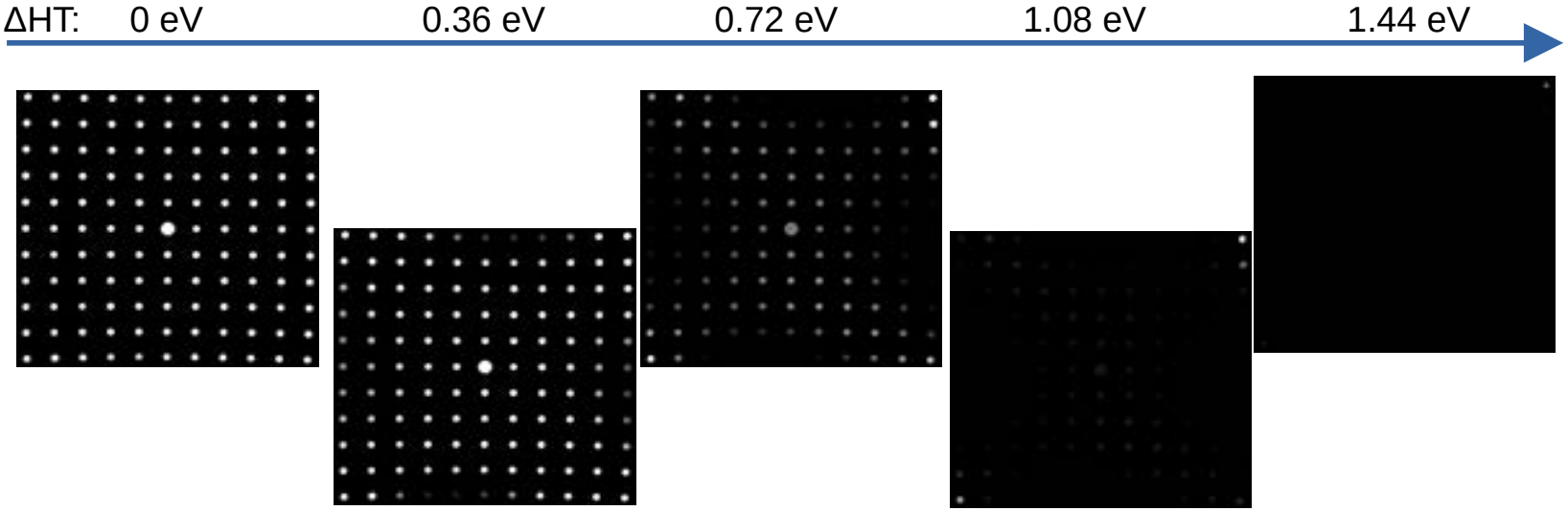

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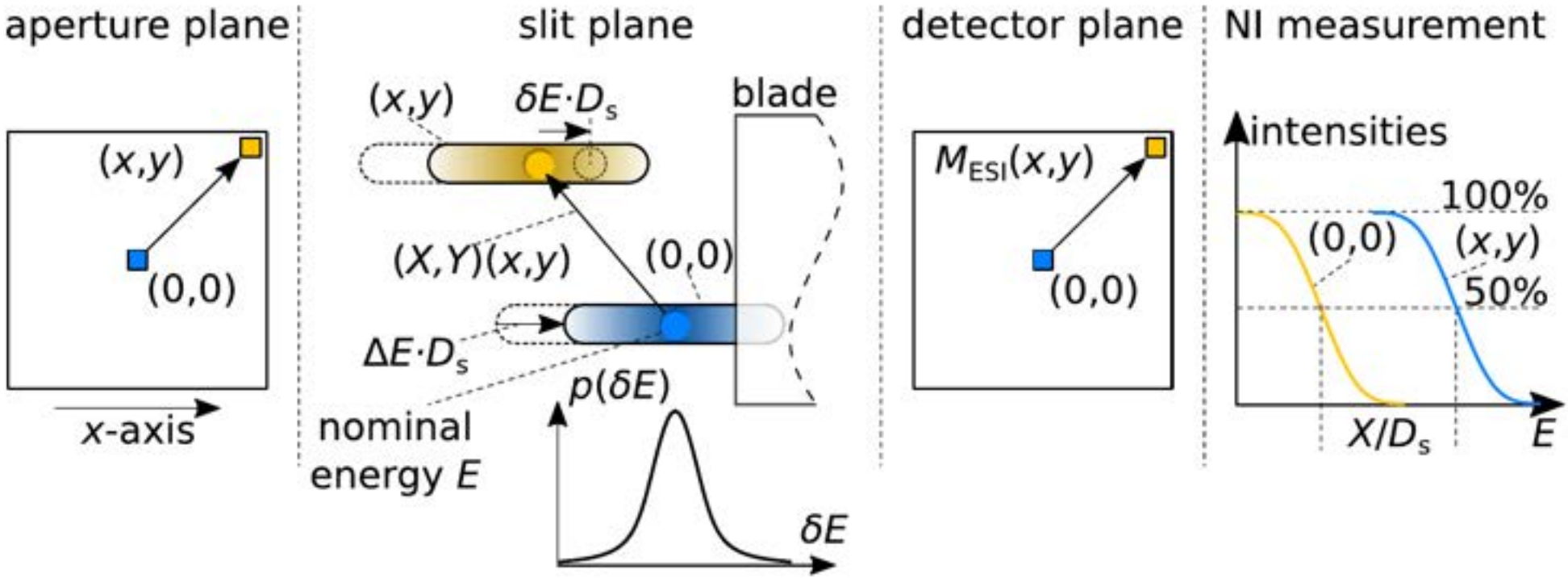

$$E(x, y, \Delta E) = \Delta E + \sum_{r \geq 0} \sum_{\substack{m=0 \\ n=r-m}}^{r} E_{nm} x^n y^m \,,$$

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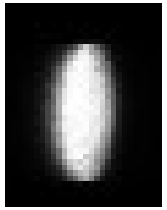
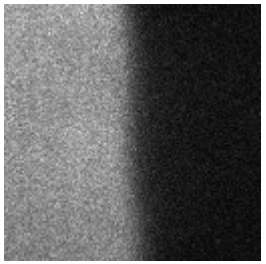
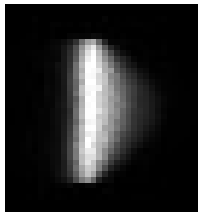
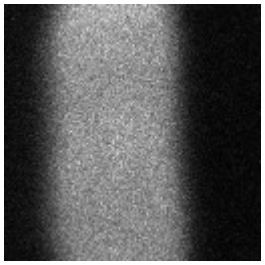
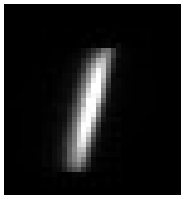
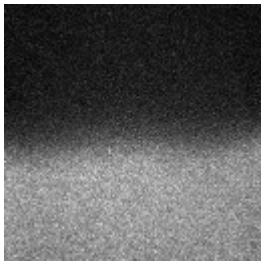
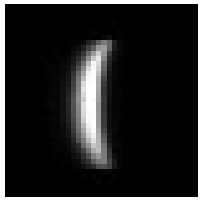
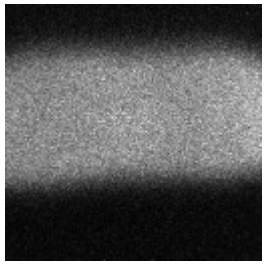
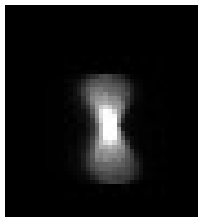
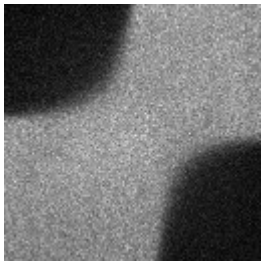
ZLP	⟷	NI at EA	ZLP	⟷	NI at EA
					
SX10		E10	SX20		E20
					
SX01		E01	SX02		E02
					
			SX11		E11

Measurement of pre-slit aberrations in imaging (ESI) mode is more robust and quantitative than in EELS mode

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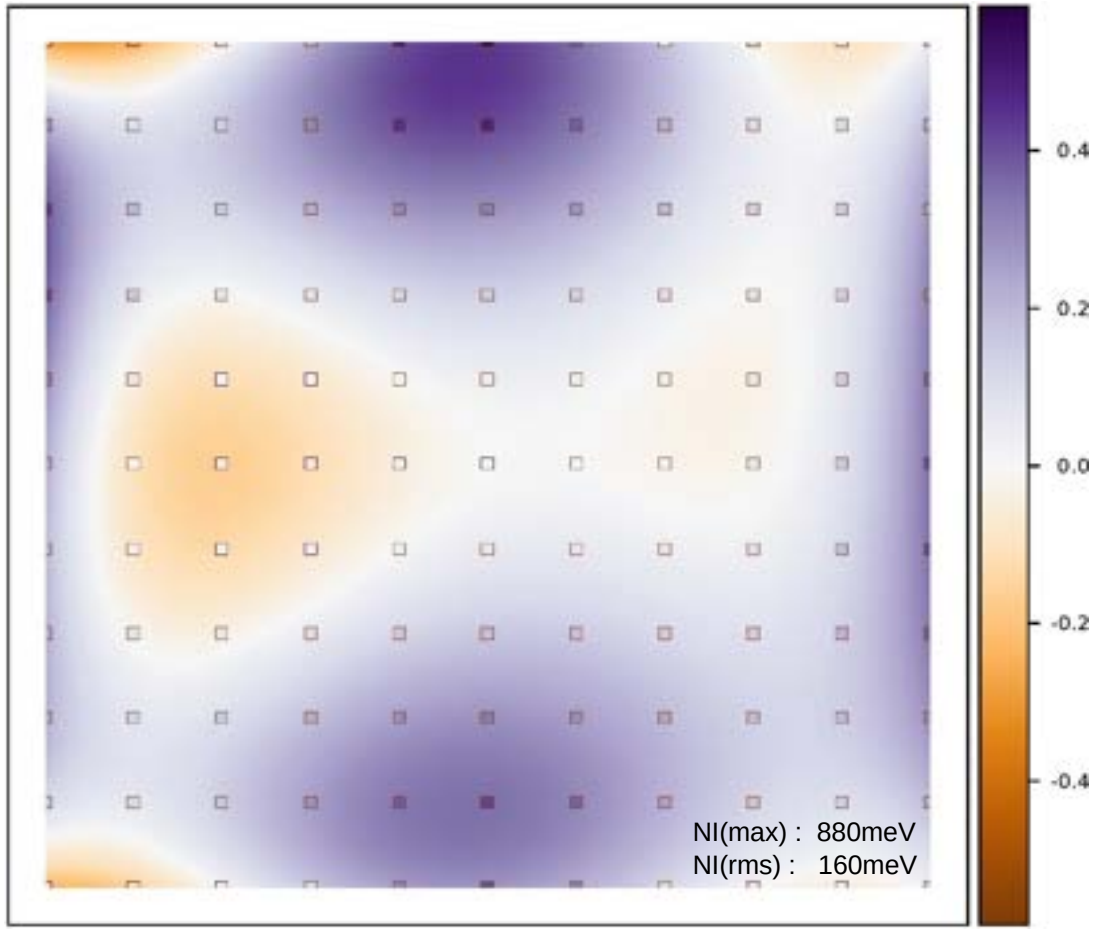
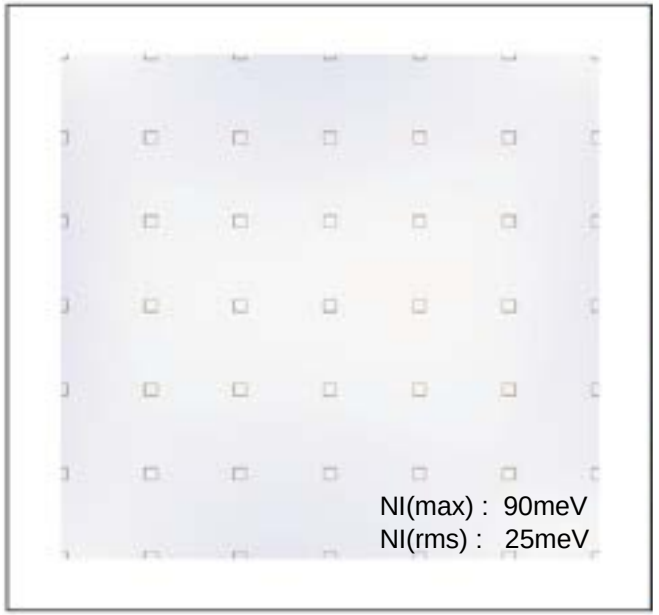
CEFID Isochromaticity at 200kV



ESI 12mm 11x11



ESI 8mm 7x7

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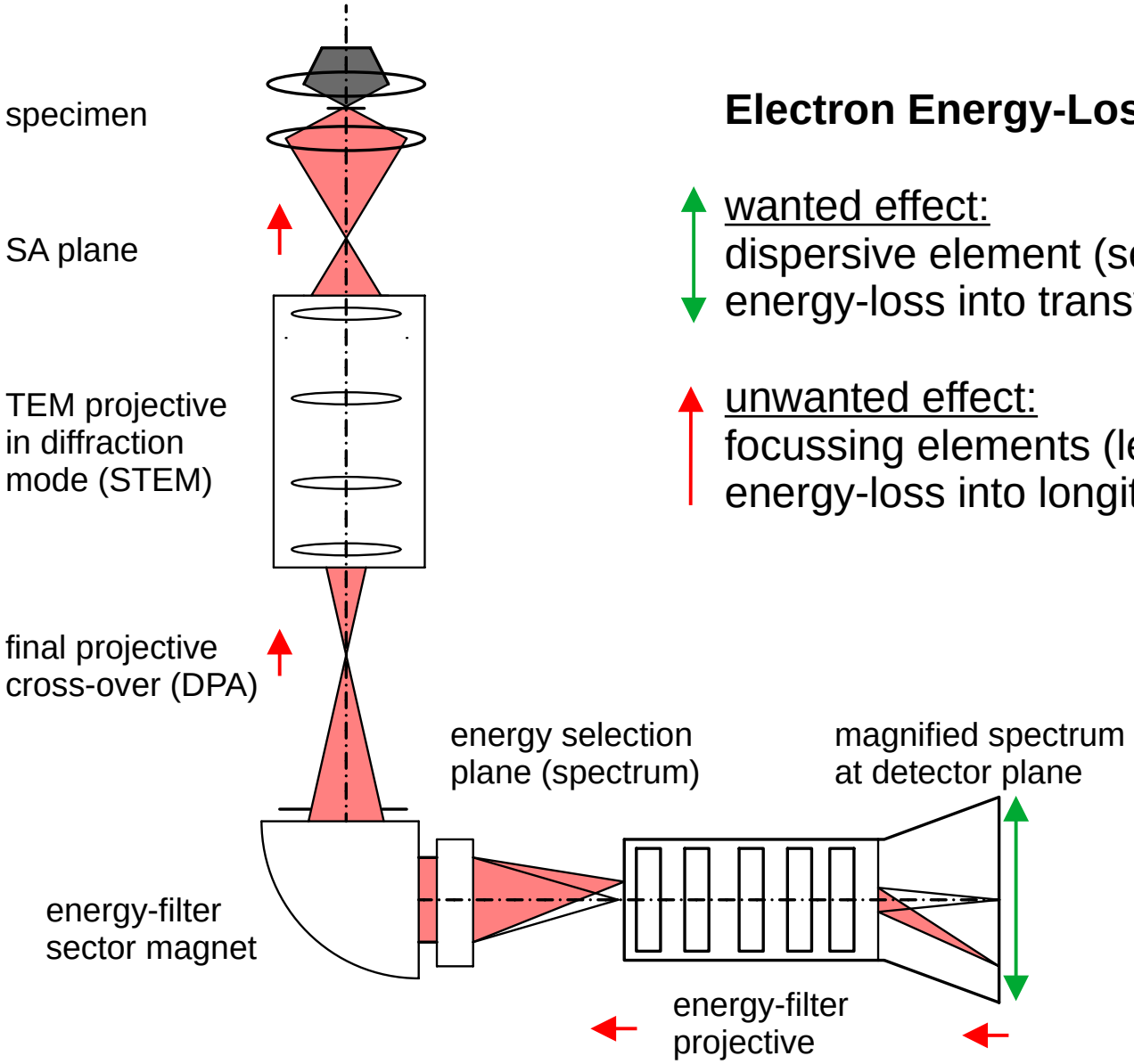

Electron Energy-Loss Spectroscopy

<u>wanted effect:</u>
dispersive element (sector magnet) translates energy-loss into transversal displacement

<u>unwanted effect:</u>
focussing elements (lenses, quadrupoles) translate energy-loss into longitudial shift of focus plane

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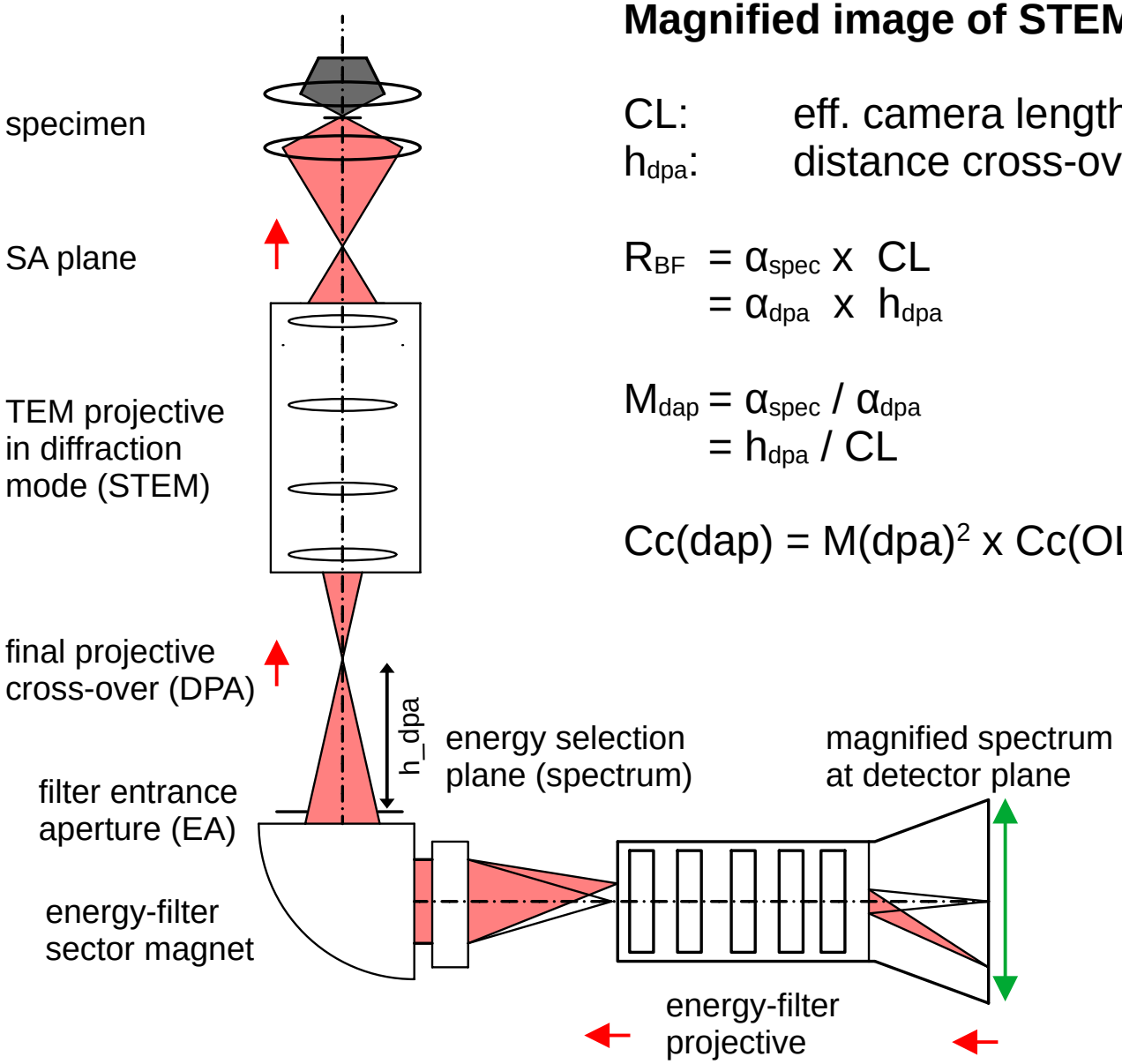

Magnified image of STEM probe at DPA plane:

CL: eff. camera length w.r.t EA
h_{dpa}: distance cross-over to EA

$$R_{BF} = \alpha_{spec} \times CL = \alpha_{dpa} \times h_{dpa}$$

$$M_{dap} = \alpha_{spec} / \alpha_{dpa} = h_{dpa} / CL$$

$$Cc(dap) = M(dpa)^2 \times Cc(OL)$$

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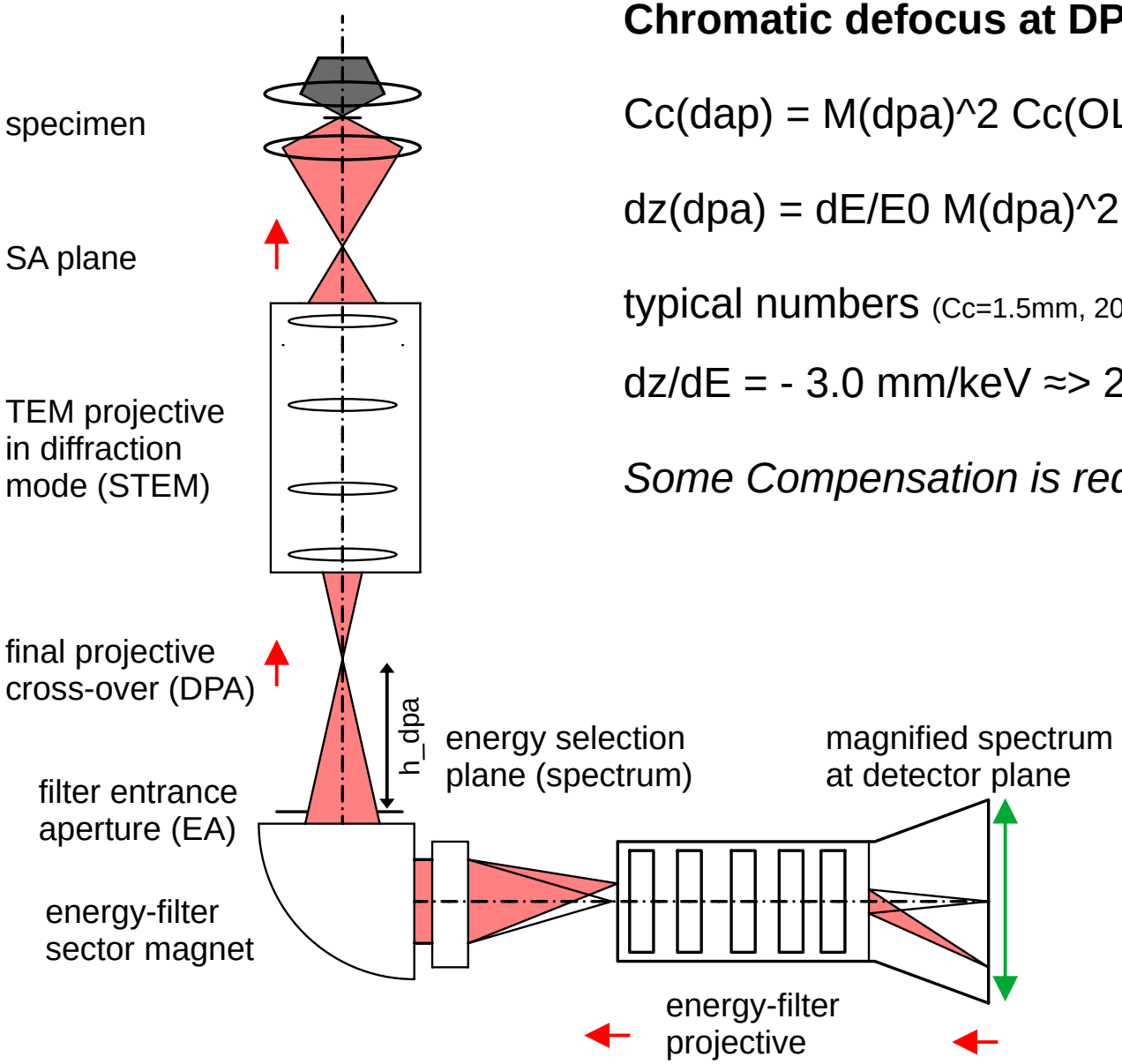

Chromatic defocus at DPA plane:

Cc(dap) = M(dpa)^2 Cc(OL)

dz(dpa) = dE/E0 M(dpa)^2 Cc(OL)

typical numbers (Cc=1.5mm, 200kV, CL=30mm, hDPA=600mm):

dz/dE = - 3.0 mm/keV ≈> 2.6 eV/keV (30mrad)

Some Compensation is required!

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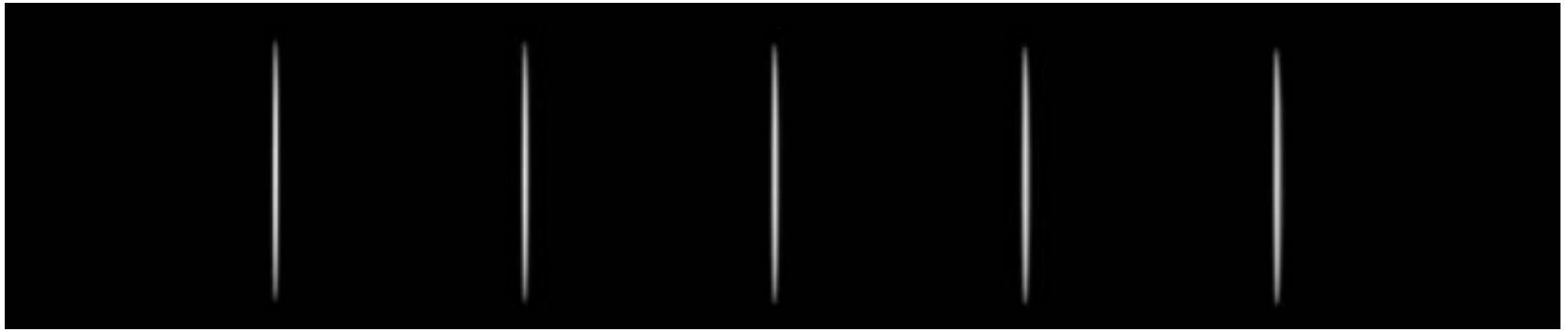
Focussed but spectrum inclination not corrected:

Focussed and spectrum inclination corrected:



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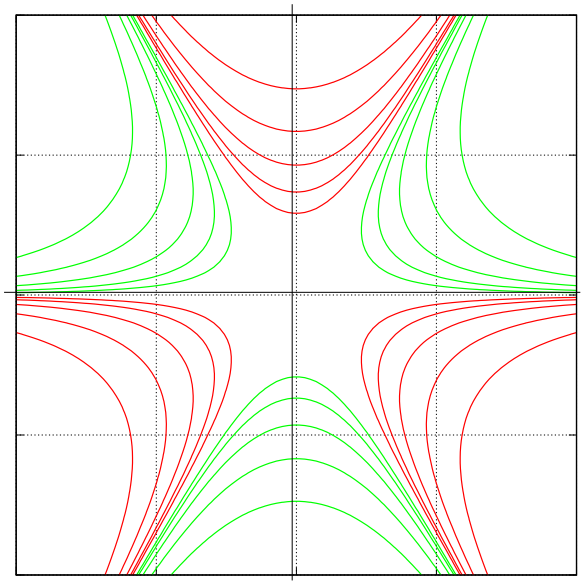
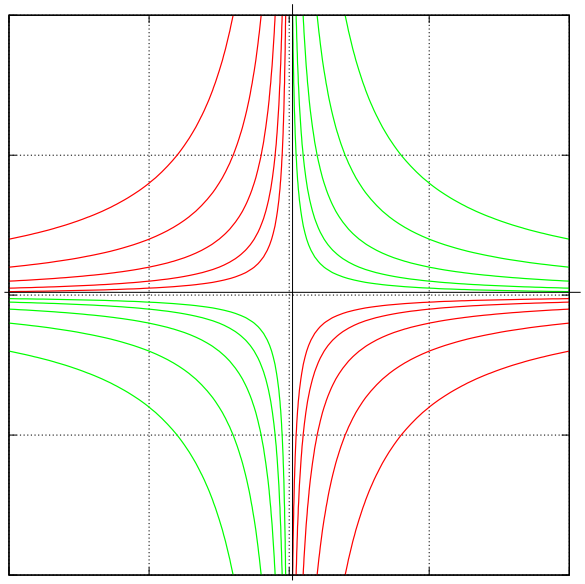
hexpole potential



+

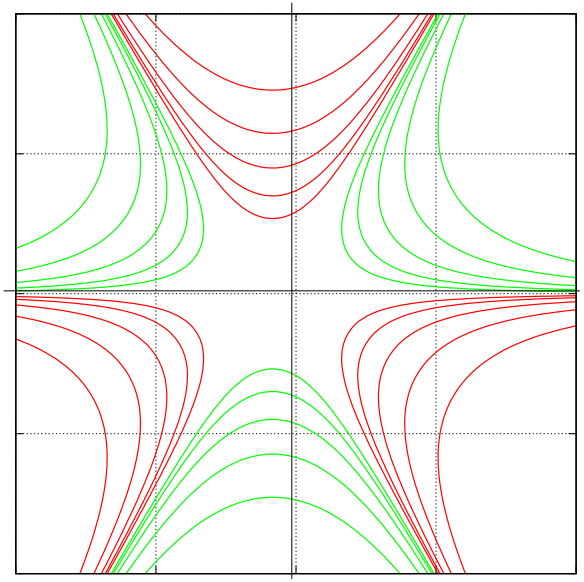


quadrupole potential

shifted potential

or

superimposed quadruole



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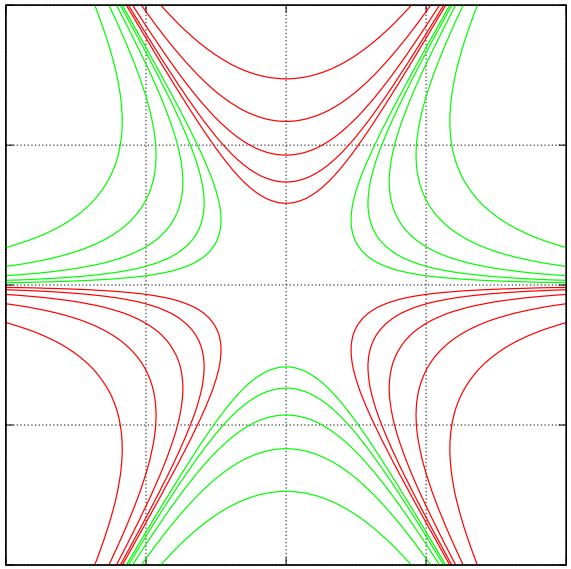

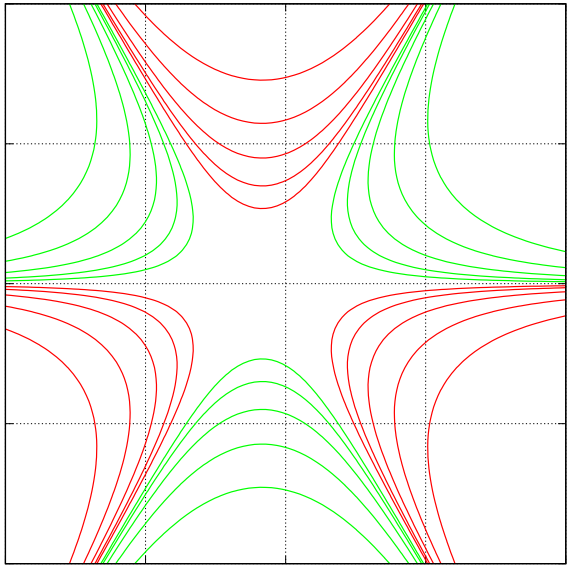

quadrupole potential:

$$\psi_2 = 2\Psi_{2s}xy$$

hexapole potential:

$$\psi_3 = \Psi_{3s}\left(y^3 + 3x^2y\right)$$

shift of optic axis:

$$\begin{aligned}\psi &= \Psi_{3s}\left(y^3 + 3\left(x+\Delta x\right)^2 y\right)\\ &\approx \Psi_{3s}\left(y^3 + 3x^2y\right) + 6\Delta x\Psi_{3s}xy\end{aligned}$$

shift-induced quadruple strength:

$$\psi_{2s} = 3\Delta x\Psi_{3s}$$

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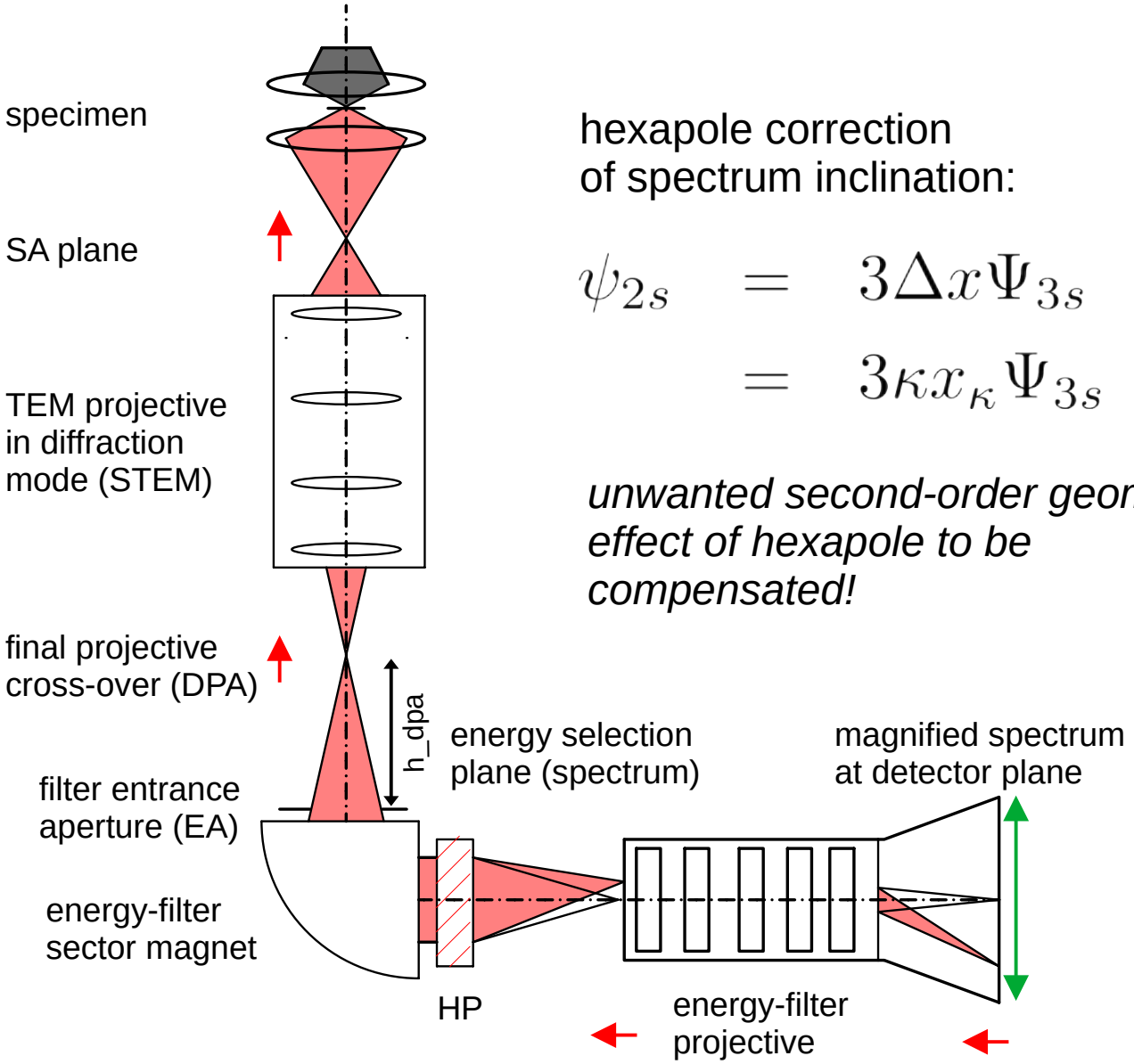
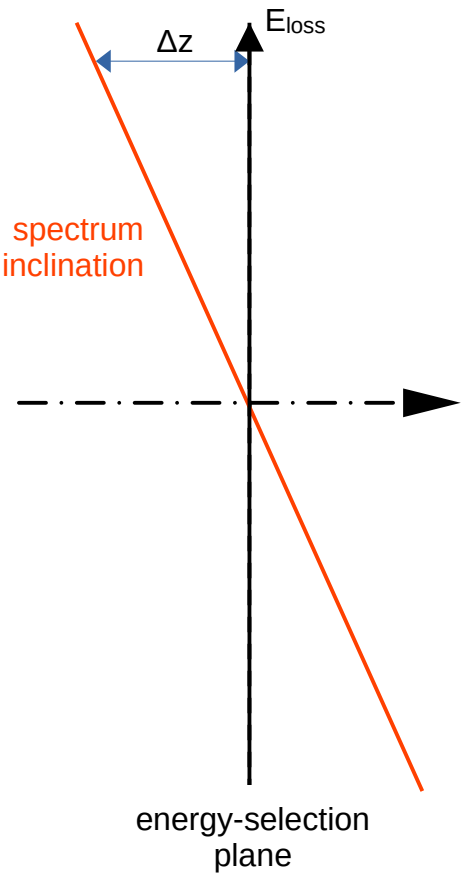


hexapole correction of spectrum inclination:

$$\psi_{2s} = 3\Delta x \Psi_{3s} = 3\kappa x_\kappa \Psi_{3s}$$

unwanted second-order geom. effect of hexapole to be compensated!



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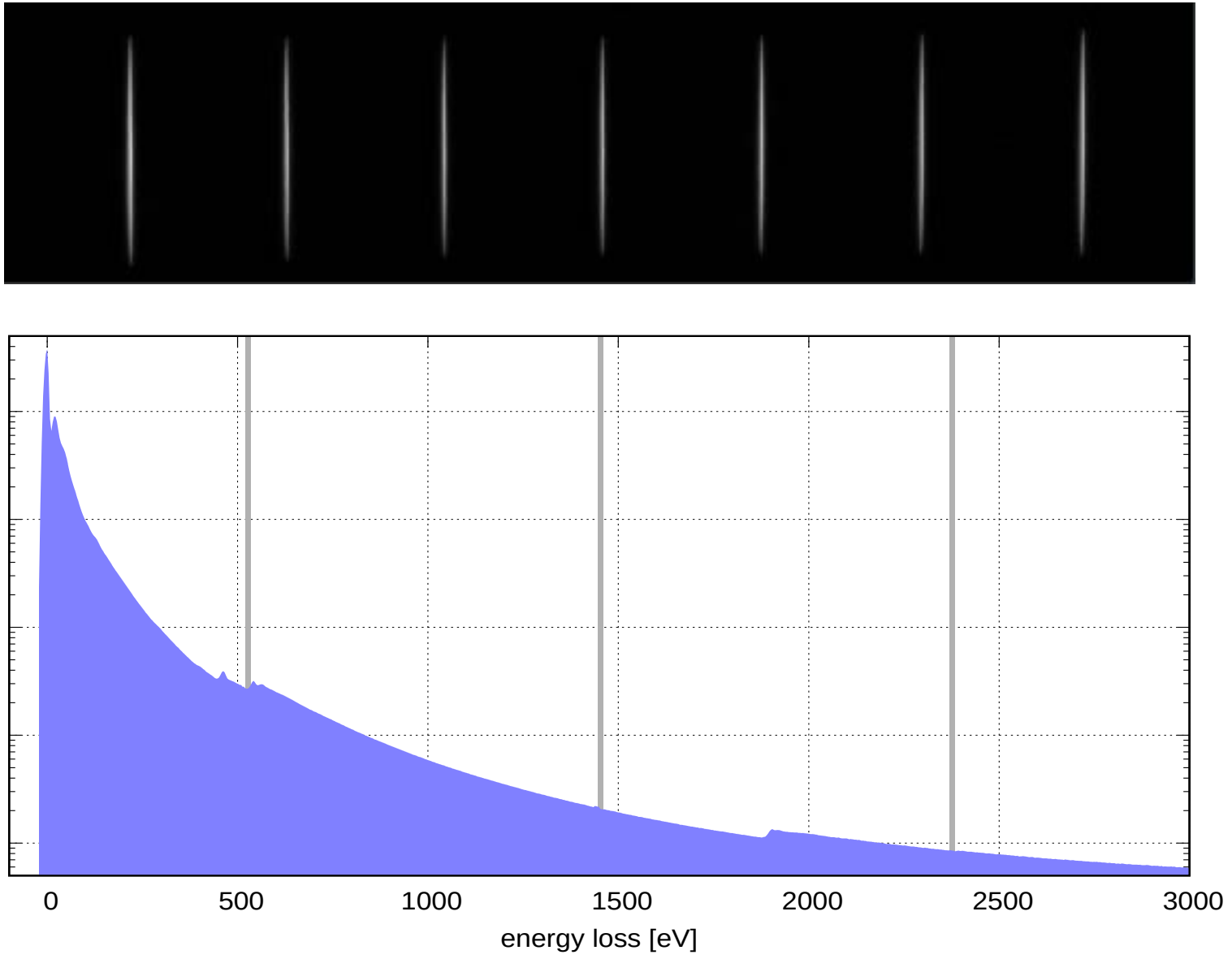

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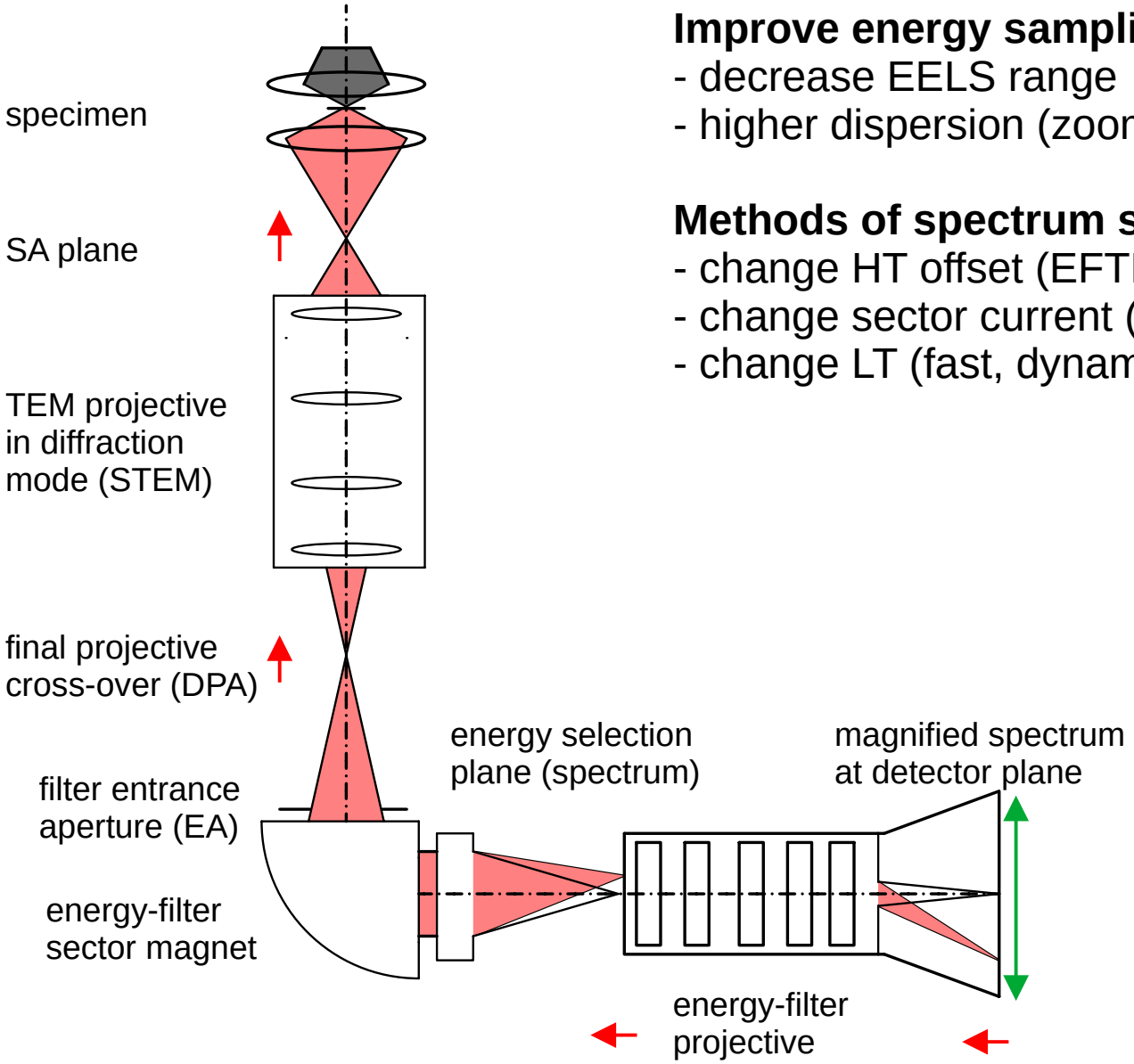

Improve energy sampling:
- decrease EELS range
- higher dispersion (zoom in)

Methods of spectrum shift:
- change HT offset (EFTEM)
- change sector current (high-loss, slow)
- change LT (fast, dynamic EELS)

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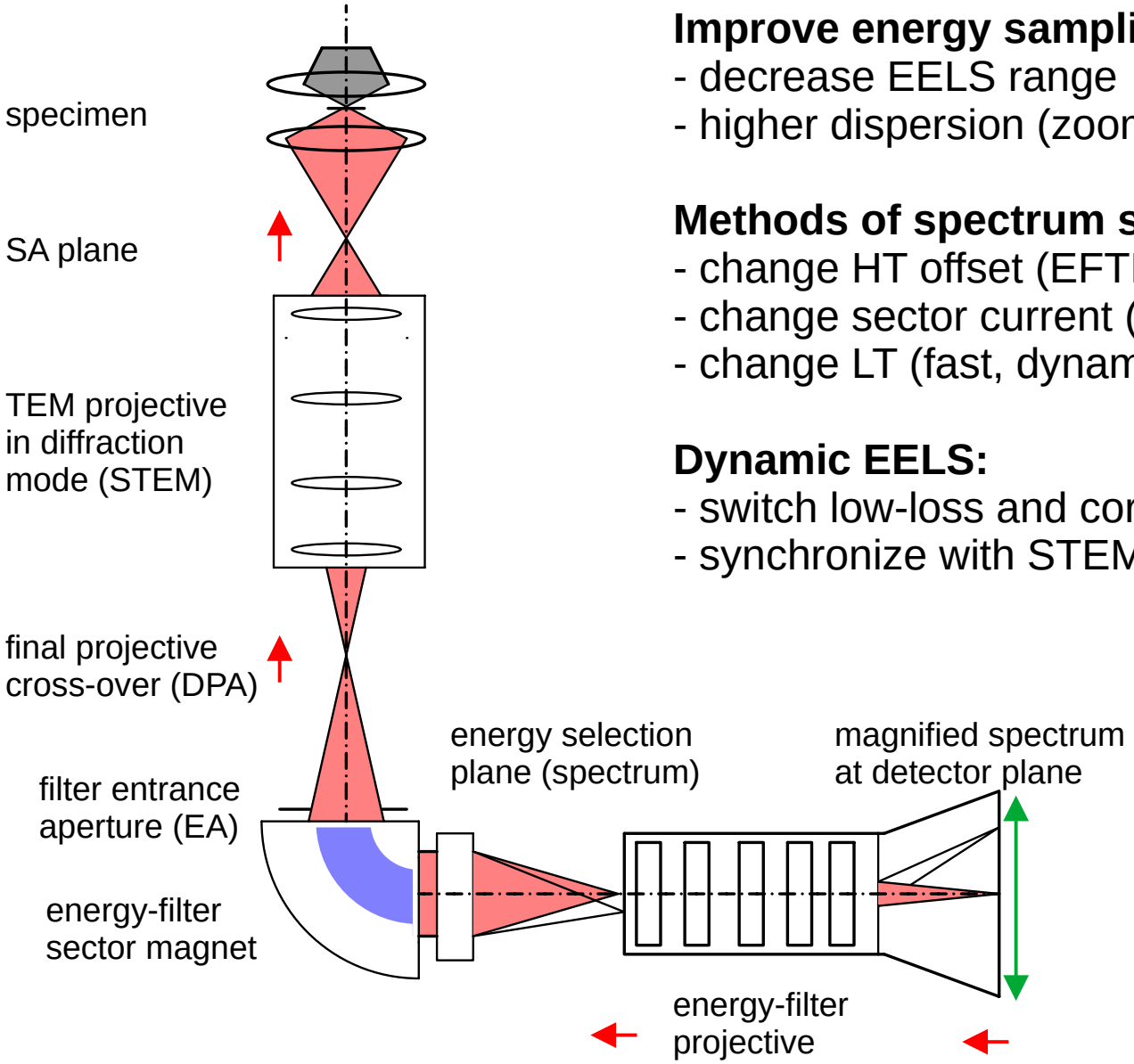

Improve energy sampling:
- decrease EELS range
- higher dispersion (zoom in)

Methods of spectrum shift:
- change HT offset (EFTEM)
- change sector current (high-loss, slow)
- change LT (fast, dynamic EELS)

Dynamic EELS:
- switch low-loss and core-loss
- synchronize with STEM scan

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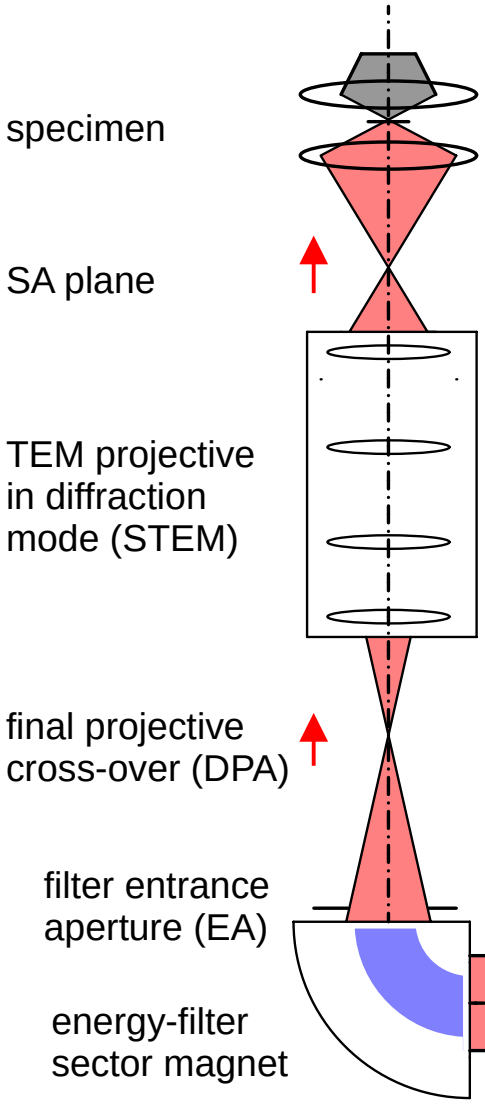

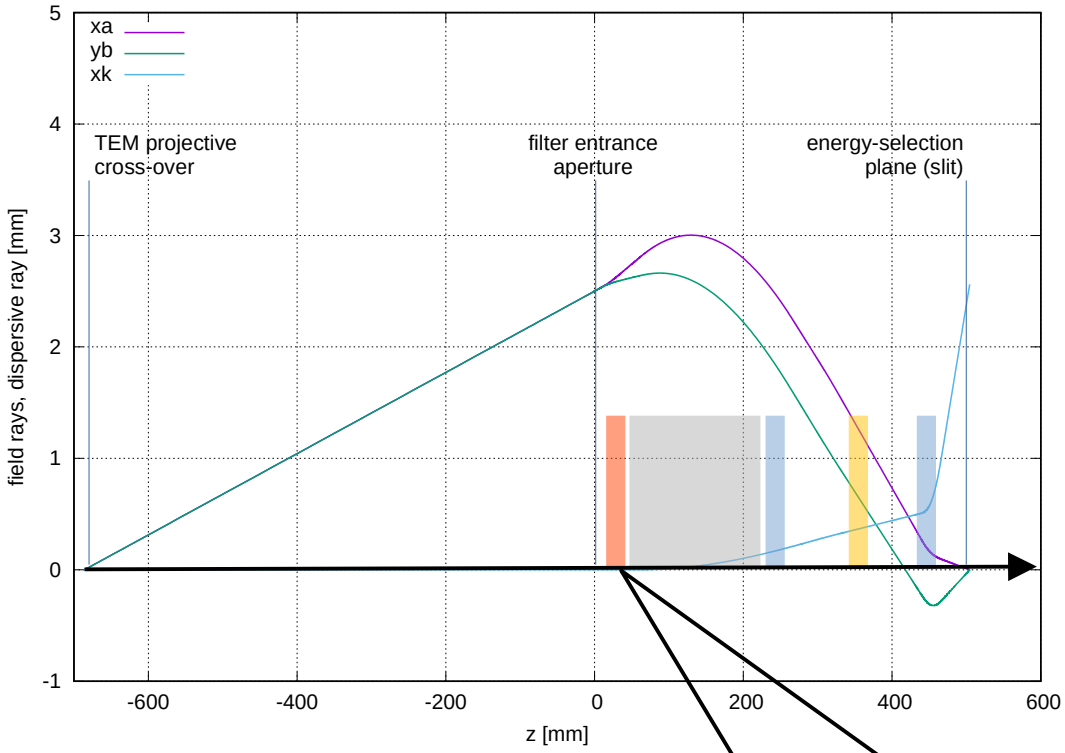

energy selection plane (spectrum)

magnified spectrum at detector plane

energy-filter projective

Change of initial cross-over due to energy-shift can be compensated by a weak change of e.g. the first quadrupole.

Tweston et al. (2015) implemeted a fast electro-static stigmator for dynamic re-focussing for Multiple Range EELS applications.

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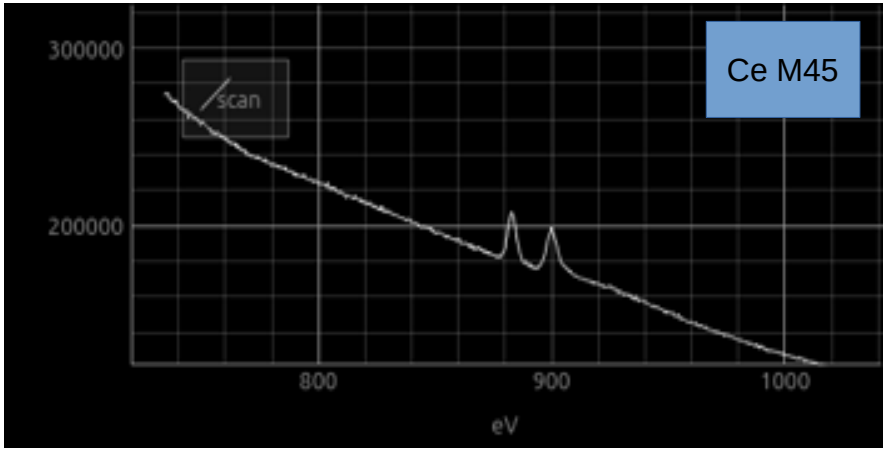
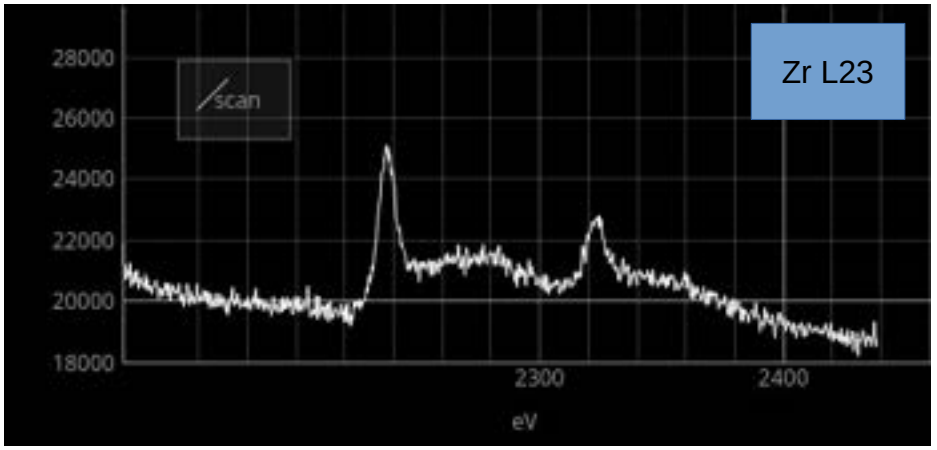
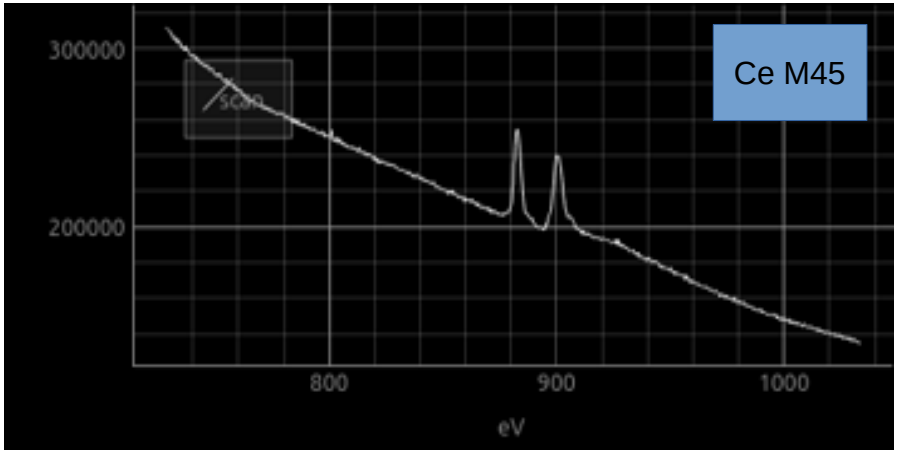
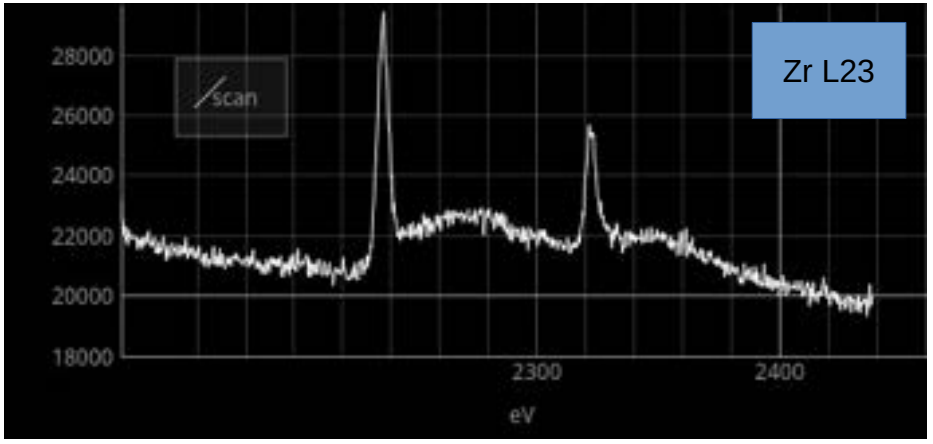




MP1-2y
+1mA

MP1-2y
+2.5mA





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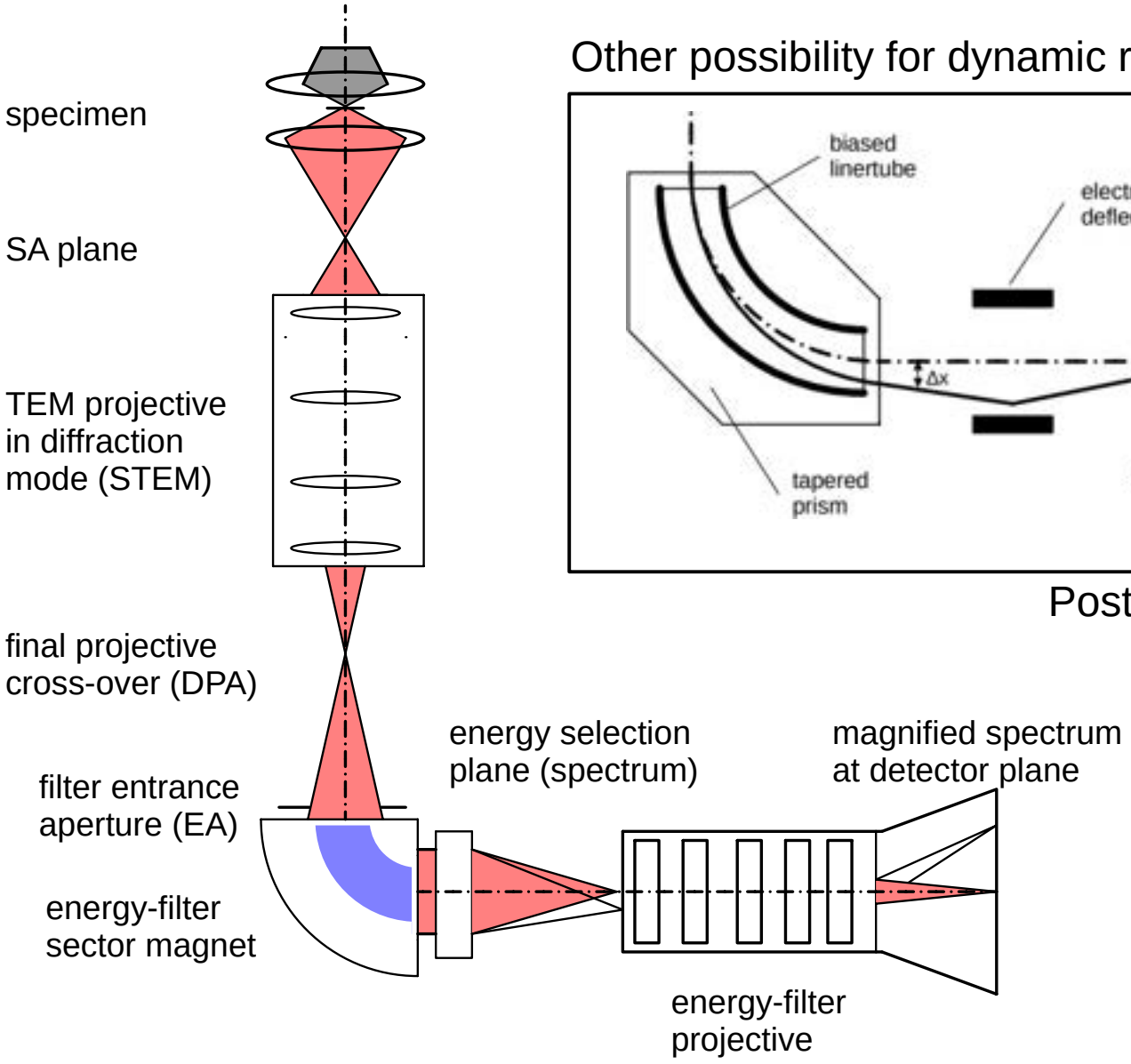
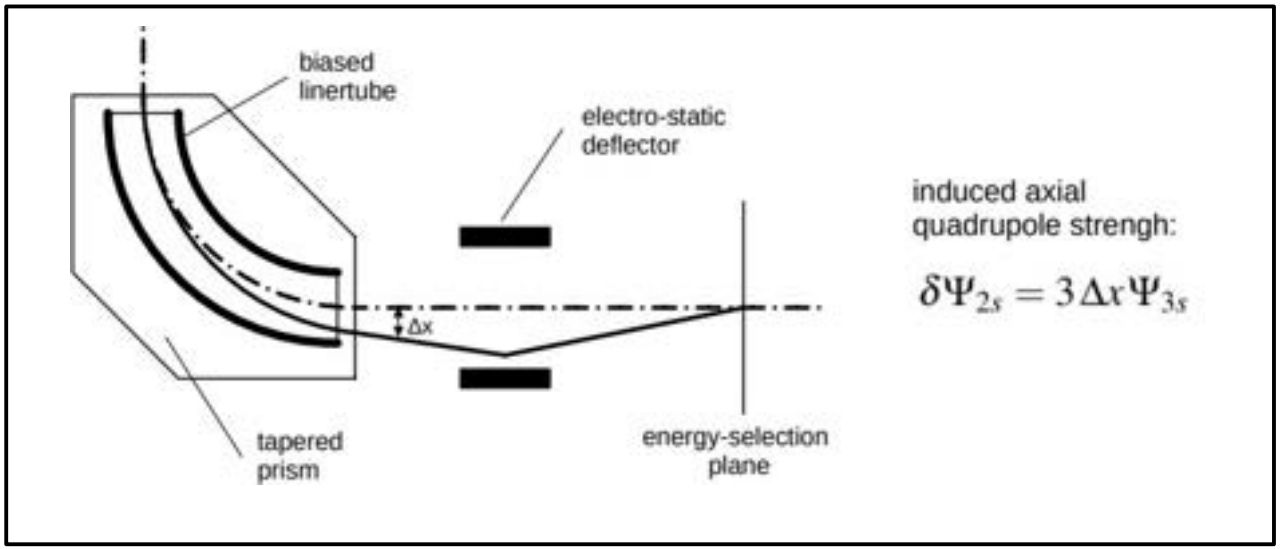


Other possibility for dynamic re-focussing w/o stigmator



Poster: IM1.P01 Mo. 14:00-16:00

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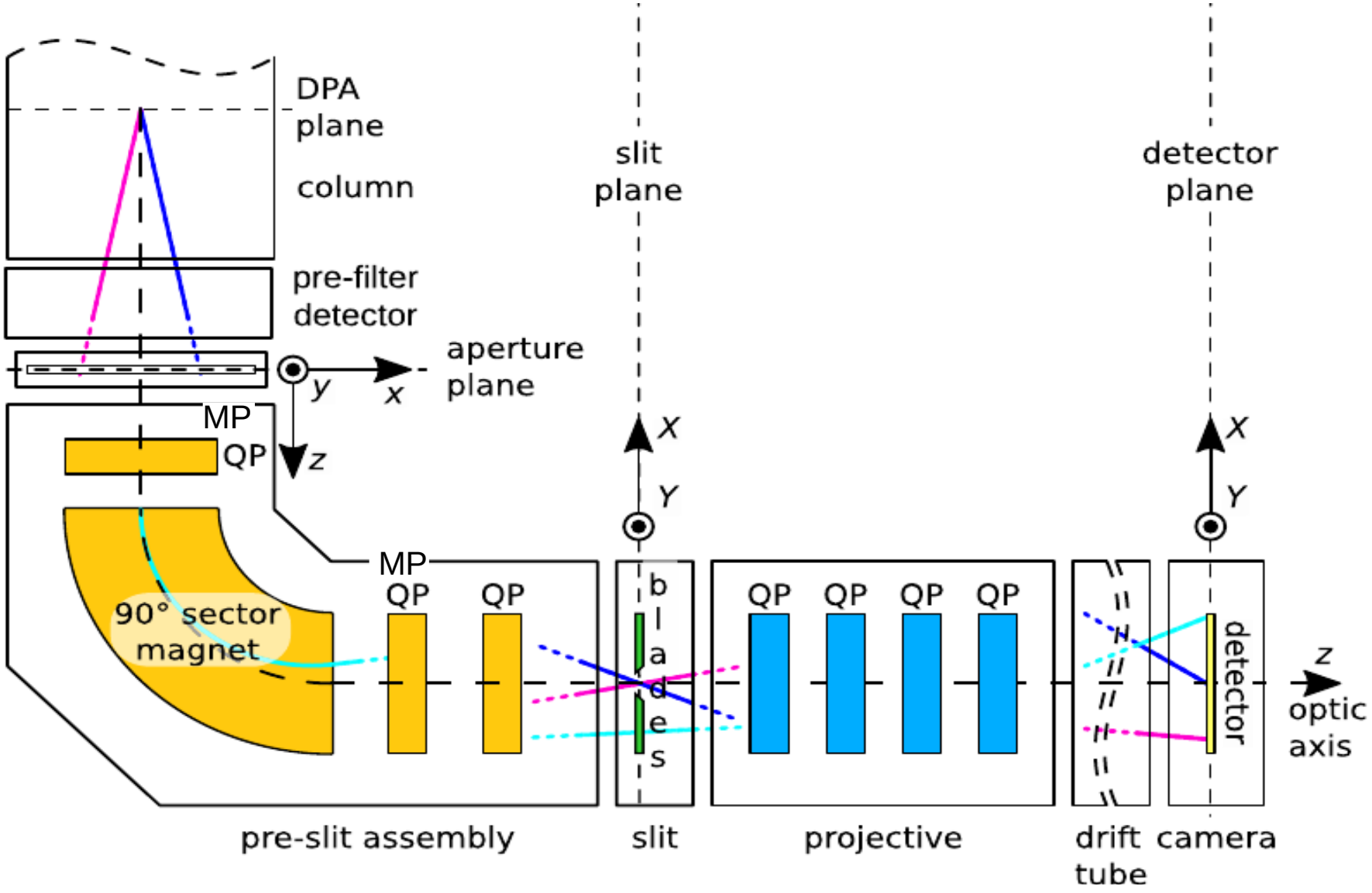
EELS Alignment



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MC 2025 Karlsruhe
WS1: Electron optics and new approaches for spectroscopy in the TEM

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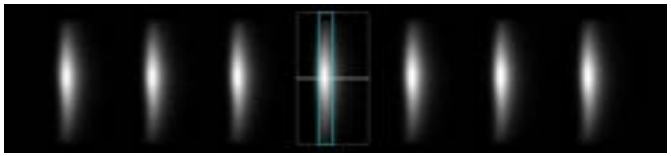
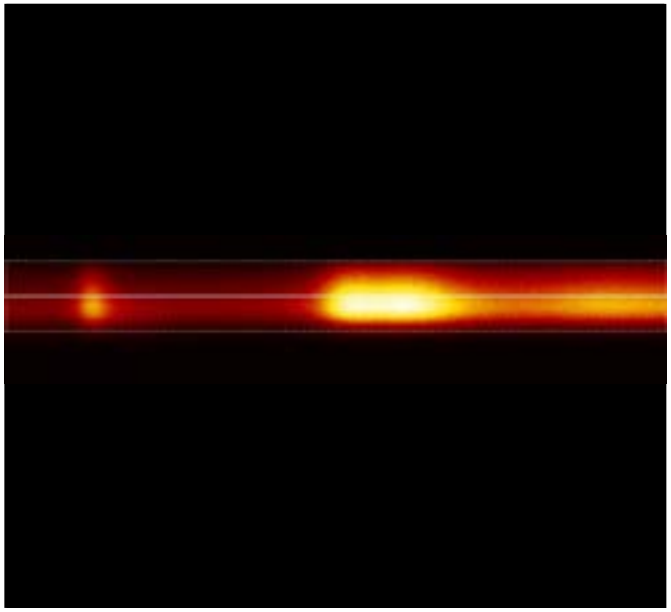
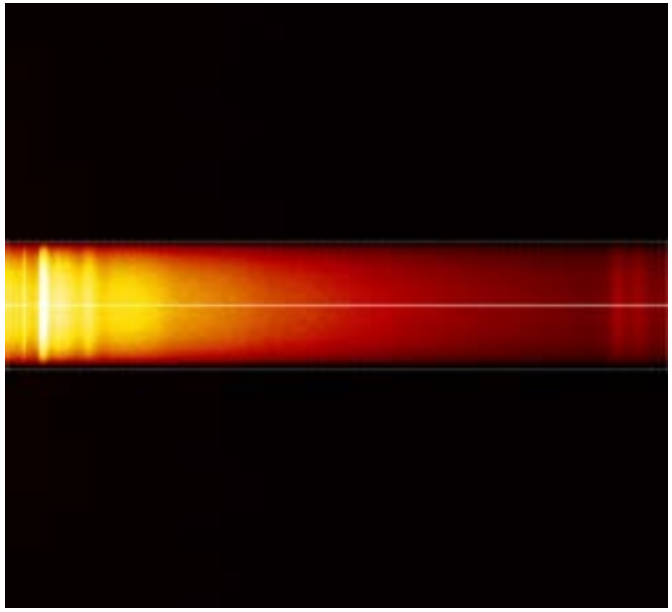
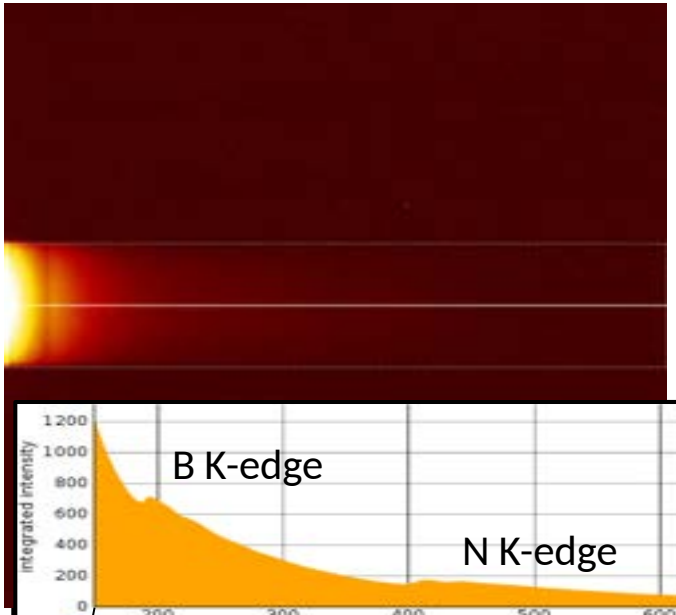
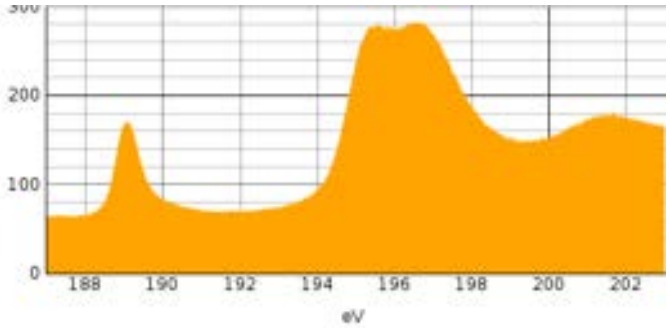
16 eV range, 7.8 meV/pix

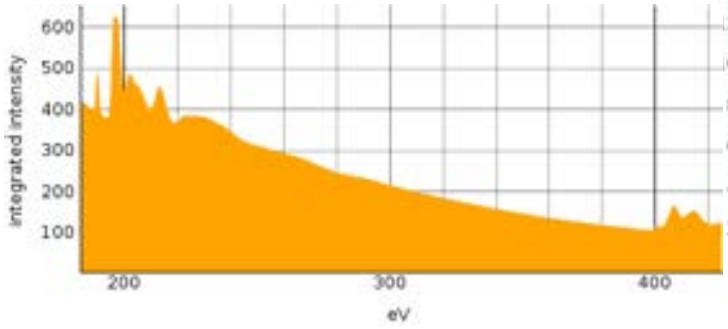
256 eV range, 125 meV/pix

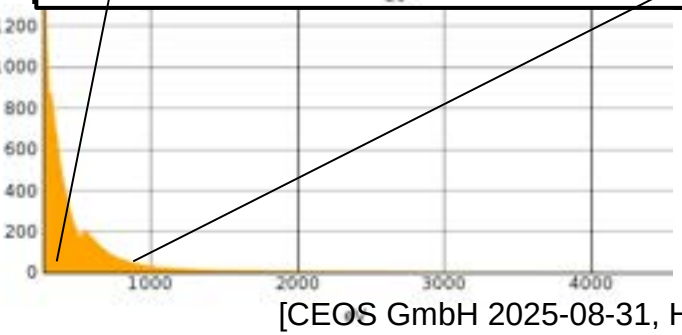
4 keV range, 2 eV/pix









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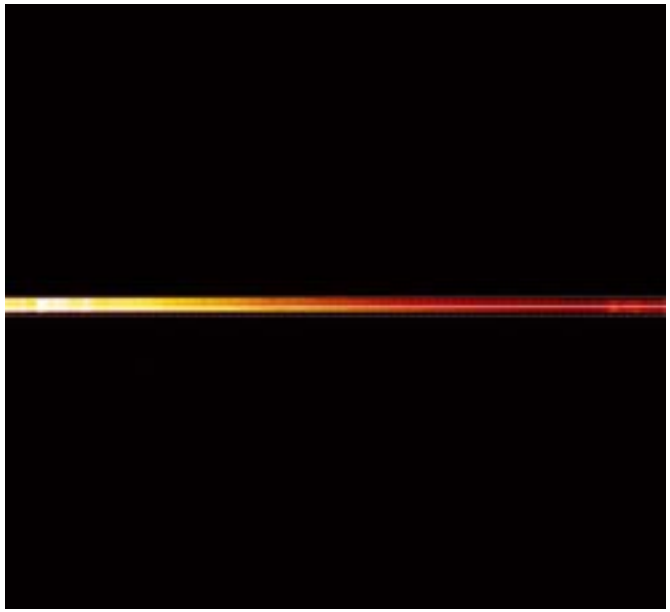
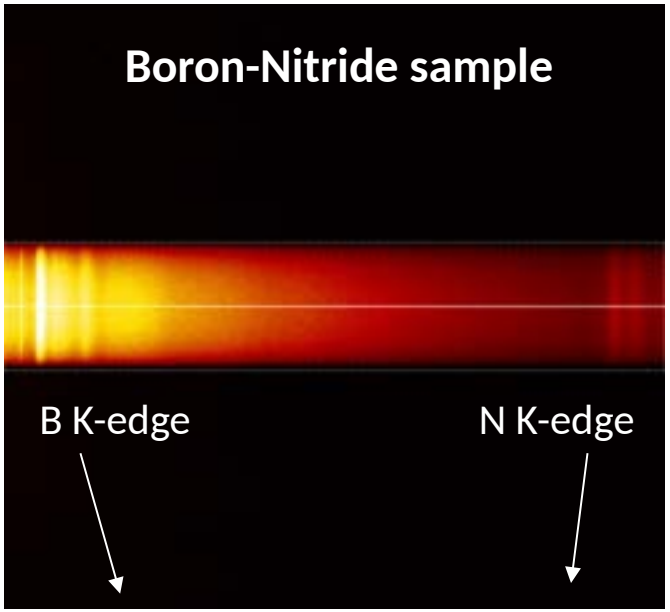
Adjustable spectrum height:

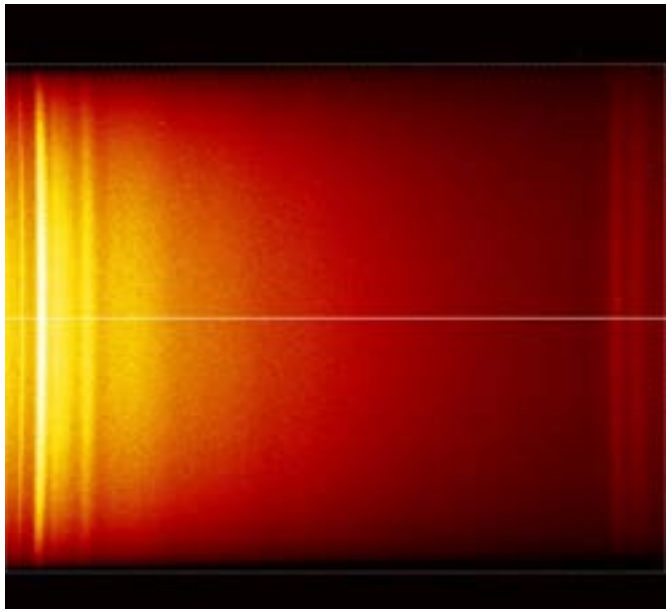
50 pix (2.5% of detector)

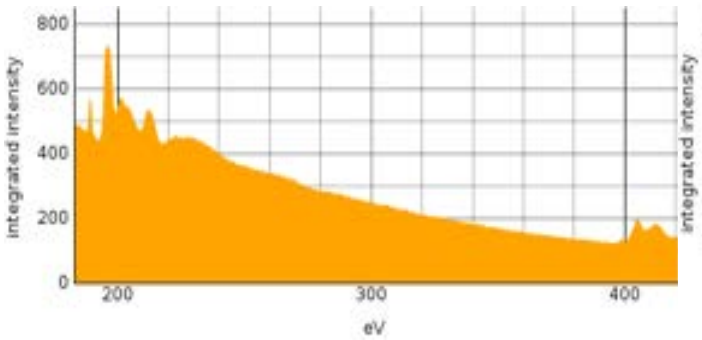
400 pix (20% of detector)

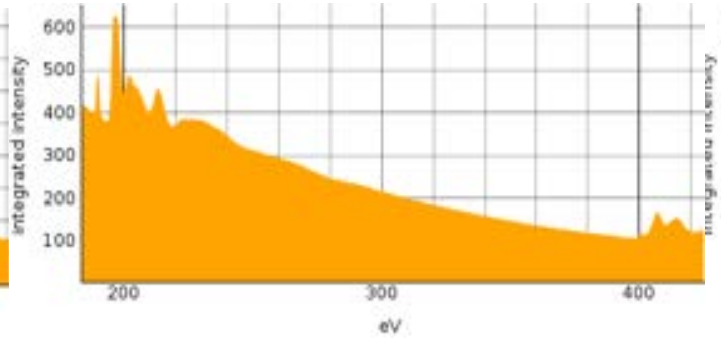
1800 pix (90% of detector)

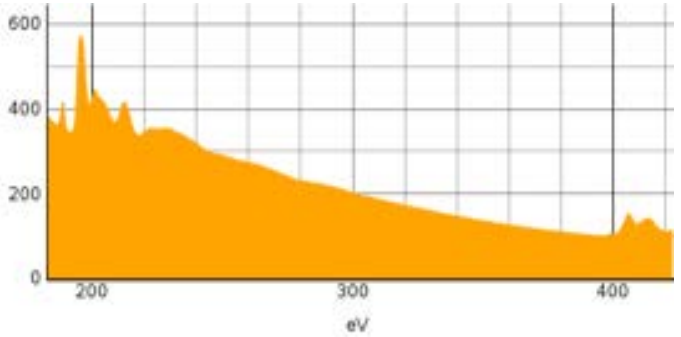












[CEOS GmbH 2025-08-31, HM]

EELS: Three degrees of freedom (Quadrupoles)

* Dispersion at detector (EELS magnification)

* Spectrum height (defocus in y-direction)

* Spectrum focus (SX10)

Momentum resolved EELS:

* focus entrance aperture at detector in y-direction
  x: Energy coordinate (dispersion scale)
  y: conjugated to entrance aperture (e.g. momentum in y-direction)

* momentum space in projected (averaged) in x-direction and resolved in y-direction

  => use slit-shpaed aperture to confine momentum in x-direction

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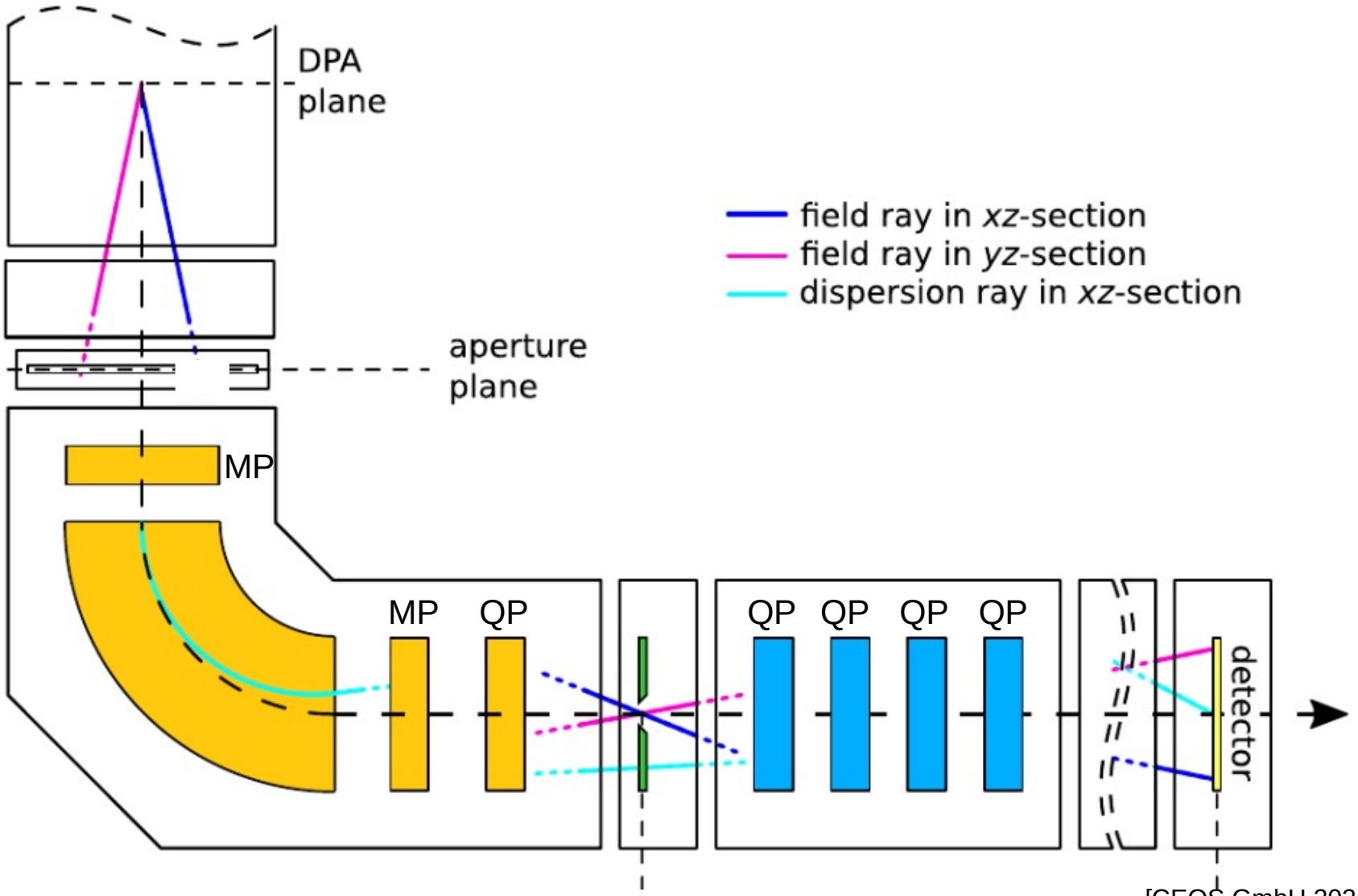
ESI Alignment



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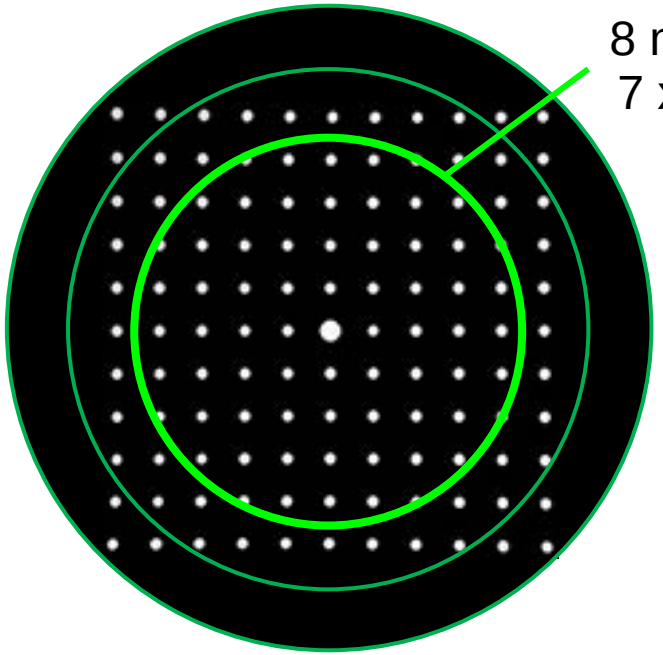
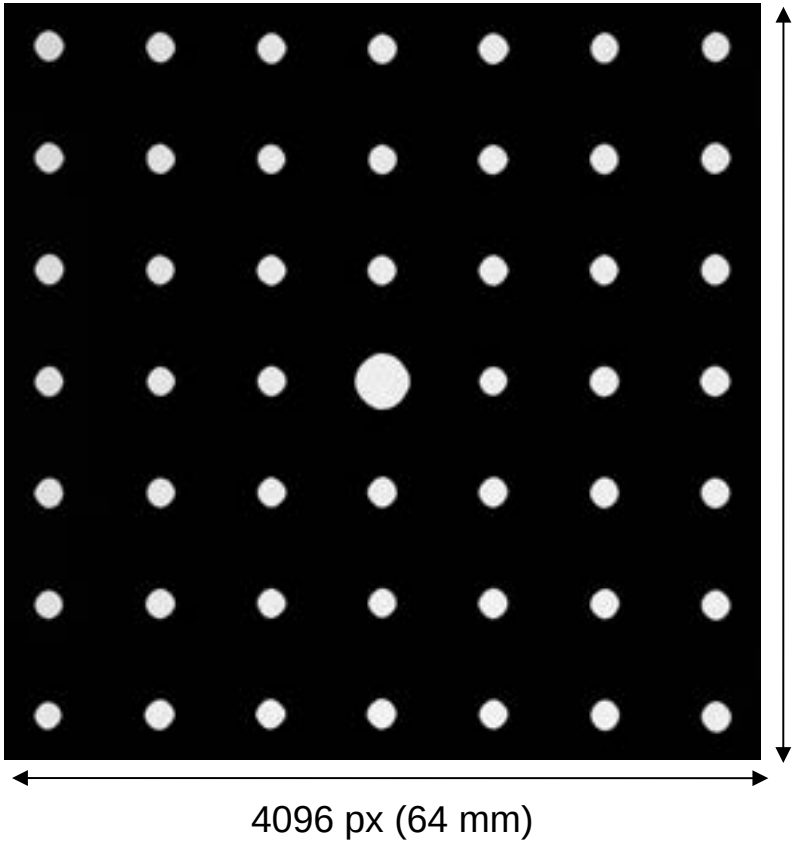
Flexible post-magnification

alignment mask in entrance aperture



detector (TVIPS XF416)



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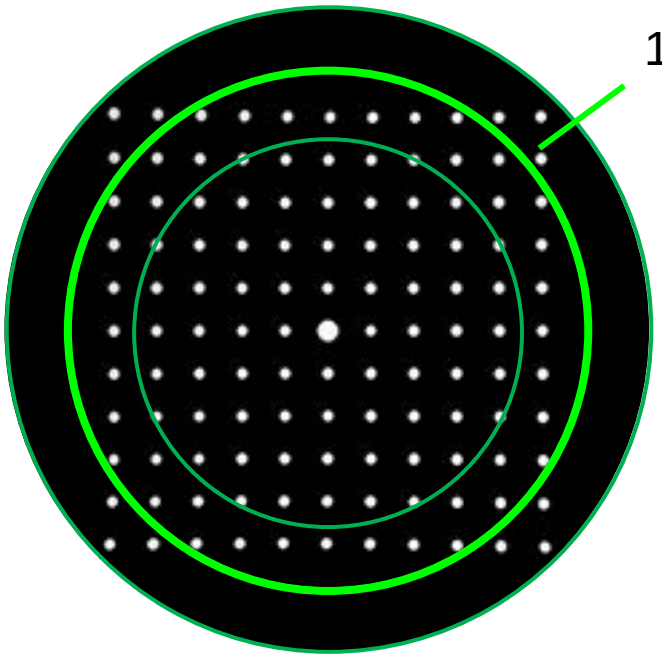
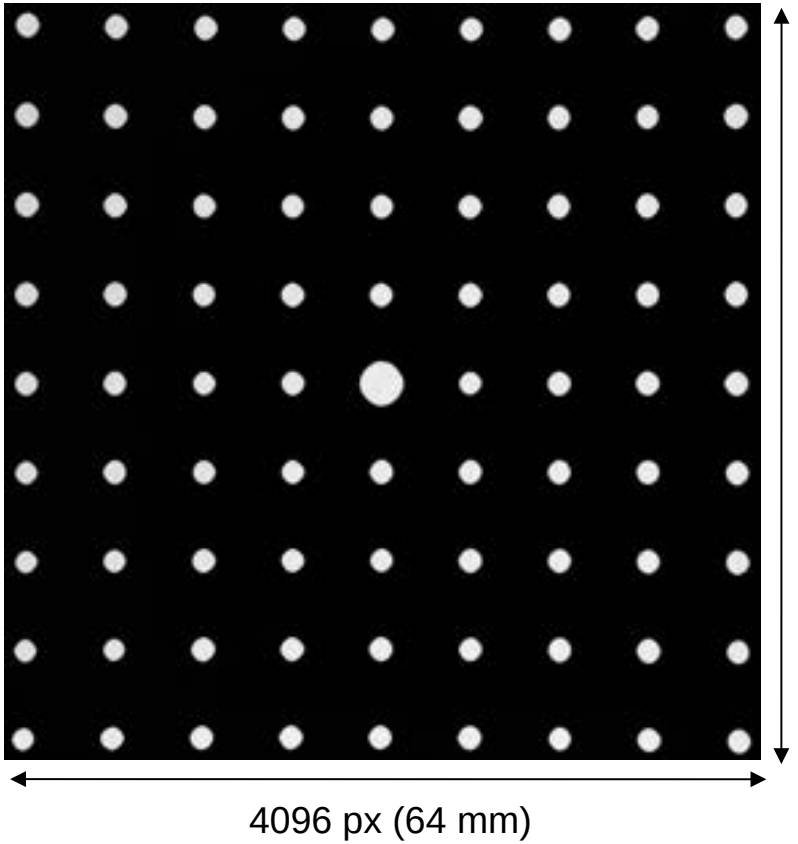
Flexible post-magnification

alignment mask in entrance aperture



detector (TVIPS XF416)



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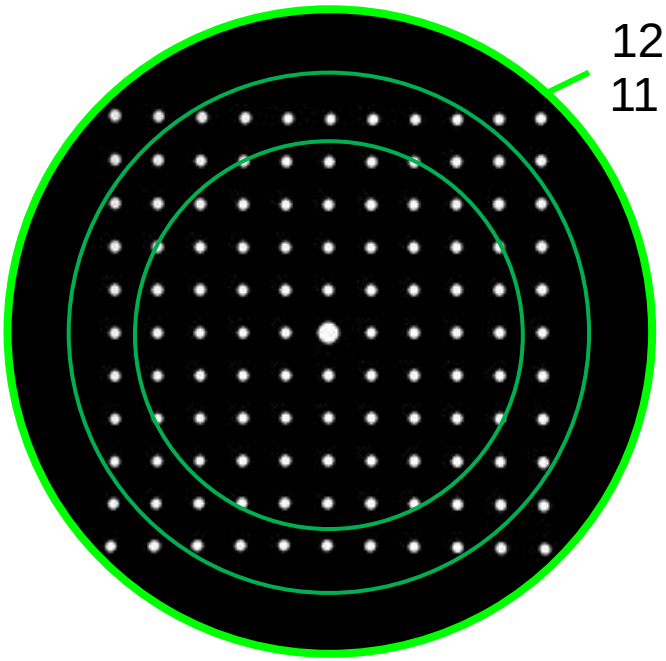
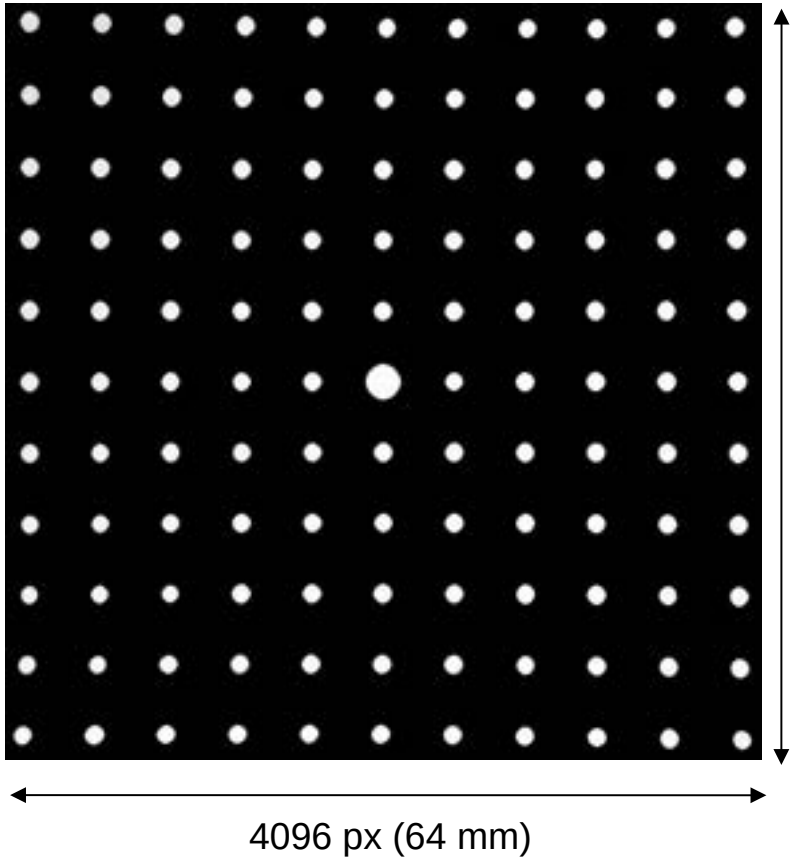
Flexible post-magnification

alignment mask in entrance aperture



detector (TVIPS XF416)



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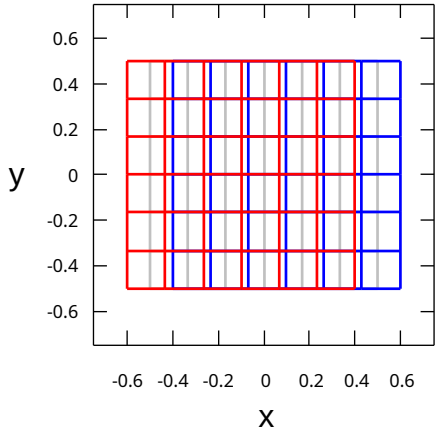
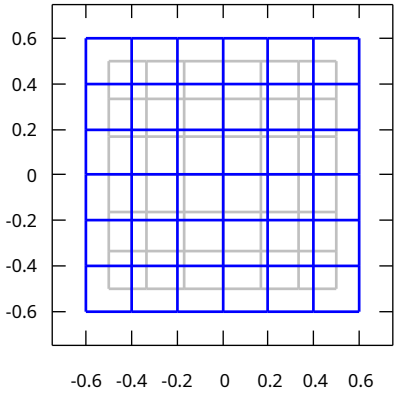
ESI: Correction of Dispersion and Distortions

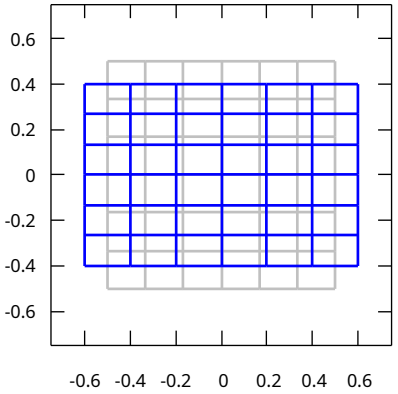
CX001



Magnification



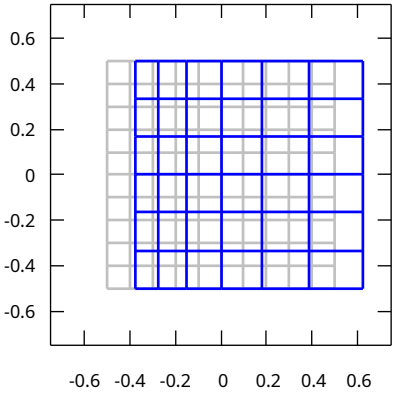
Aspect



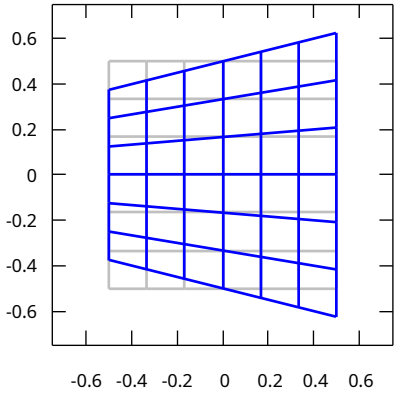
Three first-rank degrees of freedom

"Quadruples"

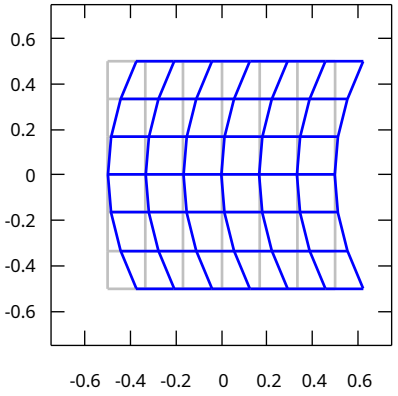
DX20



DY11



DX02



Three second-order degrees of freedom

"Hexapoles"

[CEOS GmbH 2025-08-31, HM]

Non-Linear Mapping of Entrance aperture onto Detector:

$$\begin{pmatrix} X \\ Y \end{pmatrix} = \begin{pmatrix} X_{00} \\ Y_{00} \end{pmatrix} + \begin{pmatrix} X_{10} & X_{01} \\ Y_{10} & Y_{01} \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} + \begin{pmatrix} X_{001} \\ Y_{001} \end{pmatrix} \Delta E + \begin{pmatrix} \Delta X(x, y, \Delta E) \\ \Delta Y(x, y, \Delta E) \end{pmatrix} \quad (2)$$

with the non-linear term

$$\begin{pmatrix} \Delta X \\ \Delta Y \end{pmatrix} = \sum_{R>1} \sum_{k=0}^{R} \sum_{\substack{m=0 \\ n=R-k-m}}^{R-k} \begin{pmatrix} X_{nmk} \\ Y_{nmk} \end{pmatrix} x^n y^m \Delta E^k . \quad (3)$$

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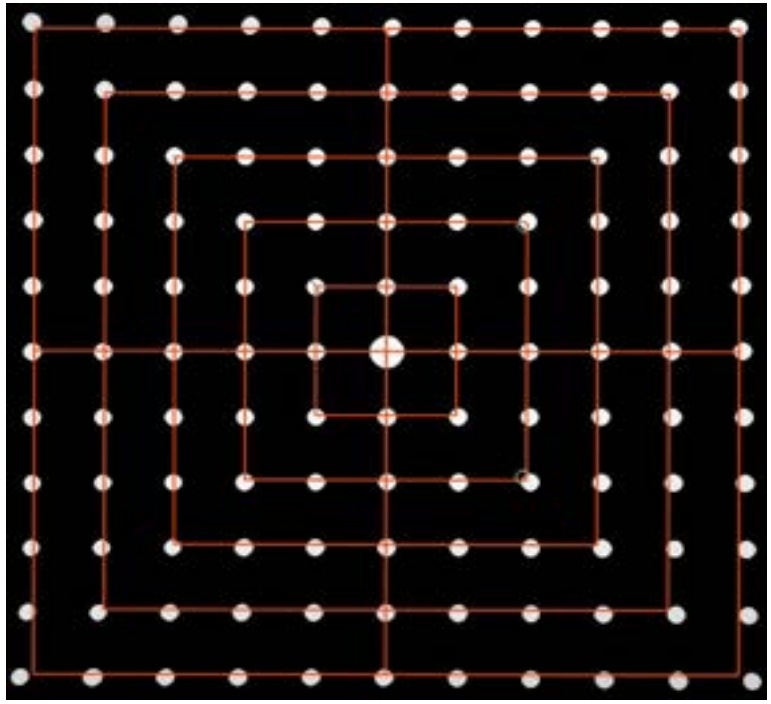
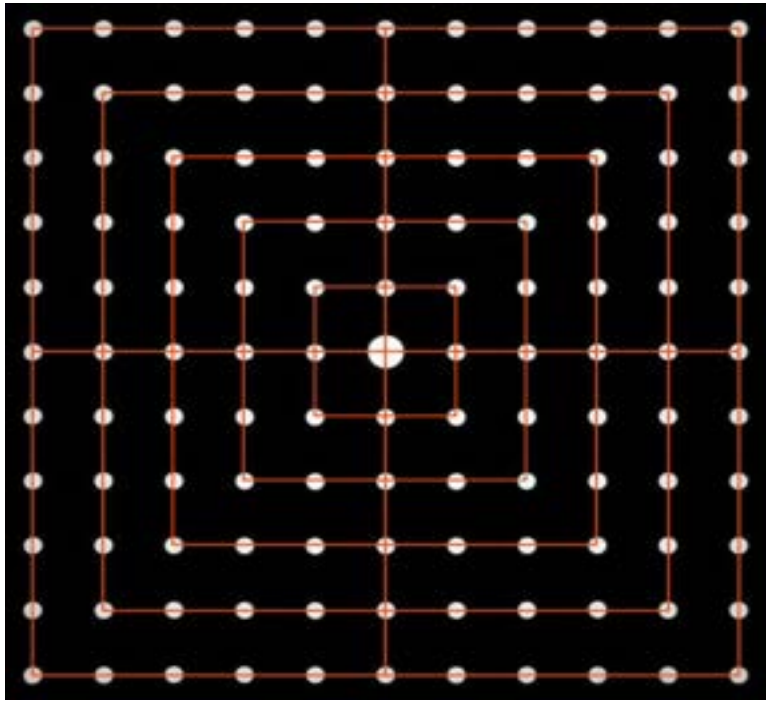
Dewarping

$$\vec{R}_{ij} = \sum_{r=0}^{R} d_{\mathrm{m}}^{r} \sum_{\substack{m=0 \\ n=r-m}}^{r} \begin{pmatrix} X_{nm} \\ Y_{nm} \end{pmatrix} i^n j^m$$





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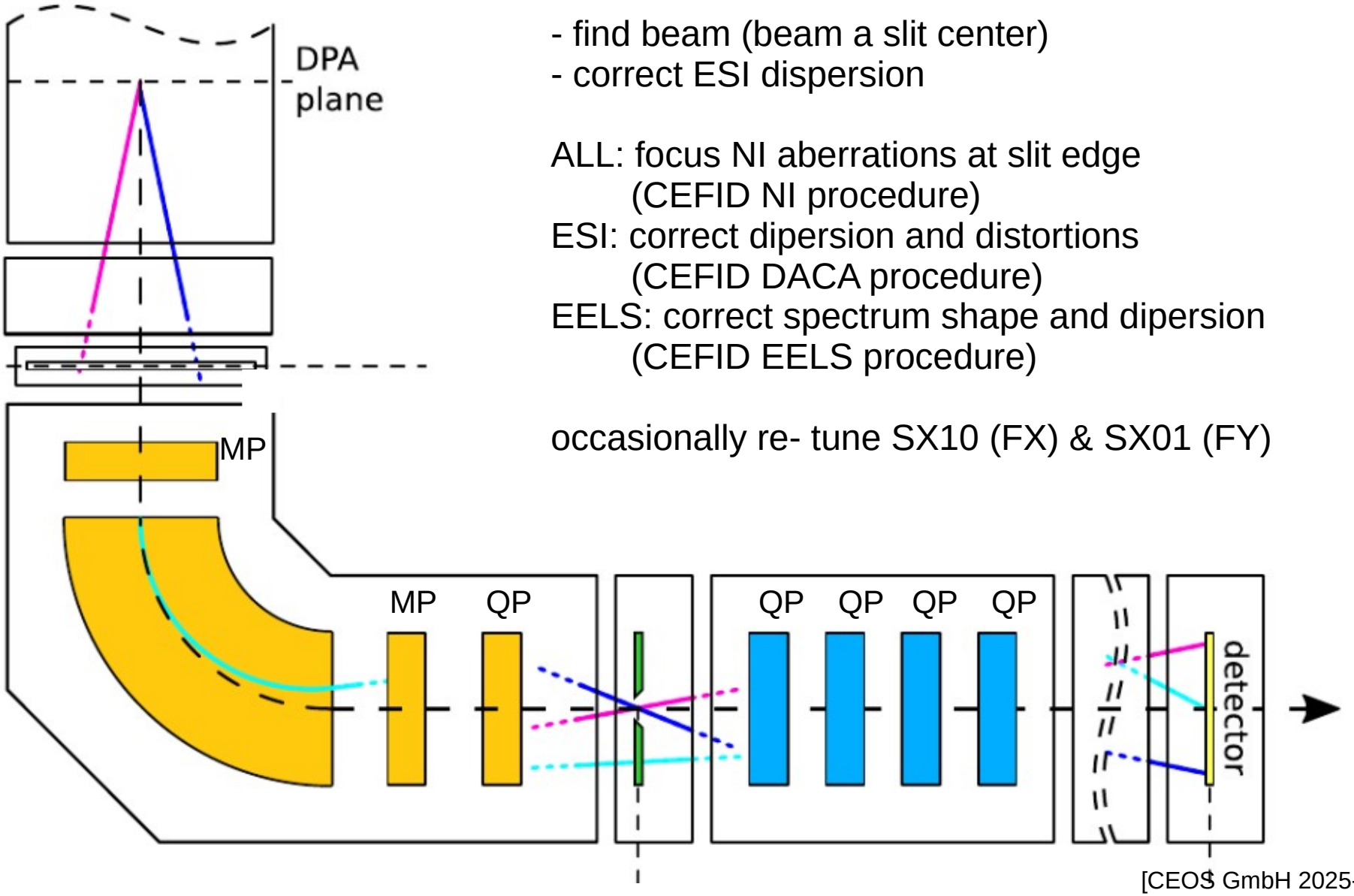
Summary of Alignment Strategy:

- find beam (beam a slit center)
- correct ESI dispersion

ALL: focus NI aberrations at slit edge
(CEFID NI procedure)
ESI: correct dipersion and distortions
(CEFID DACA procedure)
EELS: correct spectrum shape and dipersion
(CEFID EELS procedure)

occasionally re- tune SX10 (FX) & SX01 (FY)



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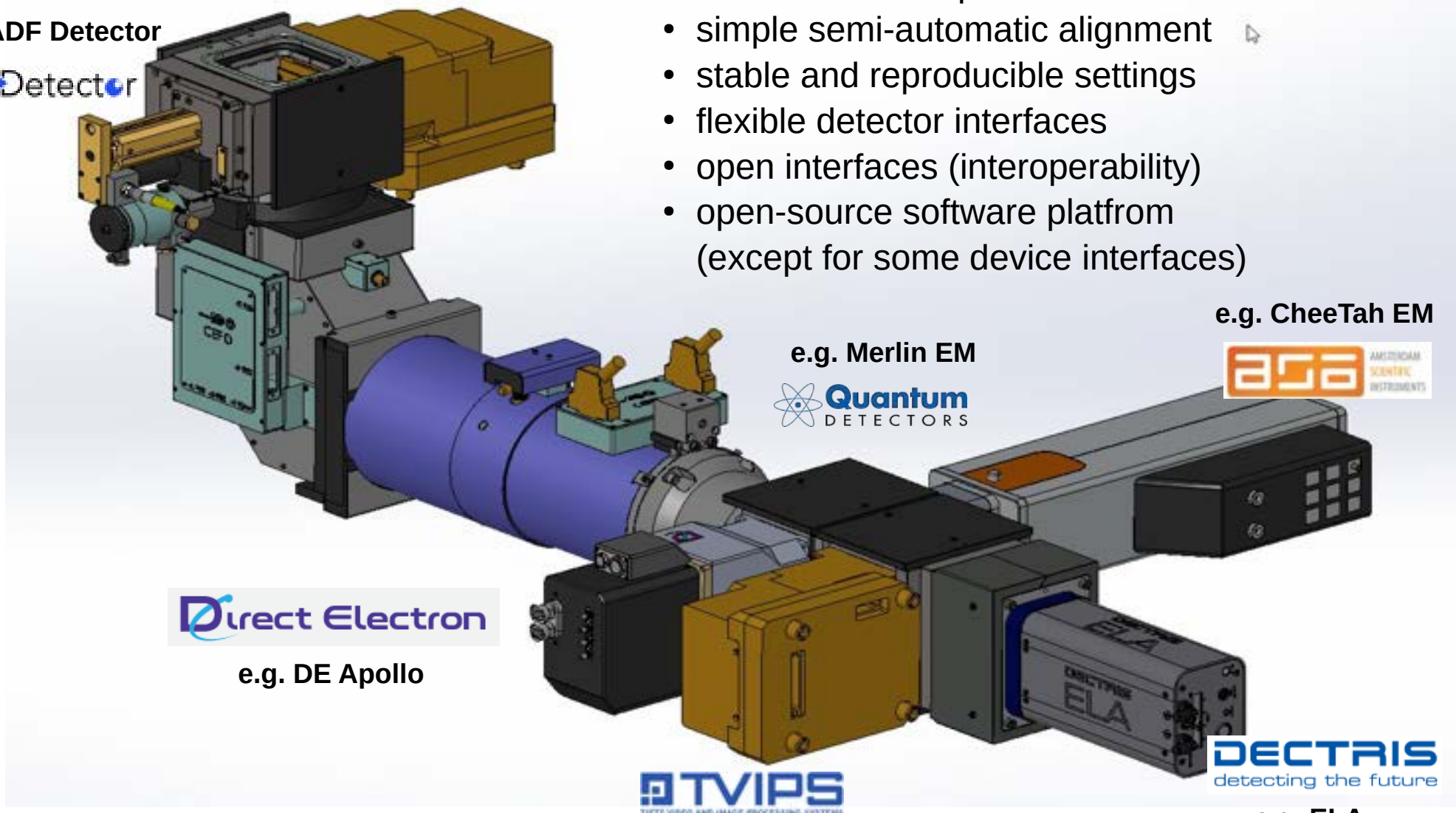
CEOS Energy-Filter and Imaging Device (CEFID)

e.g. ADF Detector

PNDetector



Direct Electron

e.g. DE Apollo

e.g. Merlin EM

Quantum DETECTORS

e.g. CheeTah EM

ASI

TVIPS

e.g. XF416R

DECTRIS
detecting the future

e.g. ELA

Efforts spend by CEOS:

- state-of-the-art optics
- simple semi-automatic alignment
- stable and reproducible settings
- flexible detector interfaces
- open interfaces (interoperability)
- open-source software platfrom (except for some device interfaces)

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