# SELECTROLUX: THEORY AND OPERATION

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DRAFT 1

This document explains the operation of the Selectrolux electron energy loss spectrometer.

## 1. How It Works

The information in this section is mostly based on Kahl et al. [1], who describe the design of the CEFID energy filter which shares some of its design history with the Selectrolux. We will use their notation for the trajectories and path deviations. Lazar et al [2] describe the unique ability of the Selectrolux to probe very high energy losses (but give little detail of the optics).

[1] Kahl, F., Gerheim, V., Linck, M., Müller, H., Schillinger, R., and Uhlemann, S. (2019) *Test and Characterization of a New Post-Column Imaging Energy Filter*

The primary trajectories of the electron beam through the spectrometer are shown for imaging (ESI) and EELS modes in Figure 1. The (curved) $Z$ axis is defined by the trajectory of an axial electron of nominal energy. The $X$ direction (also referred to as the dispersive direction) always points perpendicular to the $Z$-axis and in the plane of the sector magnet, and the non-dispersive $Y$ direction is perpendicular to the sector magnet plane.

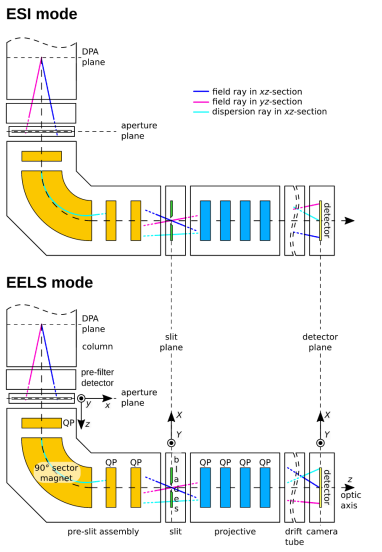


Figure 1. Trajectories in imaging (ESI) and EELS modes, taken from [1]. In the Selectrolux, all of the "QP" elements are instead dodecapoles, and additional weak post-slit elements are present to bring the total count to 10 multipoles.

We generally consider the system to comprise two separate sections: the pre-slit optics and the post-slit optics. The pre-slit contains primarily the prism and three multipole elements, referred to as MP1-MP3 in the Selectrolux covention. The prism serves to disperse the incoming beam, transferring electrons of different energy to a different position in the slit plane, as well as focus it, transferring electrons originating from a point in the object plane to a point in the slit plane. The setup of the pre-slit optics is essentially identical for spectroscopy and imaging modes.

The precise shape of the prism and its fringing fields at the entrance and exit faces govern the focusing properties—see

Egerton [3, §2.2] for a detailed discussion of the origins of the aberrations of the prism. In short, inclination of the faces of the prism produces a first-order focusing effect (an effective quadrupole at the entrance and exit faces), and curvature of the faces produces second-order aberration (an effective sextupole). We will not concern ourselves with the details of the prism design, as modern spectrometers place multipole electromagnetic elements at the entrance (MP1 in the Selectrolux) and exit (MP2) faces, which allow for adjustment of the focusing strength and compensation of the prism aberrations [4].

[3] Egerton, R. F. (2011) *Electron Energy-Loss Spectroscopy in the Electron Microscope*

The slit plane contains two movable knife edges which can block portions of the beam. In imaging mode, the slit blades are brought close together so that only a narrow window of the dispersive direction is permitted to pass, thus filtering out electrons that have been dispersed outside the window. The post-slit optics are configured to project an image of the differential pumping plane onto the detector, producing an energy-filtered image. Incorrect tuning of the pre-slit lenses produces *non-isochromaticity*, or nonuniformity in the energy range selected by the slit over the field of view. Aberrations in the post-slit optics produce geometric and chromatic distortions of the image.

In spectroscopy mode, the setting of the pre-slit lenses is identical to imaging mode[1]. The slits are withdrawn to allow a large range of energies to pass through (but are kept partly inserted to cut off electrons outside the energy range of the detector and prevent them from scattering off of the beam tube). The post-slit lenses are reconfigured to project an image of the slit plane on the detector. The magnification of this image is varied independently in the $X$ and $Y$ directions to control the dispersion and spectrum height, respectively. The different dispersion settings result from different $X$-direction magnification of the slit plane. The intrinsic dispersion of the prism is dependent on the primary beam energy, leading to a different total dispersion for a given post-slit configuration and a different range of dispersions available at each high tension setting (Table II).

[1] The "XXL" dispersions use a different setup of the pre-slit optics that does not produce a crossover at the slit plane. This avoids the need for large quadrupole strengths in the post-slit optics to produce a large dispersion, leading to lower aberrations[5].

## *1.1. Trajectories and Aberrations*

Consider an electron passing through the differential pumping aperture of the microscope projective at an angle $(\theta_x, \theta_y)$, ar-

riving at the spectrometer entrance aperture at position $(x, y)$, with energy loss $\Delta E$. The position $(X, Y)$ this electron arrives on the spectrometer camera[2] is given by

$$\begin{pmatrix} X \\ Y \end{pmatrix} = \begin{pmatrix} X_{00} \\ Y_{00} \end{pmatrix} + \begin{pmatrix} X_{10} & X_{01} \\ Y_{10} & Y_{01} \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} + \begin{pmatrix} X_{001} \\ Y_{001} \end{pmatrix} \Delta E + \begin{pmatrix} \Delta X(x, y, \Delta E) \\ \Delta Y(x, y, \Delta E) \end{pmatrix} \tag{1}$$

where the final, non-linear term is given by

$$\begin{pmatrix} \Delta X \\ \Delta Y \end{pmatrix} = \sum_{R>1} \sum_{k=0}^{R} \sum_{\substack{m=0 \\ n=R-k-m}} \begin{pmatrix} X_{nmk} \\ Y_{nmk} \end{pmatrix} x^n y^m \Delta E^k \tag{2}$$

The coefficients $X_{nm}$ implicitly have $k$ set to zero and are referred to as geometric distortion aberrations of order $N = n + m$, while the $X_{nmk}$ are referred to as chromatic aberrations of rank $R = n + m + k$ and degree $k$.

In spectroscopy mode, the ideal behavior of the system is that an electron entering the spectrometer will arrive on the detector such that:

- The $X$ position depends solely on its energy loss. This implies that the dispersion $X_{001}$ is nonzero, and all other $X_{nmk}$ are zero.
- The $Y$ position depends linearly on its position along the $y$ axis at the spectrometer entrance, with the maximum $Y$ position on the detector being slightly smaller than the width[3] of the detector[4]. This implies that the spectrum height $Y_{01}$ is nonzero, and all other $Y_{nmk}$ are zero.

The meaning of the coefficients are summarized in Table I, along with their common names in the Gatan and Selectrolux conventions. The measurement of the coefficients in Sherpa follows the basic scheme described by Kahl et al [1, Figure 4], where the geometric aberrations are determined by fitting the shape of the ZLP and the chromatic aberrations are determined by measuring the ZLP at several high tension offsets and fitting the energy dependence with a polynomial.

## *1.2. Available Configurations*

The spectrometer is tuned at 60, 120, and 300 kV accelerating voltages. The detector performance is optimal at 120 kV.

[2] Kahl et al [1] prefix the coefficients in these equations with an $S$ when referring to spectroscopy mode. As I am ignoring imaging mode and the intermediate trajectories at the slit plane, I will drop this prefix and all aberrations should simply be understood to refer to spectroscopy mode.

Confusingly, Sherpa uses the term "order" to mean both "order" and "rank."

[3] *Height* and *width* are confusing terms in the context of the spectrometer because the dispersion direction is vertical in the microscope coordinate system but is represented as the horizontal axis on all plots.

[4] This is tuned to the size of the Zebra strip detectors, is equal to about 40 pixels on the 2D alignment camera

Table I. Notable coefficients. Shaded entries are non-zero for the ideal system, others are aberrations and ideally null.

| Symbol | Common name(s) | Description |
|---|---|---|
| $X_{001} = D_s$ | Dispersion | First-order dispersion, determines eV/ch. |
| $X_{00k}$ | Nonlinear dispersion of degree $k$ | Stretch/squish of the energy scale across detector |
| $X_{10}$ | Focus, FX | ZLP width |
| $X_{01}$ | Tilt, FY | Rotation of the ZLP |
| $Y_{01}$ | Height | Height of the ZLP |
| $Y_{001}$ | Spectrum rotation | Energy axis not perfectly horizontal on detector |
| $X_{101}$ | Spectrum Inclination | Change of focus across energy scale |
| $X_{02}$ | Banana, SX | C-shaped ZLP |
| $X_{20}$ | Asymmetry | D-shaped ZLP |
| $X_{11}$ | Propeller, SY | Figure-of-eight shaped ZLP |

The available dispersion settings are shown in Table II for each accelerating voltage. The dispersions in each row of the table share the same basic alignment of the projective, and the difference at each high tension is due to the change of the intrinsic dispersion of the prism (about 3.6 µm/eV at 300 kV). The normal dispersions have a crossover at the slit plane, while the XXL dispersions do not—therefore the pre-slit optics of the XXL dispersions are rather different and so switching between normal and XXL dispersions will require more realignment.

Table II. Dispersions available at each high tension setting, in eV per channel.

| Index | 300 kV | 120 kV | 60 kV |
|---|---|---|---|
| 1 | 0.017 | 0.0074 | 0.0039 |
| 2 | 0.035 | 0.016 | 0.0081 |
| 3 | 0.085 | 0.038 | 0.02 |
| 4 | 0.17 | 0.075 | 0.039 |
| 5 | 0.25 | 0.11 | 0.059 |
| 6 | 0.42 | 0.19 | 0.098 |
| XXL 1 | 1 | 0.44 | 0.23 |
| XXL 2 | 2 | 0.89 | 0.46 |
| XXL 3 | 4 | 2 | 0.93 |

## 2. Operation Procedure

### *2.1. Set-up*

1. Operation of the spectrometer is split across several programs:
   - **Velox** is used for acquisition of data

- **Sherpa** is used for all automated alignments and also allows first-order hand tuning
- **Energy Filter Monitor** is used to load the alignment file, check the status of the communications, and to access the individual multipole elements directly. *Non-expert users should only use this to load the alignment file.*
- Reference Image Manager (Supervisor) is used to acquire dark and gain references for the detector
- Acquisition Service Tool is used to check and set the temperature of the detector
- Acquisition Monitor[5] allows you to check the connection to the EELS camera controller.

The ones listed in **bold** here are necessary to open every time, the others are mostly for troubleshooting.

2. In Energy Filter Monitor, click `Load...` and (re-)load the alignment file for the current accelerating voltage.

[5] Acquisition Monitor and Acquisition Service Tool are normally service-only tools, but we have shortcuts on the desktop.

## *2.2. Initial Tuning (once daily)*

The initial tuning serves mostly to align the pre-slit optics, which are stable over a long period and not changed by most settings. Perform the steps in this section:

- When the alignment file is reloaded
- Daily
- When switching between normal and XXL dispersions

Pre-slit tuning requires the beam to go through vacuum, and a current of 50 pA or more is desirable.

1. In Energy Filter Monitor or Velox[6], select the dispersion you intend to operate at.[7]
2. Open Sherpa, go to the Energy Filter app, and select the EELS tab
3. Ensure the beam is evenly illuminating the *imaging* aperture. The "EF" annotation on the FluCam is the 5 mm entrance aperture, so the beam needs to be twice as big as the green circle in order to fill the imaging aperture.
4. In Sherpa, run `Daily Tune`.
    - The automatic procedure will raise the screen, locate the zero-loss, optimize the exposure time, per-

[6] Velox shows both the dispersion and the full energy range for each setting, EFM only shows the dispersion per pixel.

[7] You do not need to repeat `Daily Tune` when switching dispersions, but it saves time to pick one first since the procedure will also automatically perform some of the other alignments that do depend on dispersion.

form the isochromaticity alignment, switch to EELS mode, perform a `Zero Loss: Tune first`, and execute `Spectrum: Measure`.

5. `Daily Tune` will not perform Spectrum tuning. If the `Spectrum: Measure` reports high distortion values (red or yellow values), run `Spectrum: Tune first` or `Spectrum: Tune All`[8].
6. Switch to the camera length you will use for acquisition (see Table III for the acceptance angle at each CL). Insert the screen and center the beam in the 5mm entrance aperture (green circle in FluCam). Raise the screen.
7. Adjust the exposure time in Sherpa to target a maximum of 10–20,000 counts. If the detector is overexposed, the color bar on the live view will turn solid red.
8. Run **only** `Zero Loss: Tune first`.[9] If any values are still yellow, run `Zero Loss: Tune First` again[10]

The system is now tuned and ready for acquisition (Section 2.4).

[8] If the only red values are in the second column (linear in $E$), tuning only first order is more stable than trying to tune all.

[9] When the entrance aperture is not fully illuminated the height measured here will be red, but this is correct. We want to map *the entire entrance aperture* to the height of the strips, and if we adjust the (now smaller) beam to fill this height then scattered electrons will now land off of the strip.

[10] The procedure will only run a maximum of 4 iterations each time, even if the tuning isn't within spec.

## *2.3. Operational Tuning (as needed)*

This section details the tuning that may be performed during a session in case the system drifts or different operating conditions are selected.

Most tuning is done automatically using Sherpa. It is preferable to run these automated alignments over vacuum, but the system seems tolerant to having some inelastic scattering present. If a sample is present, it seems safe to run `Zero Loss: Tune first`.

Note: The `Super` checkbox simply sets a more conservative threshold for some of the aberration targets. Always leave it enabled (we have not struggled to achieve even the more restrictive values).

### *2.3.1. Automated Tuning*

The automated alignments in Sherpa are the main way to keep the spectrometer tuned during a session. Tune the ZLP (typically only to first order) when changing camera length or if you notice the spectrum defocus has changed. Perform Spectrum tuning after changing dispersions (but see the note below).

When the entrance aperture is not evenly illuminated (such as when you are at a short camera legnth for achieving a high collection angle in STEM) the only automated alignment you should use is `Zero Loss: Tune first`. If you use any other tool the routine will stretch the spectrum height too high, which causes part of the beam to fall outside the strip detectors when acquiring.

### *2.3.2. Hand Tuning*

Manual hand tuning of the first order controls is possible in Sherpa by pressing `Manual Fine` and scrolling on the boxes that appear. Hand tuning is rarely needed when the system is performing properly. No refocusing of the core-loss portion of the spectrum should be necessary, as the optics are normally able to fully compensate the spectrum inclination $X_{101}$.

## *2.4. Acquisition*

Velox is used for all acquisition.

1. Use the DF-S detector for imaging when in spectroscopy mode, as its inner opening is just slightly larger than the entrance aperture and we have ensured that they are mechanically well aligned to one another.
2. Adjust the contrast and brightness of the DF-S detector, if you haven't already.
3. In the Spectrum menu on the ribbon, select EELS.
4. Select the energy range(s)[11] to acquire and set the dwell time for each range. Typical times are 1 µs for the ZLP and 1 ms for a moderate energy core loss.
5. View the spectrum live or acquire a single spectrum with the buttons in the Spectrum menu[12].
6. To acquire a spectrum image, use the SI menu of the ribbon. The pixel size of the SI always matches the STEM image, so adjust the step size with magnification or the number of pixels in the STEM scan. Drag a box to select an area, and the acquisition time is displayed above the box.
7. To navigate the spectrum in the processing window, use `Shift+drag` *on the plot area* to draw a box to zoom in. `Shift+drag` *on the axes* to shift the scale. Press

[11] See Section 2.4.3 for information on choosing the number of strips to use to avoid ZLP afterglow artifacts. See Section 2.4.1 for information on shifting the available energy range.

[12] Unfortunately, the dwell times are shared for view, acquire, and SI.

`Shift+Home` to auto-scale only the intensity axis, or press `Home` to zoom all the way out. Press `Shift+[left/right arrow]` to navigate between energy ranges in the spectrum.

8. Select elements in the periodic table to mark edges and produce maps. The regions for background subtraction can be adjusted, but this is currently odd.

*2.4.1. Energy Ranges*

When using multiEELS in Velox, the different energy ranges are reached by biasing the drift tube (as this is electrostatic and thus can be changed rapidly). The bias supply on the drift tube has a limit of 2,500 V, which sets the limit for the greatest shift between energy ranges in a scan. To measure higher losses, use the prism to shift the overall energy range by adjusting `Spectrum Start` in Energy Filter Monitor. The ranges shown in Velox will update to show the new accessible window.

*2.4.2. Collection Angle*

The acceptance angle of the spectrometer at each camera length is shown in Table III. The inner angle of the DF-S detector is slightly larger (by about 10%) than the spectrometer acceptance, so this is the ideal detector to use for elastic imaging when at the CL needed for spectroscopy.

Table III. Filter acceptance angle using 5 mm entrance aperture at 120kV[13].

| CL (mm) | $\beta$ (mrad) | CL (mm) | $\beta$ (mrad) |
|---|---|---|---|
| 9 | 132 | 46 | 26 |
| 12 | 102 | 59 | 20 |
| 15 | 80 | 76 | 16 |
| 19 | 65 | 95 | 13 |
| 24 | 52 | 115 | 10 |
| 30 | 41 | 150 | 8 |
| 37 | 33 | 190 | 7 |

[13] These may differ slightly at other voltages due to differences in the true CL. You can view the calibrated value in the metadata of an SI.

*2.4.3. Energy Ranges*

The Zebra detector contains 5 separate 1×2048 pixel "strip" detectors, allowing readout of one strip to occur while the beam is exposing another strip and thus enabling faster acquisition of many energy ranges. *The system always uses all of the strips, in*

*sequence, regardless of how many energy ranges you select.* If one of your energy ranges contains the ZLP, and it is exposed for long enough, there will be some afterglow in the scintillator. In this case, it is beneficial to ensure that the ZLP is only ever located on one of the strips, so that the afterglow does not affect the other energy ranges. To ensure the ZLP and core-loss never occupy the same strips, it is recommended that **if you are capturing the ZLP, use either 1 energy range or all 5**. You can set all the core-loss ranges to the same energy, or to different ones, but they should all be checked so that every strip gets the same energy range on every exposure[14].

[14] There's no benefit to setting all 5 to the same energy range, as it results in the same behavior as selecting just one range.

## *2.5. End of Session*

1. No end-of-session actions are needed.

## *2.6. Detector Normalizations*

The strip detectors and the alignment area have separate dark and gain references, which are stored per high tension setting. The references for the alignment area are not critical unless they are very poor, which we do not expect to happen with any regularity. We are not yet certain of the frequency calibration of the strip detectors will be needed, or the long term effects of oversaturation. It is not recommended, at this time, to take a new gain or dark reference on the detector in each session. Please alert staff if you notice a detector artifact.

To acquire gain or dark references:

1. Open **Reference Image Manager (Supervisor)** from the Microscope Software Launcher.
2. The Zebra detector and the alignment area will show their current status, and the time of the last reference acquisition at the current HT setting.
3. Click the Dark or Gain buttons to acquire a new reference.
4. The guided procedure will open. Follow the steps on the screen. Make sure the DF detector is retracted, as it partially blocks the imaging aperture.
    - Following a dark reference, the mean counts should be less than 10 and the traces should be featureless.

- In order to perform a gain reference, the spectrometer must be fully tuned in imaging mode. Use the Imaging tab in Sherpa and run a `Daily Tune`, ensuring the distortions are within spec.
- Gain references require increasing the beam current to around 1 nA. For the strip detectors, target a mean intensity of 7,000 counts and use the Medium setting to acquire a sufficient number of images for averaging. This will take about 15 minutes.
- The left-right variation should be less than 5 counts after gain normalization.

For the alignment area, 100 images is sufficient.

# 3. Troubleshooting

## *3.1. Can't view EELS detector*

If the alignment area or the strips cannot be viewed in Sherpa, first check if you can start/stop a view of the spectrum in Velox. Sometimes this resolves a software glitch on the readout pipeline.

If Velox also cannot view the spectrum, check the status of the EELS detectors in Acquisition Monitor[15]. If they are red here, first try rebooting the detector server (this is in the rack at the very back of the room). Wait 5 minutes for it to reconnect. If this does not resolve the problem, restart the microscope server.

[15] This is usually on the desktop, or can be opened from Microscope Software Launcher in Service mode.

## *3.2. Invalid dispersion message in Velox*

If you are unable to switch dispersions from Velox, close Velox and open it again. This is a bug (present as of version 3.16.1). Velox needs to be restarted after a high tension change to update the dispersions menu.

## *3.3. EELS missing from Velox*

If there is any error with the EELS detector or the spectrometer, the EELS menu will not populate in Velox. Check the system status in Energy Filter Monitor (should be two green lights) and

in Acquisition Monitor (both detectors green). Solve any problems you find, then restart Velox.

### *3.4. RTOM errors*

If the RTOM connection light in Energy Filter Monitor goes red, you can usually solve this by restarting the system service that runs the optics. Open Task Manager, go to Services, and restart `RTOMControlService`.

### *3.5. Camera Temperature*

The detector cooling is controlled in **Acquisition Service Tool**, which is launched from Microscope Software Launcher when in service mode or from the shortcut on the desktop. The temperature is normally set to −20°C. Sometimes other programs will not read the temperature correctly, or you will see temperature warnings. These seem to be bugs.

## References

[1] F. Kahl, V. Gerheim, M. Linck, H. Müller, R. Schillinger, and S. Uhlemann, "Test and Characterization of a New Post-Column Imaging Energy Filter," *Advances in Imaging and Electron Physics*, vol. 212. Elsevier, pp. 35–70, 2019. doi: 10.1016/bs.aiep.2019.08.005.

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[3] R. F. Egerton, *Electron Energy-Loss Spectroscopy in the Electron Microscope*, 3d edition. in The Language of Science. New York: Springer, 2011.

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