MA-XRF Scanner: Implementation of Image Reconstruction Algorithms Based on Single Photon Detection for Cultural Heritage Studies

1st Mesoamerican Workshop on Reconfigurable X-ray Scientific Instrumentation for Cultural Heritage

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IAEA
International Atomic Energy Agency
Atoms for Peace and Development

IUPAP Centenary
YEARS 1922 - 2022

ICTP
The Abdus Salam
International Centre
for Theoretical Physics

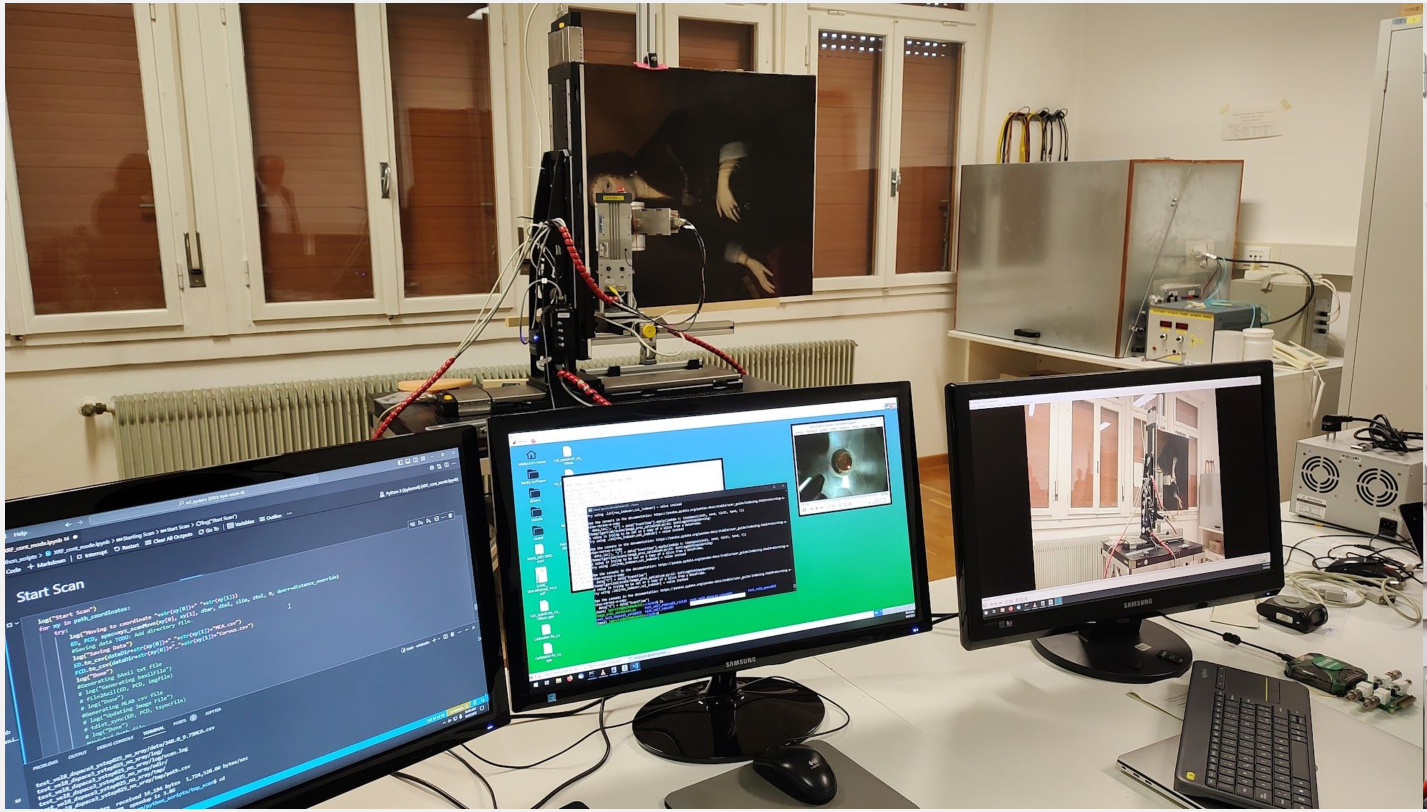
Motivation

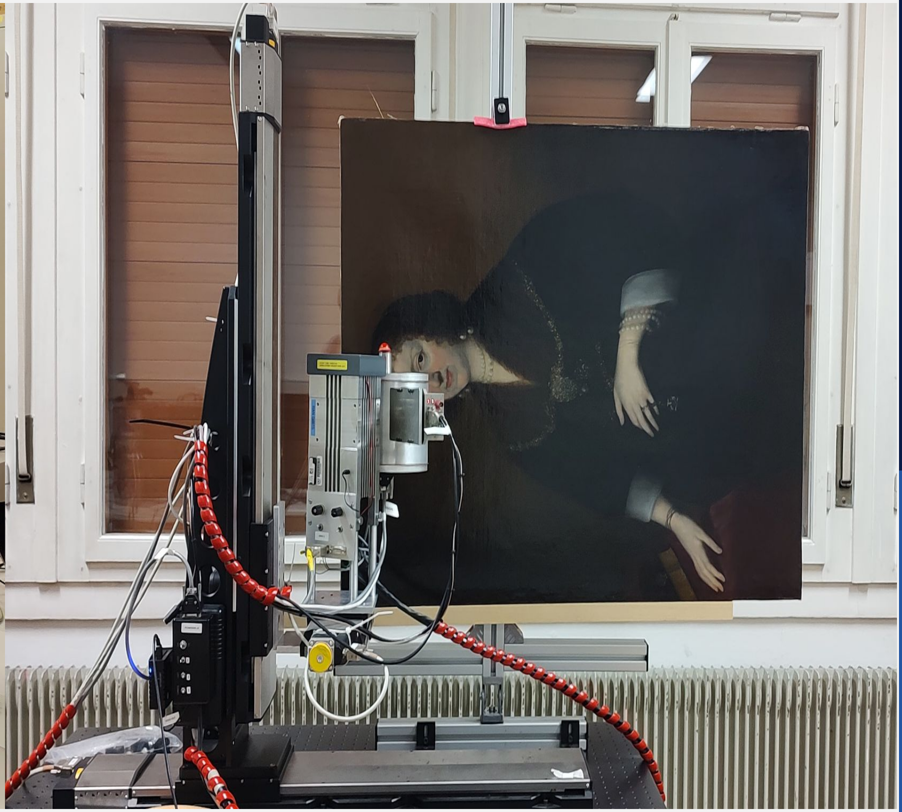
- Transportable MA-XRF scanner for research and training prioritizing cultural heritage studies, in a joint collaboration between MLAB/ICTP and NSIL/IAEA

- Versatile elemental map reconstruction with variable pixel resolutions taking advantage of:
    - Nanosecond timestamping
    - Precise positioning system

- Data compression analysis for efficient storage and distribution

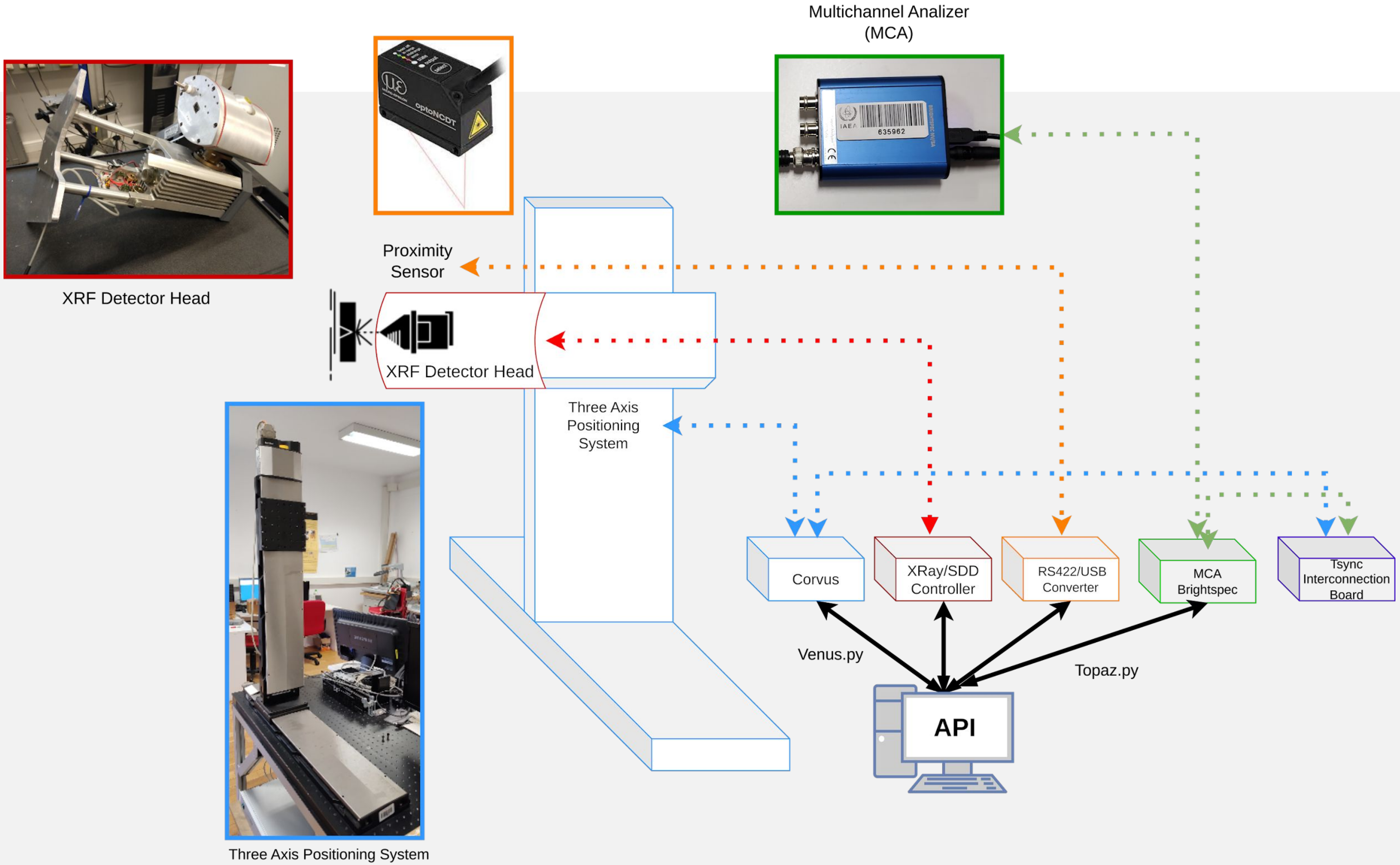
ICTP-IAEA MA-XRF Scanner





ICTP-IAEA MA-XRF Scanner

Main subsystems



ICTP-IAEA MA-XRF Scanner

Main specifications

Scan velocity: 1-20 mm/s

Scan acceleration: 1-40 mm/s^2

DTS sensor range: 0.1-5.0* mm

X and Y scan ranges: 510 mm

Z scan range: 50 mm

Step in X, Y, and Z axes: 1 µm

Energy range:
S (2.308 keV) - Ba (32.19 keV)

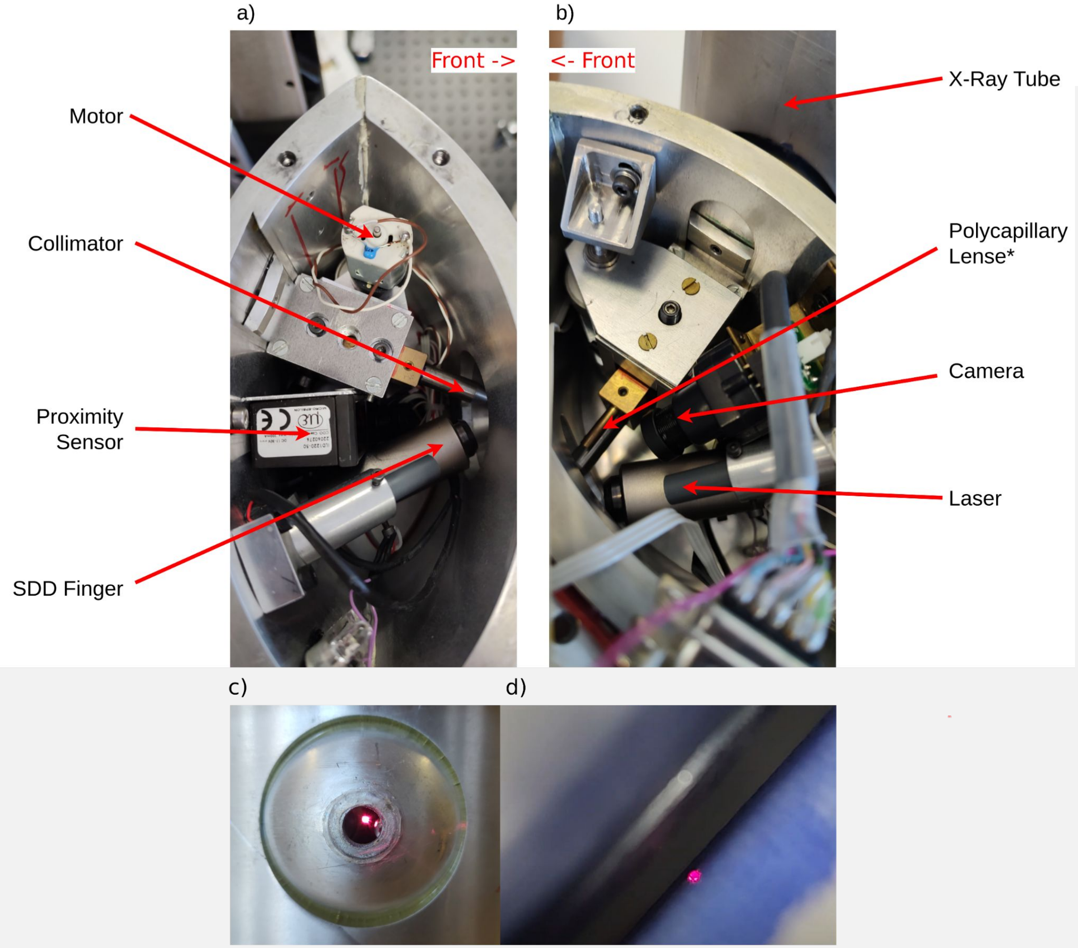
X-Ray source:
Pd Anode, 50 W max power
(50 kV @ 1 mA). Oxford XTF5011.

X-Ray spot size:
500 µm (collimated), 50 µm (PCL)

Detector: KETEK AXAS X1391 Silicon drift detector (SDD). FWHM Mn-Ka ~150 eV.

MCA: Brightspec Topaz-X, 40 ns TLIST mode

*Range for effective automatic DTS adjustment

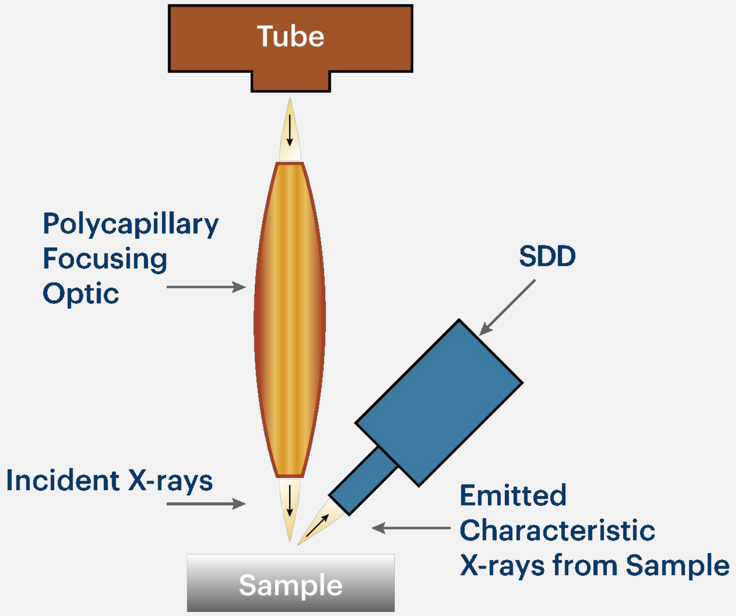


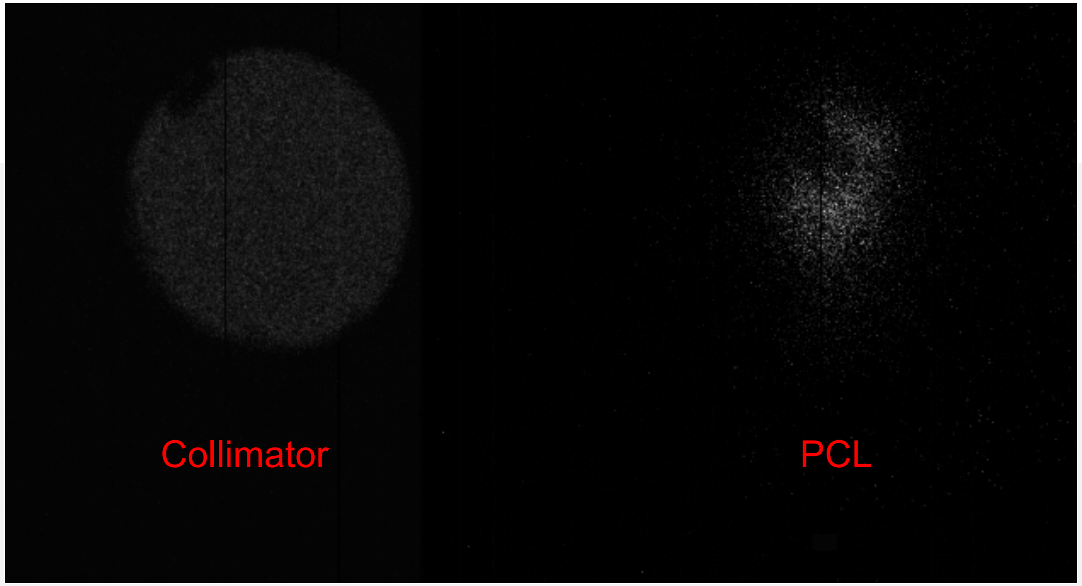
MA-XRF Scanner: detector head

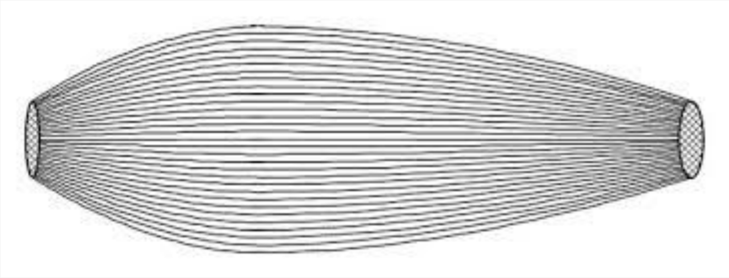
Upper (left) and lower (right) views

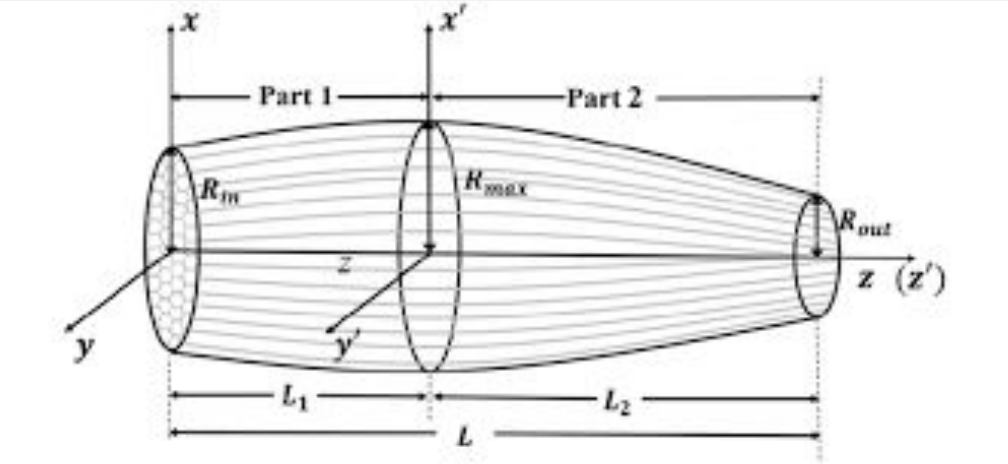
ICTP-IAEA MA-XRF Scanner

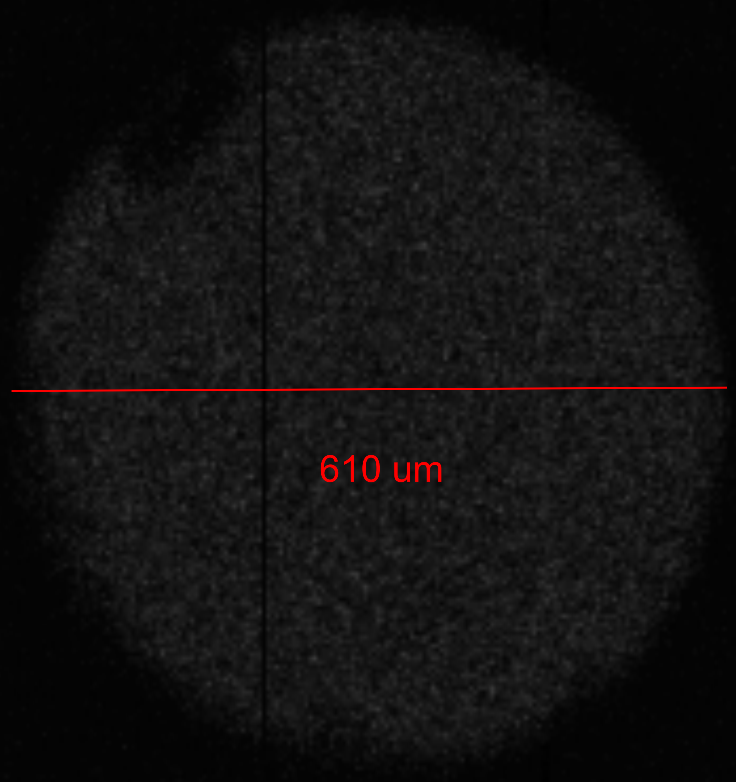
Polycapillary Lense



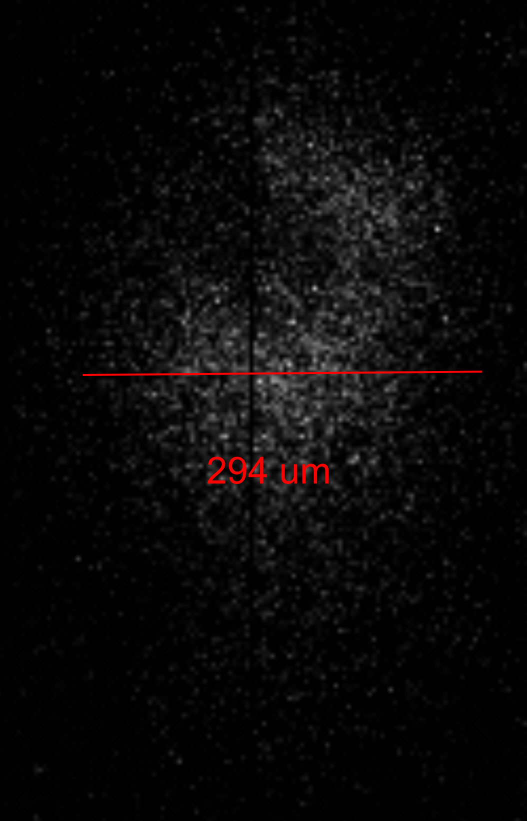




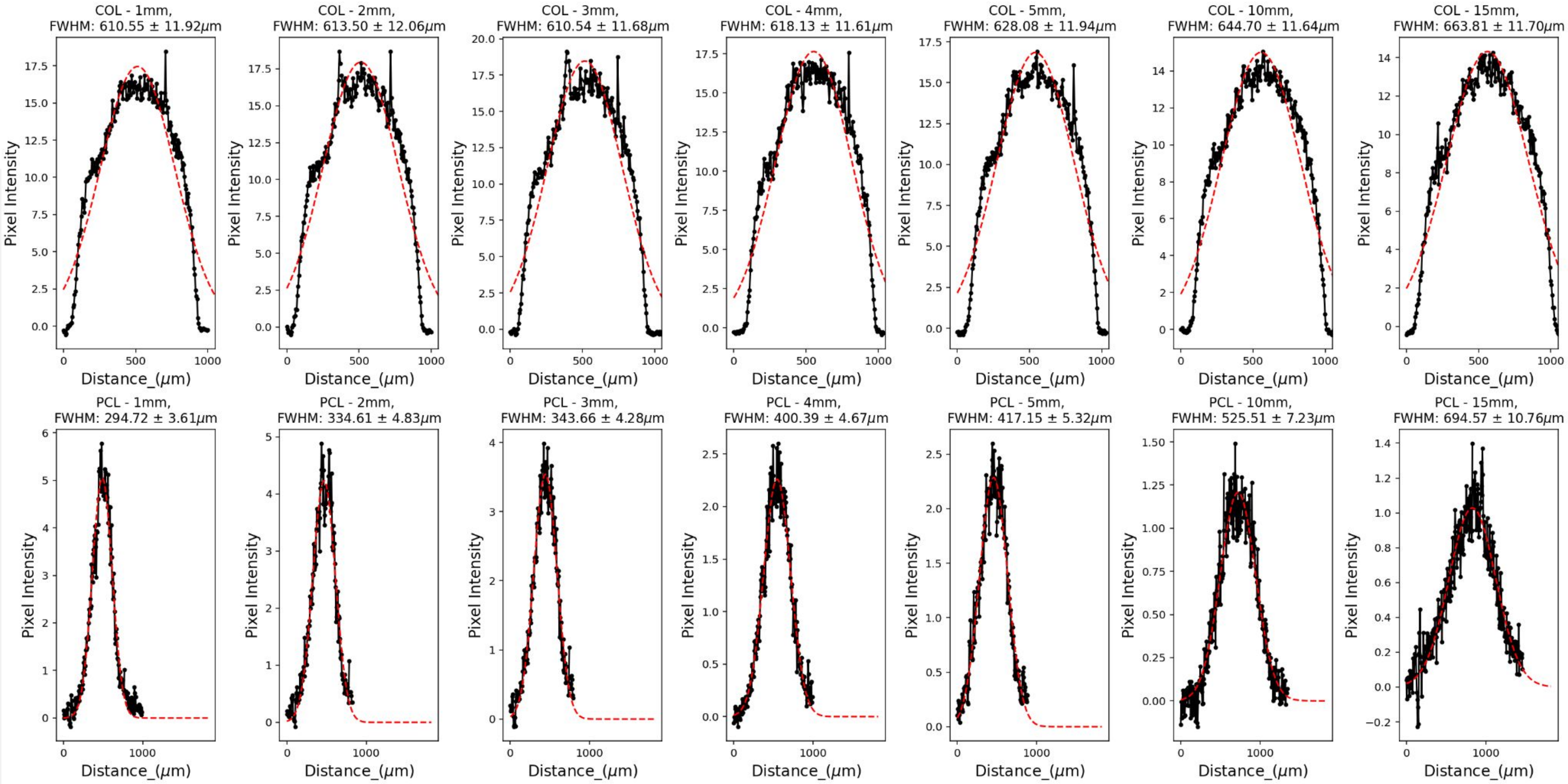




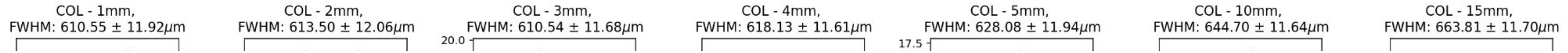
Collimator

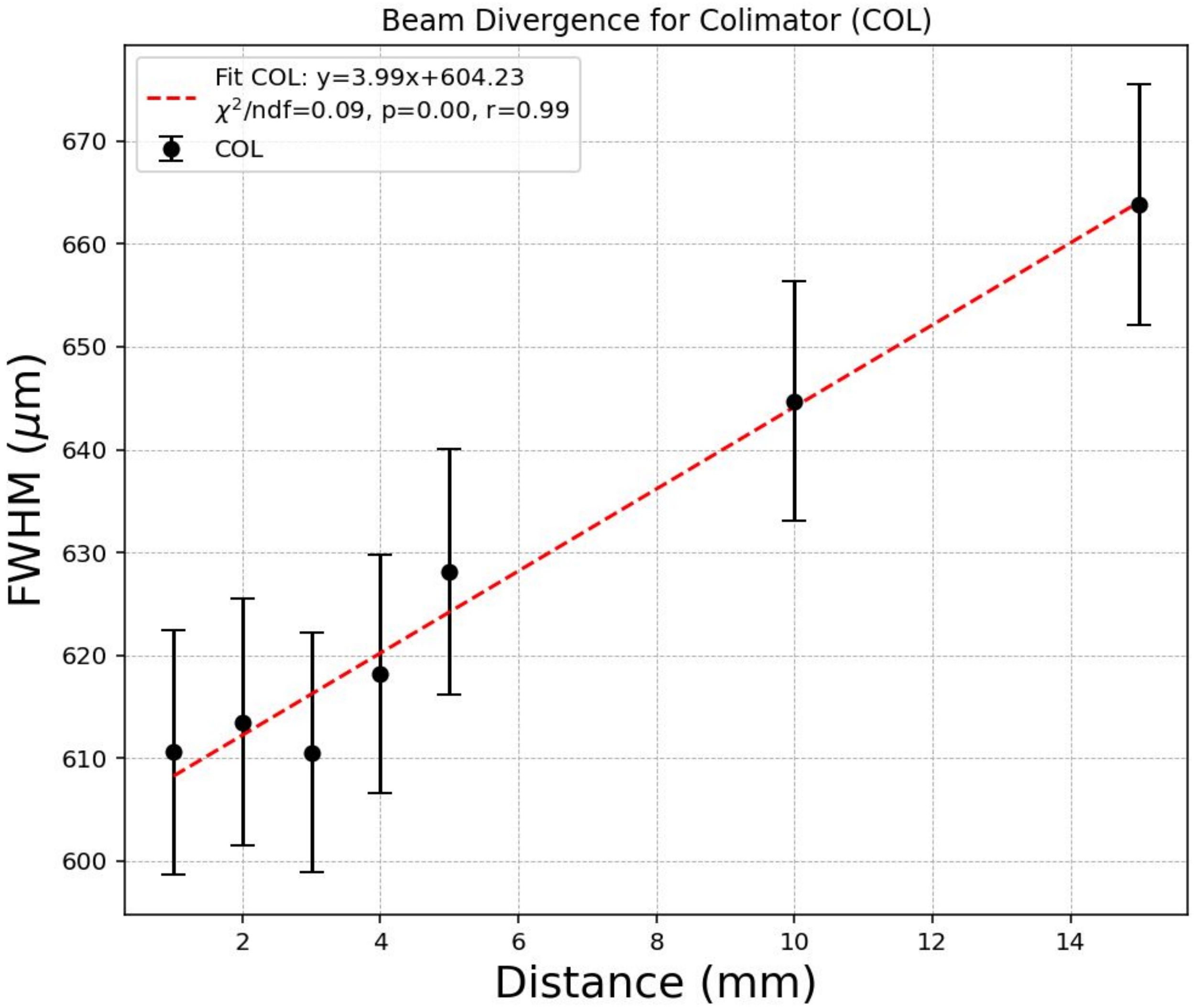


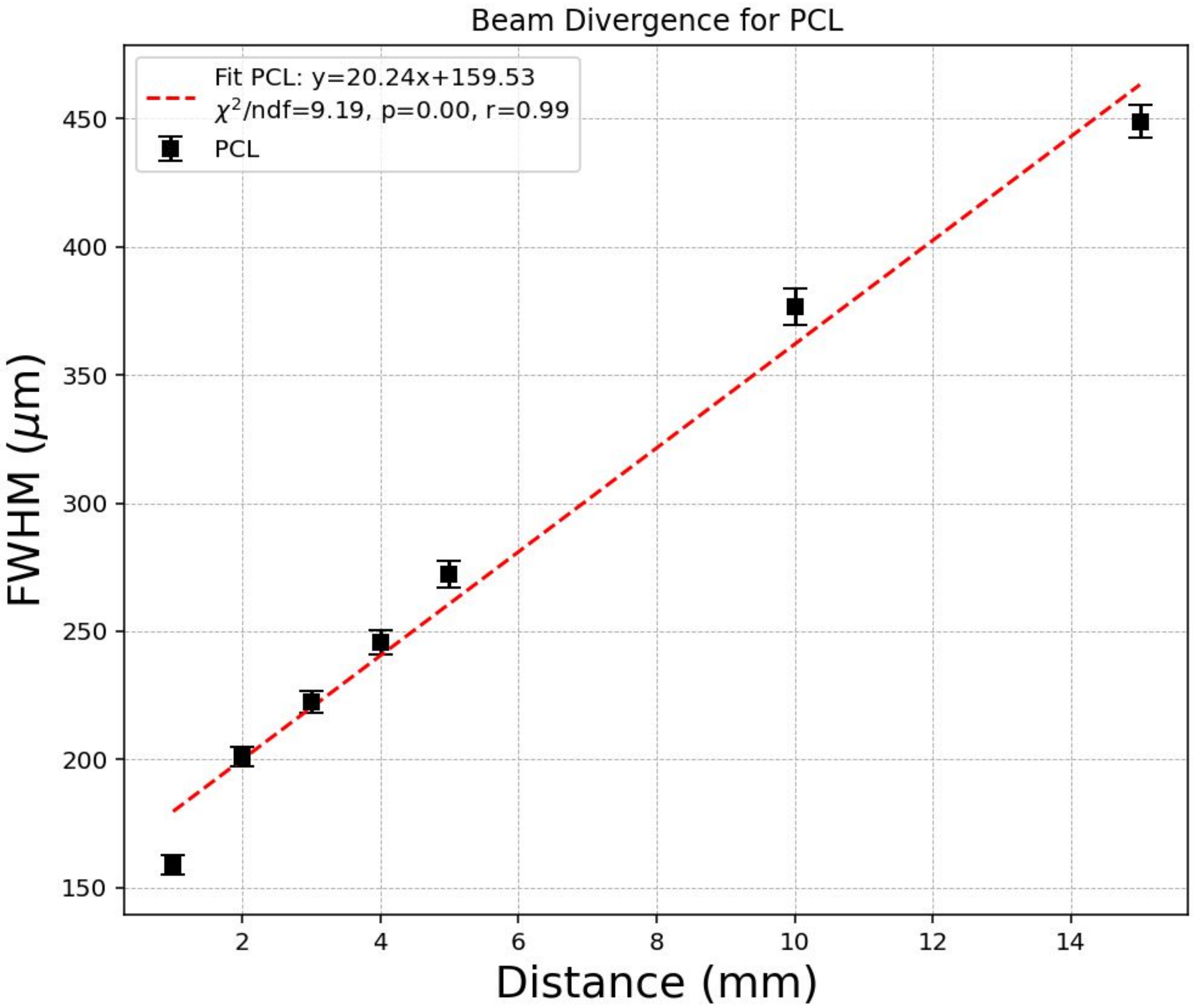
PCL



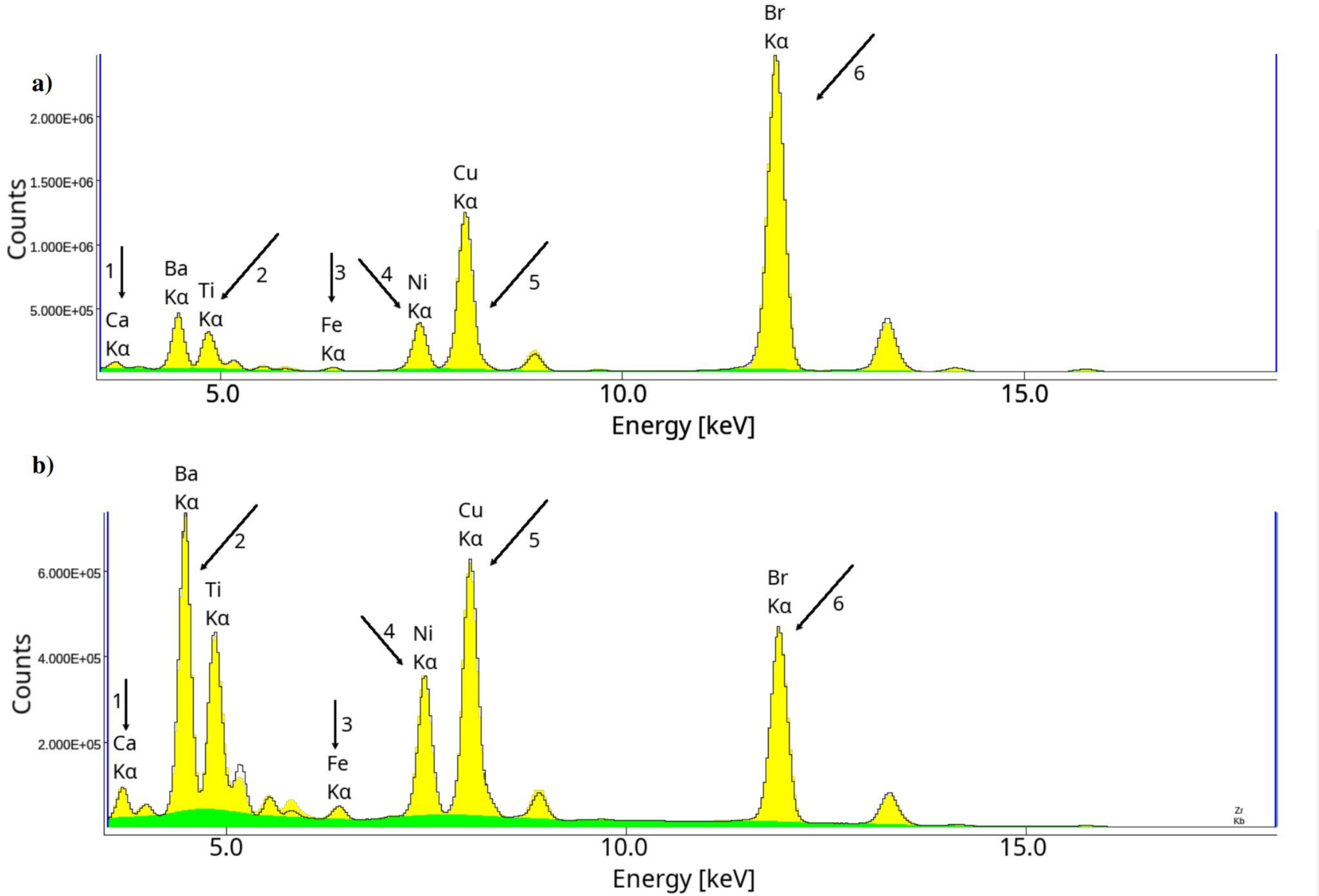
Horizontal beam profile after baseline correction, for the collimator (up) and PCL (down) at different distances between detector head and the CMOS detector.







head and the CMOS detector.



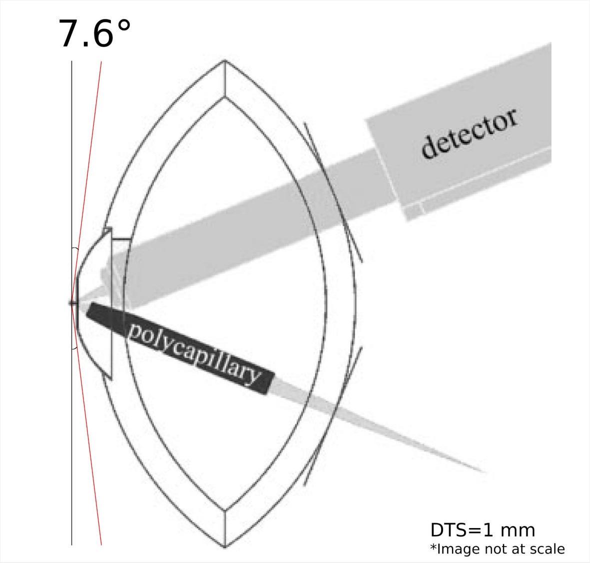
Comparison of energy spectra using collimator (a) and PCL (b) scanned under the same conditions. Scan velocity 5 mm/s, vertical step size, 0.1 mm, and 0.2 mm of distance to the surface of the object. Ca (1), Ba, Ti (2), Fe (3), Ni (4), Cu (5) and Br (6)

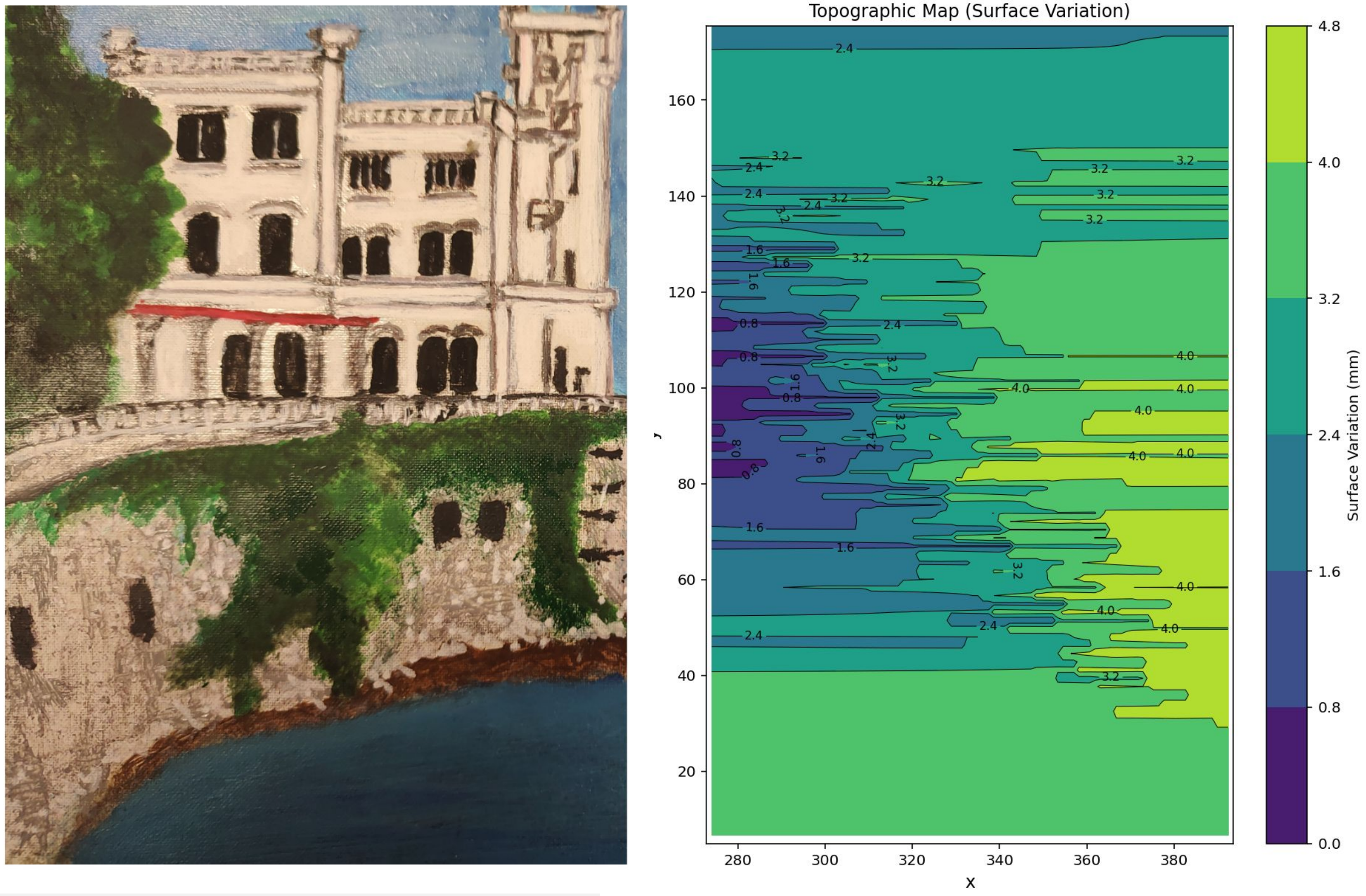
ICTP-IAEA MA-XRF Scanner

Automatic distance adjustment

On-the-fly distance tracking and adjustment w/proximity sensor

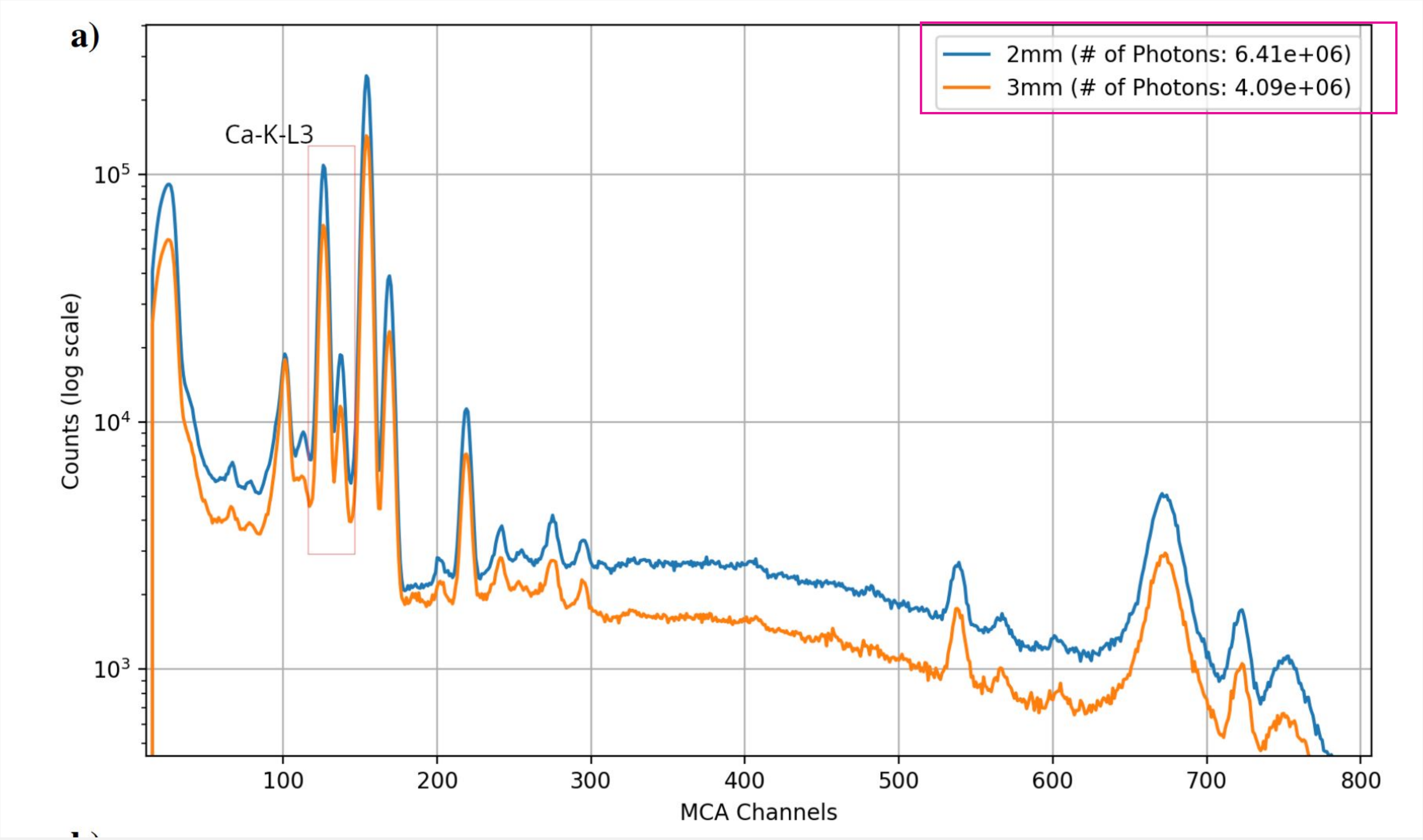
- Keeps DTS steady (uneven surfaces)
- Collision avoidance
- Resolution 10 μm
- Max. DTS 5 mm





DTS variations (in mm) of the surface of a painting

Test case: painting scan at 5 mm/s at two different DTS



Scan Characteristics:

Painting Size: 220x170 mm

Scan Velocity: 5 mm/s

YStep Size: 0.25 mm

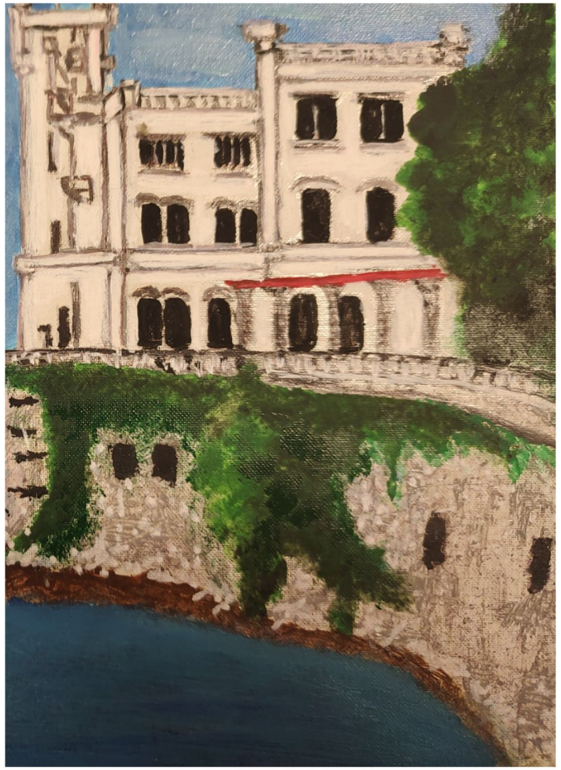
Scan Sweep: Raster

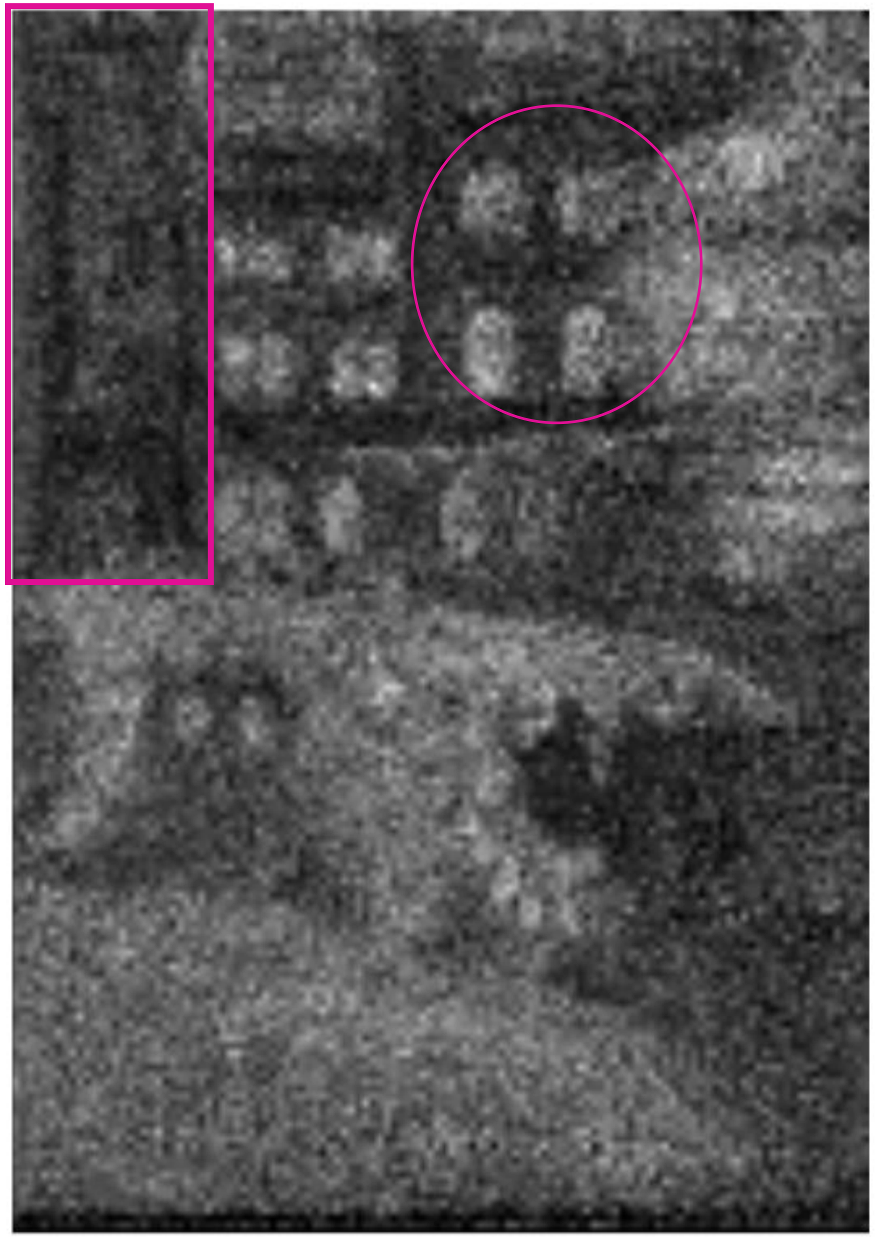
Pixel Size: 0.5x0.5 mm

Element: Titanium

3 mm ~4.1 M photons

2 mm ~6.4 M photons





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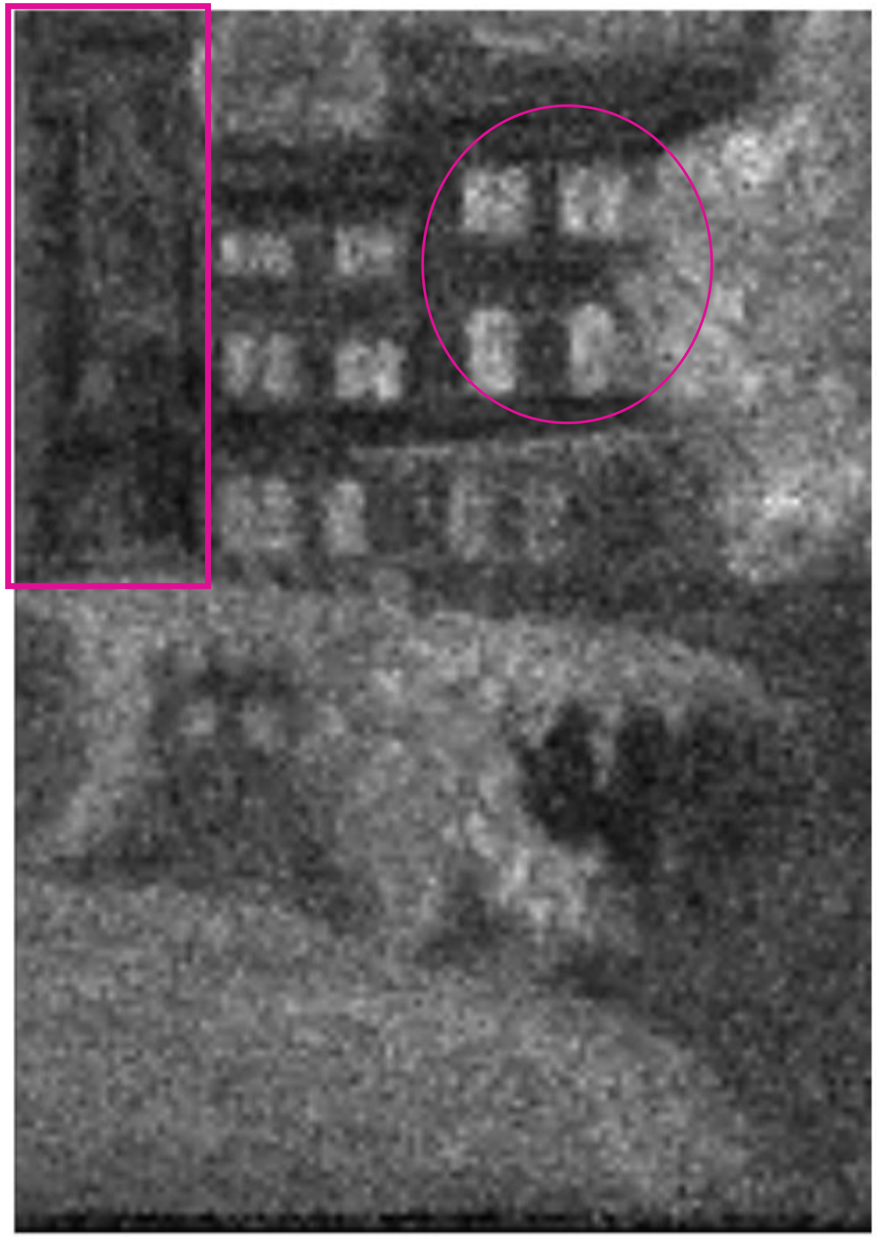

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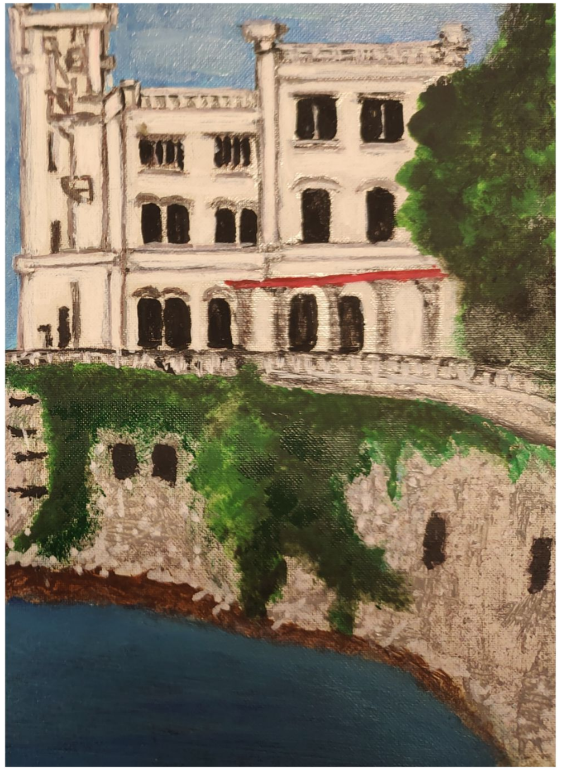
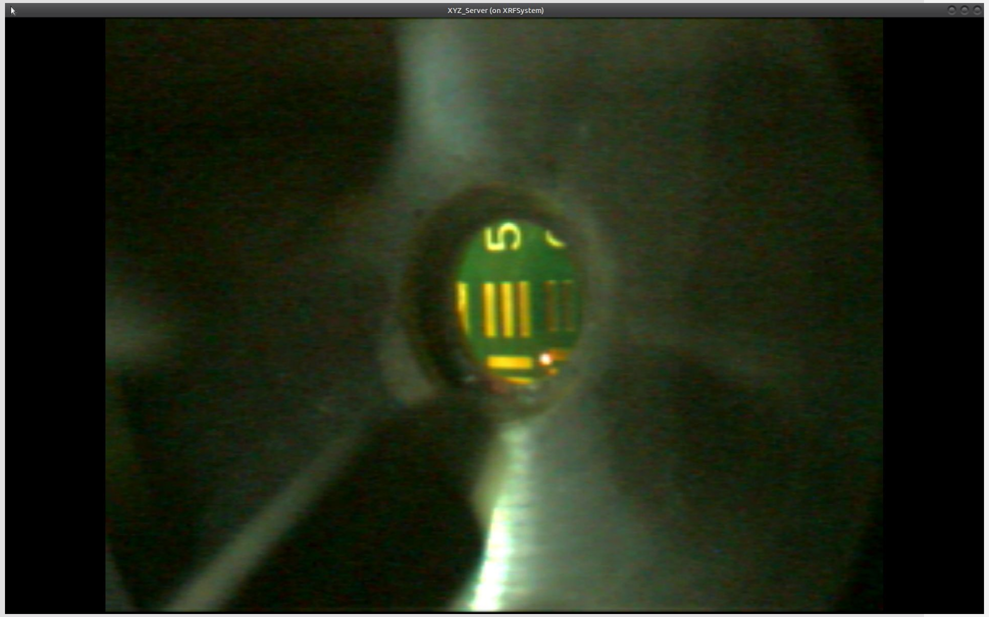
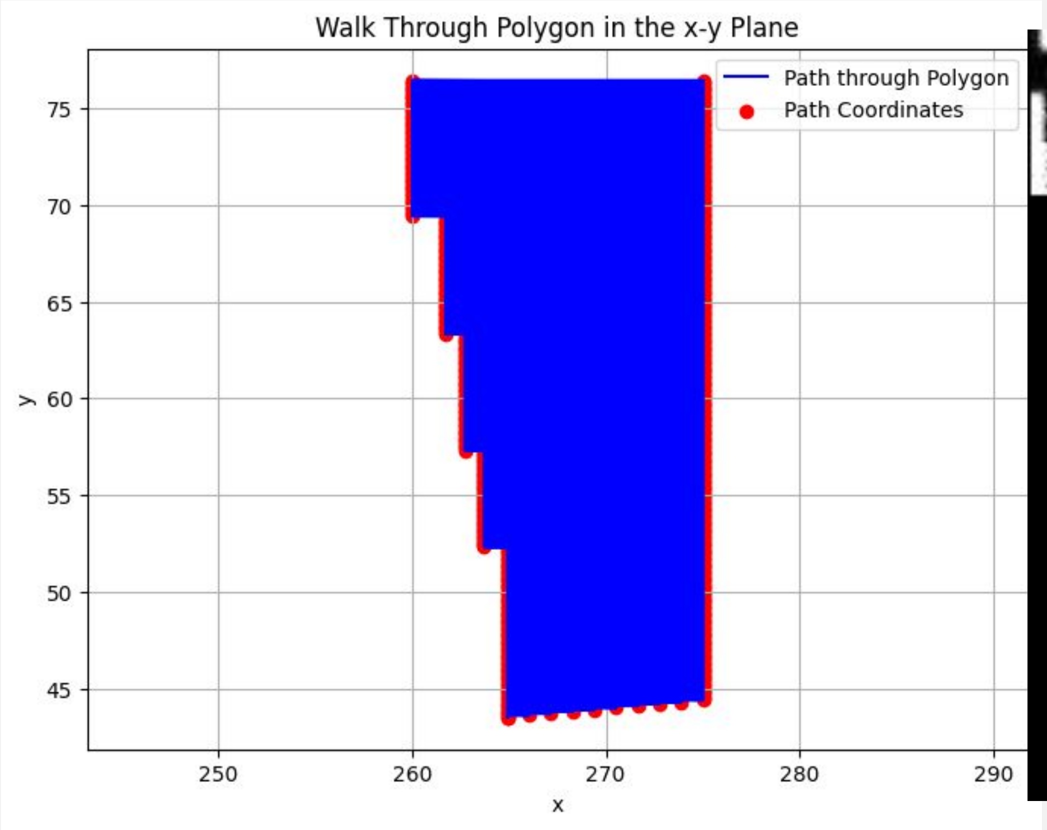


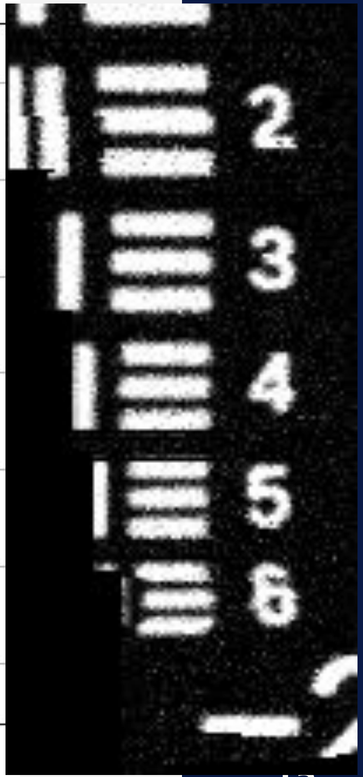
Other Features

- Custom scan areas: variable velocity and irregular shape
- XYZ position replicability down to 10 µm
- Vacuum-ready detector head (0.1 mbar)



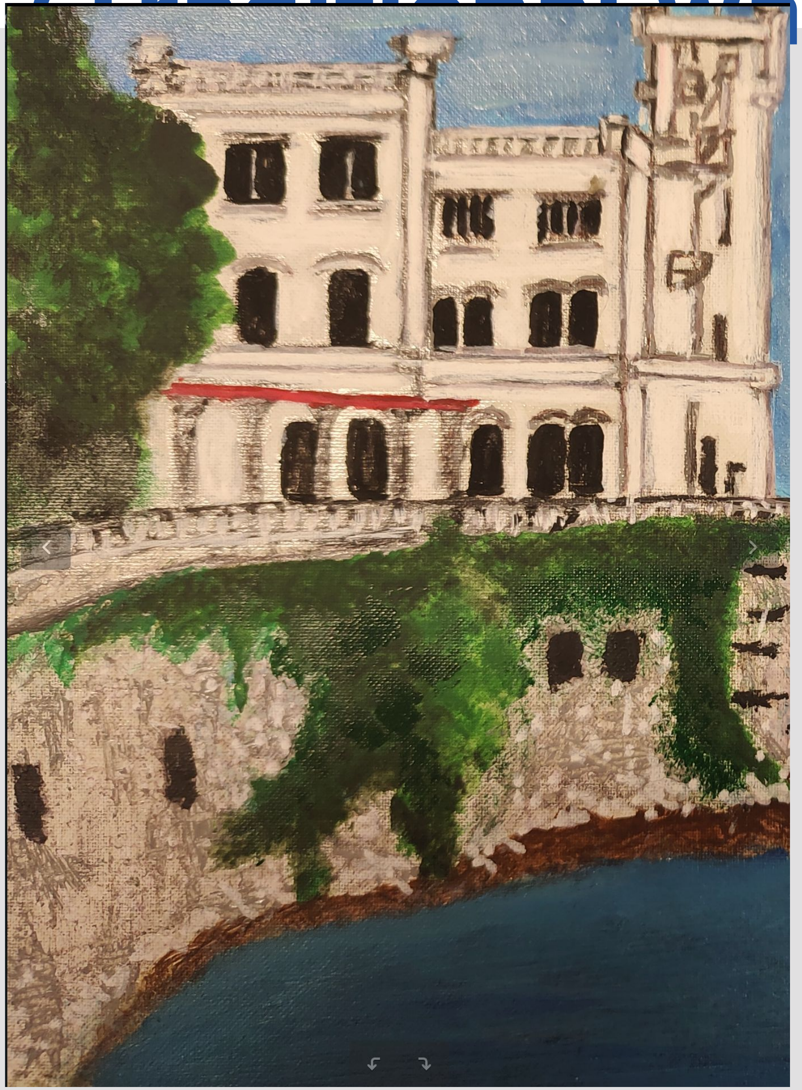
Detector head camera view: USAF 1951 phantom



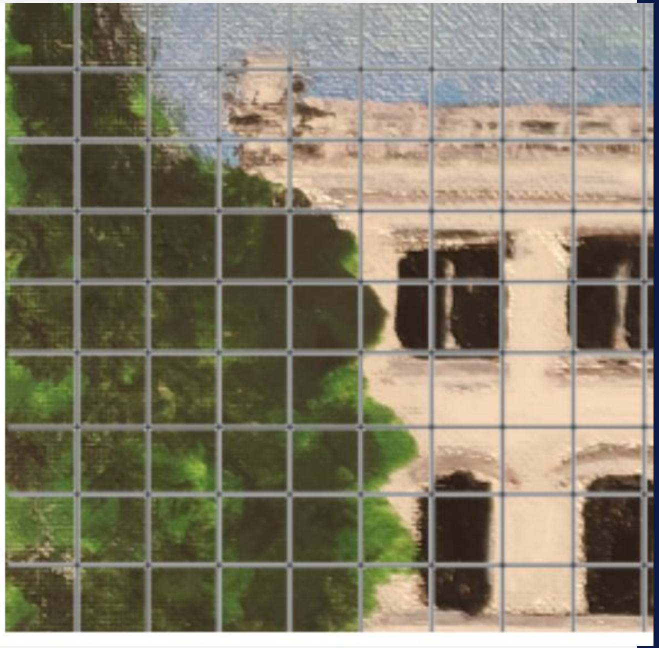


Custom scanning area definition and result

Elemental Map Reconstruction (Traditional way)



1. Select a grid size (usually spot size)



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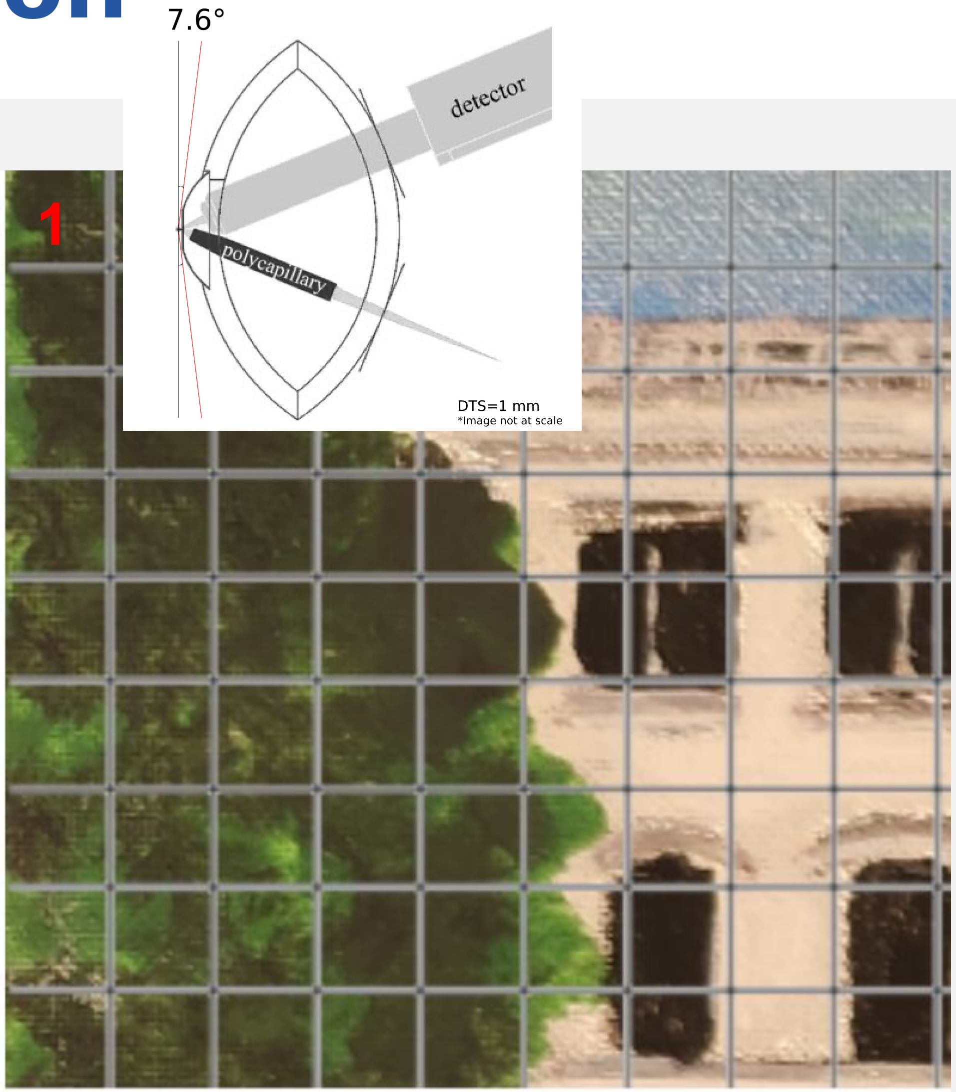
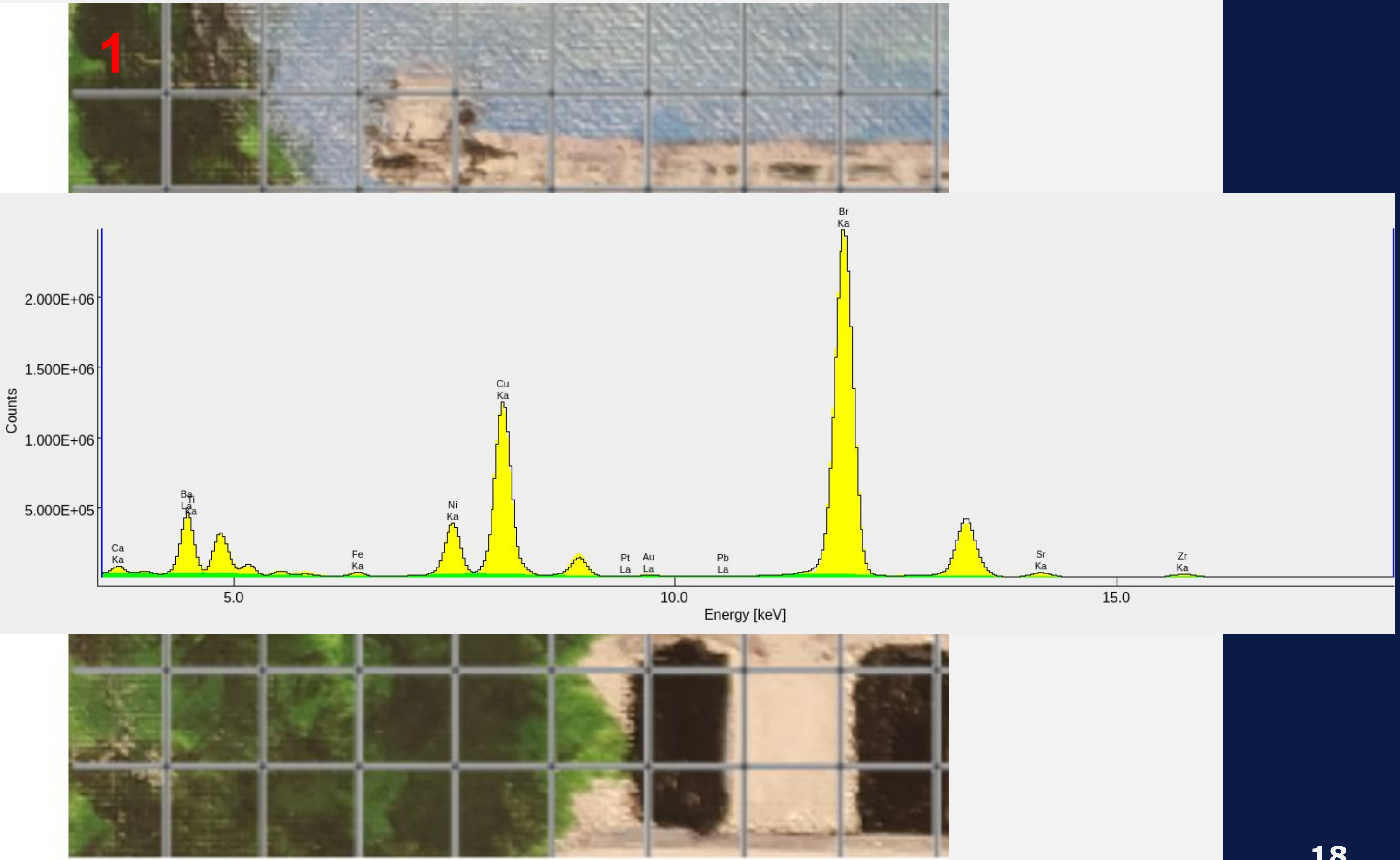


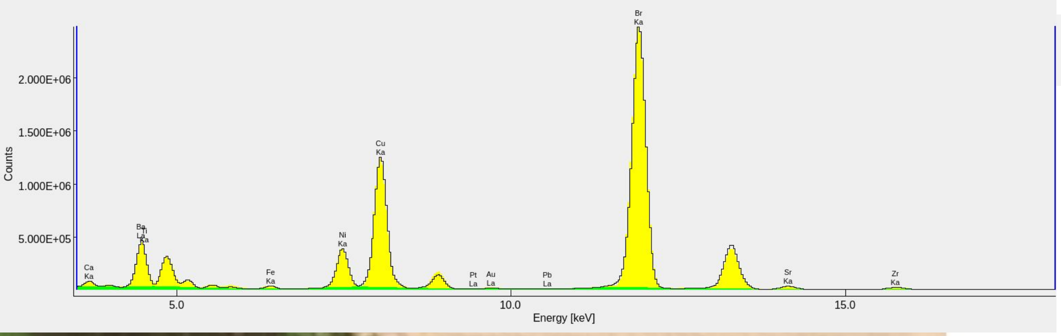
2. Move your detector to Pixel 1.

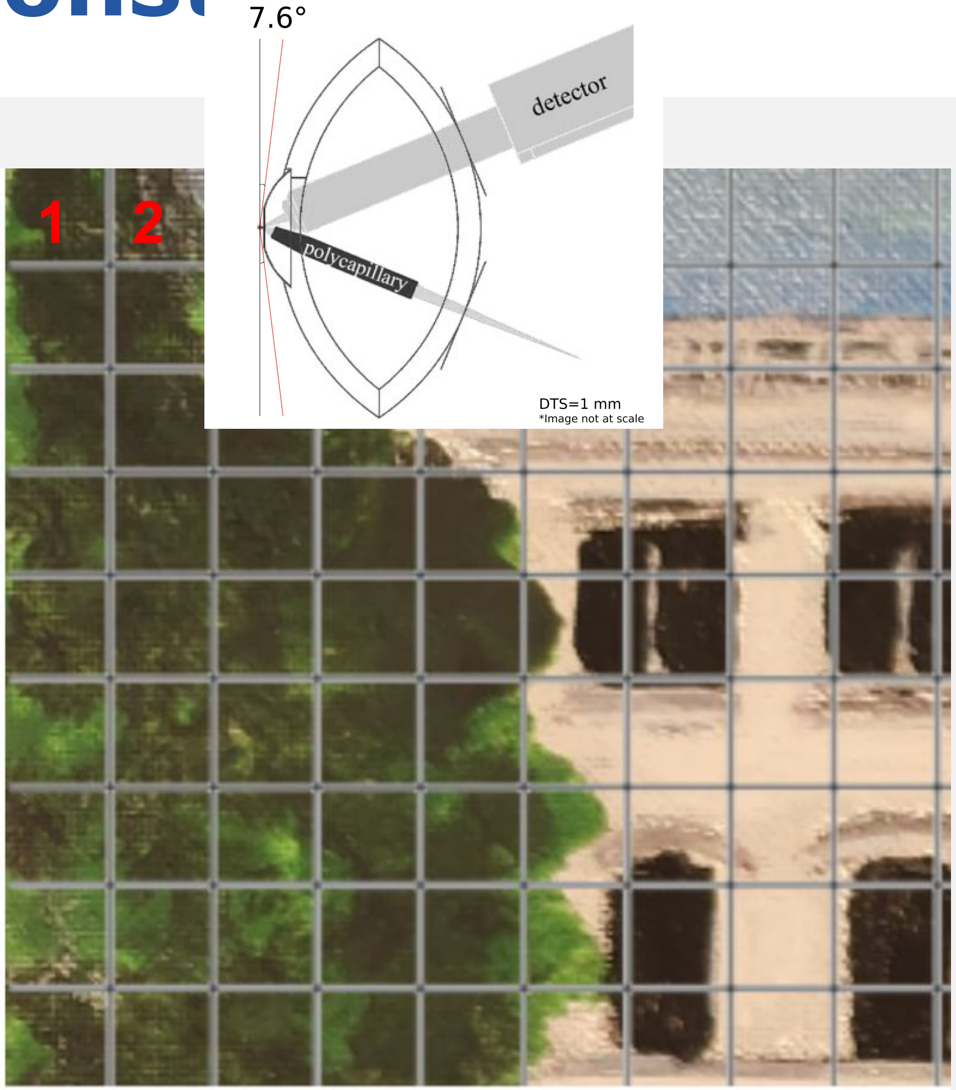
Elemental Map Reconstruction (Traditional way)

3. Scan for few seconds and get the spectrum.



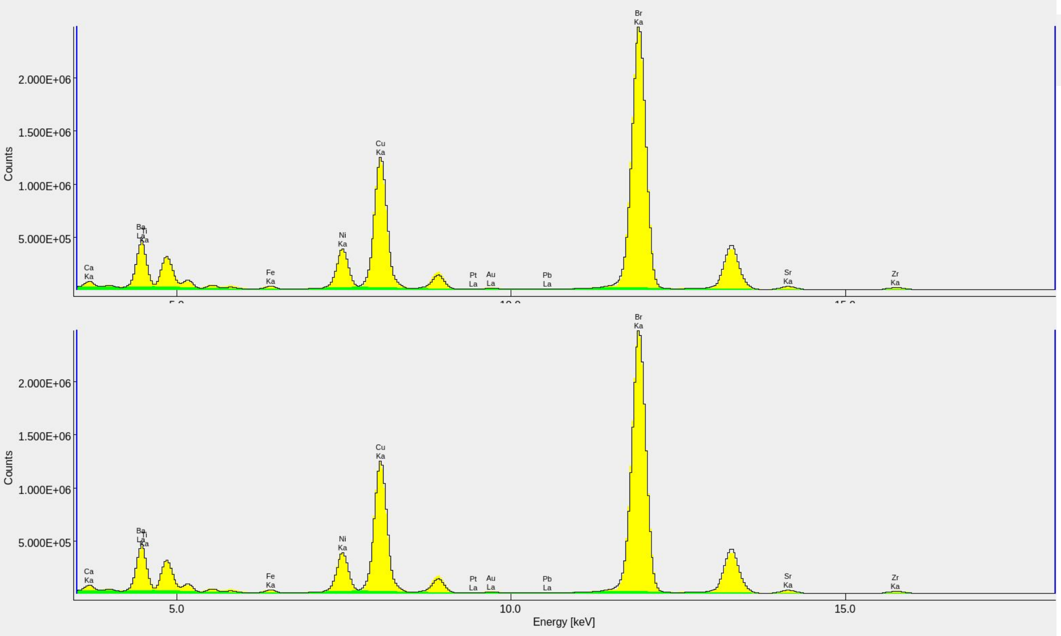
Elemental Map Reconstruction (Traditional way)

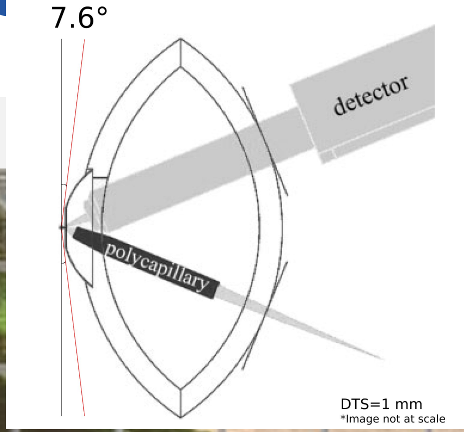


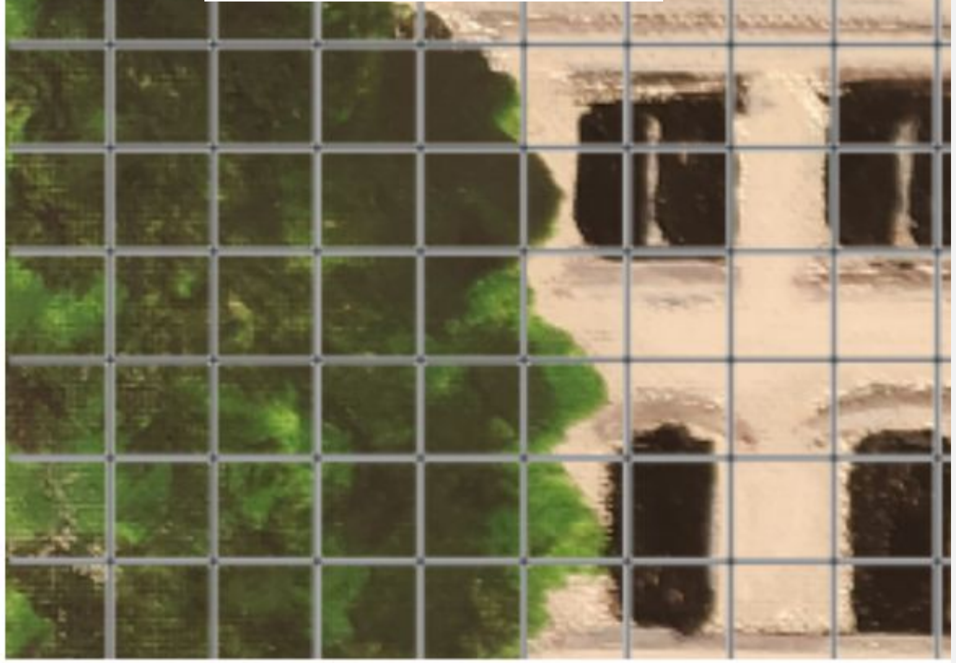


4. Store your spectrum and move to pixel 2.

Elemental Map Reconstruction (Traditional way)

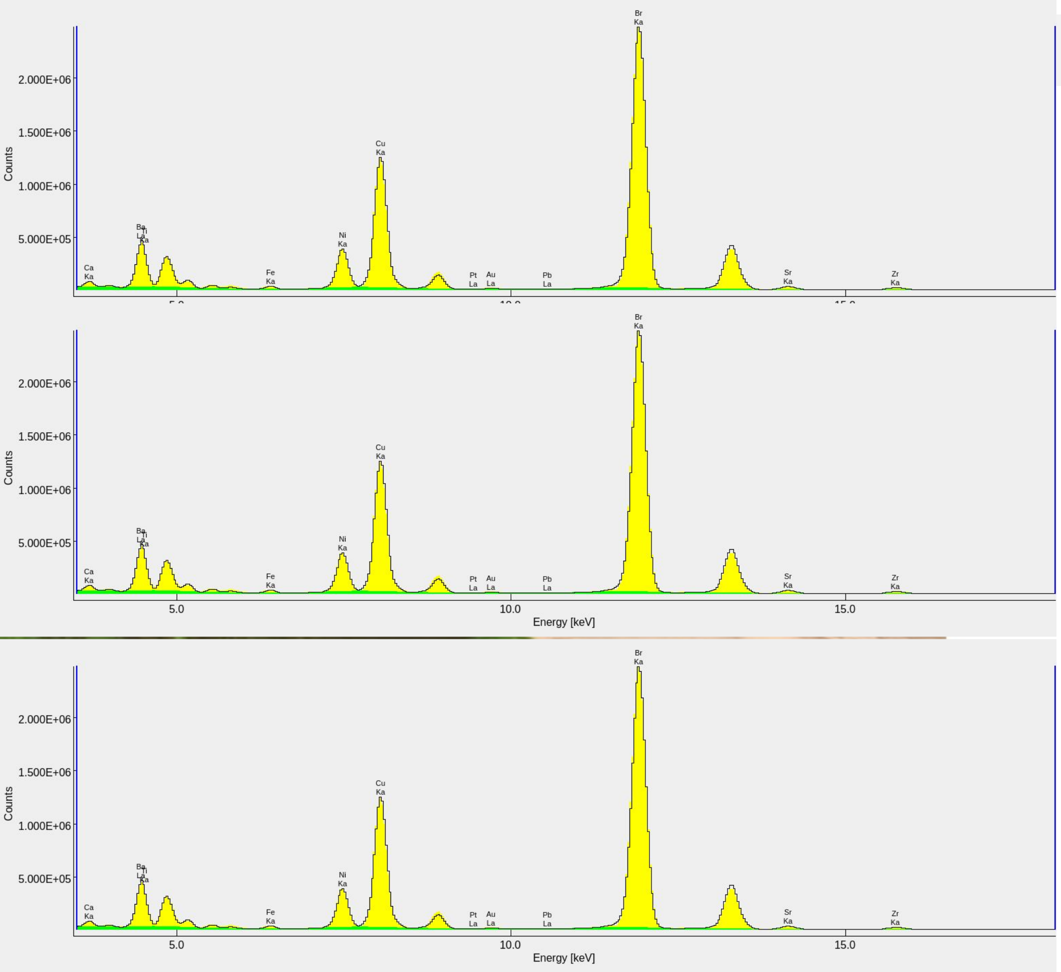


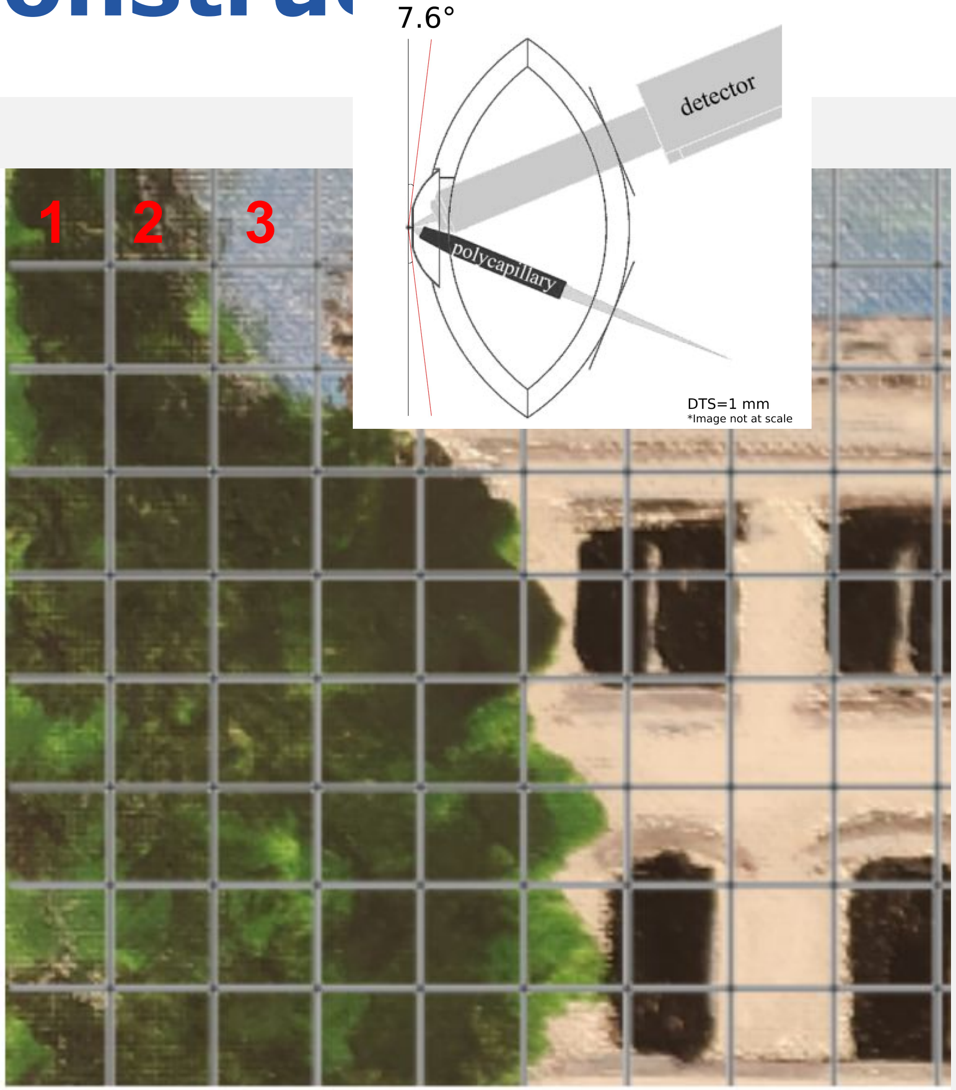




5. Repeat

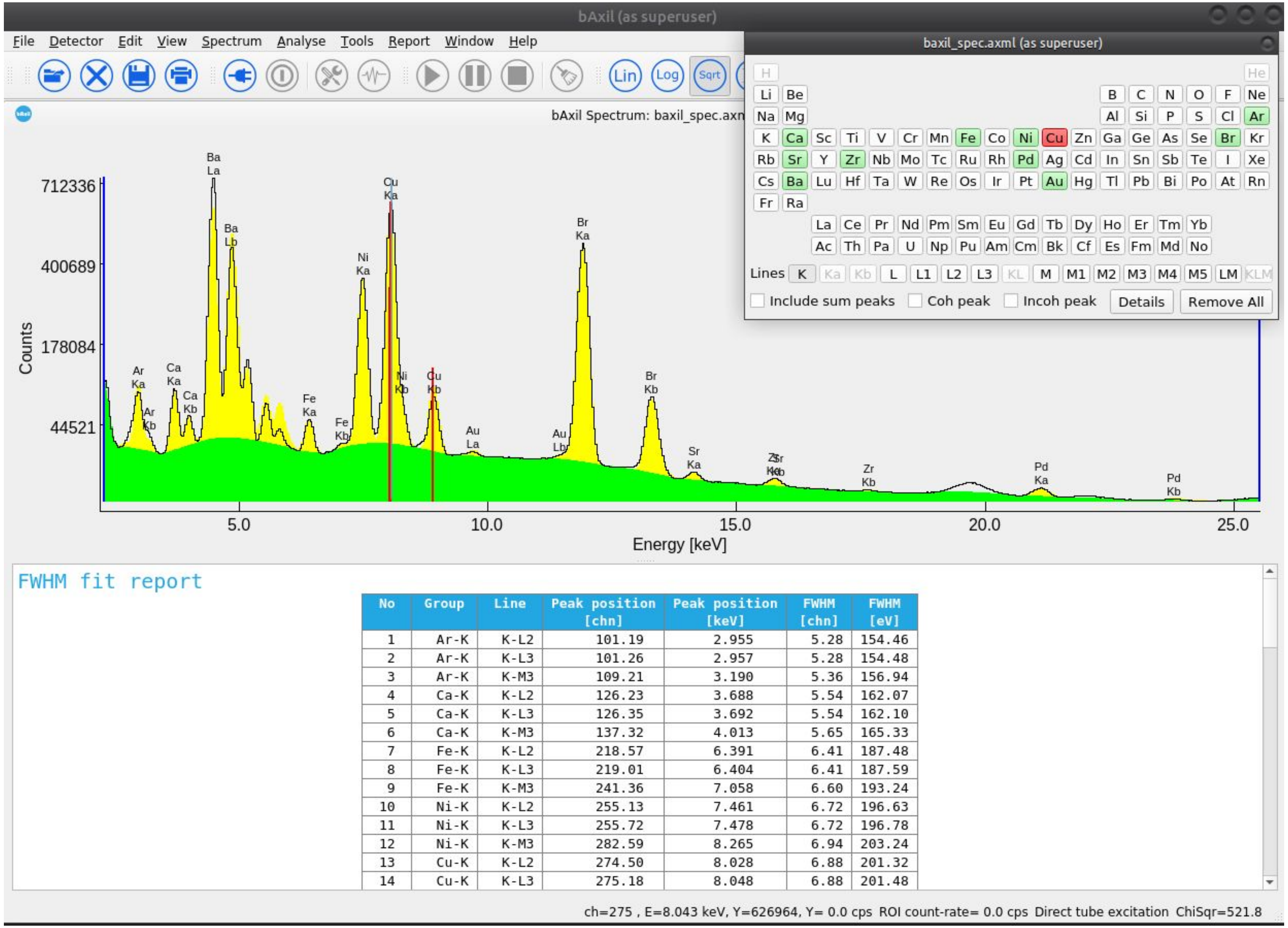
Elemental Map Reconstruction (Traditional way)





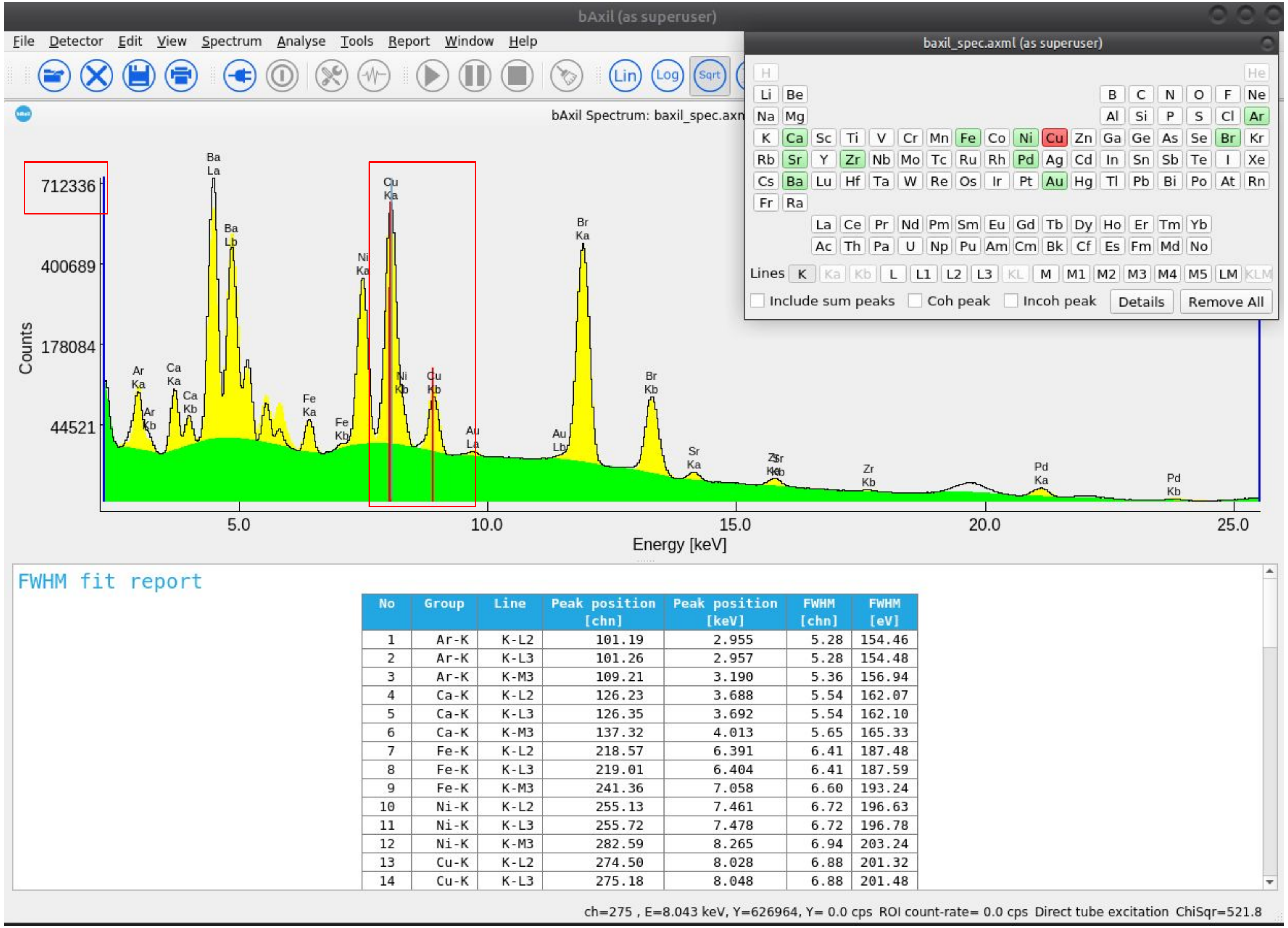
5. Repeat

Region-of-Interest (ROI) selection



No	Group	Line	Peak position [chn]	Peak position [keV]	FWHM [chn]	FWHM [eV]
1	Ar-K	K-L2	101.19	2.955	5.28	154.46
2	Ar-K	K-L3	101.26	2.957	5.28	154.48
3	Ar-K	K-M3	109.21	3.190	5.36	156.94
4	Ca-K	K-L2	126.23	3.688	5.54	162.07
5	Ca-K	K-L3	126.35	3.692	5.54	162.10
6	Ca-K	K-M3	137.32	4.013	5.65	165.33
7	Fe-K	K-L2	218.57	6.391	6.41	187.48
8	Fe-K	K-L3	219.01	6.404	6.41	187.59
9	Fe-K	K-M3	241.36	7.058	6.60	193.24
10	Ni-K	K-L2	255.13	7.461	6.72	196.63
11	Ni-K	K-L3	255.72	7.478	6.72	196.78
12	Ni-K	K-M3	282.59	8.265	6.94	203.24
13	Cu-K	K-L2	274.50	8.028	6.88	201.32
14	Cu-K	K-L3	275.18	8.048	6.88	201.48

Region-of-Interest (ROI) selection



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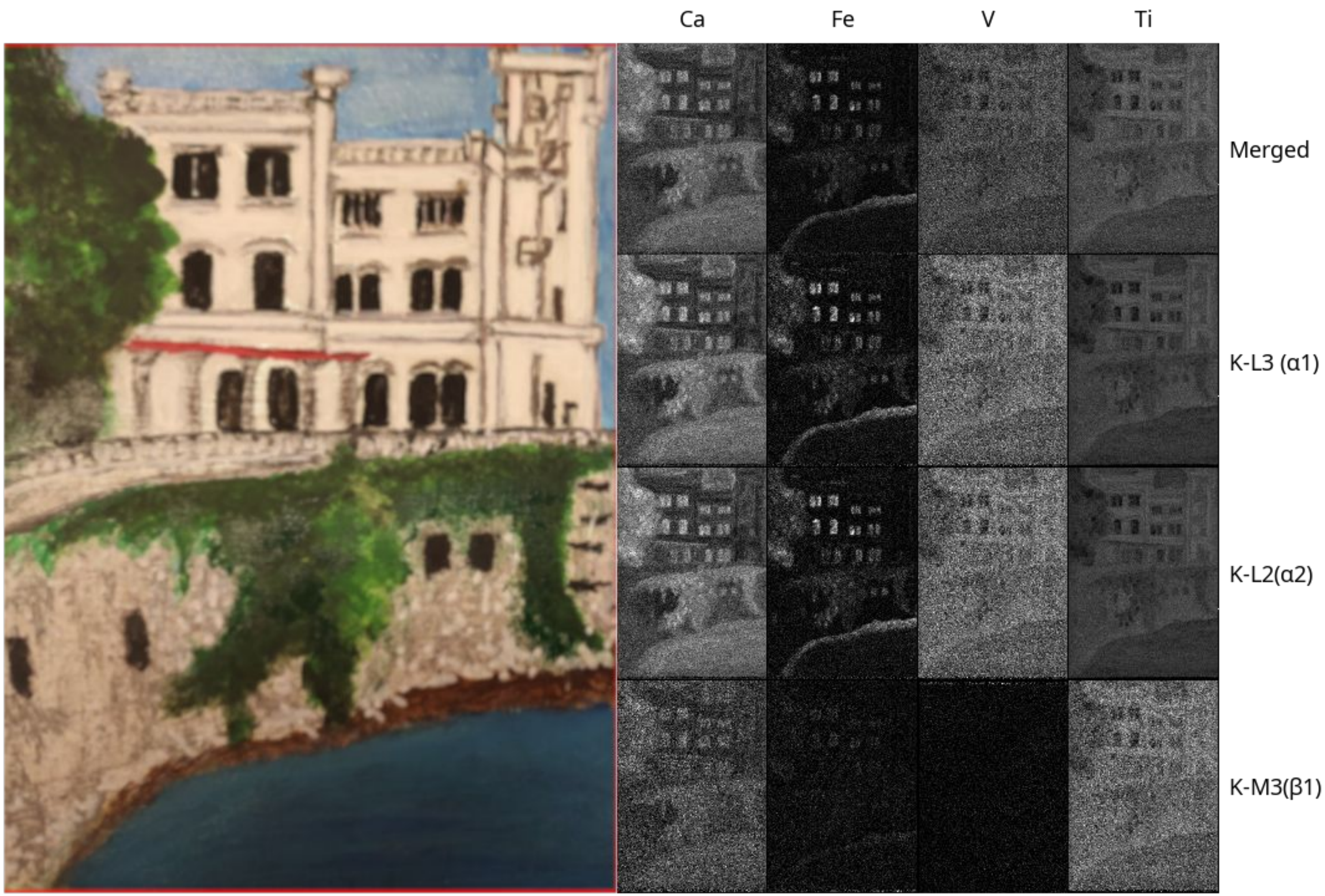
Ca
Fe
V
Ti
Merged
K-L3 (α1)
K-L2(α2)
K-M3(β1)

Elemental Map Reconstruction (Traditional way)

Pros:

- **Homogeneous time of scan**
- **Precise spatial resolution***
- **Reduced motion artifacts**
- **Accurate Quantitative Analysis**

Cons:

- **Long scanning time**
- **Large data files**
- **Spatial precision depends on mechanical system capabilities.**

Elemental Map Reconstruction (Traditional way)

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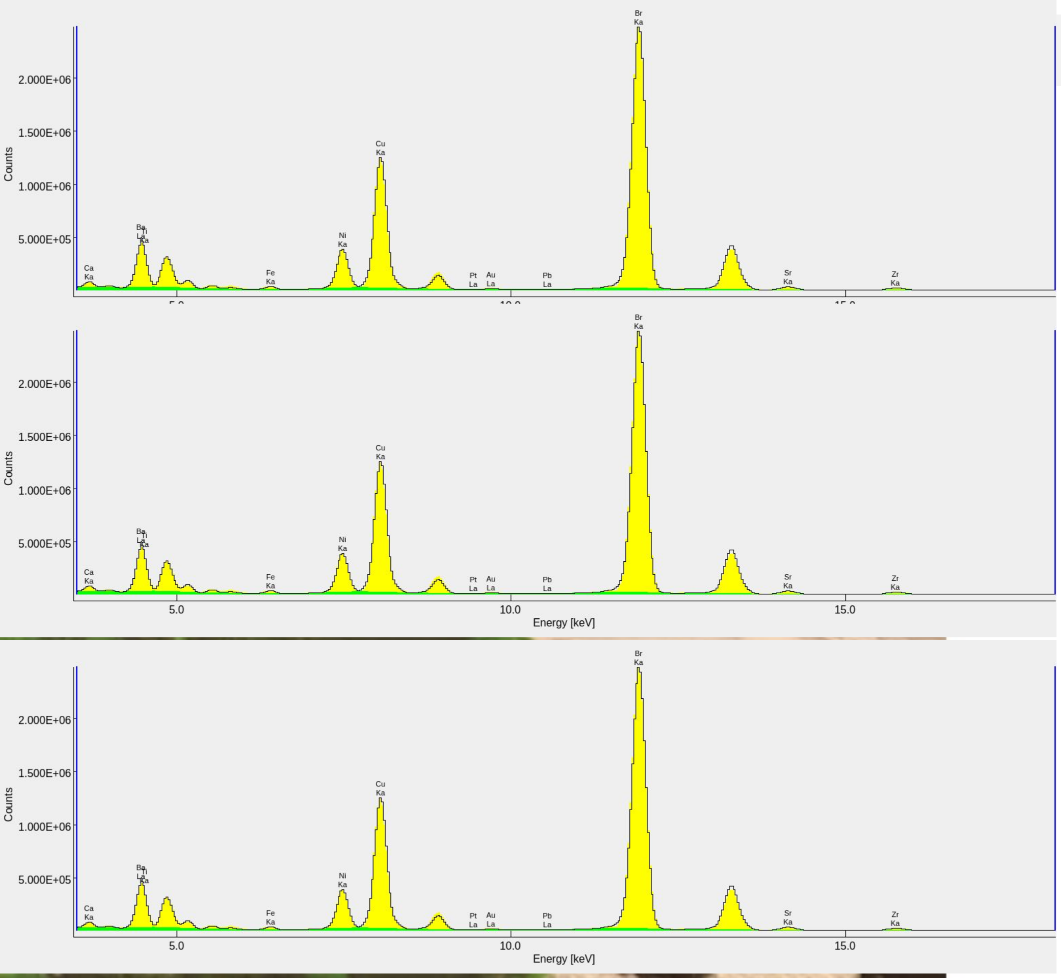
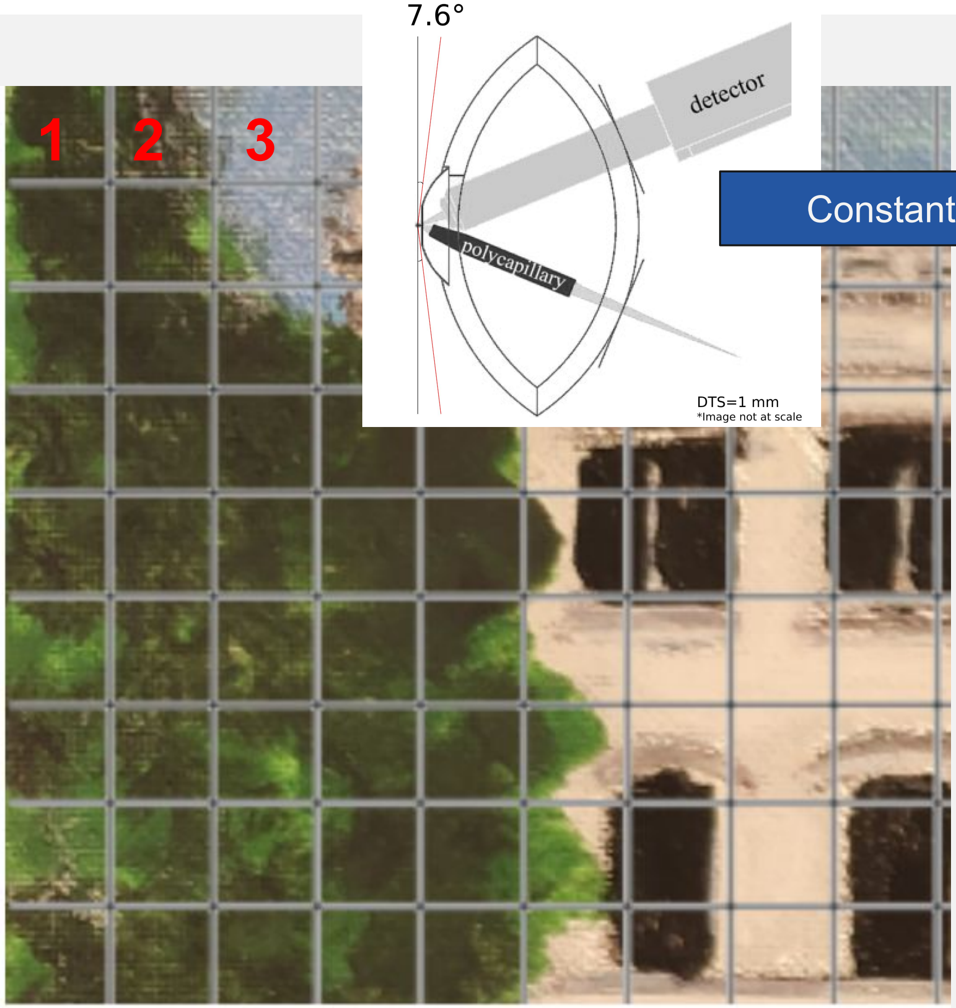
Cons:

- Long scanning time
- Large data files
- Spatial precision depends on mechanical system capabilities.
- Fixed Pixel Size

Elemental Map Reconstruction (Fly Scan)





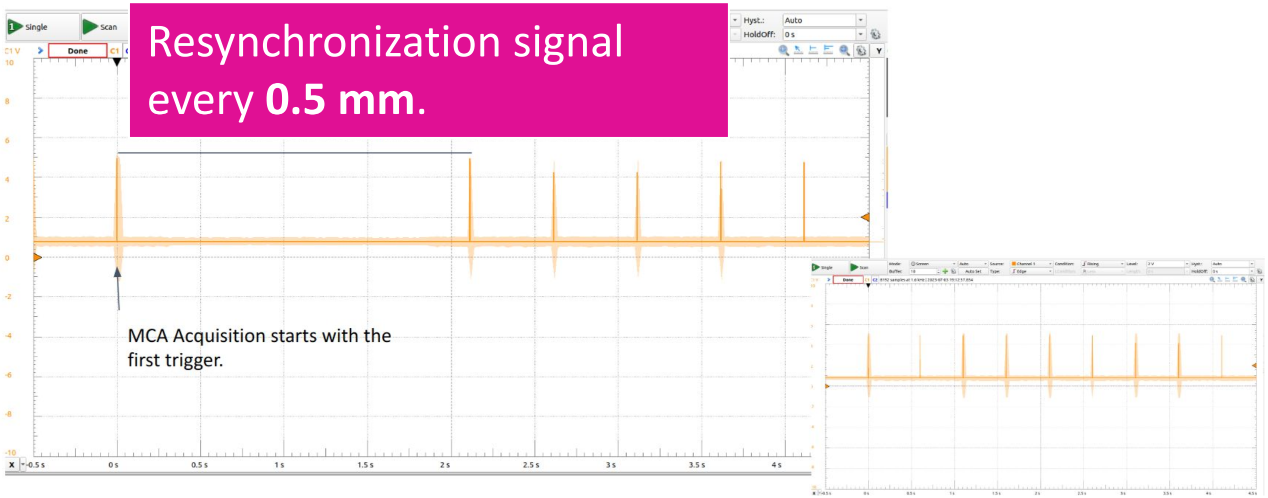
Constant V

5. Repeat

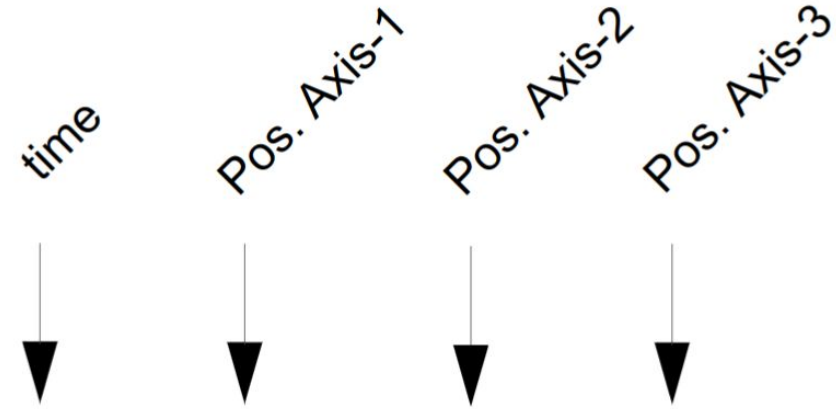
Single-photon mapping (SPM)

By interpolating each photon within each "tick" from the mechanical system, we can map every photon with a single x,y coordinate.

Resynchronization signal every **0.5 mm**.



Corvus XYZ: 250 µs tick



296149	9.749368	9.749368	0.000000
296151	9.749868	9.749868	0.000000
296153	9.750368	9.750368	0.000000
296155	9.750868	9.750868	0.000000
296157	9.751368	9.751368	0.000000
296159	9.751868	9.751868	0.000000
296161	9.752368	9.752368	0.000000
296163	9.752868	9.752868	0.000000
296165	9.753368	9.753368	0.000000
296167	9.753868	9.753868	0.000000

BS-Topaz-X: TLIST mode with 40 ns resolution

```
Start Acquisition
Energy Event: channel=1304, timestamp=0.00065724 sec
Energy Event: channel=1309, timestamp=0.0016572800000000001 sec
Energy Event: channel=255, timestamp=0.00165836 sec
Energy Event: channel=128, timestamp=0.0016602400000000001 sec
Energy Event: channel=1307, timestamp=0.0026571200000000002 sec
Energy Event: channel=58, timestamp=0.00266192 sec
Energy Event: channel=28, timestamp=0.00266344 sec
Energy Event: channel=1310, timestamp=0.00365716 sec
Energy Event: channel=1305, timestamp=0.0046572 sec
```

Elemental map reconstruction

Using a defined ROI and FWHM (bAxil)

Given:

- E_{ROI} the expected value of a Gaussian fitting of the ROI, and
- σ the standard deviation of the fit, and
- Δ_{ROI} as the full with half maximum of the Gaussian fit, defined by $\Delta_{ROI} = 2\sqrt{2\ln 2}\sigma$.

Defining reconstruction space and pixel size

And the reconstruction space given by:

- x_k, y_k and E_k for $k = 1, \ldots, N$ are the coordinates and energy of the acquired photons.
- $\min_x$, $\min_y$, $\max_x$, $\max_y$ the minimum and maximum values of the x and y coordinates.
- *voxel_size* the voxel size selected by the user.

The photons corresponding to the selected ROI will be accumulated in an energy grid $E(i,j)$ and normalized by the total number of photons on the voxel accumulated in a Counter Grid $C(i,j)$, both with W and H dimmensions given by:

$$W = \left\lceil \frac{\max_x - \min_x}{\text{voxel\_size}} \right\rceil \qquad E(i,j) = 0 \quad \forall i,j$$

$$H = \left\lceil \frac{\max_y - \min_y}{\text{voxel\_size}} \right\rceil \qquad C(i,j) = 0 \quad \forall i,j$$

Converting coordinates into voxels

For each point (x_k, y_k, E_k) corresponds a voxel pair of coordinates v_x and v_y given by:

$$v_x = \left\lceil \frac{x_k - \min_x}{\text{voxel\_size}} \right\rceil \qquad v_y = \left\lceil \frac{y_k - \min_y}{\text{voxel\_size}} \right\rceil$$

Single-photon mapping

Elemental map reconstruction

If $0 \leq v_x < W$ and $0 \leq v_y < H$:

Accumulating for counting grid and energy grid

$$C(v_x, v_y) = C(v_x, v_y) + 1$$

and in similar way for the energy: $E_{ROI} - \Delta_{ROI} \leq E_k \leq E_{ROI} + \Delta_{ROI}$:

$$E(v_x, v_y) = E(v_x, v_y) + 1$$

For counter grid $C(i,j)$:

C(i,j)

$$C(i,j) = \sum_{k=1}^{N} \delta_{i,v_x} \cdot \delta_{j,v_y}$$

where δ is the Kronecker delta function. In a similar the energy grid $E(i,j)$ for each ROI can be defined by:

E(i,j)

$$E(i,j) = \sum_{k=1}^{N} \delta_{i,v_x} \cdot \delta_{j,v_y} \cdot \delta_E$$

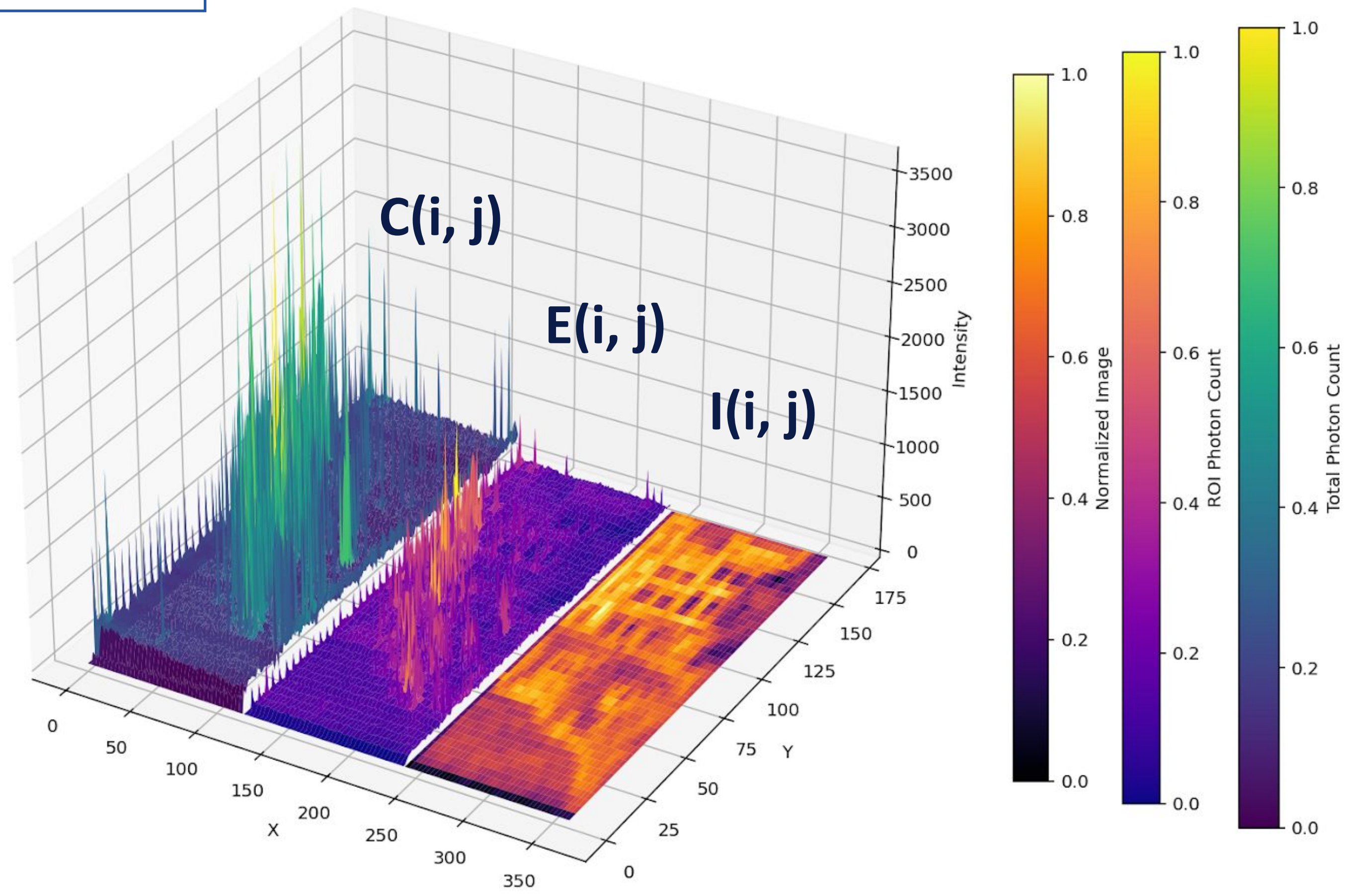
where

$$\delta_E = \begin{cases} 1 & \text{if } (E_{ROI} - \Delta_{ROI}) \leq E_k \leq (E_{ROI} + \Delta_{ROI}) \\ 0 & \text{otherwise} \end{cases}$$

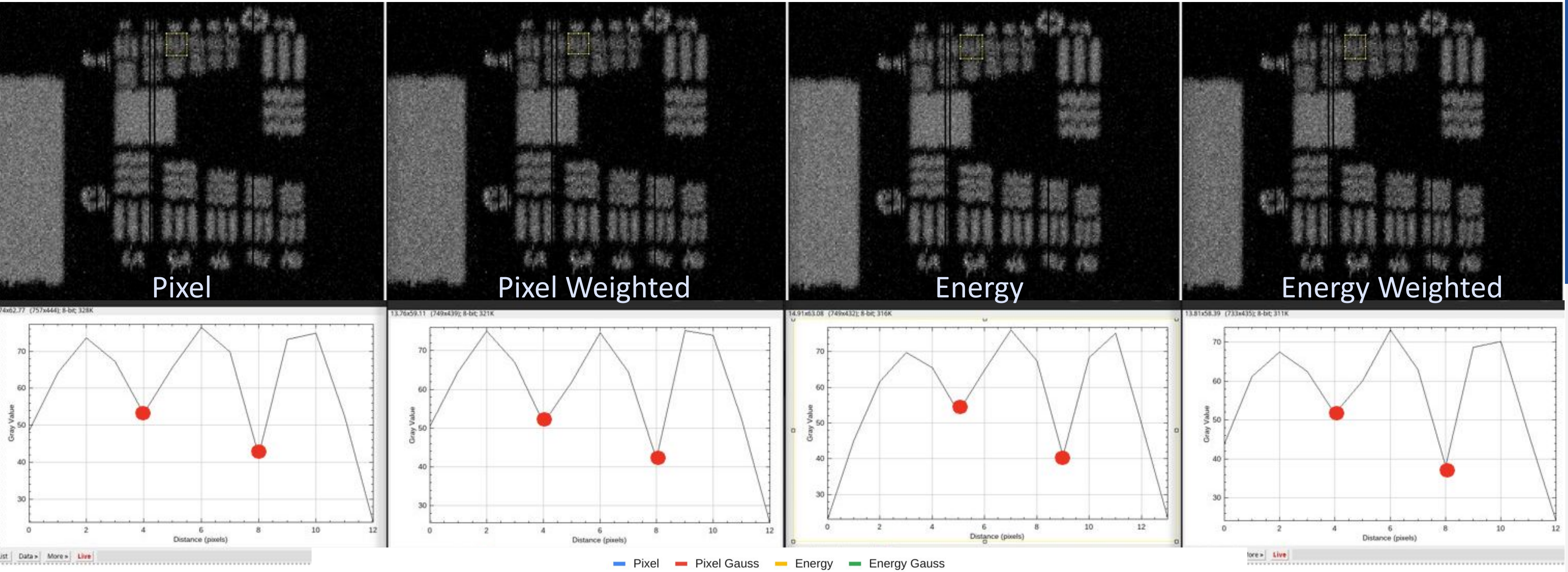
The output image for each ROI I is the ratio of E to C and is given by

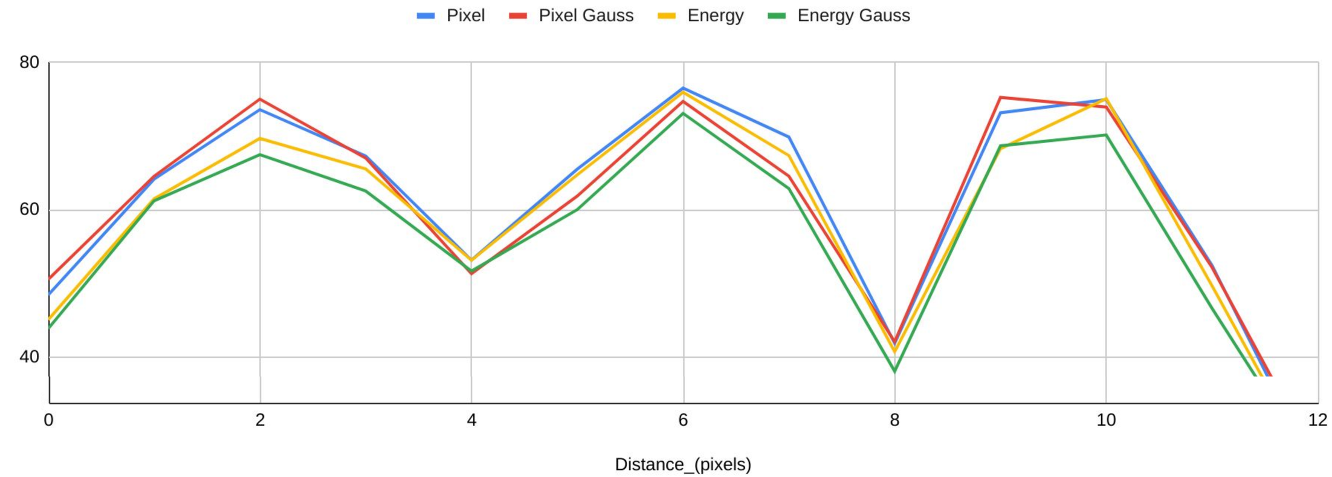
I(i,j)

$$I(i,j) = \frac{E(i,j)}{C(i,j)} \quad \forall i \quad \forall j$$



Weighted elemental map reconstruction





Single-photon mapping

Different elemental map resolutions

(a) 0.2 mm/pixel

(b) 0.5 mm/pixel

(c) 1 mm/pixel

FIGURE 11 Size comparison of image reconstruction with different pixel sizes (all scaled at 0.25 of real size). Velocity: 7 mm/s, Y-step: 0.25 mm. Element: Titanium.

Scan Characteristics:

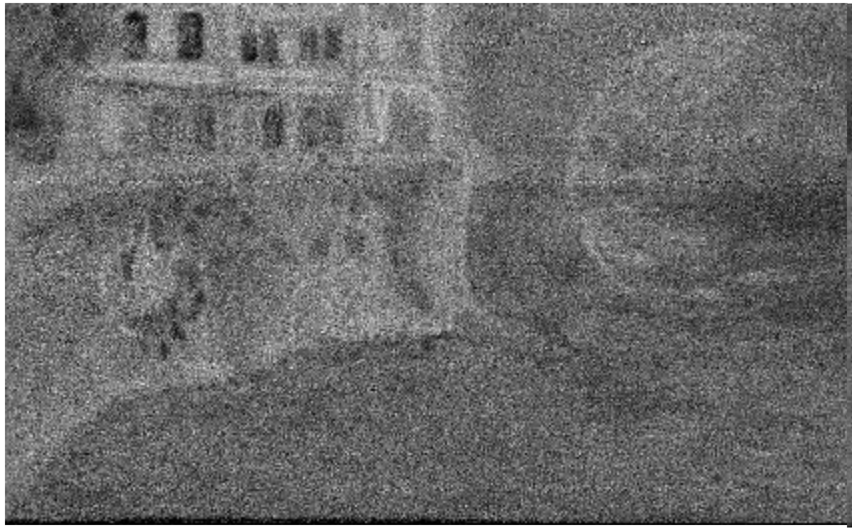
Velocity: 7 mm/s

Acceleration: 10 mm/s^2

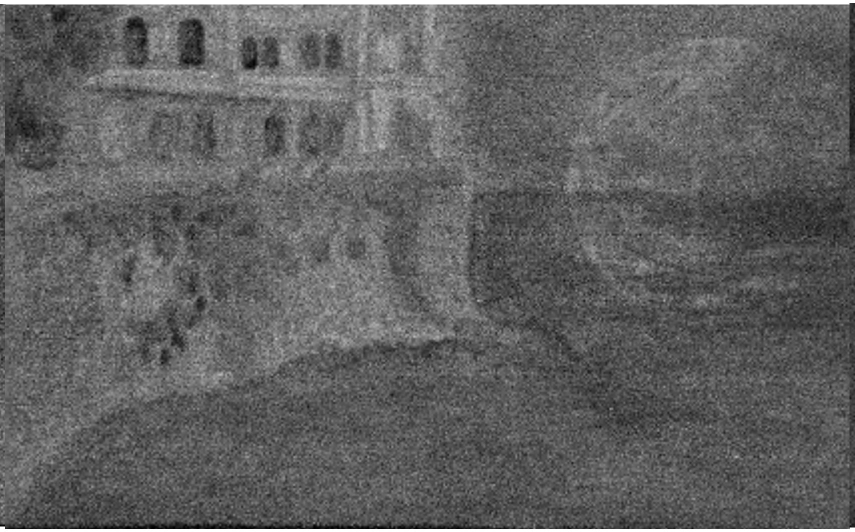
YStep Size: 0.25 mm

Element: Titanium

Tests of different scan velocities



5 mm/s (8 h)



7 mm/s (5.93 h)

8 mm/s (5.1 h)

Scan Characteristics:

Painting Size: 220x170 mm

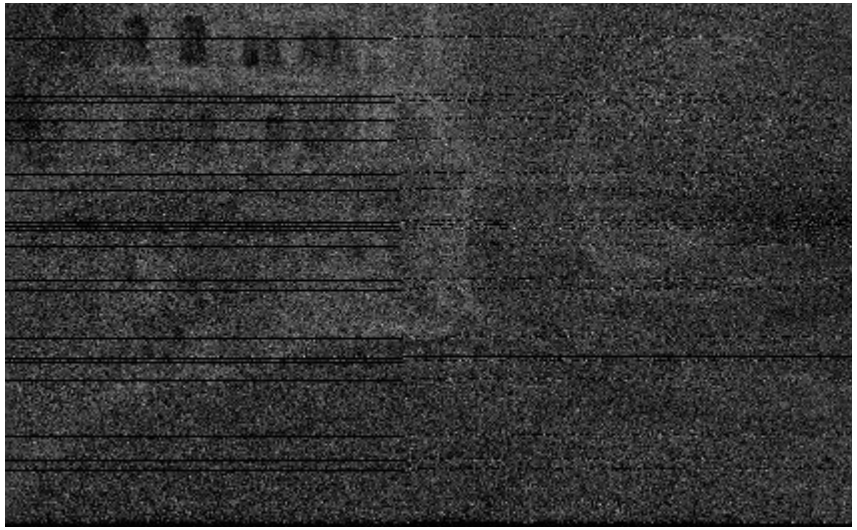
Acceleration: 10 mm/s^2

YStep Size: 0.25 mm

Scan Sweep: Zig-zag

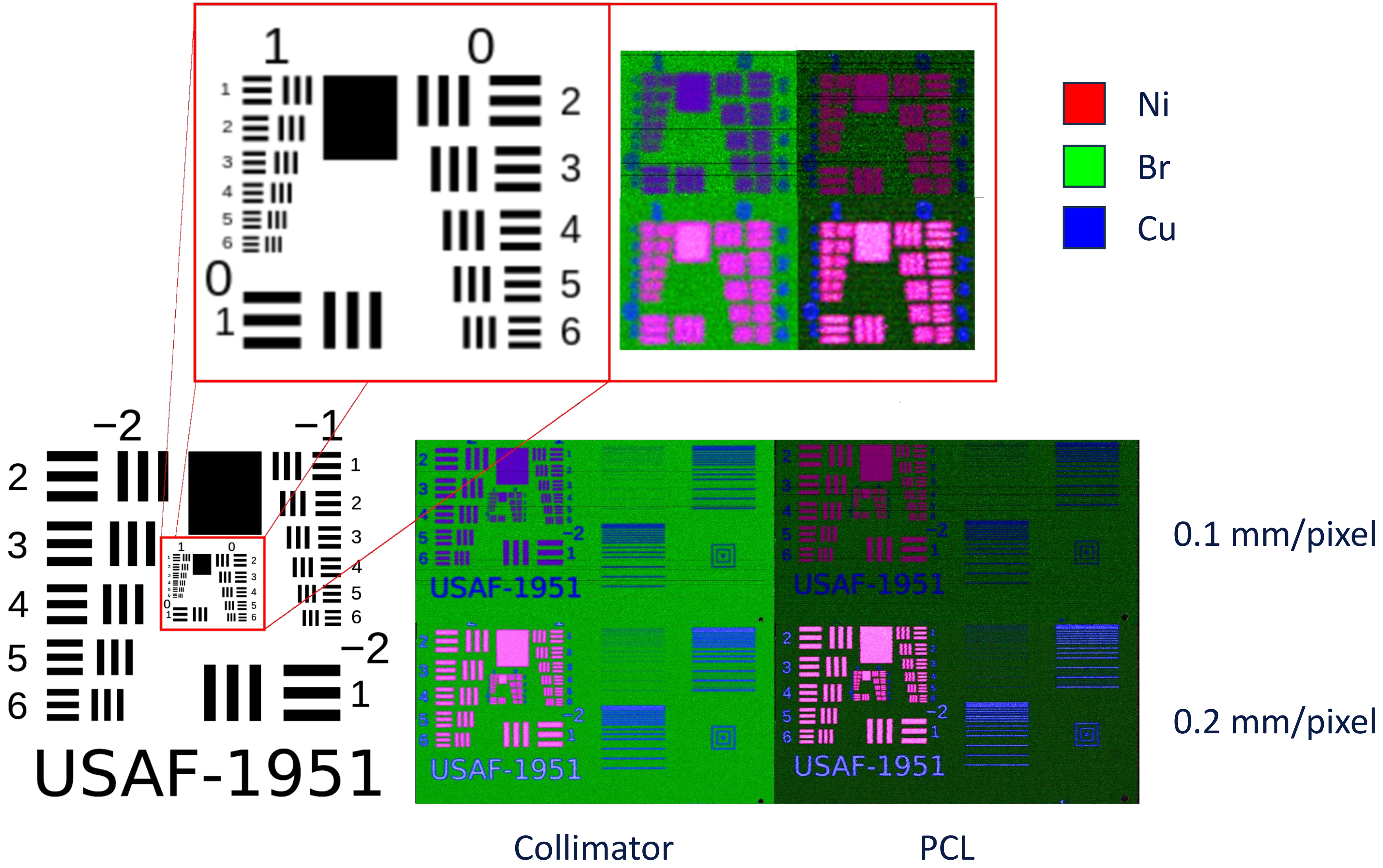
Pixel Size: 0.5x0.5 mm

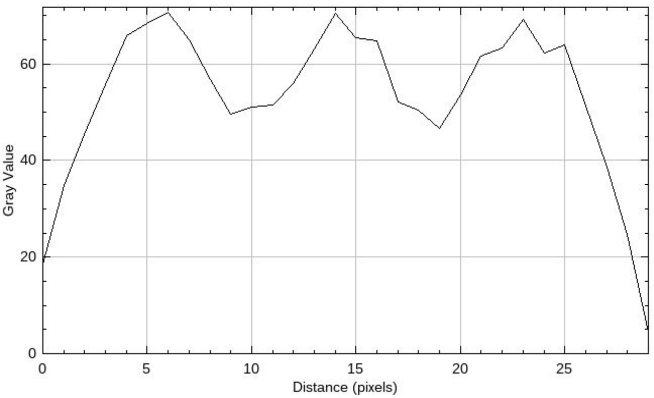
Element: Titanium



10 mm/s (4.15 h)

Different elemental map resolutions

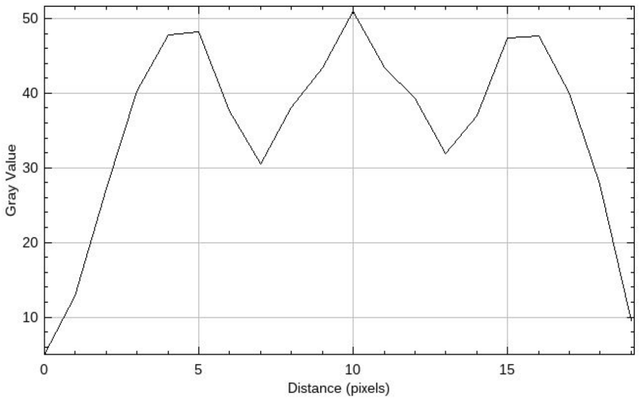


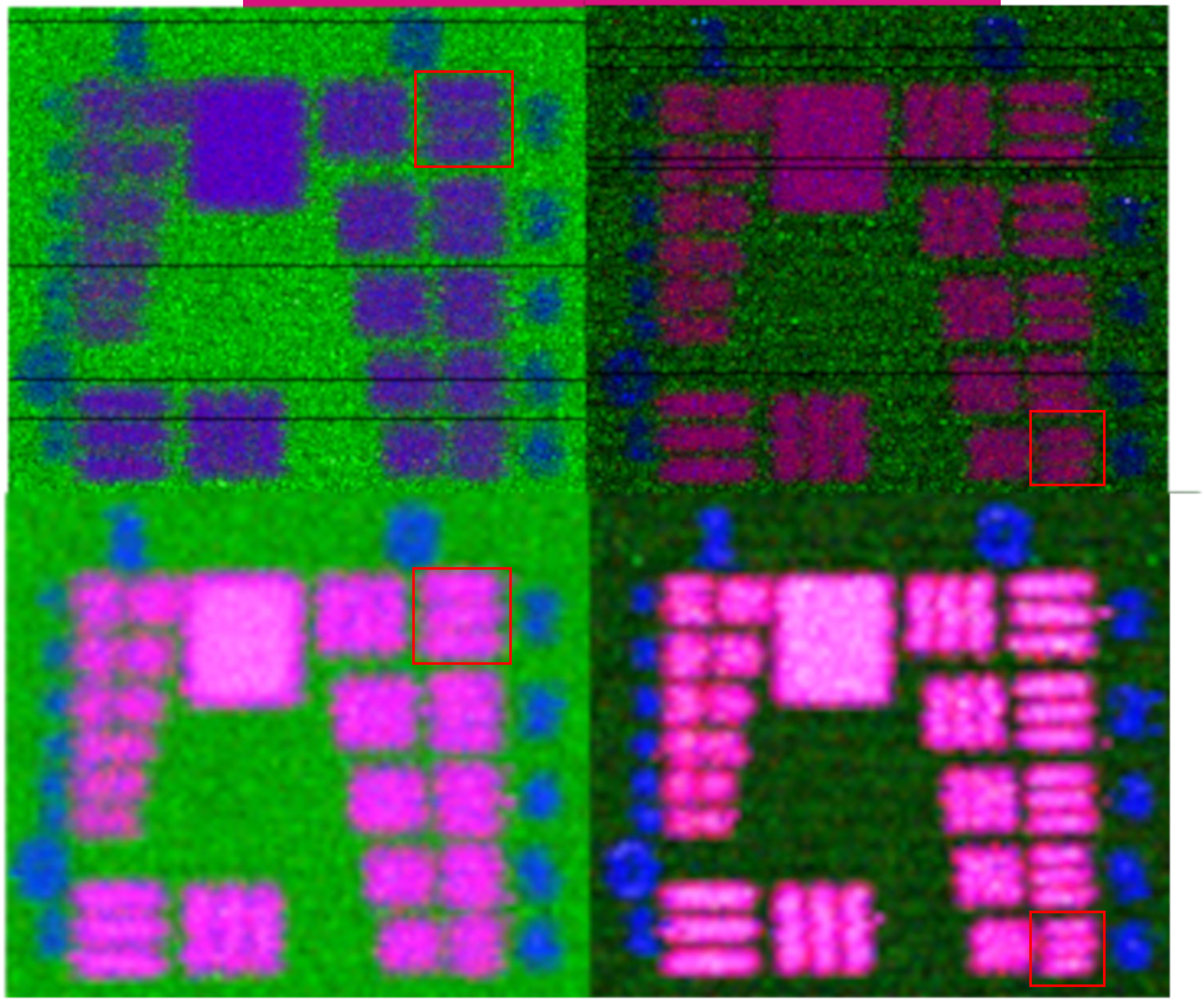


Scan Velocity: 5 mm/s

Max Col. Resolution 1 lp/mm

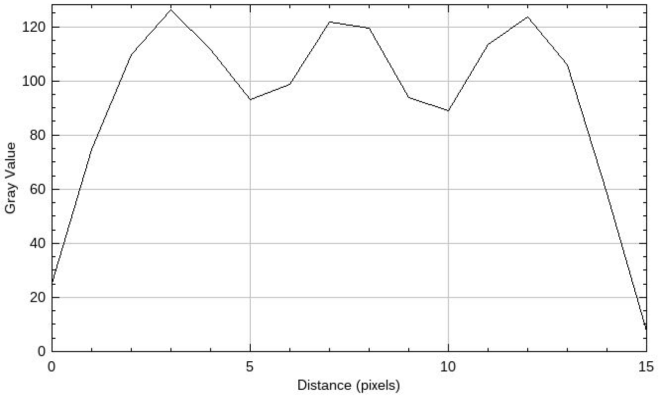
Max PCL. Resolution 1.78 lp/mm





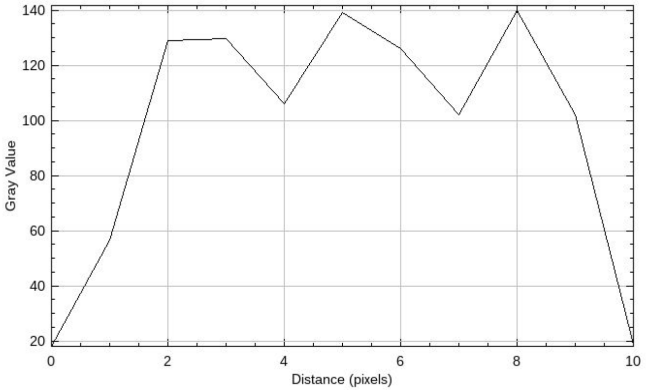
0.1 mm/pixel

0.2 mm/pixel



Collimator

PCL



Data storage compression

Format	Bytes/photon	Reference File (~34M ph.)	Compression ratio
Spectra (bAxil txt)	119	4.0 GB	1x
CSV	62	2.1 GB	1.9x
HDF5	40	1.4 GB	2.9x
CSV compressed (zip)	17	601 MB	6.7x
HDF5 Compressed (zip)	22	**745.5 MB**	**5.4x**
LAS	50	1.7 GB	2.4x
LAZ	**6.74**	**229.1 MB**	**17.5x**

Size comparison of different file storage formats

X-RAY SPECTROMETRY

RESEARCH ARTICLE

MA-XRF Scanner: Implementation of Elemental Maps Reconstruction Algorithm Based on Single Photon Detection for Cultural Heritage Studies

Luis Guillermo García Ordóñez, Crespo Maria Liz, Andres Cicuttin, Ivan Rene Morales Argueta, Romina Molina, Sergio Carrato, Piet Van Espen, Paolo Romano, Alessandro Migliori ... See all authors

First published: 02 June 2025 | https://doi-org.ezproxy.cern.ch/10.1002/xrs.3496

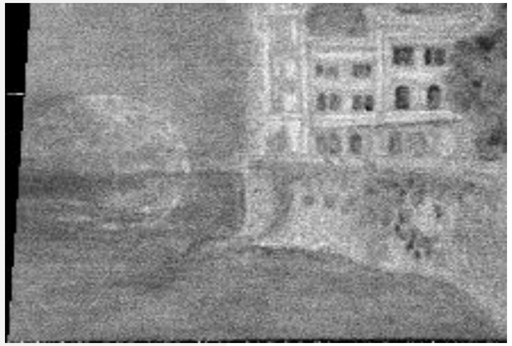
Funding: The authors received no specific funding for this work.

Preliminary Scans

First elemental analysis reconstruction
Painting Size: 220x170 mm

Ca

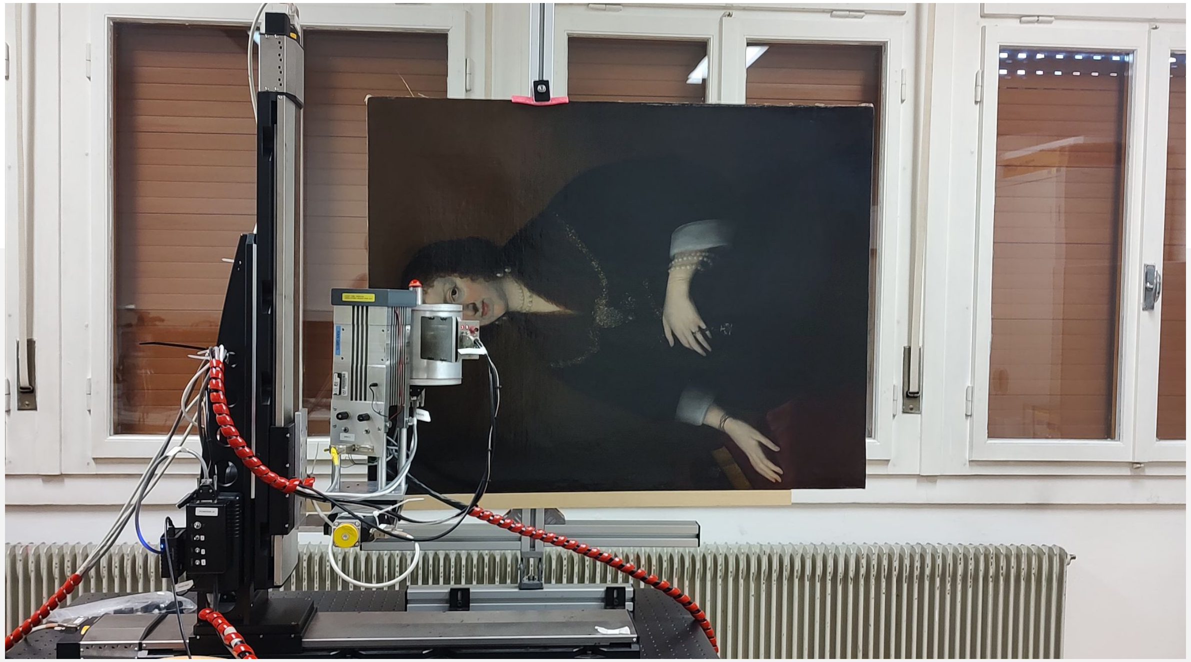
Fe

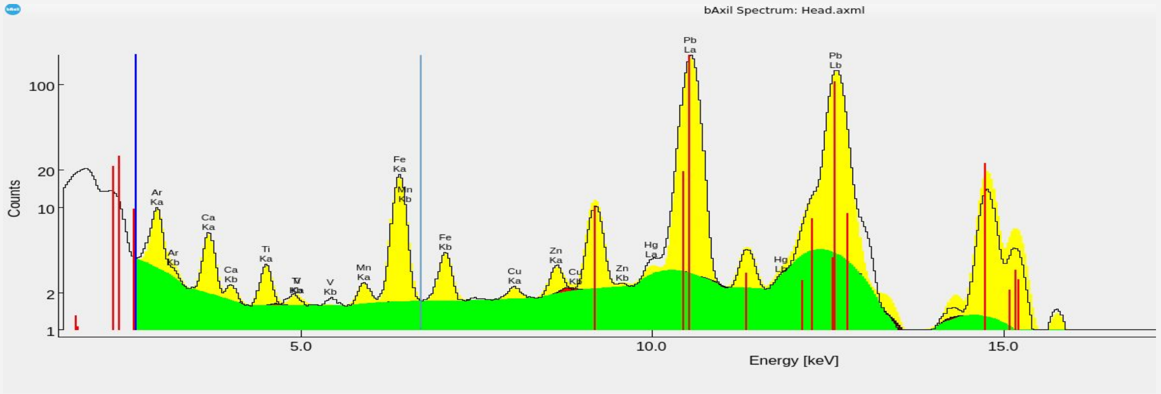


Ti

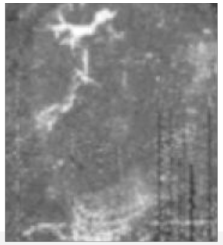
Cu

Collaboration with Elettra Synchrotron: XVIII Century Painting



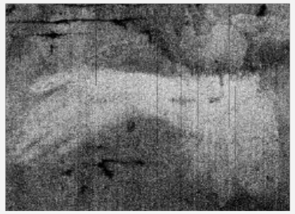


Ti-Ca



Fe

Pb



Painting Scan in collaboration with Elettra

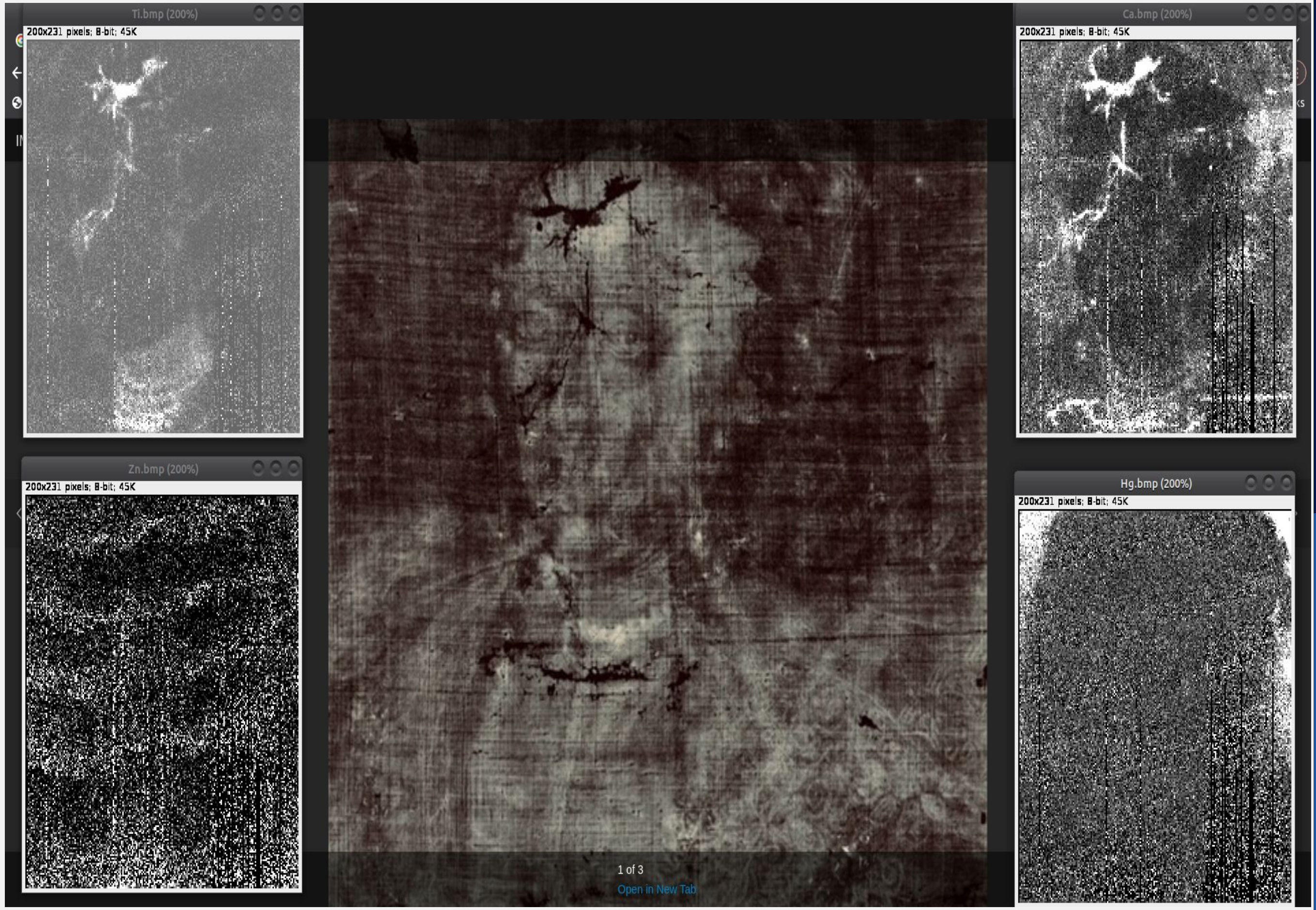
Elemental composition analysis (ongoing)

Ca

Fe

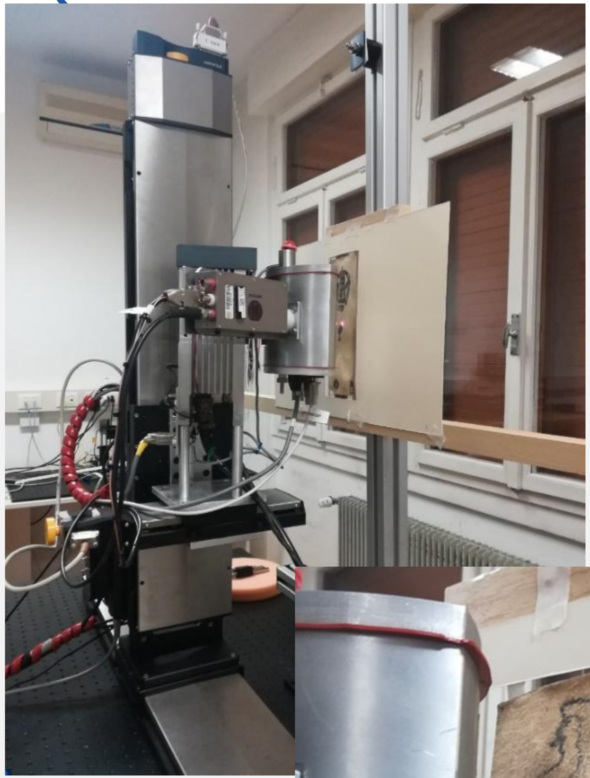
Ti

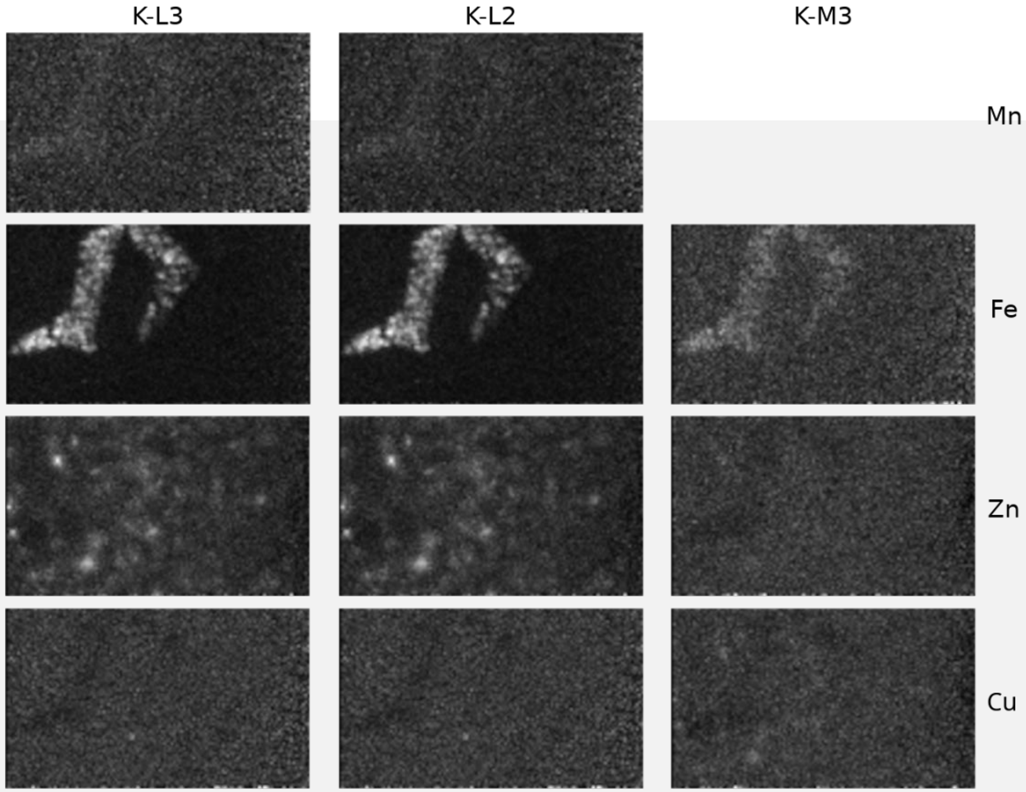
Pb

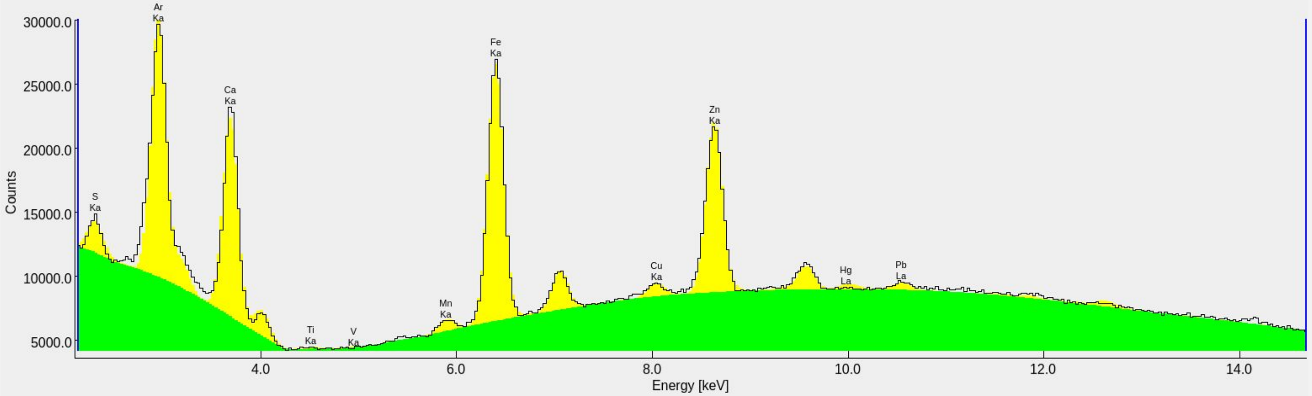


Tattooed human skin case study

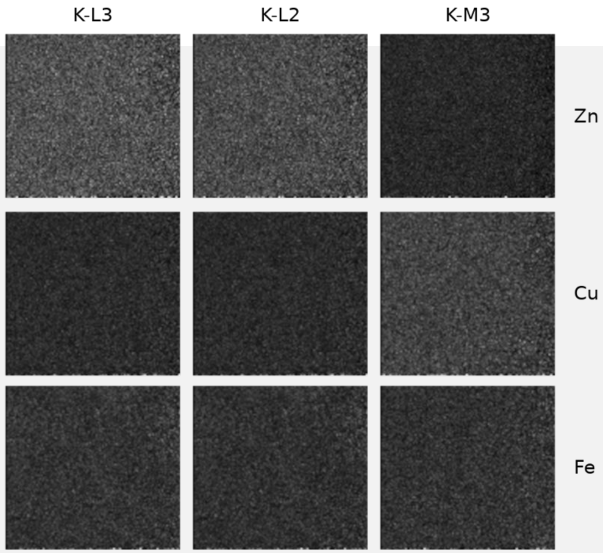
(Late 1800's – early 1900's)

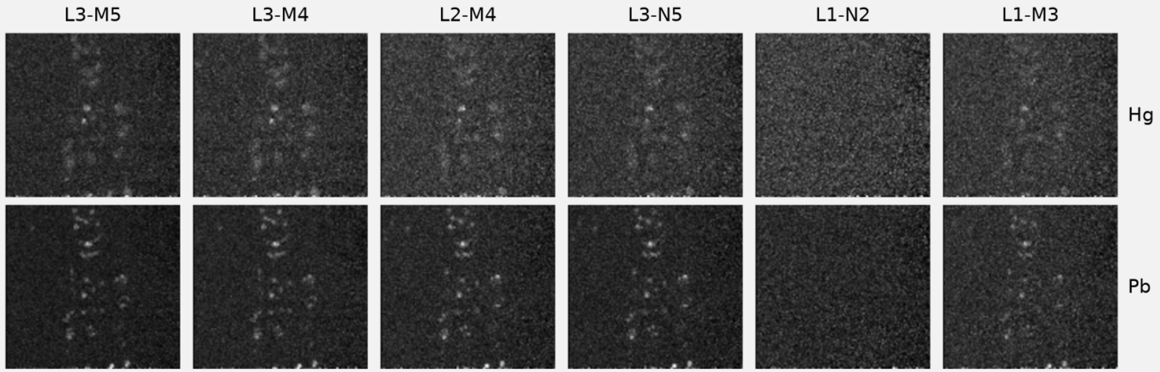


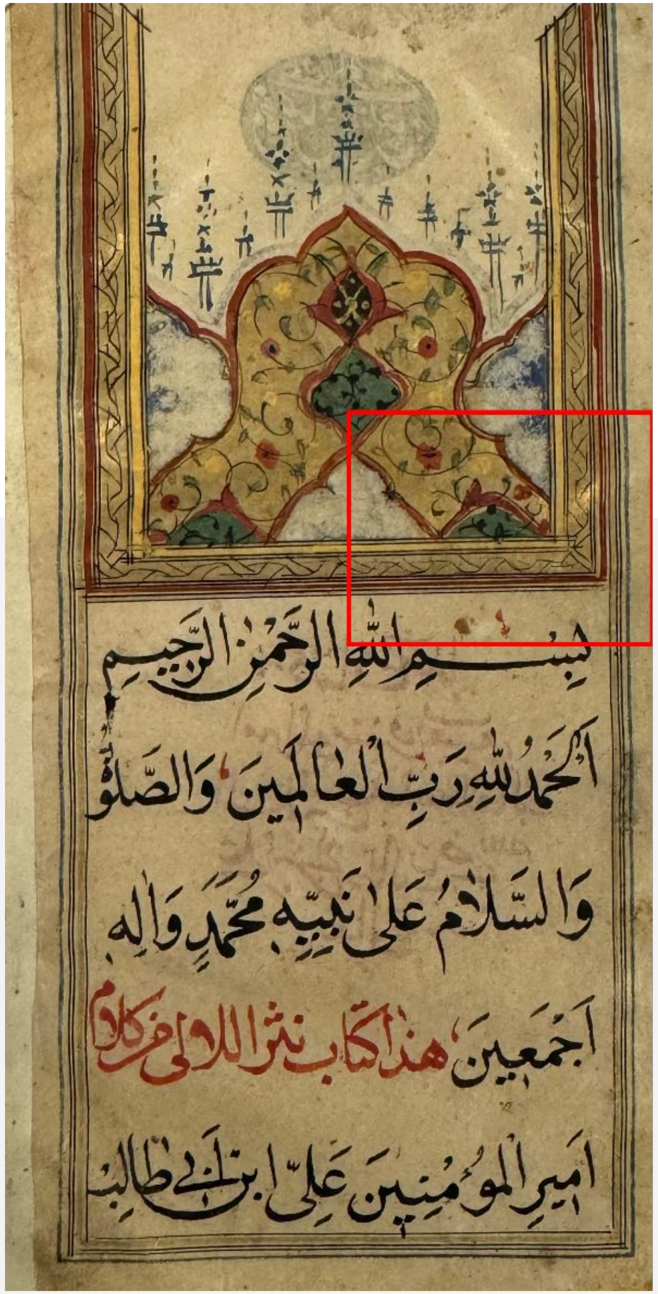


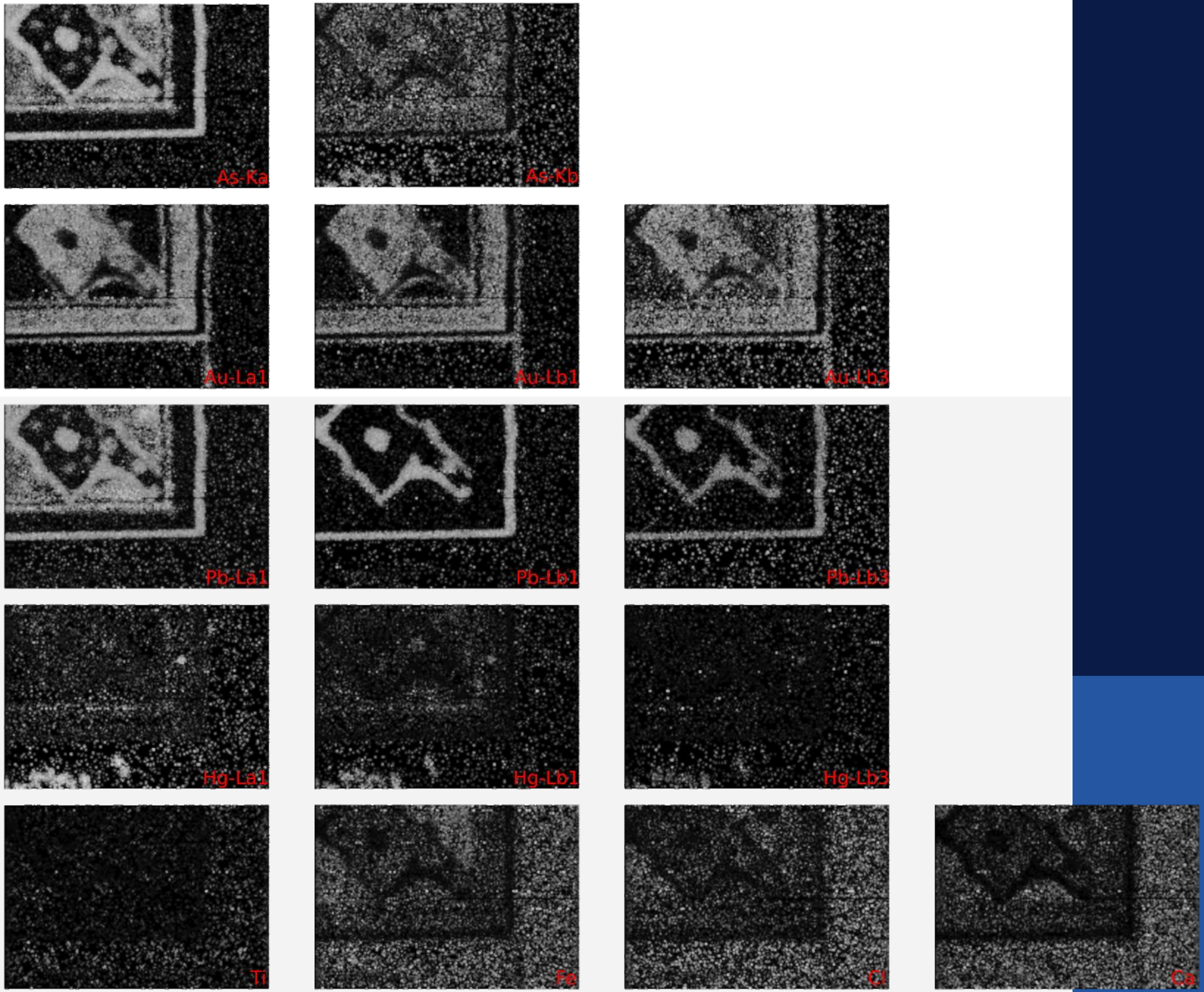


Tattooed human skin case study






بسم الله الرحمن الرحيم
الحمد لله رب العالمين والصلوة
والسلام على نبيه محمد واله
اجمعين هذا كتاب نثر اللالى من كلام
امير المومنين علي ابن ابي طالب


As-Ka
As-Kb
Au-La1
Au-Lb1
Au-Lb3
Pb-La1
Pb-Lb1
Pb-Lb3
Hg-La1
Hg-Lb1
Hg-Lb3
Ti
Fe
Cl
Ca

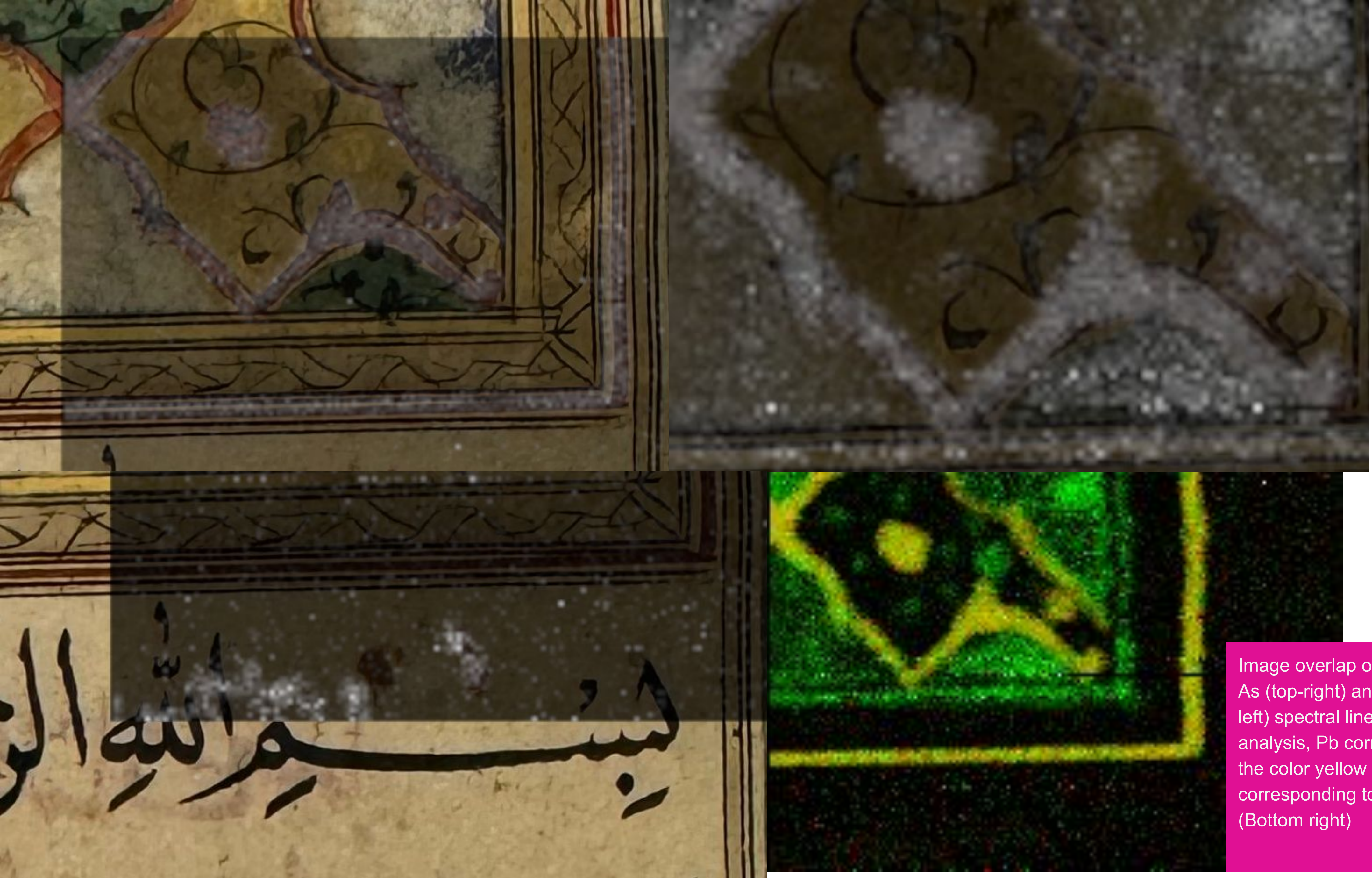


Image overlap on Pb (top-left), As (top-right) and Hg (bottom left) spectral lines. Pb-La analysis, Pb corresponding to the color yellow and As corresponding to green. (Bottom right)

Summary

The ICTP-IAEA MA-XRF Scanner enabled with the single-photon mapping features:

- **Automatic DTS adjustment** and high replicability of the positioning system to facilitate close-distance scanning, resulting in **higher photon collection rates**.
- A complete MA-XRF scan can be performed using the **PCL at the same speed as with the collimator**.
- **Custom scan polygon**, allowing for different scan velocities in specific areas of interest.
- The **single-photon mapping** algorithm reconstructs elemental maps at **custom pixel resolutions**.
- Efficient storage with the **HDF5 compressed** format, allowing to handle different scan polygons with **compression rate higher than 5x**.

Thank you!

Backup slides

Future works

- Weighted elemental map reconstruction algorithm for noise reduction (ongoing).
- Optimization on reconstruction software tools to reduce computational time.
- Correlation between optical image and elemental maps.
- Graphical User Interface.

Weighted elemental map reconstruction

Alternatively δ_E can include a weight function $w(x)$ (e.g. Gaussian):

$$w(x) = \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

if:

- μ is the peak (mean) value corresponding to E_{ROI},
- σ is the standard deviation, calculated from the Full-Width Half Maximum (FWHM) using:

$$\sigma = \frac{\text{FWHM}}{2\sqrt{2\ln(2)}}$$

Substituting the parameters $\mu = E_{ROI}$ (peak), FWHM $= \Delta_{ROI}$, and $x = E_k$, the weight function becomes:

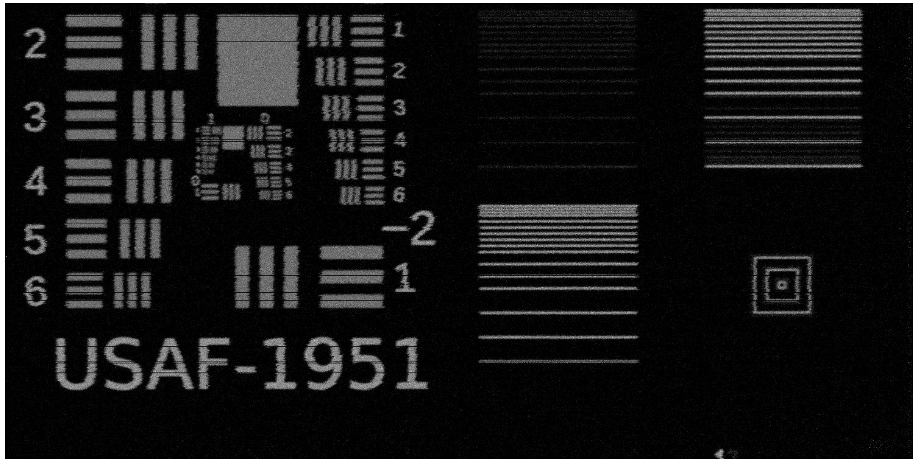
$$w(k) = \exp\left(-\frac{(E_k - E_{ROI})^2}{2\left(\frac{\Delta_{ROI}}{2\sqrt{2\ln(2)}}\right)^2}\right)$$

Hence:

$$\delta_E = \begin{cases} w(k) & \text{if } (E_{ROI} - \Delta_{ROI}) \leq E_k \leq (E_{ROI} + \Delta_{ROI}) \\ 0 & \text{otherwise} \end{cases}$$

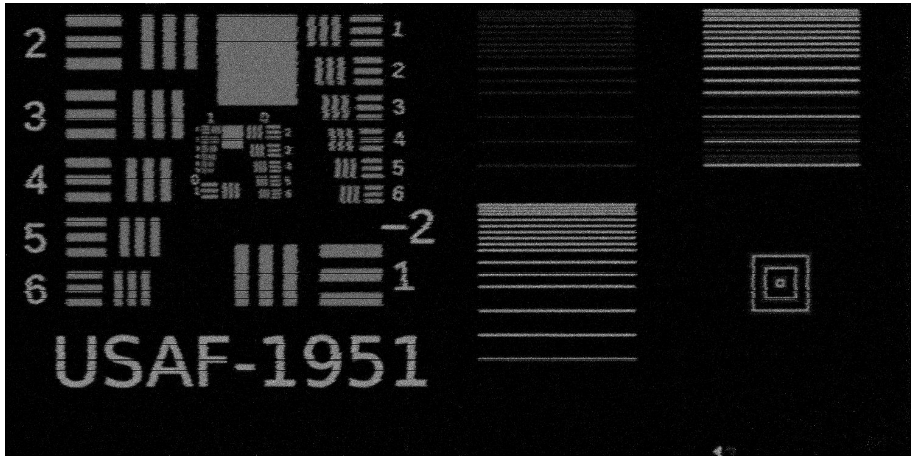
Pixel

$$\delta_E = \begin{cases} 1 & \text{if } (E_{ROI} - \Delta_{ROI}) \leq E_k \leq (E_{ROI} + \Delta_{ROI}) \\ 0 & \text{otherwise} \end{cases}$$



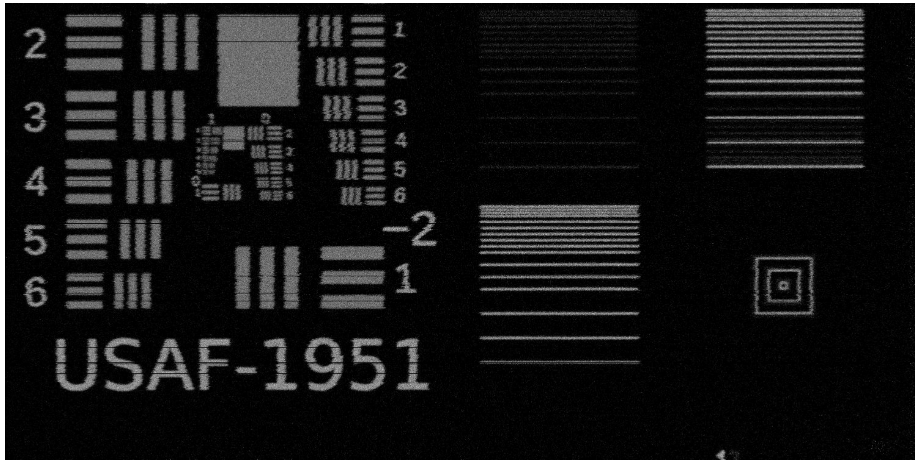
Pixel Weighted

$$\delta_E = \begin{cases} w(k) & \text{if } (E_{ROI} - \Delta_{ROI}) \leq E_k \leq (E_{ROI} + \Delta_{ROI}) \\ 0 & \text{otherwise} \end{cases}$$



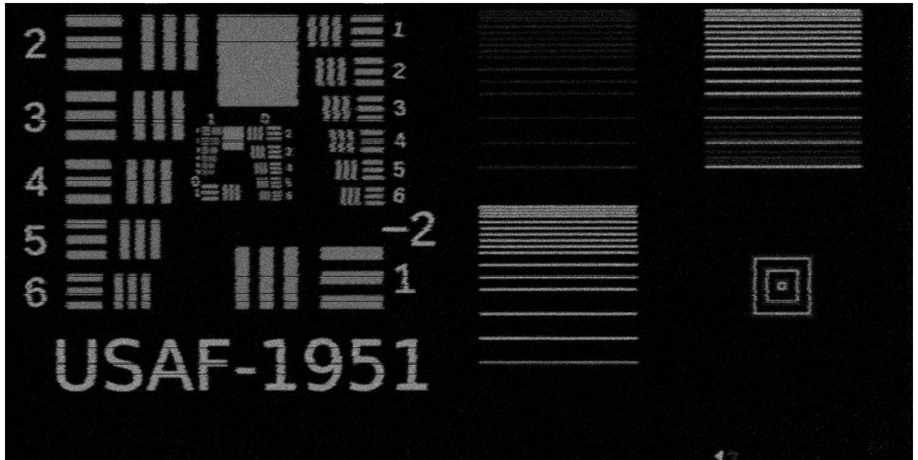
Energy

$$\delta_E = \begin{cases} E_k & \text{if } (E_{ROI} - \Delta_{ROI}) \leq E_k \leq (E_{ROI} + \Delta_{ROI}) \\ 0 & \text{otherwise} \end{cases}$$



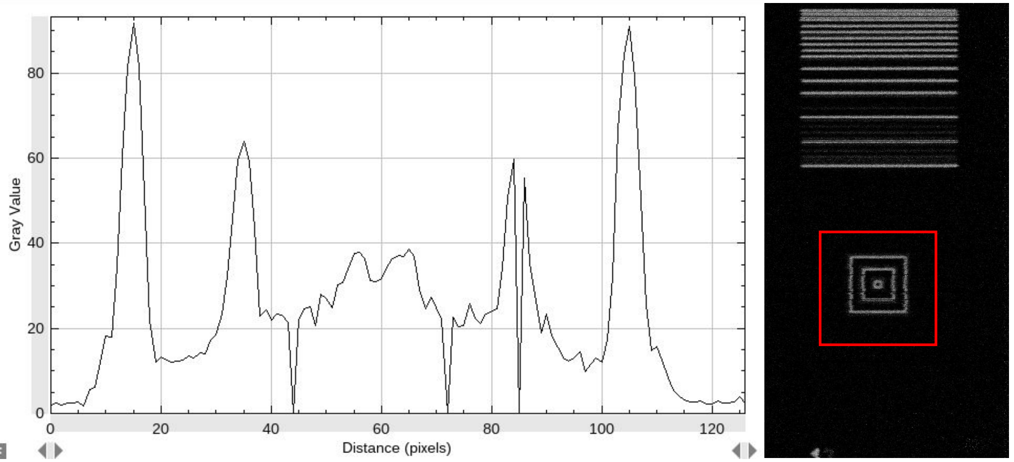
Energy Weighted

$$\delta_E = \begin{cases} E_k \cdot w(k) & \text{if } (E_{ROI} - \Delta_{ROI}) \leq E_k \leq (E_{ROI} + \Delta_{ROI}) \\ 0 & \text{otherwise} \end{cases}$$



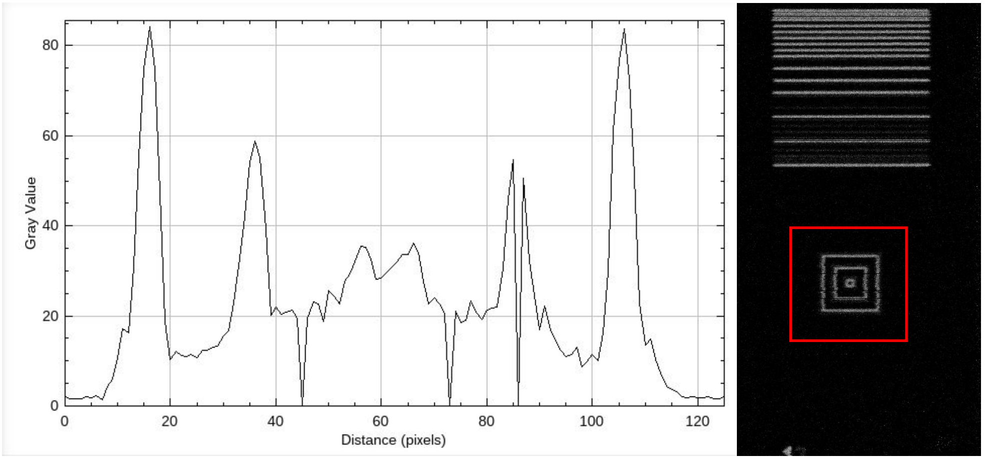
Pixel

$$\delta_E = \begin{cases} 1 & \text{if } (E_{ROI} - \Delta_{ROI}) \leq E_k \leq (E_{ROI} + \Delta_{ROI}) \\ 0 & \text{otherwise} \end{cases}$$



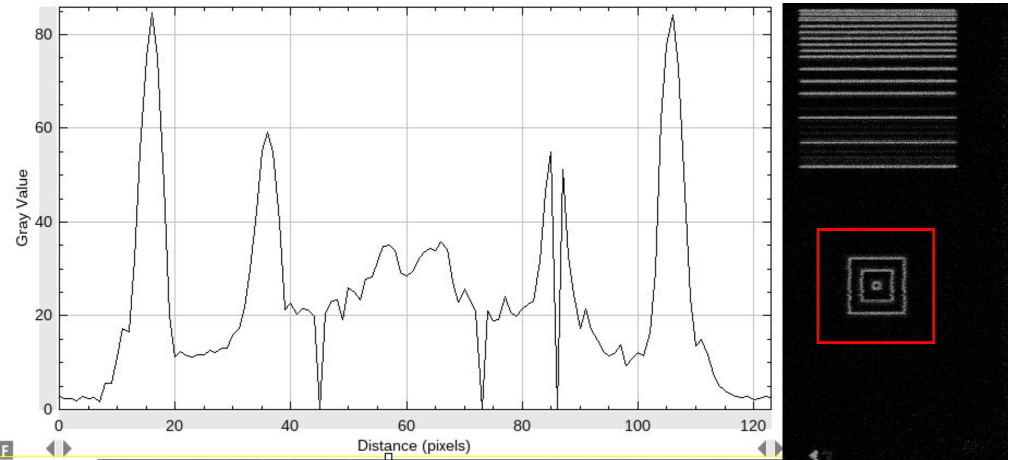
Pixel Weighted

$$\delta_E = \begin{cases} w(k) & \text{if } (E_{ROI} - \Delta_{ROI}) \leq E_k \leq (E_{ROI} + \Delta_{ROI}) \\ 0 & \text{otherwise} \end{cases}$$



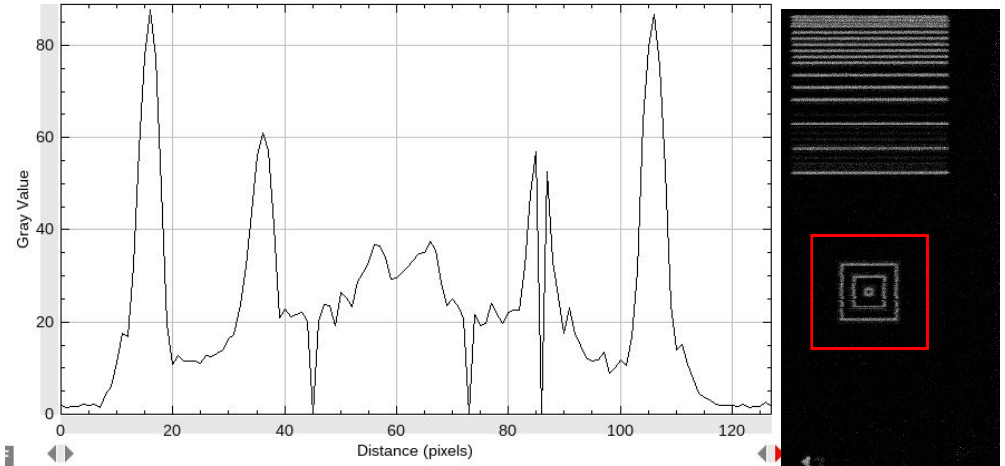
Energy

$$\delta_E = \begin{cases} E_k & \text{if } (E_{ROI} - \Delta_{ROI}) \leq E_k \leq (E_{ROI} + \Delta_{ROI}) \\ 0 & \text{otherwise} \end{cases}$$



Energy Weighted

$$\delta_E = \begin{cases} E_k \cdot w(k) & \text{if } (E_{ROI} - \Delta_{ROI}) \leq E_k \leq (E_{ROI} + \Delta_{ROI}) \\ 0 & \text{otherwise} \end{cases}$$



Elemental map reconstruction

Given:

- E_{ROI} the expected value of a Gaussian fitting of the ROI, and
- σ the standard deviation of the fit, and
- Δ_{ROI} as the full with half maximum of the Gaussian fit, defined by $\Delta_{ROI} = 2\sqrt{2\ln 2}\sigma$.

And the reconstruction space given by:

- x_k, y_k and E_k for $k = 1, \ldots, N$ are the coordinates and energy of the acquired photons.
- $\min_x$, $\min_y$, $\max_x$, $\max_y$ the minimum and maximum values of the x and y coordinates.
- *voxel_size* the voxel size selected by the user.

The photons corresponding to the selected ROI will be accumulated in an energy grid $E(i,j)$ and normalized by the total number of photons on the voxel accumulated in a Counter Grid $C(i,j)$, both with W and H dimmensions given by:

$$W = \left\lceil \frac{\max_x - \min_x}{\text{voxel\_size}} \right\rceil \qquad E(i,j) = 0 \quad \forall\, i,j$$

$$H = \left\lceil \frac{\max_y - \min_y}{\text{voxel\_size}} \right\rceil \qquad C(i,j) = 0 \quad \forall\, i,j$$

For each point (x_k, y_k, E_k) corresponds a voxel pair of coordinates v_x and v_y given by:

$$v_x = \left\lceil \frac{x_k - \min_x}{\text{voxel\_size}} \right\rceil \qquad v_y = \left\lceil \frac{y_k - \min_y}{\text{voxel\_size}} \right\rceil$$

Elemental map reconstruction

Given

1. Single-photon interpolated positions
2. Elemental map space definition ($[x_{min},x_{max}],[y_{min},y_{max}]$)
3. Processed ROIs (Energy, FWHM)
4. Pixel resolution (mm/pixel)

Reconstruction

1. Grid size computation (W, H)
2. A voxel v with coordinates (v_x, v_y) is computed for each (x_k, y_k, E_k)
3. Counter Grid **C(i,j)**:
   - Accmulates all the event counts in each voxel location
4. Energy Grid **E(i,j)** for each elemental line:
   - Accumulates each event within the ROI for the given voxel location
5. Elemental map reconstruction outcome **I(i,j)**:
   - Element-wise ratio

I(i,j) = E(i,j) / C (i,j)

If $0 \leq v_x < W$ and $0 \leq v_y < H$:

$$C(v_x, v_y) = C(v_x, v_y) + 1$$

and

$$E(v_x, v_y) = E(v_x, v_y) + 1$$

For counter grid $C(i, j)$:

$$C(i, j) = \sum_{k=1}^{N} \delta_{i,v_x} \cdot \delta_{j,v_y}$$

In a similar the energy grid $E(i, j)$

$$E(i, j) = \sum_{k=1}^{N} \delta_{i,v_x} \cdot \delta_{j,v_y} \cdot \delta_E$$

where

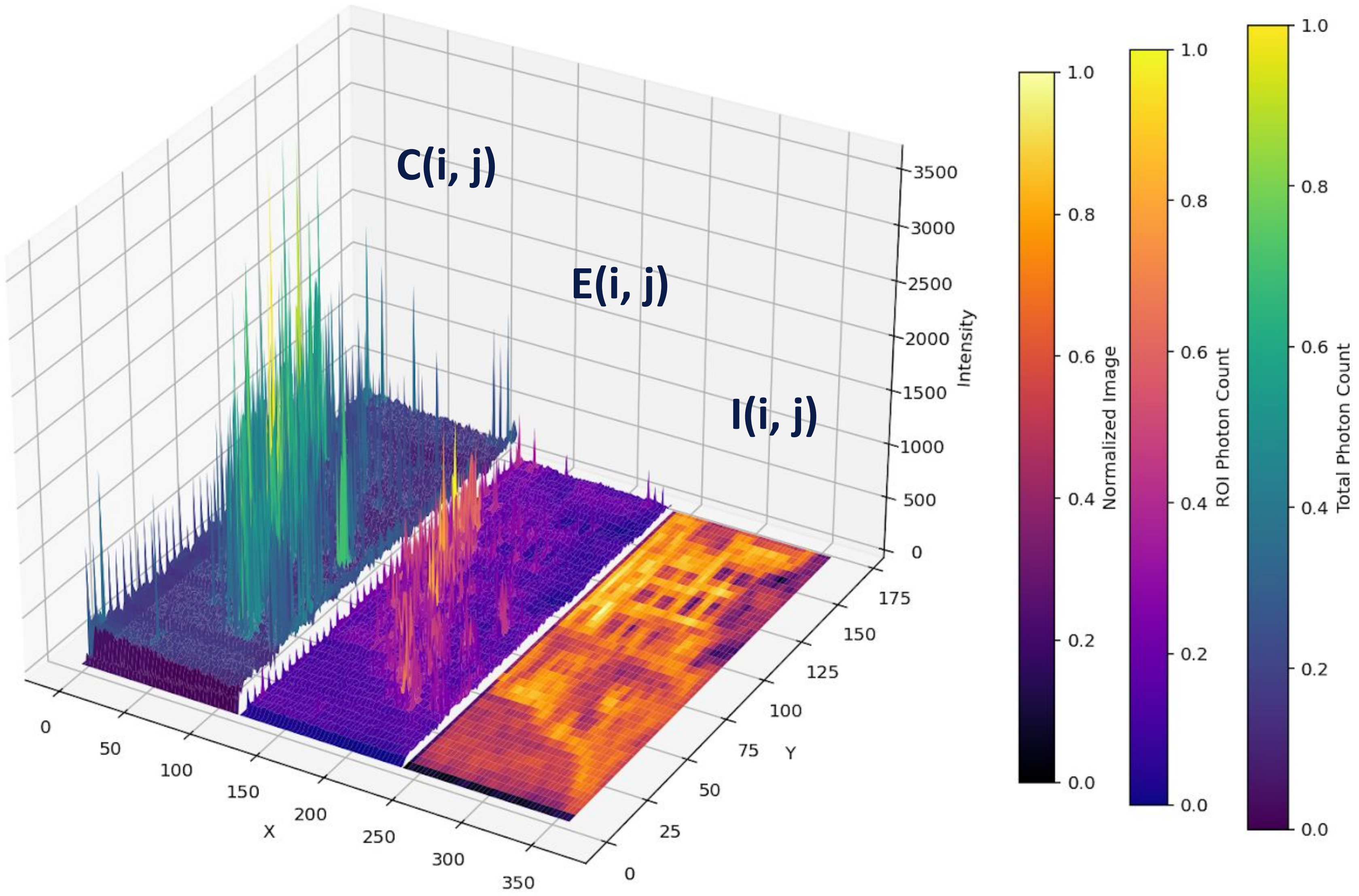
$$\delta_E = \begin{cases} 1 & \text{if } (E_{ROI} - \Delta_{ROI}) \leq E_k \leq (E_{ROI} + \Delta_{ROI}) \\ 0 & \text{otherwise} \end{cases}$$

The output image for each ROI I is the ratio of E to C and is given by

$$I(i, j) = \frac{E(i, j)}{C(i, j)} \quad \forall i \quad \forall j$$

Single-photon mapping

Elemental map reconstruction



Pixel-by Pixel vs Fly Scan

Feature	Pixel-by-Pixel Scan	Fly Scan (Continuous)
Movement	Step-wise; stage stops at each pixel	Continuous stage movement
Acquisition Time per Pixel	Longer (stationary) – more control	Shorter – limited by motion speed
Spatial Resolution	Higher; no motion blur	Slightly reduced; potential smearing at fast speeds
Spectral Quality	High; better signal-to-noise	Lower, especially at high speeds or for low-Z elements
Speed	Slower – scan time increases with resolution	Much faster – ideal for large areas
Best Use Case	High-precision imaging (e.g., overpainting, layering)	Rapid screening or large area mapping
Artifact Risk	Minimal (stationary during acquisition)	Risk of motion artifacts if not well-synchronized
Flexibility	High (can adjust dwell time, resolution locally)	Limited (fixed speed and dwell time)