



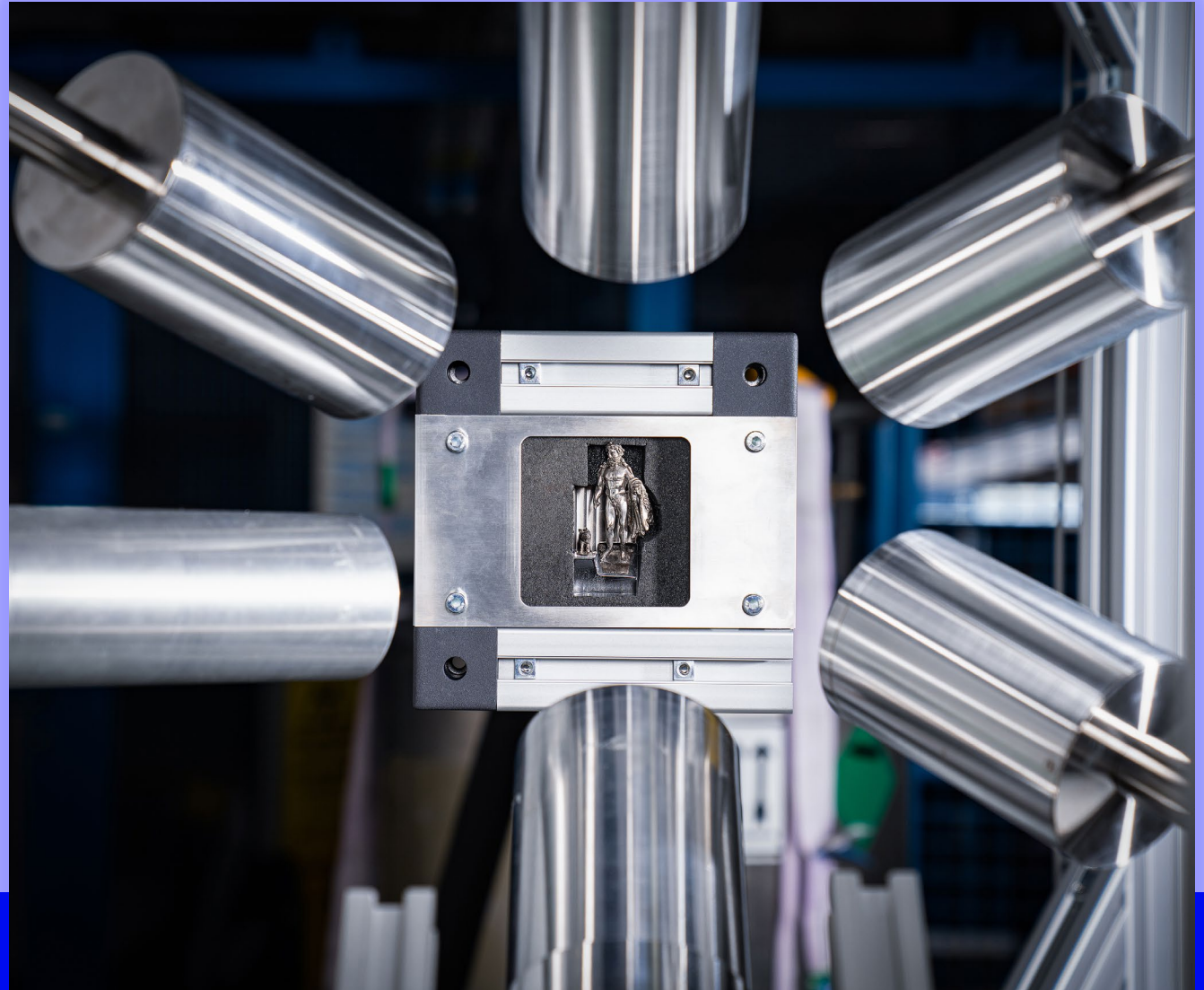
**PSI** Center for Neutron and  
Muon Sciences

# Muon-Induced X-ray Emission

## Activities at PSI

**Michael W. Heiss** (on behalf of the **MIXE** team)  
*Laboratory for Muon Spin Spectroscopy (LEM group)*

BRIDGE2025 Workshop, Tokyo, 22 October 2025



# Part I

# **Muon Induced X-ray Emission** *Technique & Instrument*

# MIXE: Muon Induced X-ray Emission – Overview



## Archeological artifacts



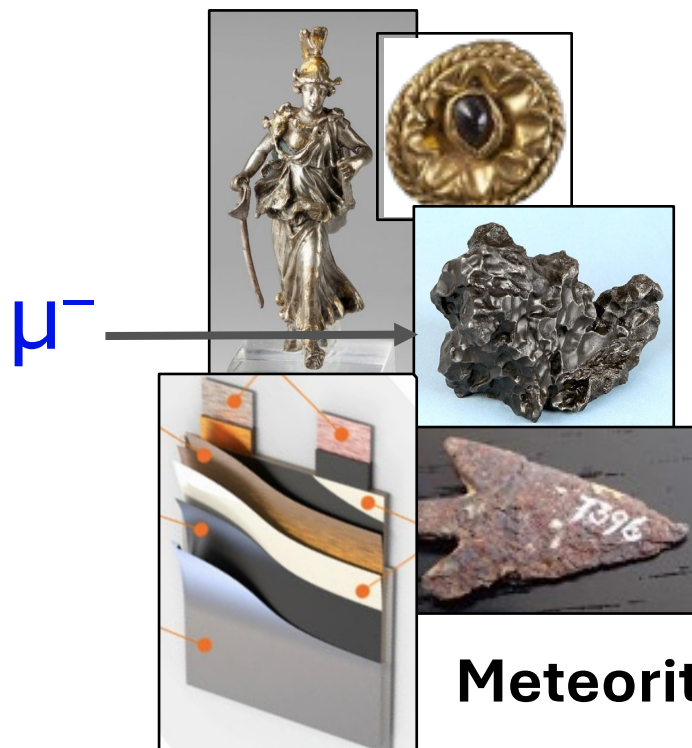
## Batteries

*and many more!*

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## Archeological artifacts



Batteries

Meteorites

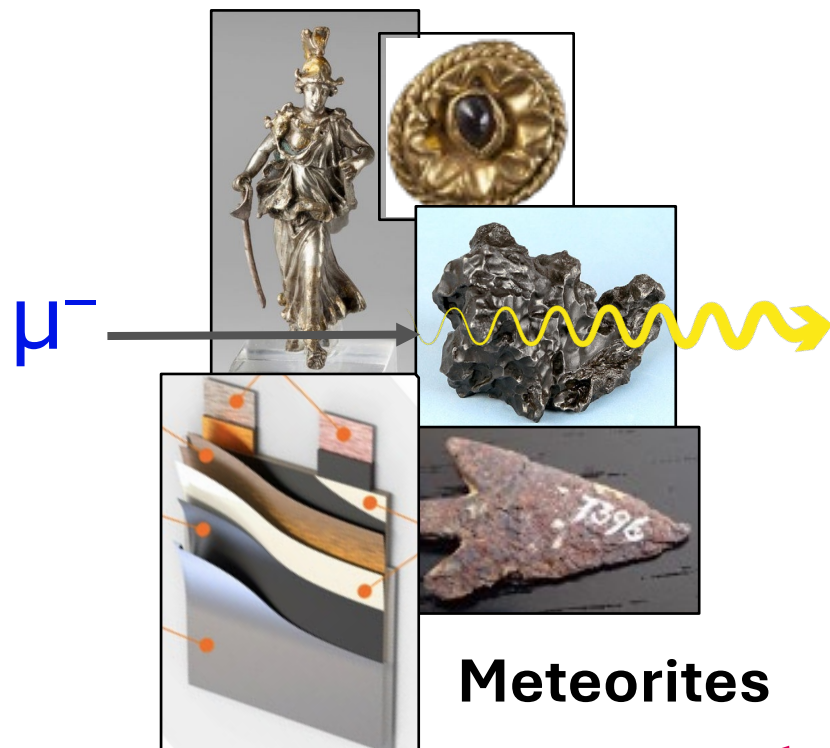
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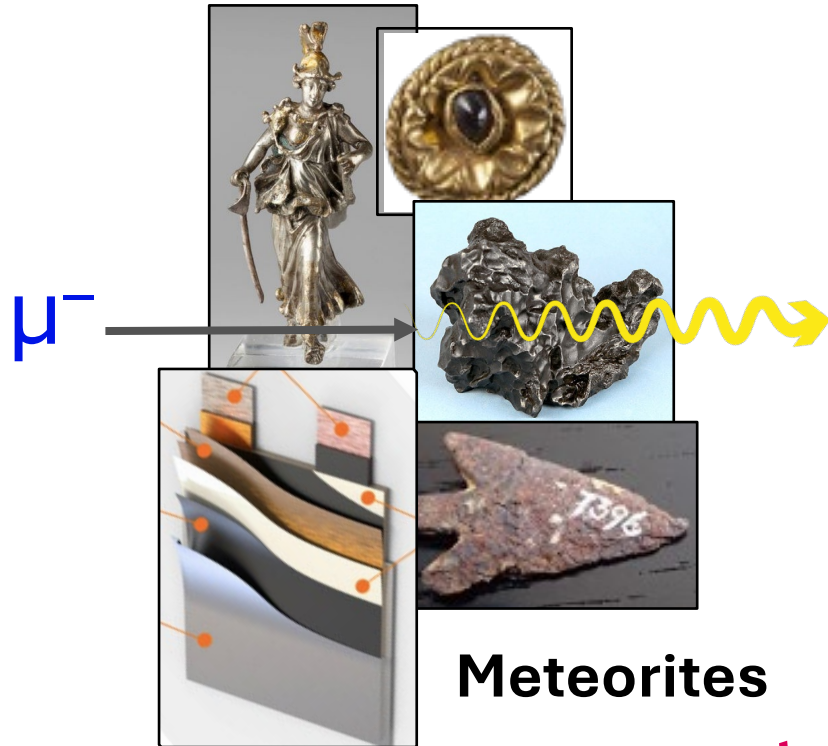
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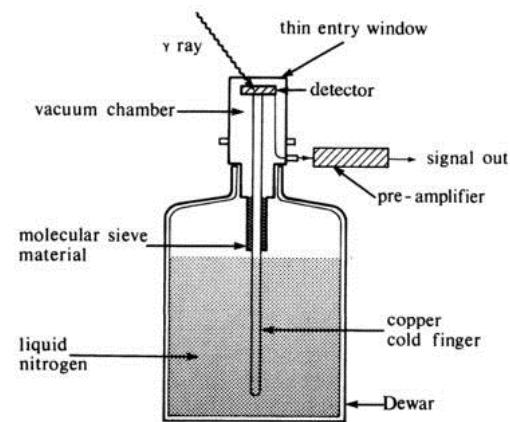


## Batteries

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## Meteorites

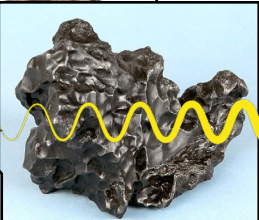
## High Purity Germanium Detectors



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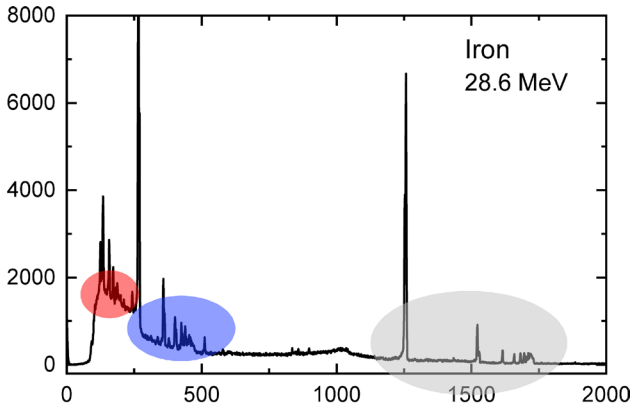
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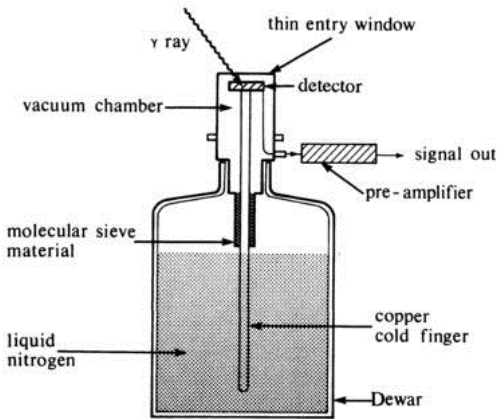
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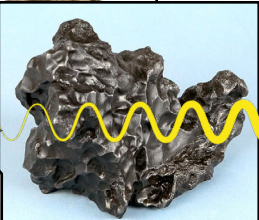
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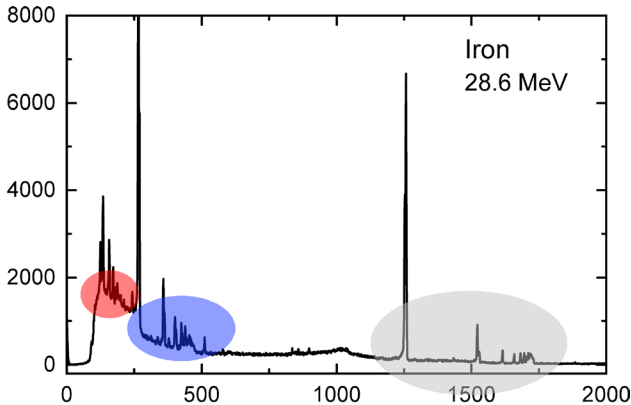
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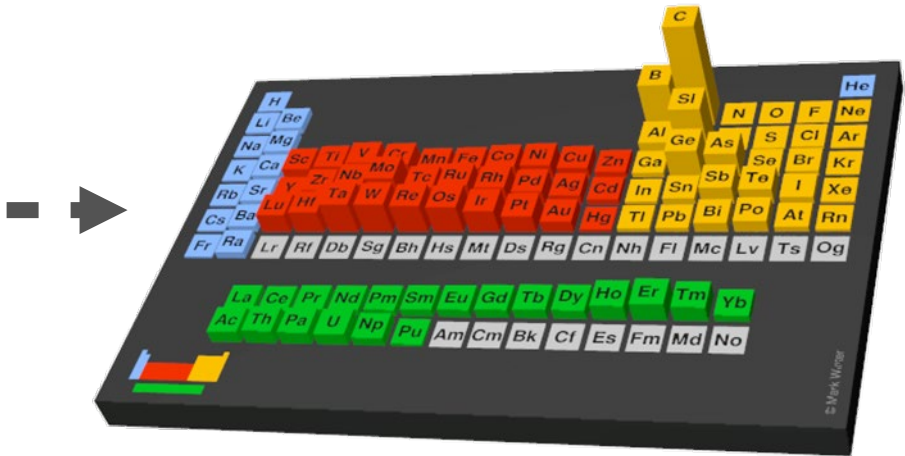
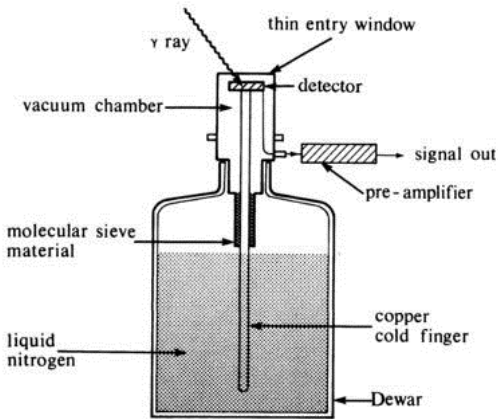
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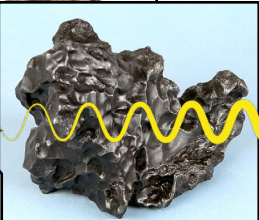




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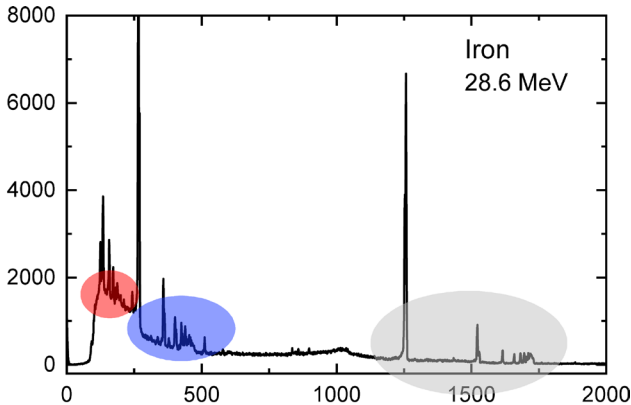
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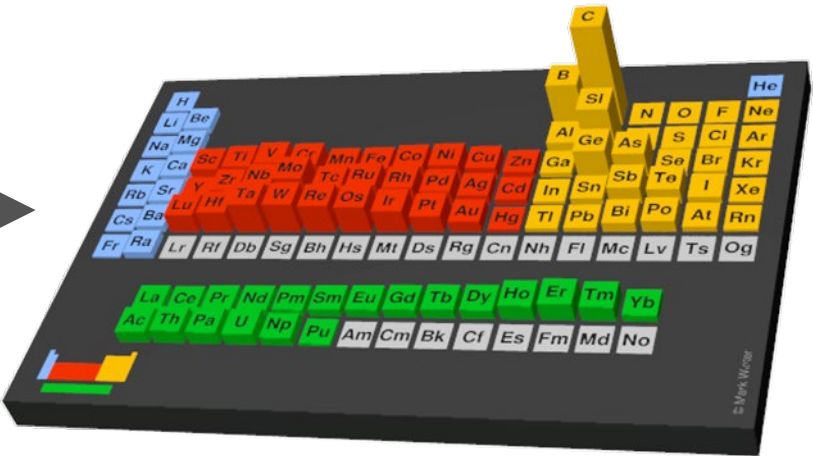
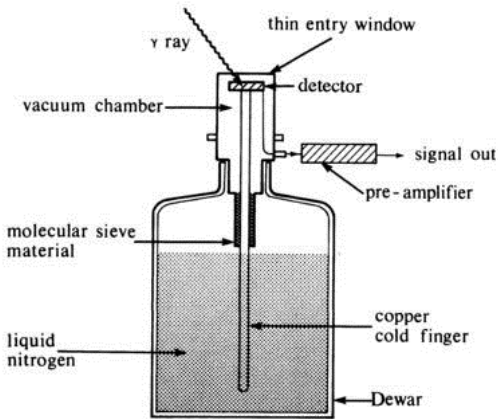
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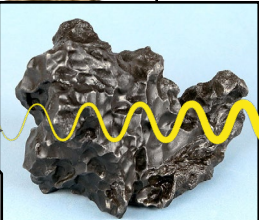
Highlights:

- Sensitive to all elements

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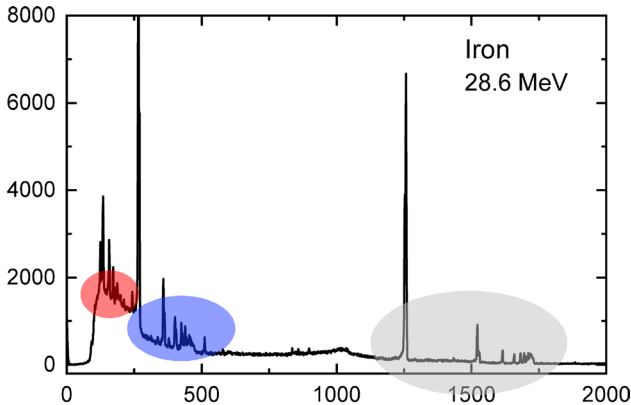
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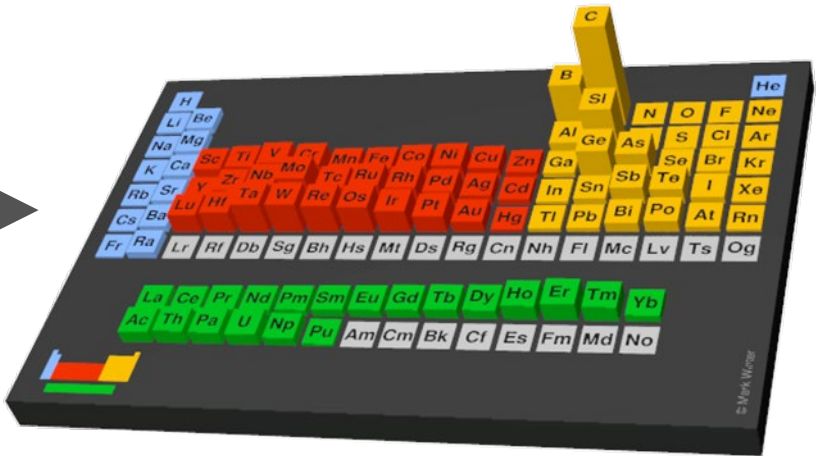
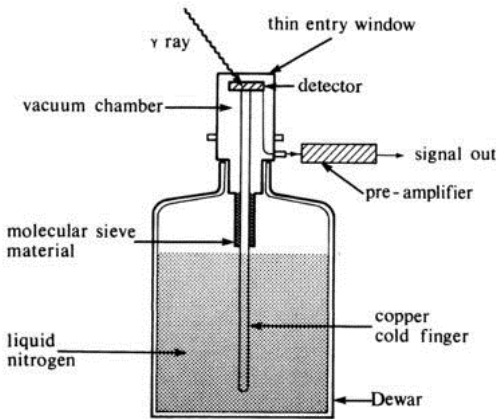
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High Purity Germanium Detectors



## Highlights:

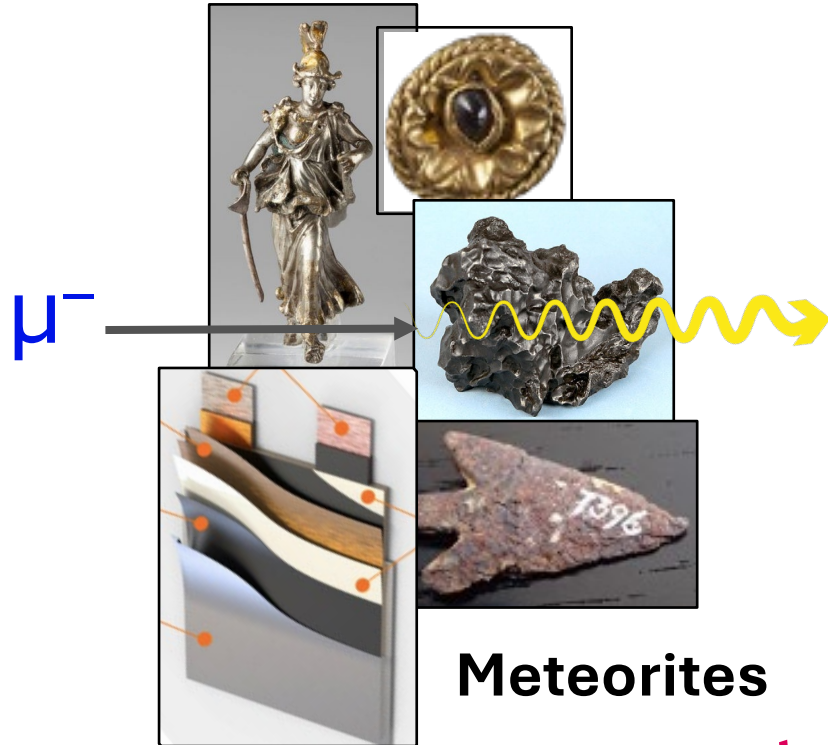
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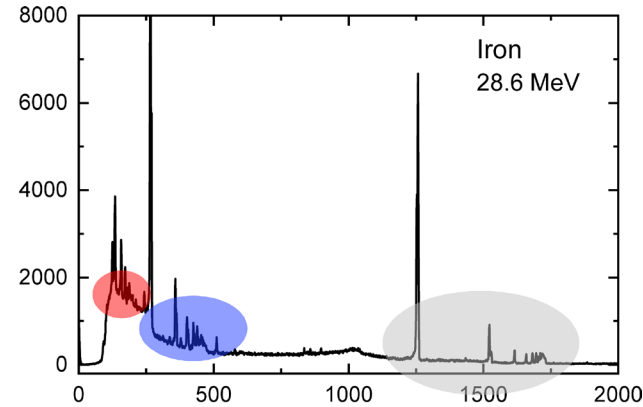
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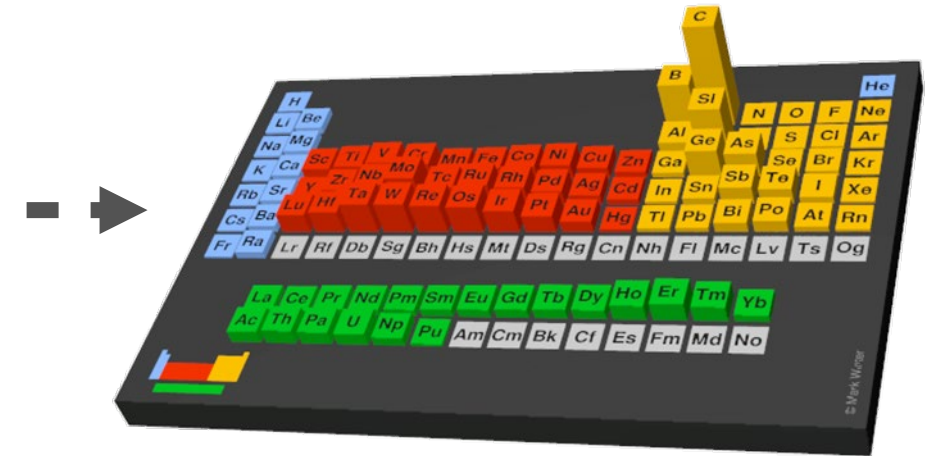
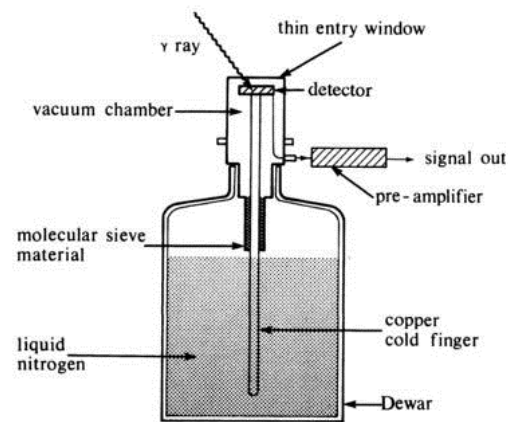
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## High Purity Germanium Detectors



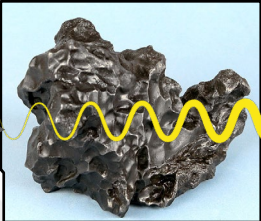
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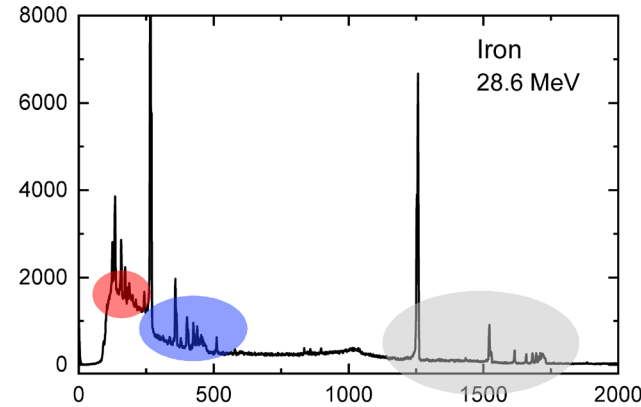
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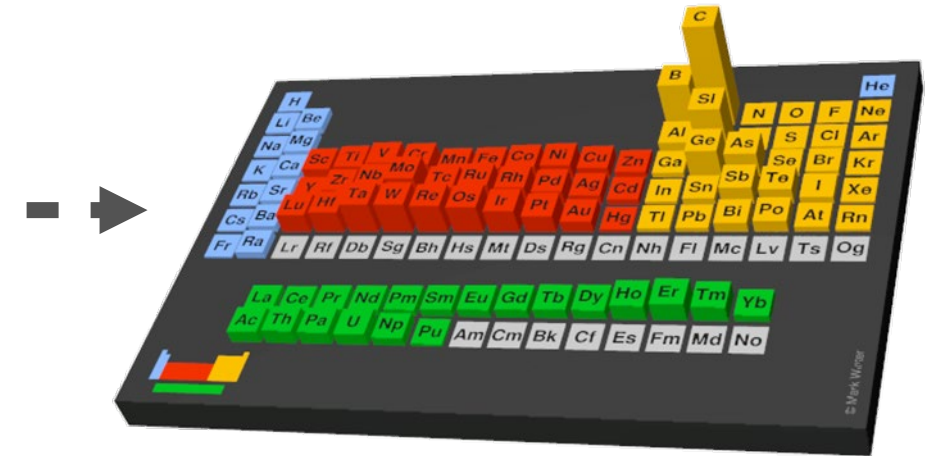
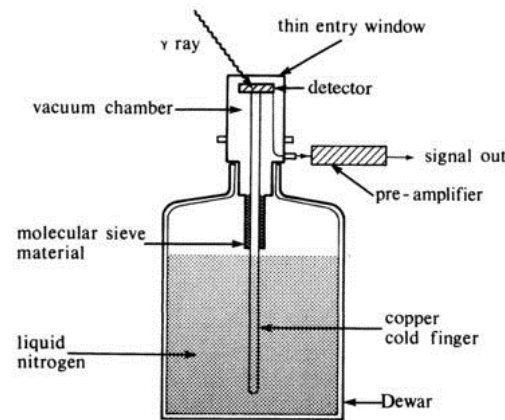
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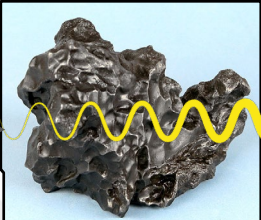
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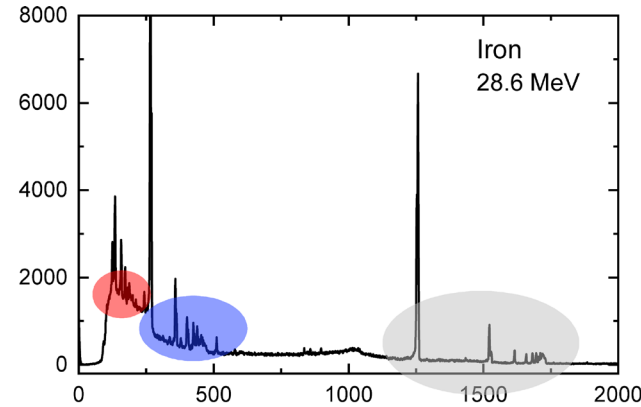
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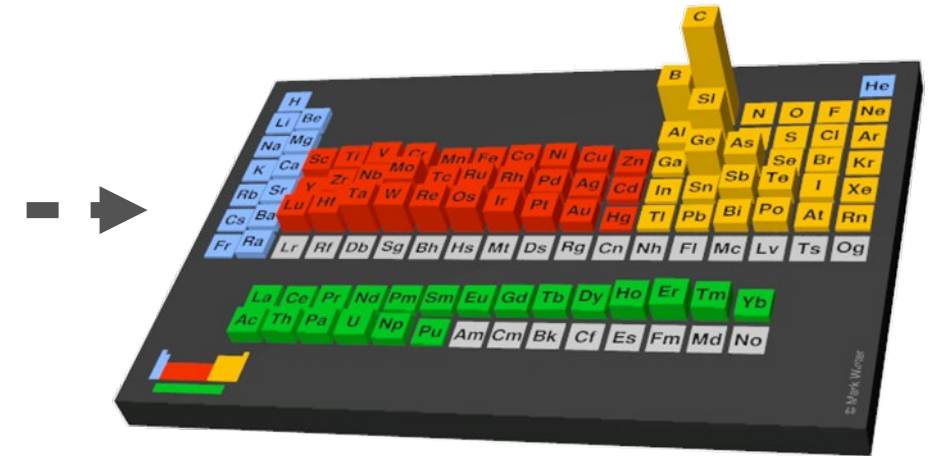
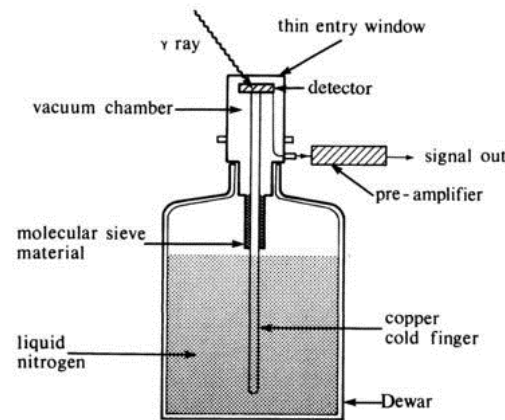
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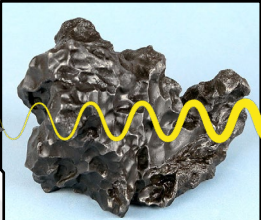
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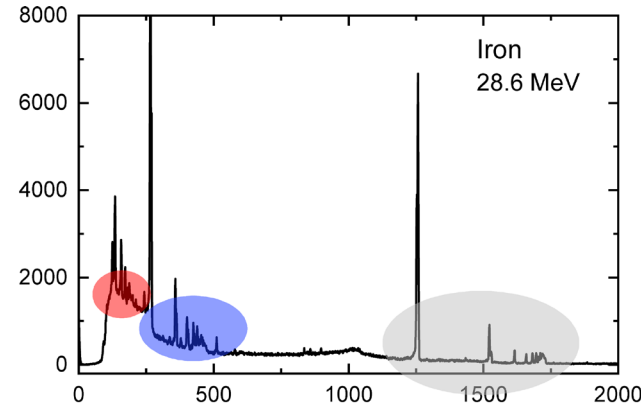
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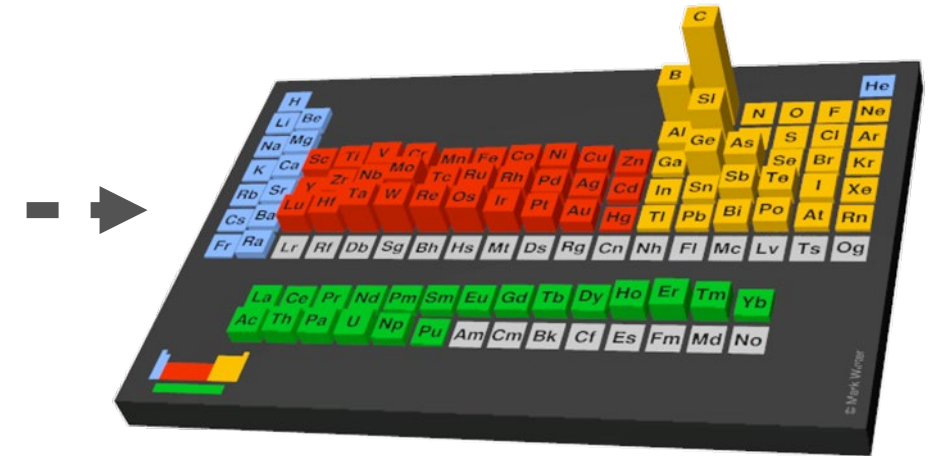
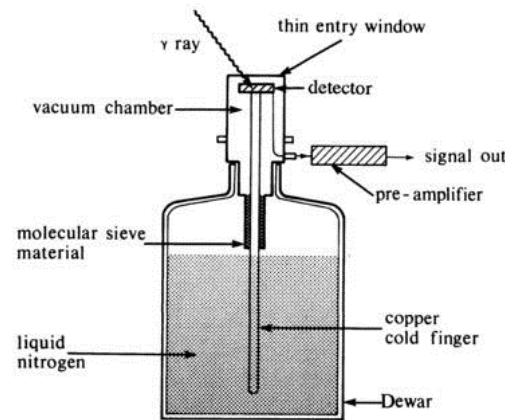
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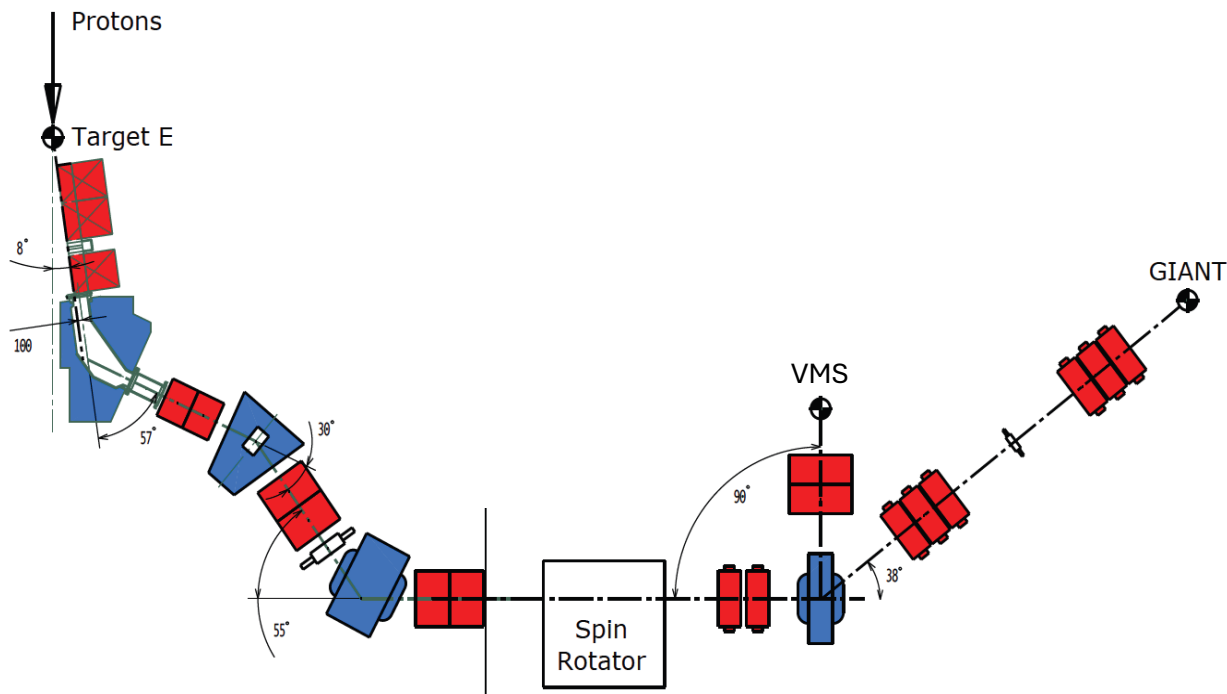
- **Sensitive to all elements**
- **Isotopic composition (high Z)**
- **Indications of chemical states**
- **Depth-resolved ( $\sim \mu\text{m}$  to  $\sim \text{cm}$ )**
  - **Completely non-destructive**
- **Tomography possible (see Part III)**

# MIXE: Muon Induced X-ray Emission – Beamlines: $\pi$ E1



**High intensity  $\pi$  beamline at target E**

- production of “cloud”  $\pi^-$  and decay to  $\mu^-$

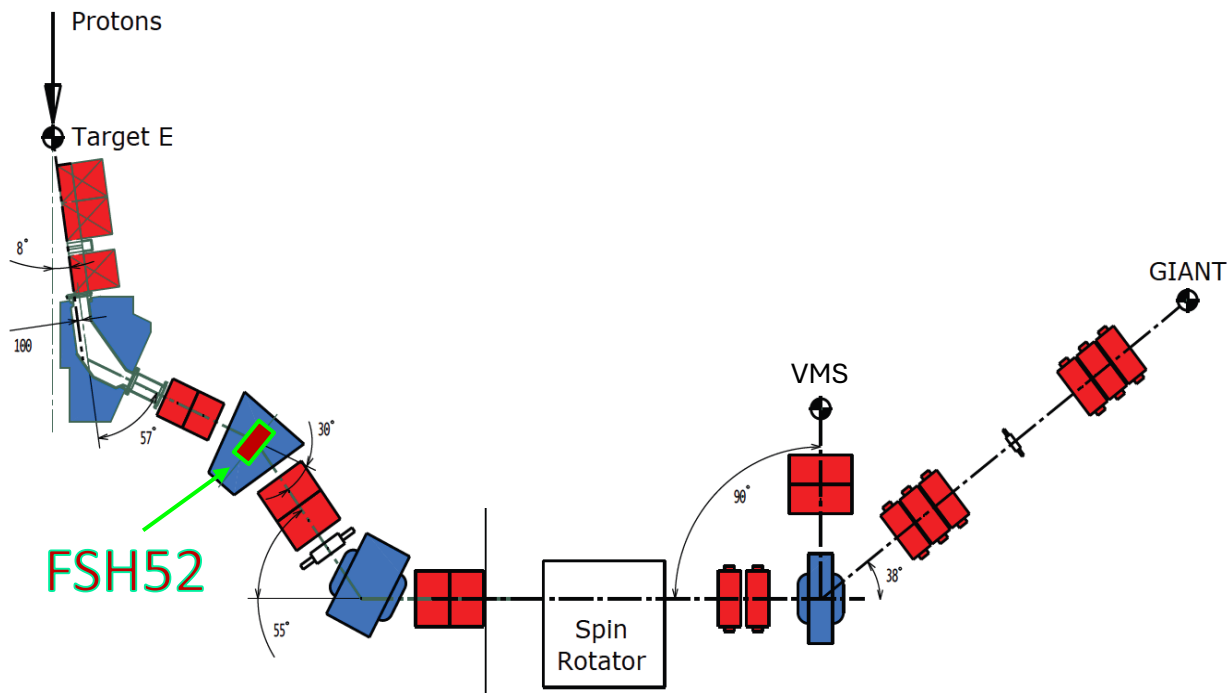


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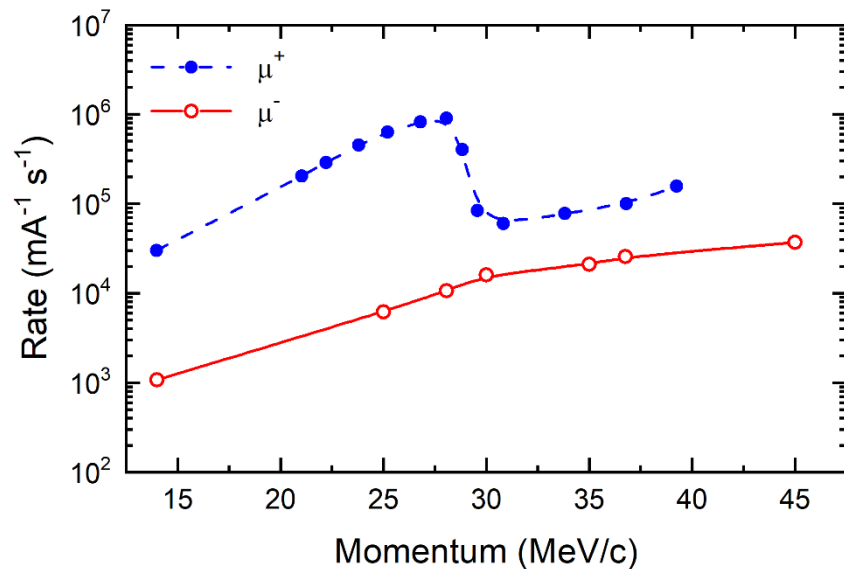
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*implantation depths: ~10 $\mu$ m to ~cm*





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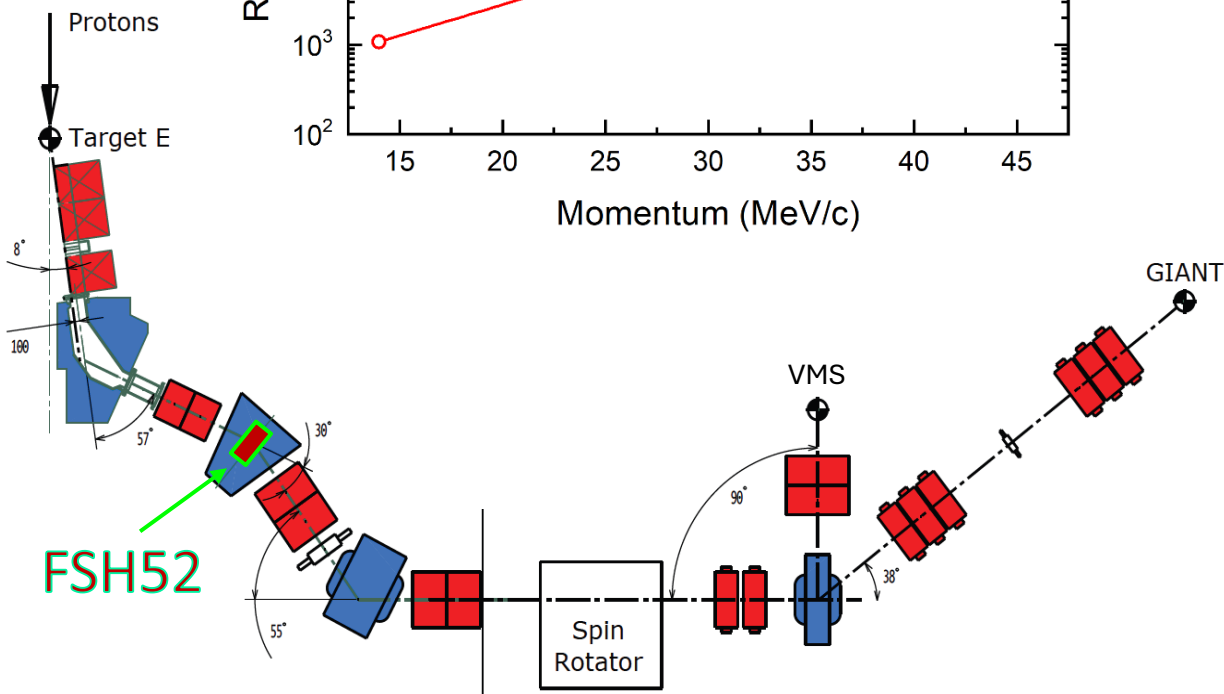
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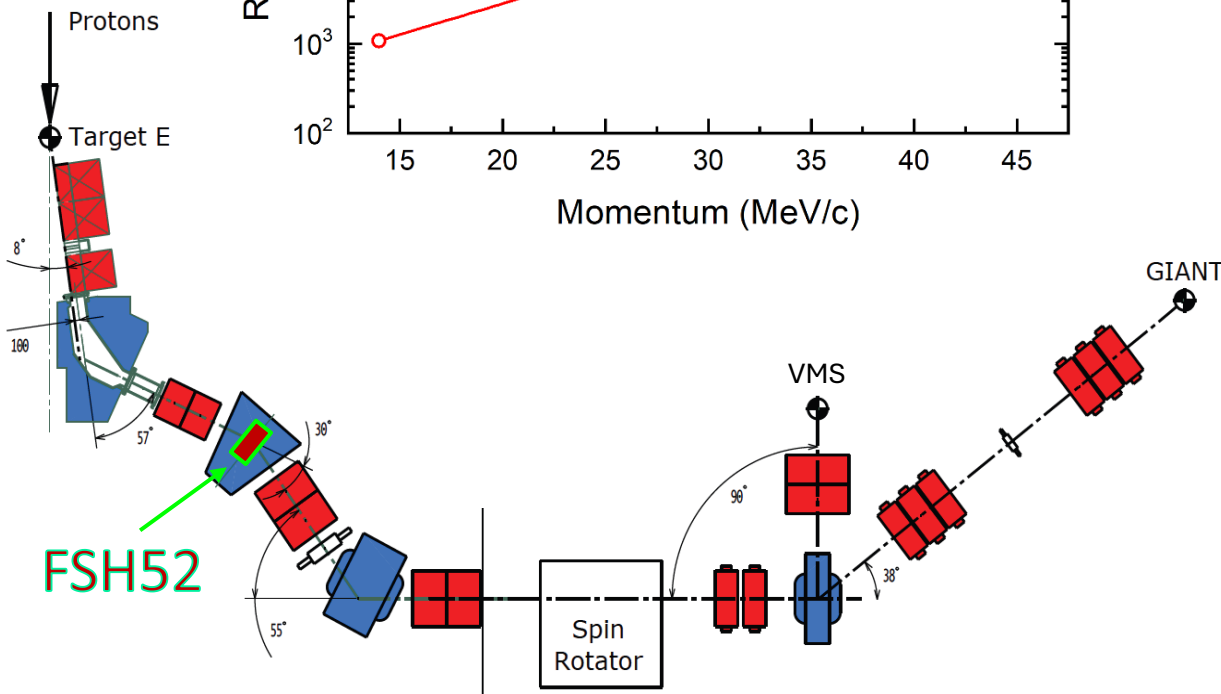
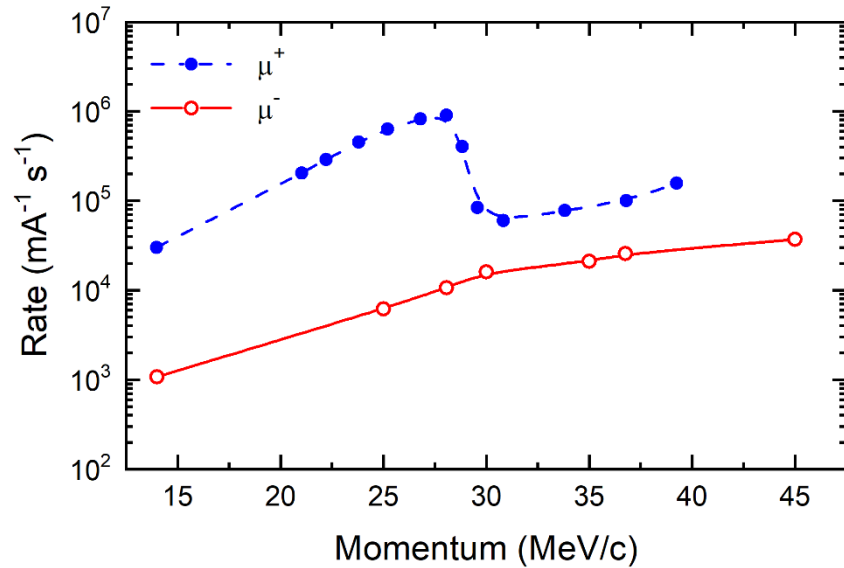
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*Rates from  $10^3$  up to  $10^5$   $\mu^-/\text{s}$  on target*



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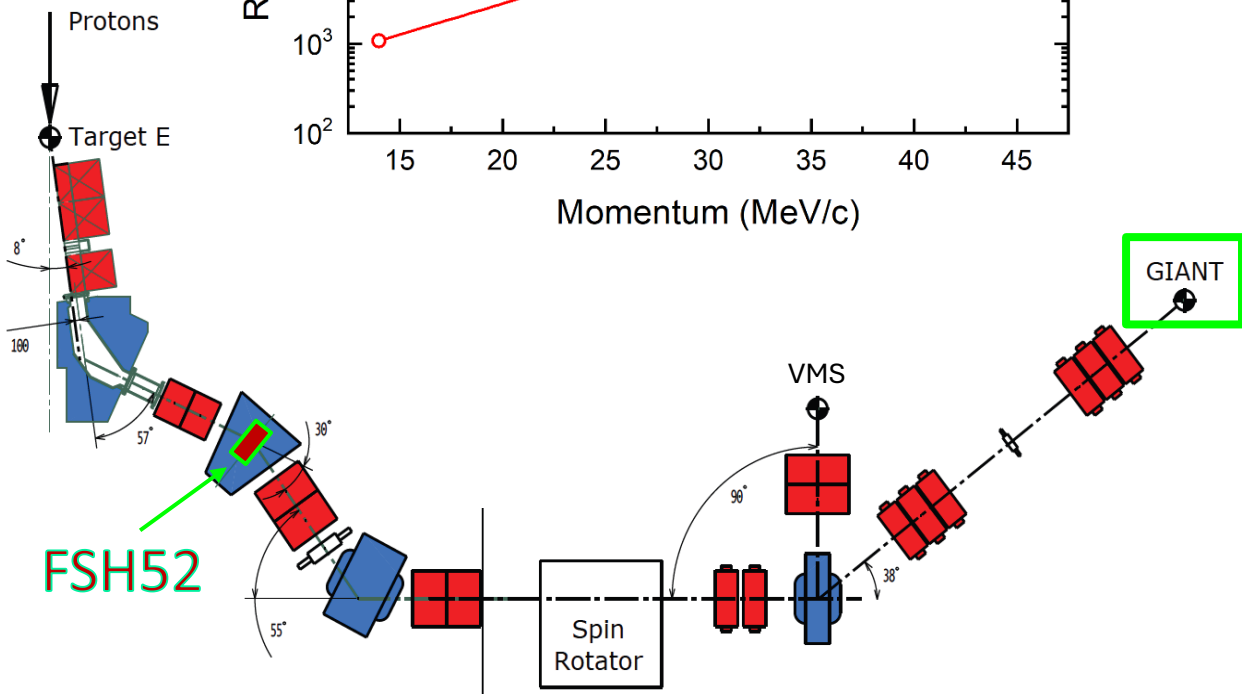
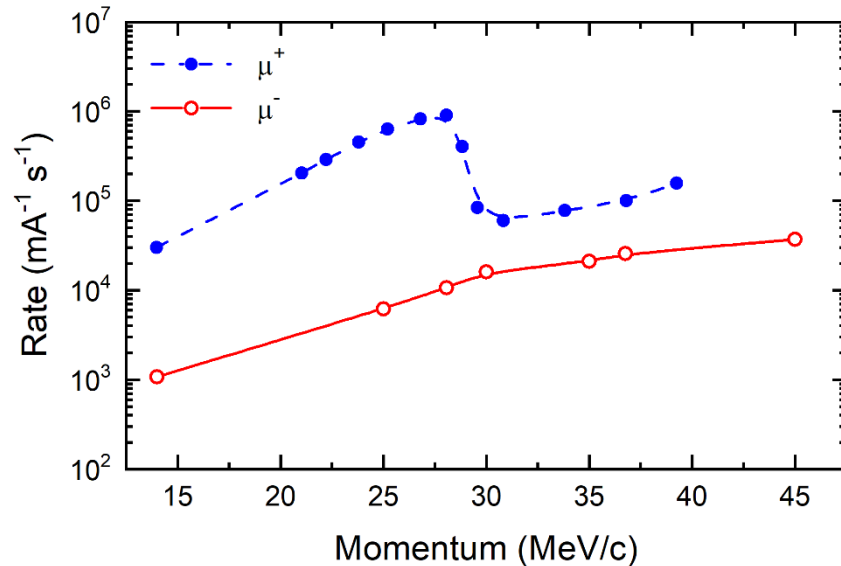
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- close to **ideal sampling rate** (cont.!)
  - *For the “average” sample, we collect enough statistics within  $\sim 1$  hour*

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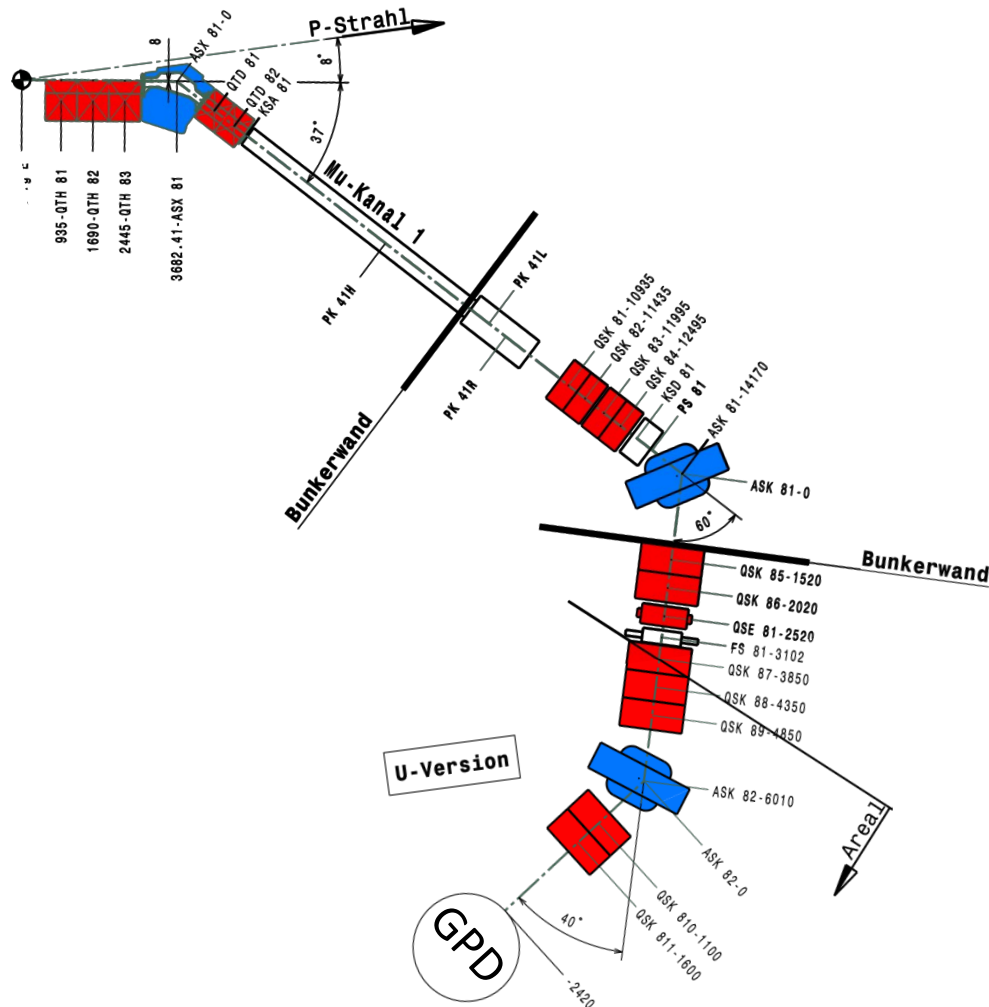
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All past MIXE campaigns hosted at  $\pi$ E1.2

- non-permanent installation
- so far ~3 weeks beam time per year

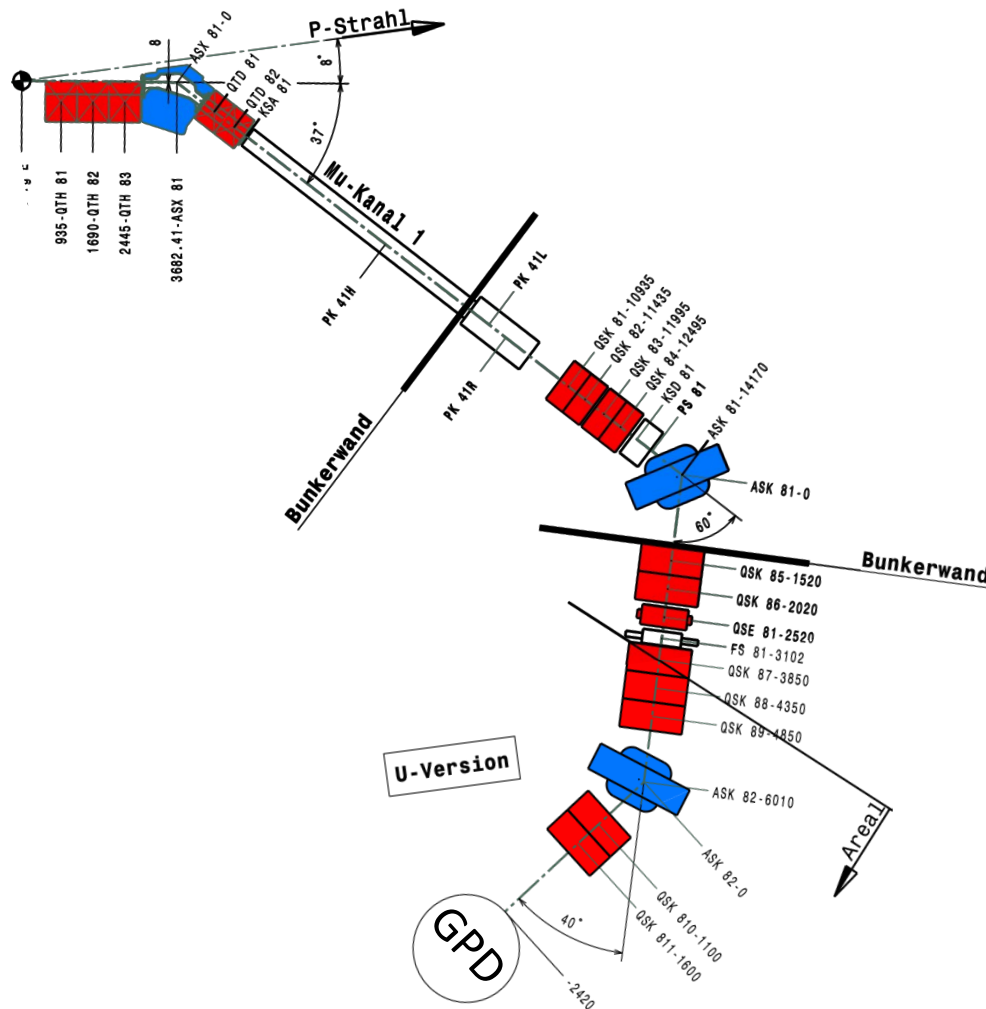
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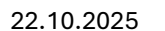
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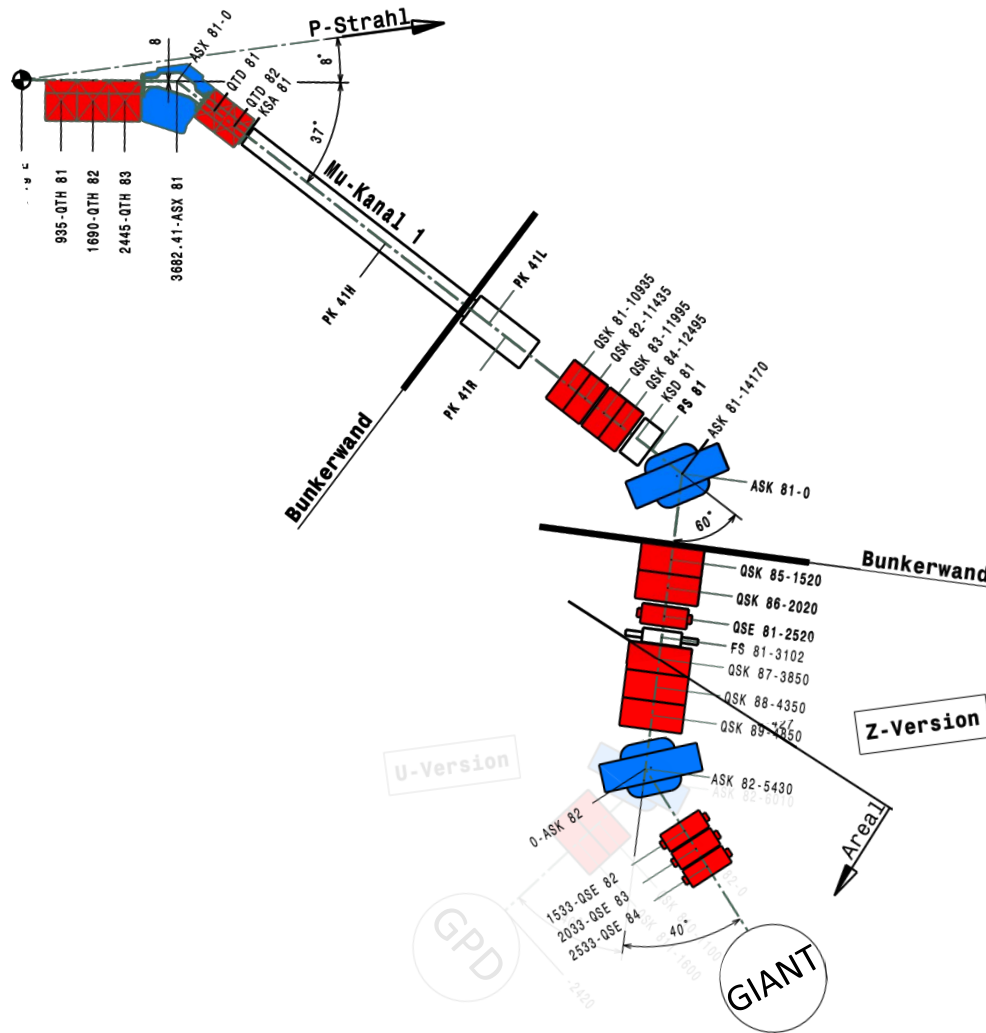








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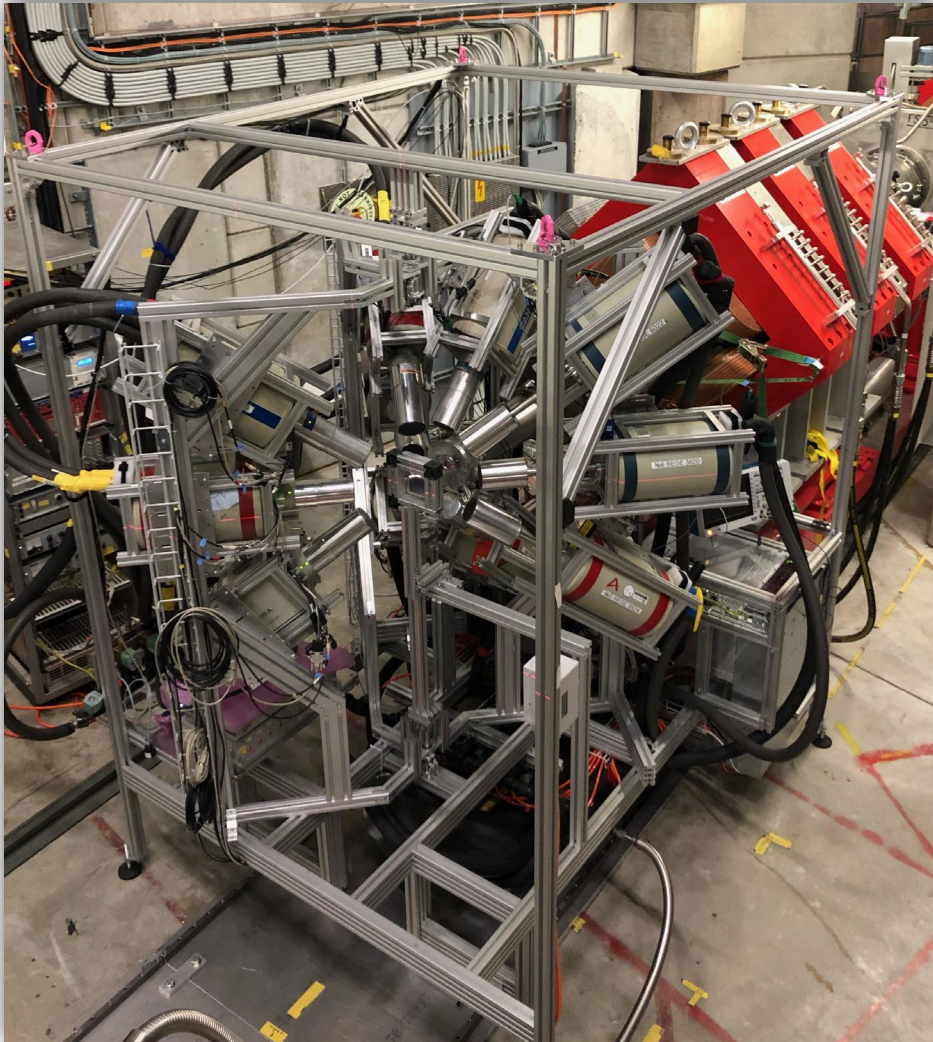
*Rates from  $10^7$  up to  $10^8 \mu^-/s$  on target*

Dual configuration: U (GPD) and Z (GIANT)

Future beam-line for MIXE

- installation during 2027/2028 shutdown (HIMB)
- high momentum / high rate studies (degrader)
- shorter  $\pi$ E1 campaign for low mom. / high res.

# GIANT: Germanium Array for Non-destructive Testing – Overview

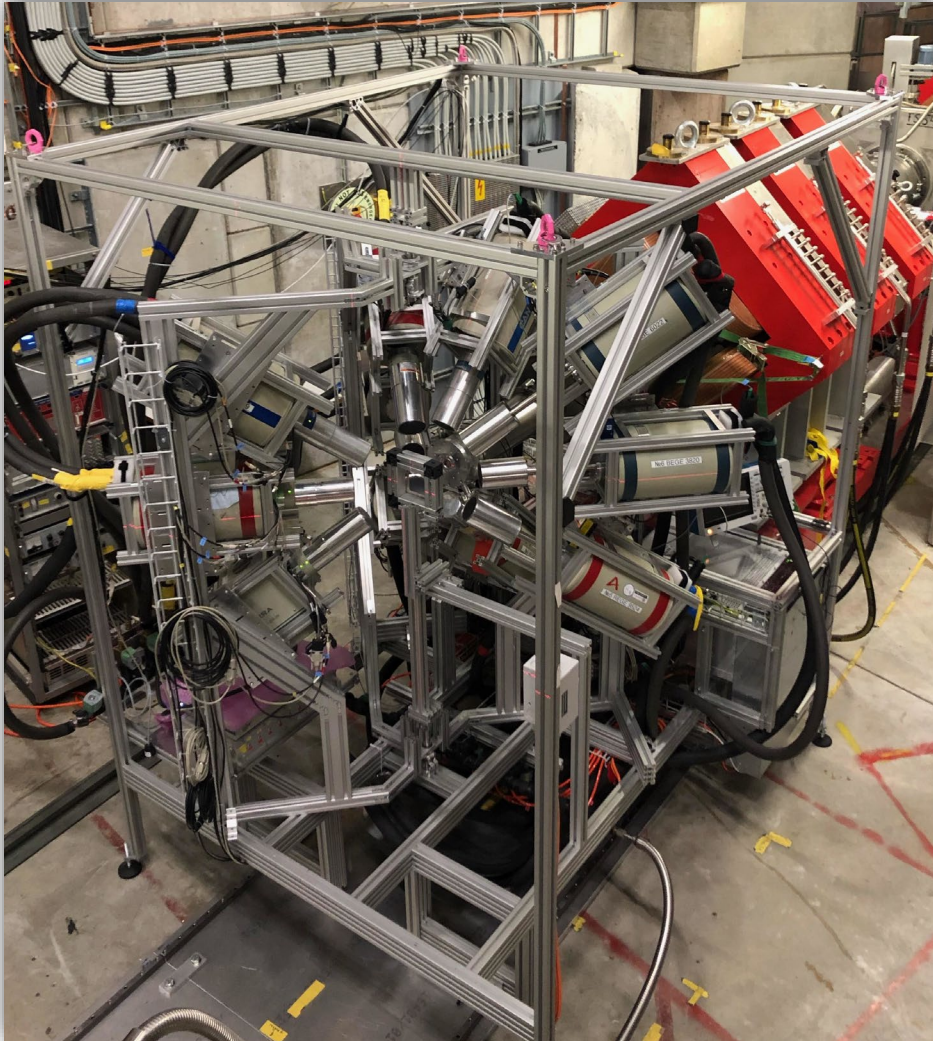


## Large solid angle detector array

- currently **~12 HPGe detectors** (up to 30)  
pooled with PP exp. (muX, Ref.Radii, MONUMENT, ...)



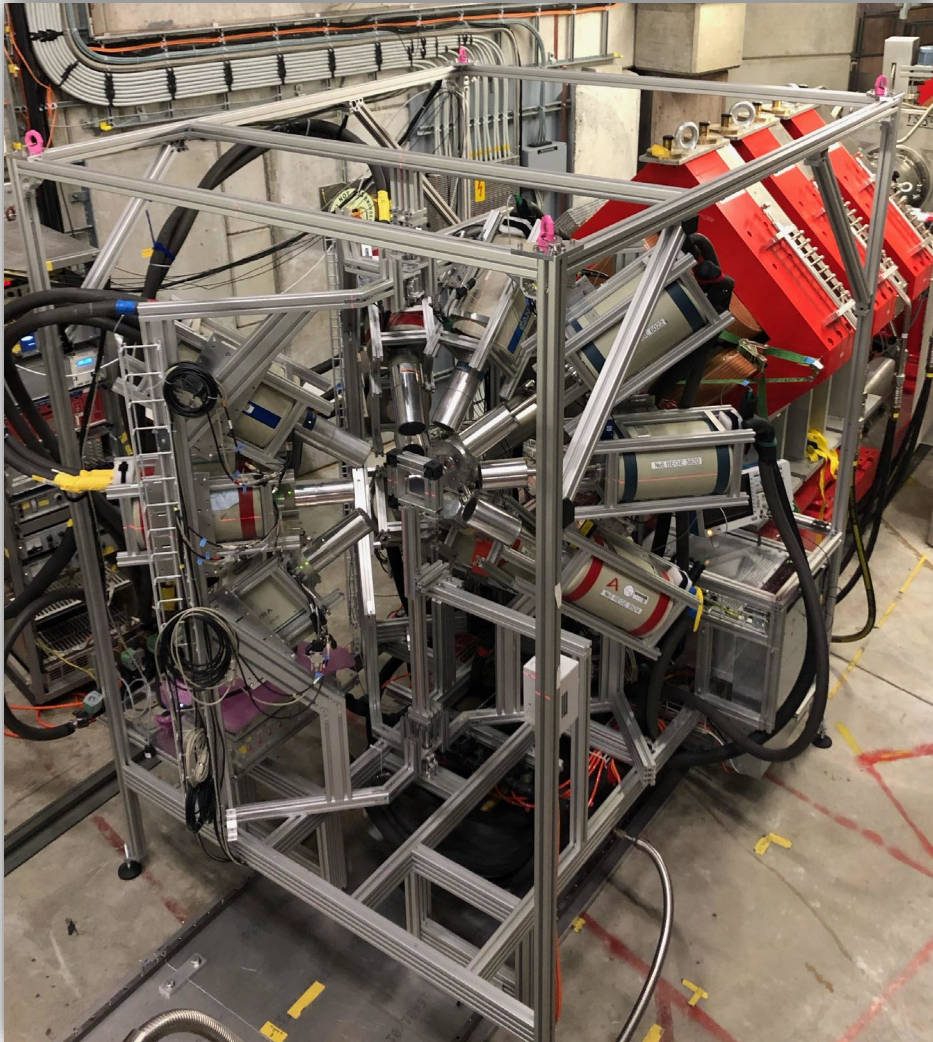
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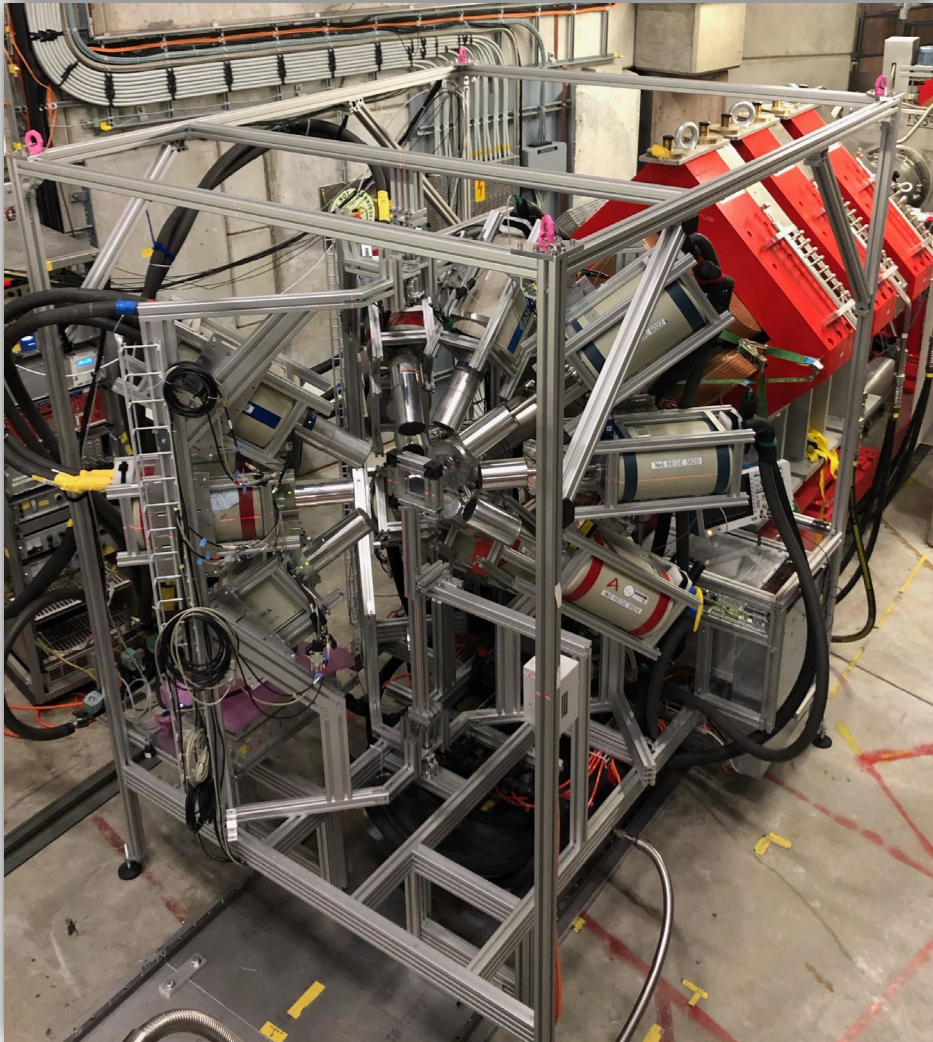


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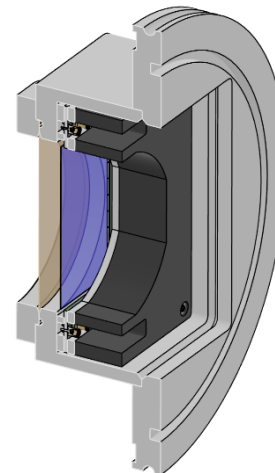


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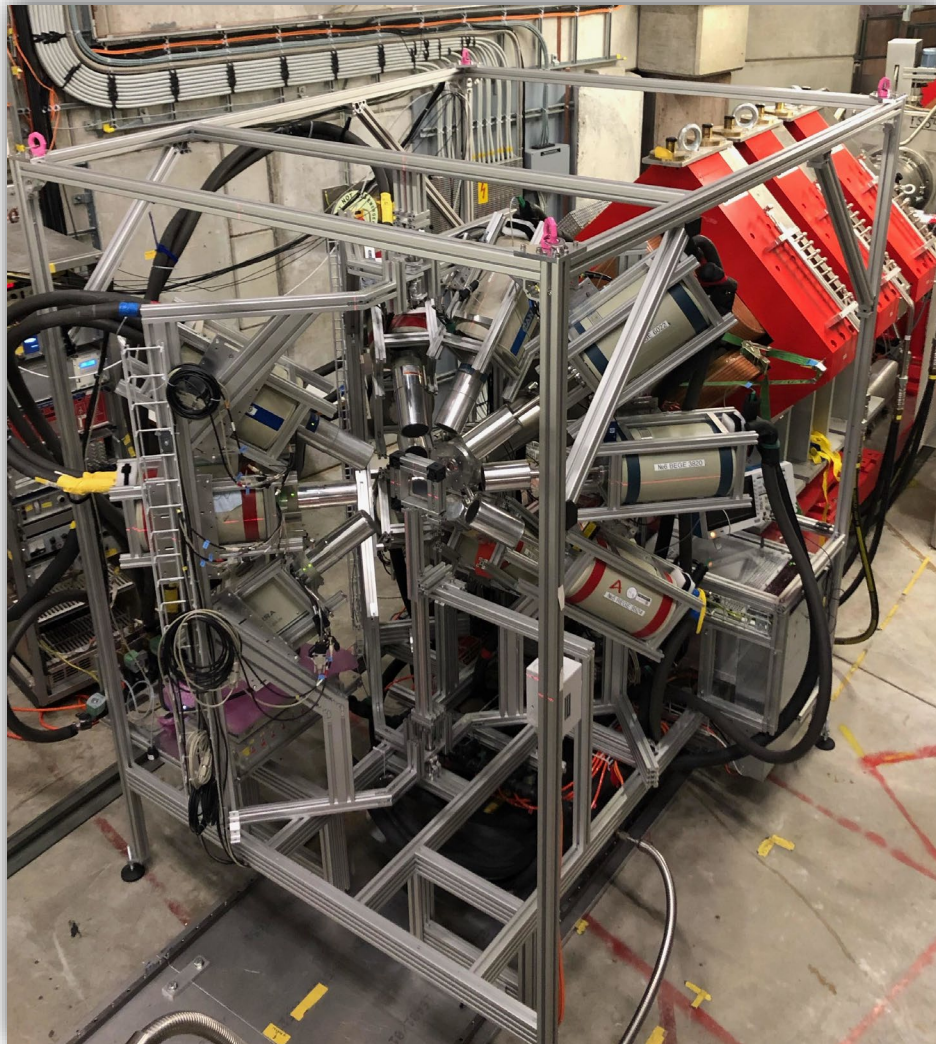
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- **low material budget** vacuum window (50 $\mu$ m mylar)





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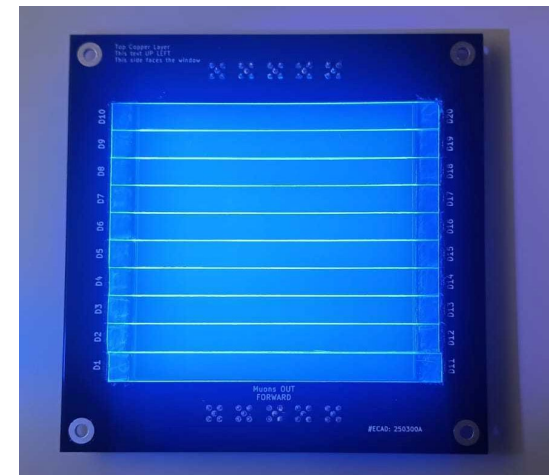
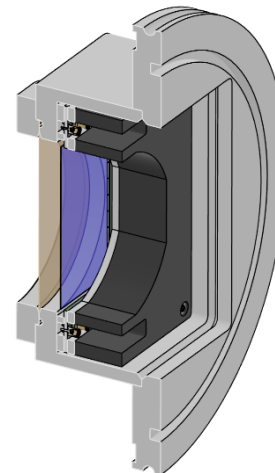


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Accessible **sample** station (~**10cm Air / He** gap to beam port)

- **low material budget** vacuum window (50μm mylar)
- **large area** (7x7cm<sup>2</sup>) **muon counter** (adaptable thickness)
- **segmented** design – facilitates higher tracking rates

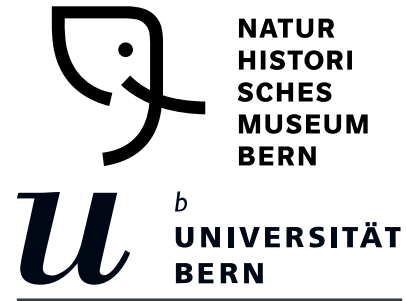


# Part II

# **Muon Induced X-ray Emission** *Showcase Studies*



# Arrowhead: Sample and Reception





# Arrowhead: Sample and Reception



Bernisches Historisches Museum  
Musée d'Histoire de Berne



Journal of Archaeological Science

Volume 157, September 2023, 105827



## An arrowhead made of meteoritic iron from the late Bronze Age settlement of Mörigen, Switzerland and its possible source

Beda A. Hofmann <sup>a b</sup> , Sabine Bolliger Schreyer <sup>c</sup>, Sayani Biswas <sup>d</sup>, Lars Gerchow <sup>d</sup>, Daniel Wiebe <sup>e</sup>, Marc Schumann <sup>e</sup>, Sebastian Lindemann <sup>e</sup>, Diego Ramírez García <sup>e</sup>, Pierre Lanari <sup>b</sup>, Frank Gfeller <sup>a b</sup>, Carlos Vigo <sup>d</sup>, Debarchan Das <sup>d</sup>, Fabian Hotz <sup>d</sup>, Katharina von Schoeler <sup>f d</sup>, Kazuhiko Ninomiya <sup>g</sup>, Megumi Niikura <sup>h</sup>, Narongrit Ritjoho <sup>i</sup>, Alex Amato <sup>d</sup>



1 cm

Archäologische Sensation

### Pfeilspitze vom Bielersee ist aus Eisen aus dem All

Rätsel um eiserne Pfeilspitze aus Bronzezeit gelöst: Das Material lieferte ein in Estland abgestürzter Meteorit.

SRF

### Diese Pfeilspitze ist nicht von dieser Welt

Forschende haben herausgefunden, dass eine bronzzeitliche Pfeilspitze aus dem Bernischen Historischen Museum aus meteoritischem Eisen hergestellt wurde. Laut Museum ein «extrem seltener» Nachweis.



### Prähistorische Pfeilspitze vom Bielersee soll aus Meteorit sein



Am Bielersee ist im 19. Jahrhundert eine prähistorische Pfeilspitze gefunden worden. Nun steht fest, dass sie aus Meteorit besteht.

Forschende weisen Herkunft nach

### Prähistorische Pfeilspitze vom Bielersee aus Meteorit hergestellt

BZ



# Arrowhead: Sample and Reception





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1 cm



# Arrowhead: The search for “Heavenly Iron”

## Bronze age

- **Metalworking** was known
- **Iron extraction** from ore *not yet discovered*





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- Iron from **meteorite** fragments
- **Production** of *jewelry, weapons, tools, ...*
- Very *rare* and *valuable* **trade goods**





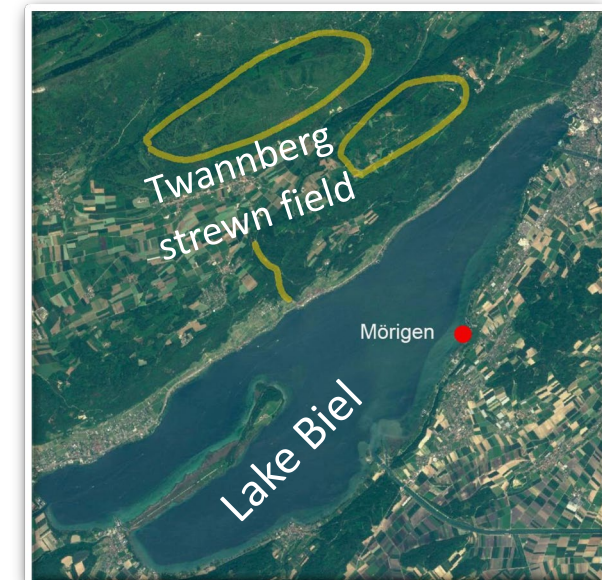
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Search in **archaeological collections** (area of *Lake Biel*)

- *Twannberg*: largest **meteorite find** in Switzerland



# Arrowhead: The search for “Heavenly Iron”

## Bronze age

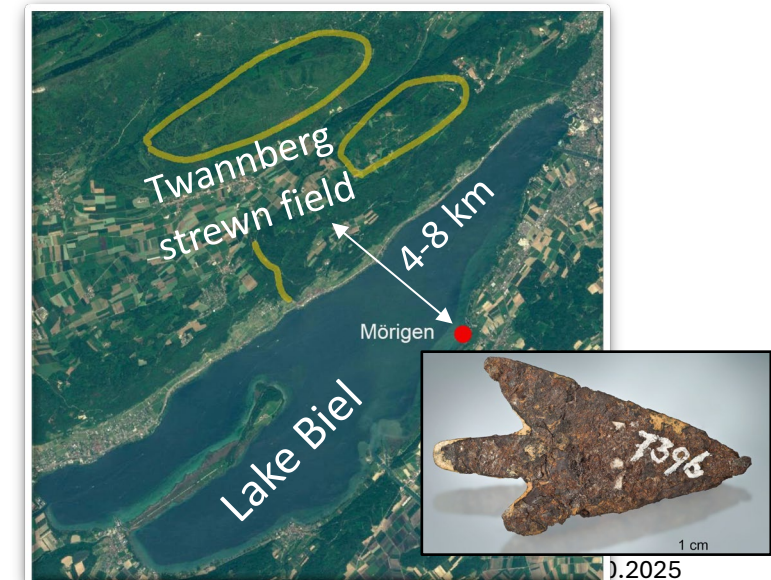
- **Metalworking** was known
- **Iron extraction** from ore *not yet discovered*
- „**Heavenly Iron**”
- Iron from **meteorite** fragments
- **Production** of *jewelry, weapons, tools, ...*
- Very *rare* and *valuable* **trade goods**

Search in **archaeological collections** (area of *Lake Biel*)

- *Twannberg*: largest **meteorite find** in Switzerland

Such an artifact identified: An **arrowhead**

- Find site: *Pile-dwelling settlement* in **Mörigen**
- Era: **Bronze Age** (900-800 BCE)
- Made from a large **iron meteorite** (>2 tons)



# Arrowhead: The surprise!

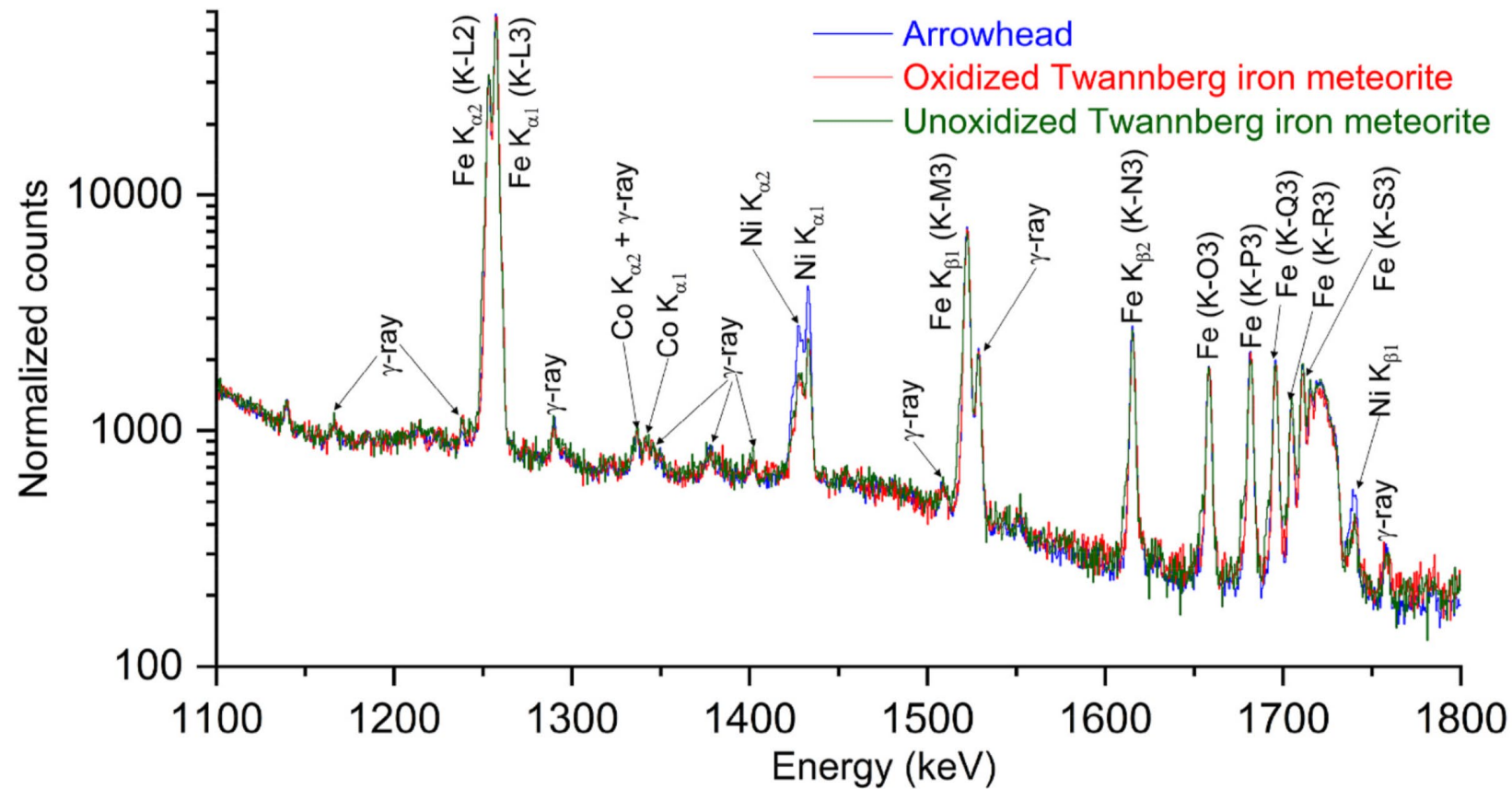


**MIXE** Study: Comparison to **Twannberg** reference meteorite for *Iron, Nickel, and Cobalt*



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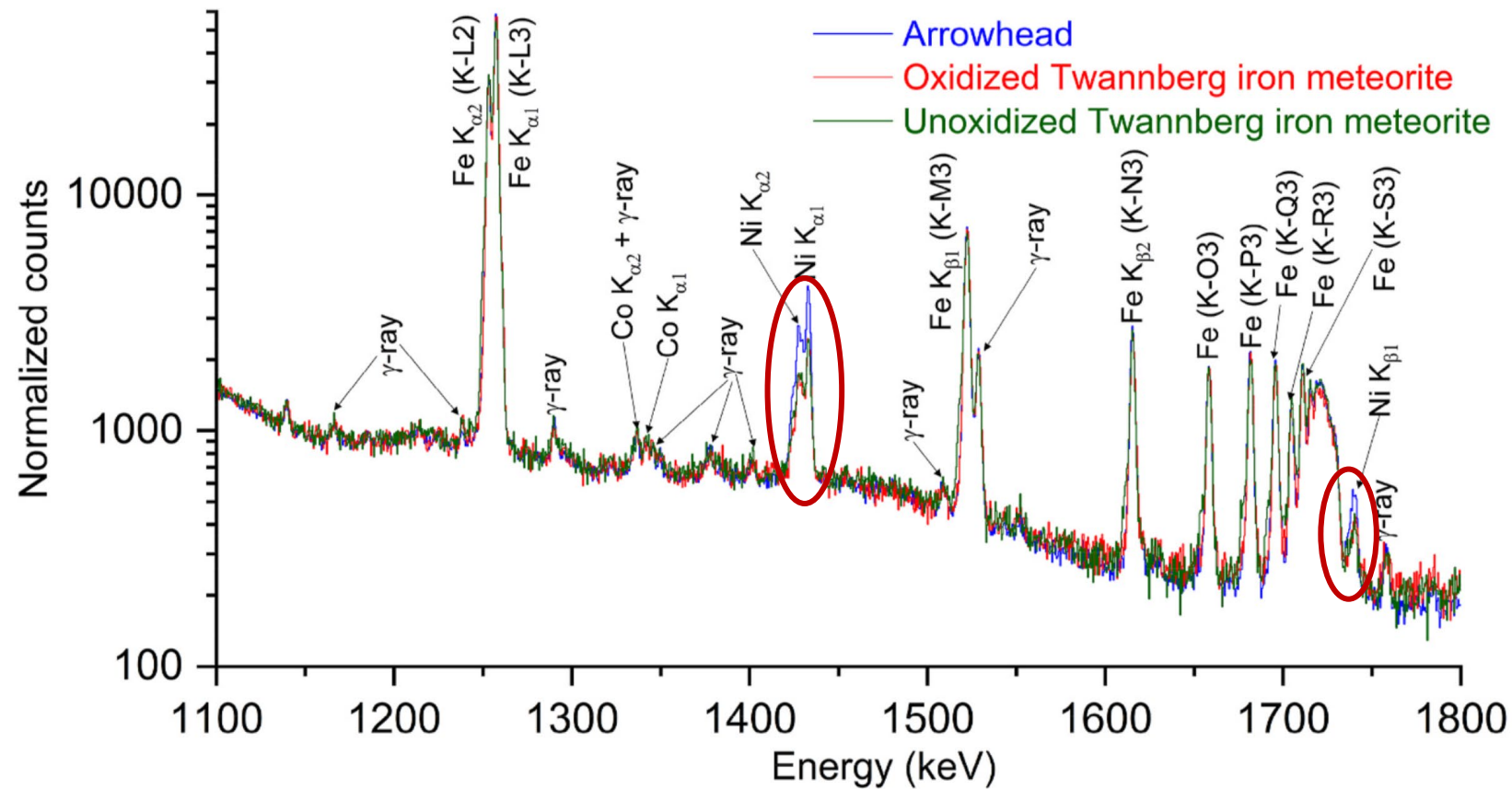
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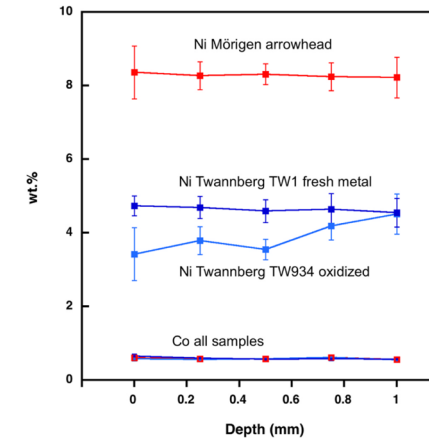
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- **Arrowhead not made of Twannberg meteorite!**



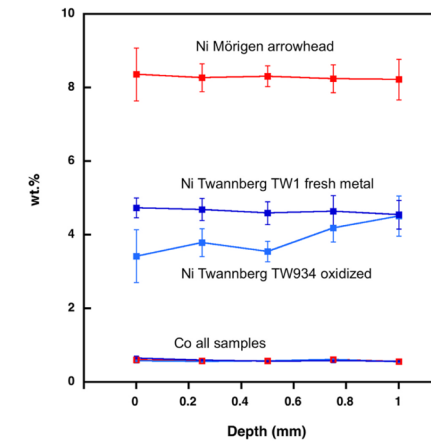
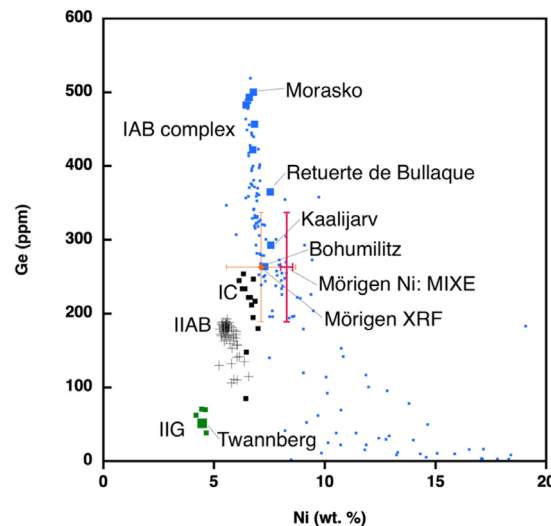
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- Retuerte de Bullaque (Spain)
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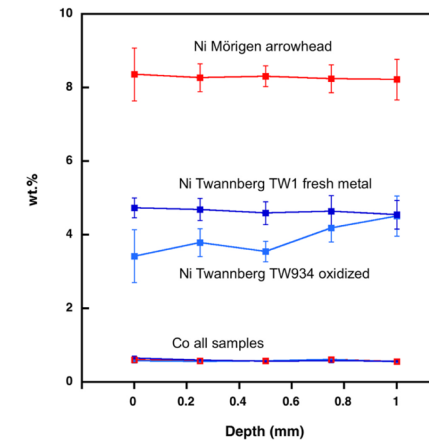
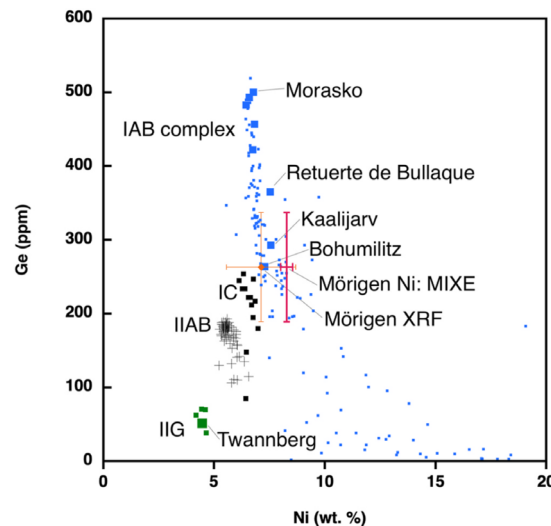
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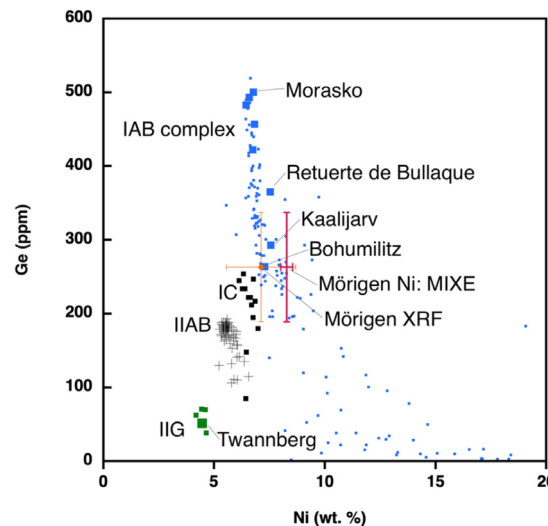
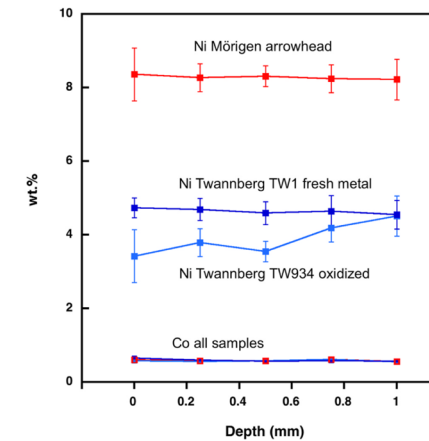
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- **Use and trade of iron meteorites** in Europe as early as the *Bronze Age* – 800 BCE (or earlier)
- **Transport and trade over 1.600 kilometers**
- Probably brought to Switzerland via **amber trade routes** from the Baltic region
- *High likelihood of additional similar discoveries!*

# Fibula: Sample and Study



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## Late-antique knob-bow fibula

- **excavated 2018** at Augusta Raurica (CH)
- **Leutkirch-type** fibula, **400-500 CE**

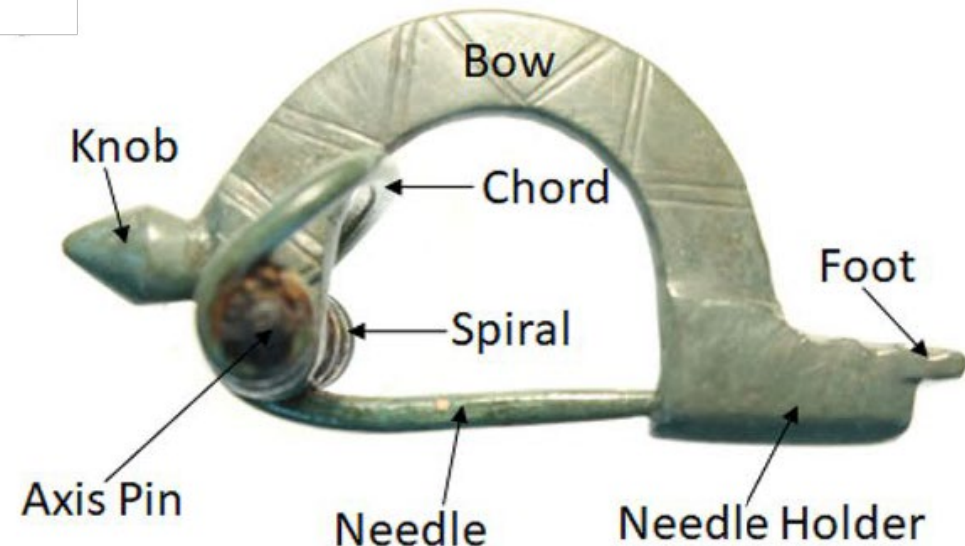
Biswas et al. *Heritage Science* (2023) 11:43  
<https://doi.org/10.1186/s40494-023-00880-0>

Heritage Science



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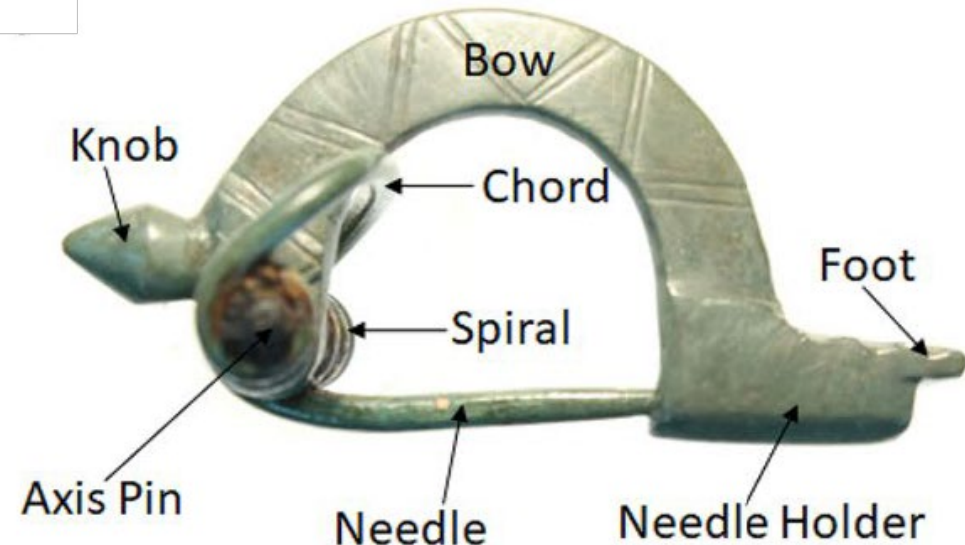
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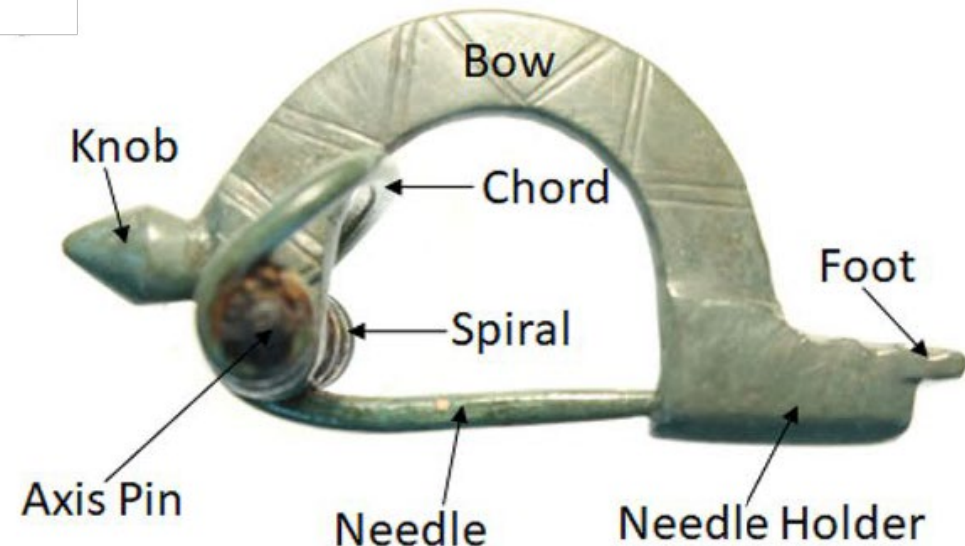
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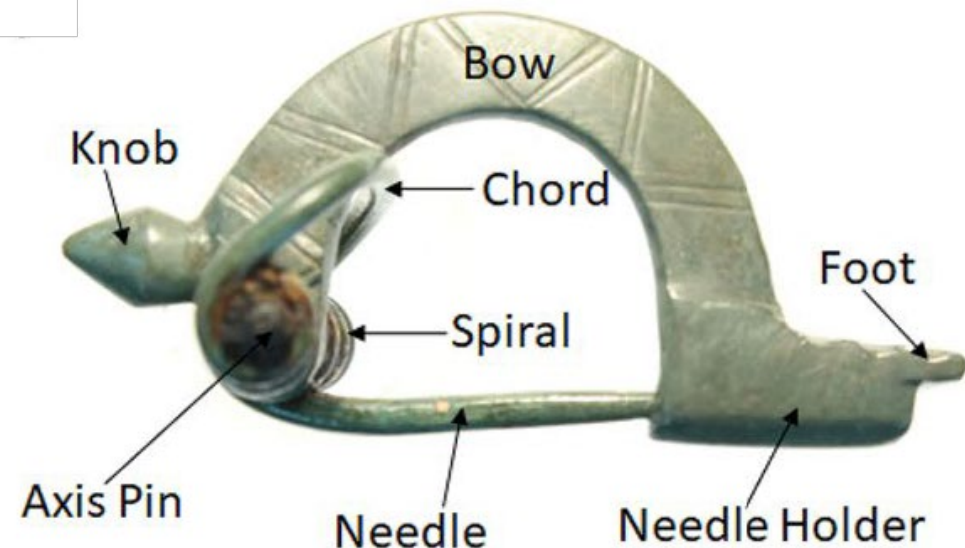
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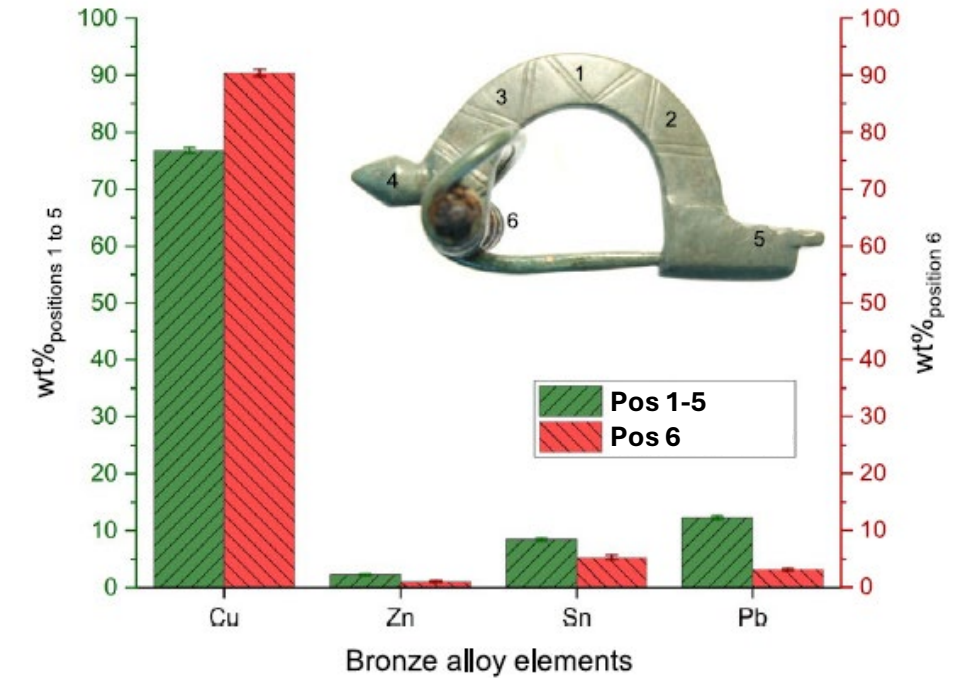


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## Elemental Composition

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- Position 6: **Low ratio of alloyants**



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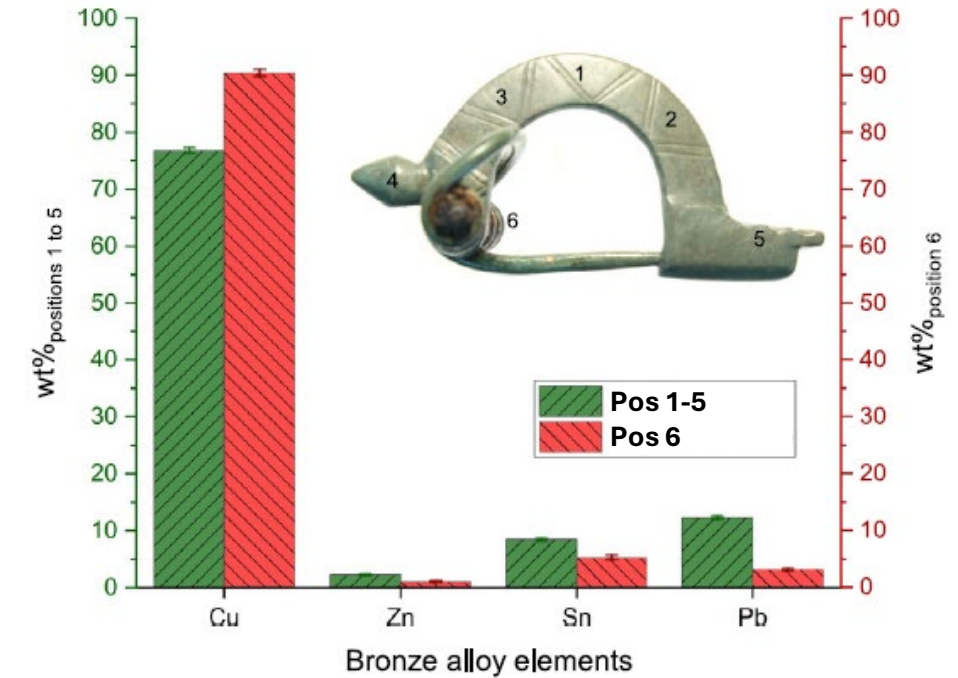
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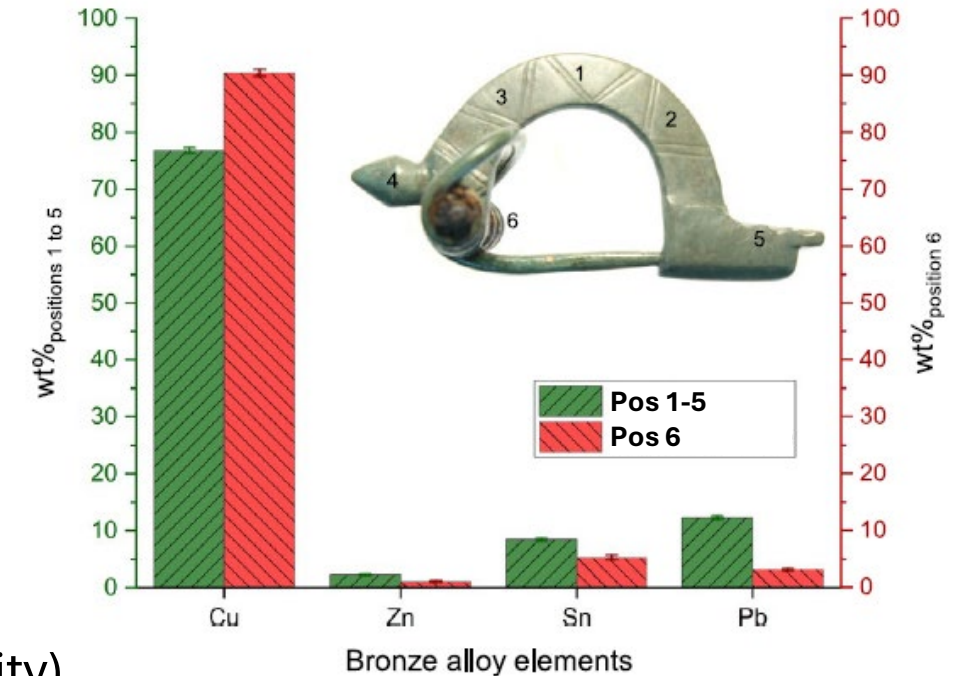
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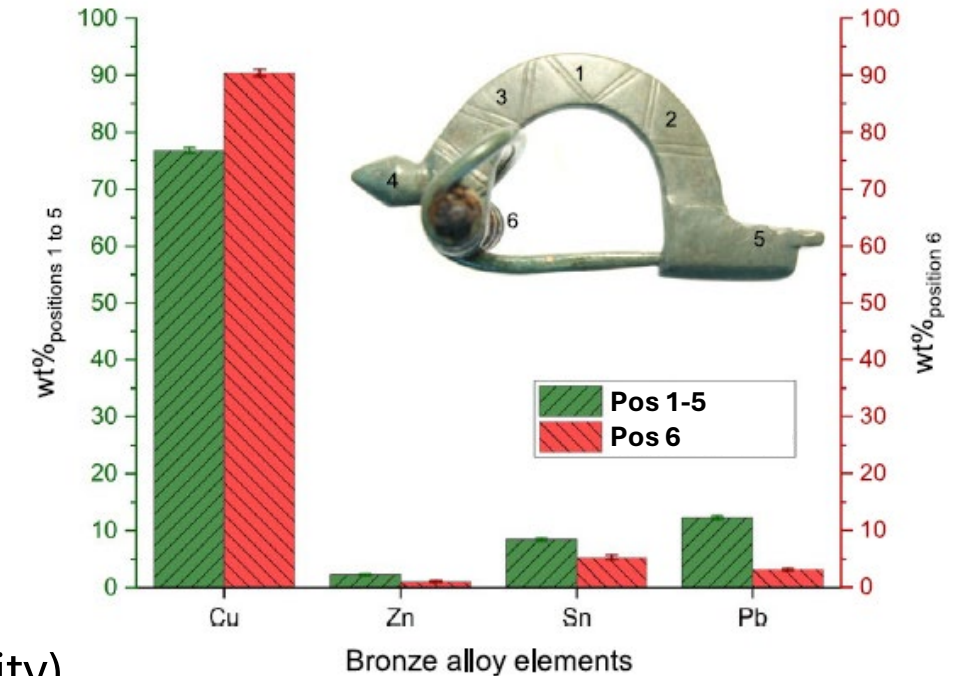
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## Conclusions

- **two-workpiece construction** reflecting **conscious alloy selection**
- **decentralized workshop** practice with **recycling** and **local mixing** of source metals



# MIXE 4 Batteries: Charge Carrier Ion Transport



## Goals:

- Tracking **charge carrier** ion **distributions**
- Mapping **parasitic ion** depositions (e.g. dendrite formation)

Journal of  
Materials Chemistry A



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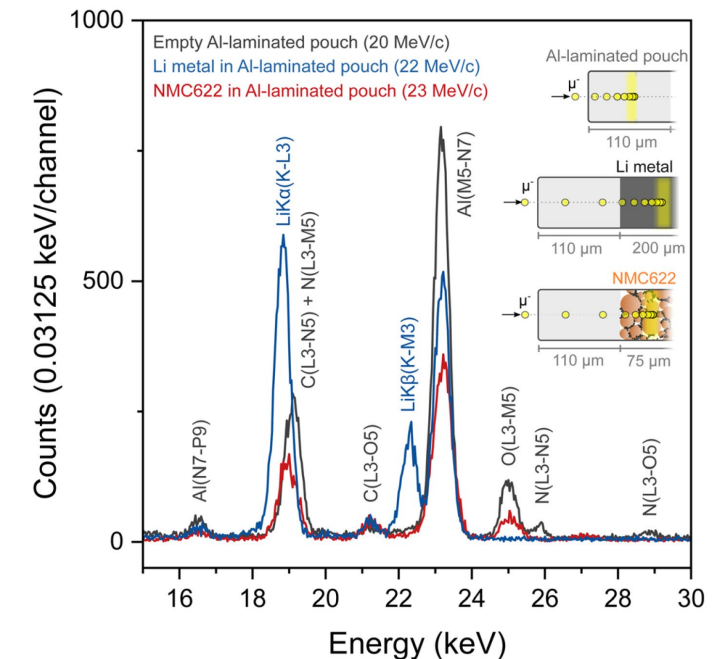
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- Li tracking in electrode material very challenging**
  - Low efficiency and capture probability** (e.g. ~16 in Ni vs. Li)
  - Masked by C-L<sub>β</sub> and N-L<sub>α</sub>**
  - Very promising first results for Na cells** (see also Part III)

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Materials Chemistry A



**Overcoming the probing-depth dilemma in spectroscopic analyses of batteries with muon-induced X-ray emission (MIXE)†**

Edouard Quérel,<sup>a</sup> Sayani Biswas,<sup>a,b</sup> Michael W. Heiss,<sup>b</sup> Lars Gerchow,<sup>b</sup> Qing Wang,<sup>a</sup> Ryo Asakura,<sup>a</sup> Gian Müller,<sup>a</sup> Debarchan Das,<sup>b</sup> Zurab Guguchia,<sup>b</sup> Fabian Hotz,<sup>b</sup> Gianluca Janka,<sup>b</sup> Andreas Knecht,<sup>b</sup> Hubertus Luetkens,<sup>b</sup> Charles Mielke, III,<sup>b</sup> Carlos Vigo,<sup>b</sup> Chennan Wang,<sup>b</sup> Stergiani Marina Vogiatzi,<sup>b,c</sup> Toni Shiroka,<sup>b</sup> Thomas Prokscha,<sup>b</sup> Katharina von Schoeler,<sup>c</sup> Shunsuke Asari,<sup>d</sup> I.-Huan Chiu,<sup>d</sup> Akira Sato,<sup>d</sup> Kazuhiko Ninomiya,<sup>e</sup> Megumi Niikura,<sup>f</sup> Corsin Battaglia,<sup>agh</sup> Alex Amato,<sup>b</sup> and Arndt Remhof<sup>b</sup>



# MIXE 4 Batteries: Stoichiometry of Electrodes



## Goal:

- Accurate **in-situ elemental quantification** of **electrode layers**



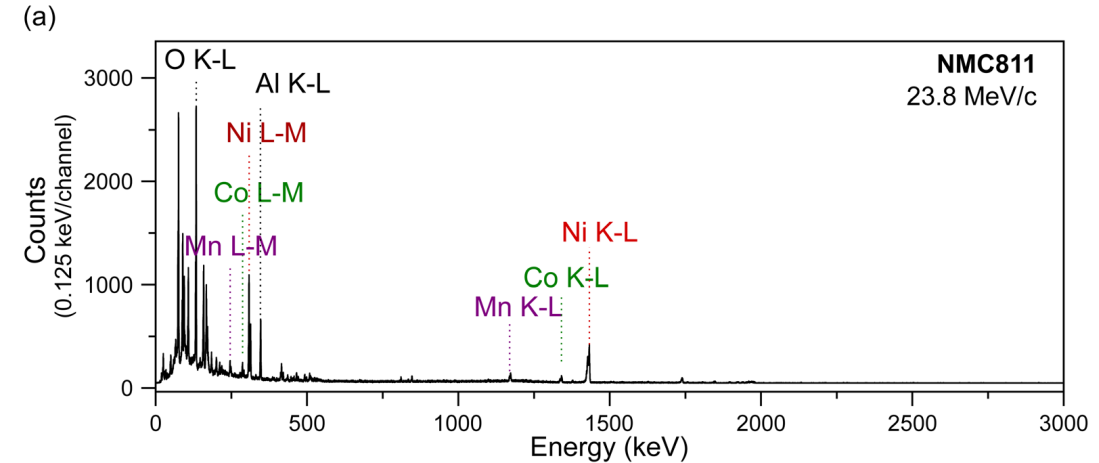
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- 3x **NMC** (1h each) with **different Ni:Mn:Co ratios**



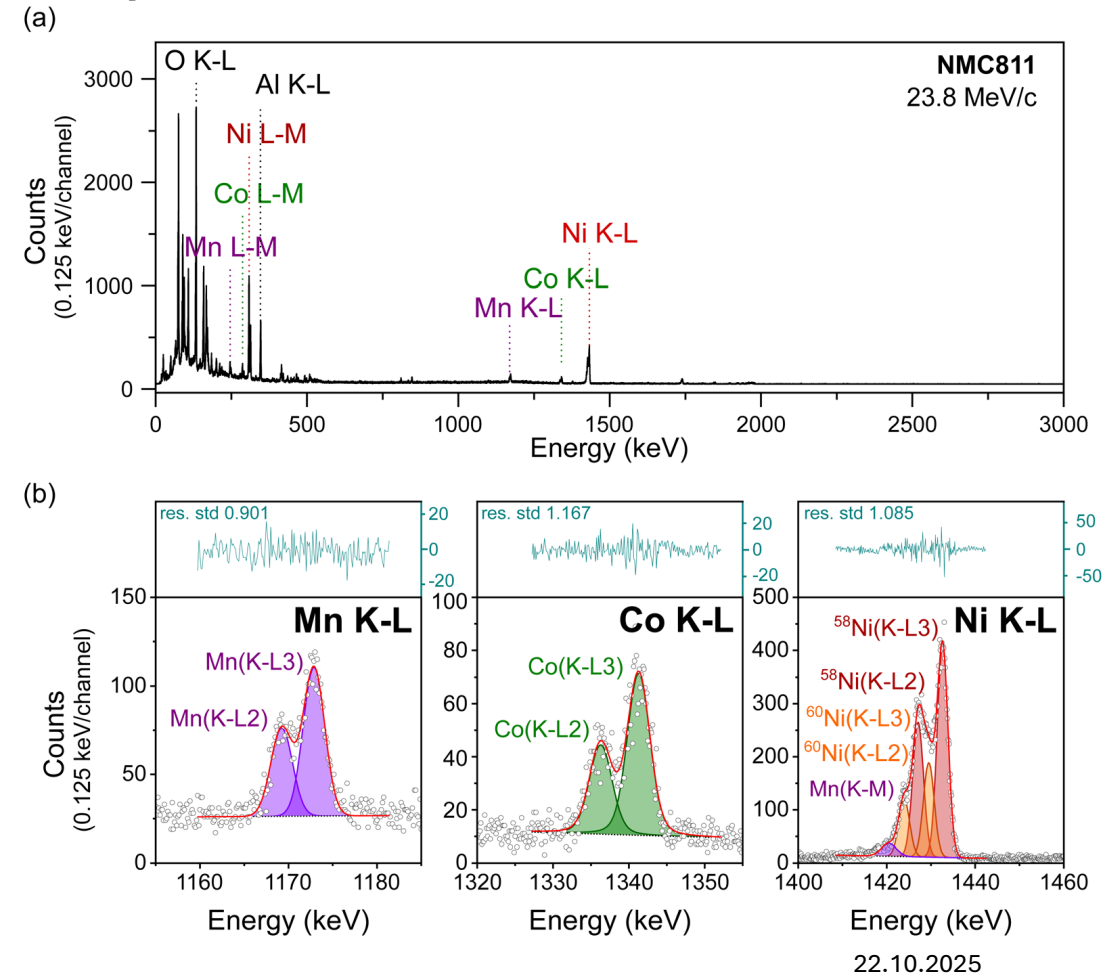
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**Result reproduces known elemental composition with high accuracy!**

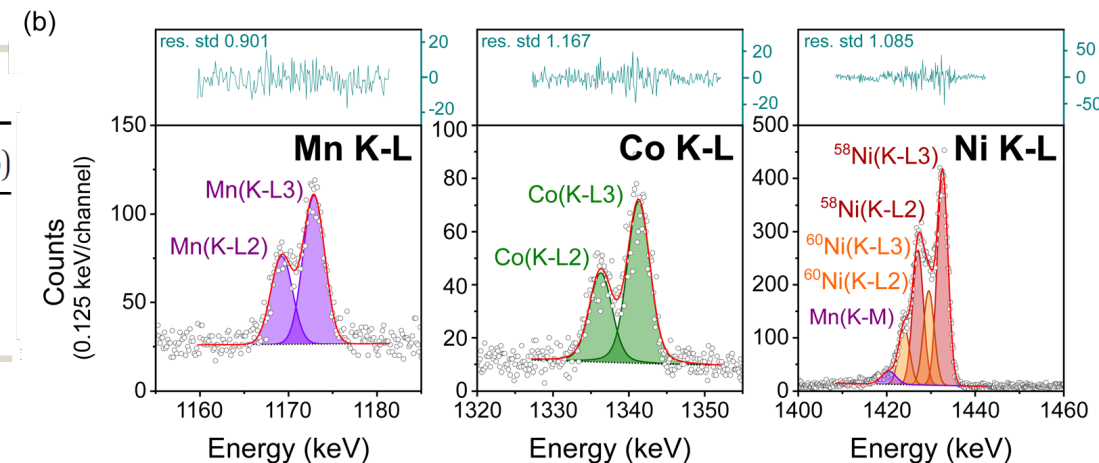
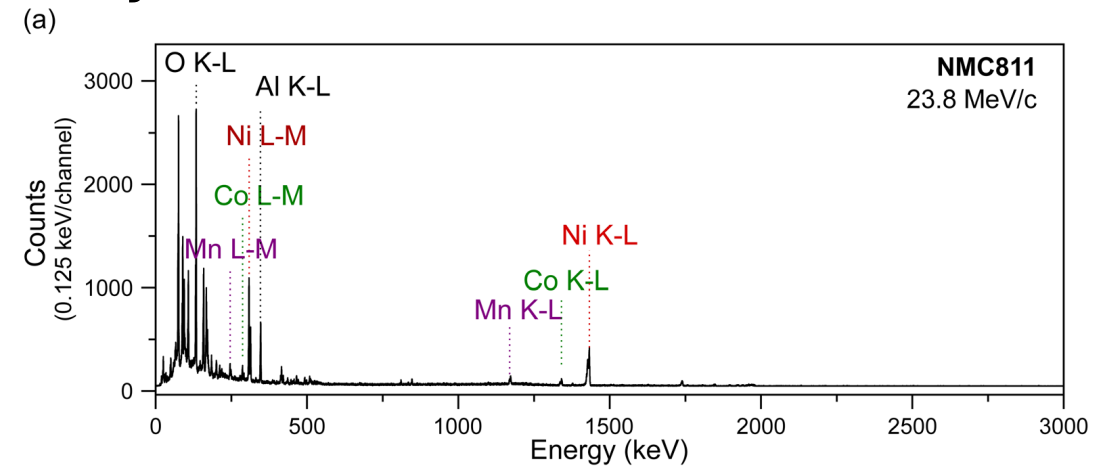


Table 1 Experimentally measured ratios for three different NMC electrodes

| NMC type | Nominal composition                                                         | Ni/(Ni + Mn + Co) | Mn/(Ni + Mn + Co) | Co/(Ni + Mn + Co) |
|----------|-----------------------------------------------------------------------------|-------------------|-------------------|-------------------|
| NMC111   | $\text{Li}_{1-x}\text{Ni}_{0.33}\text{Mn}_{0.33}\text{Co}_{0.33}\text{O}_2$ | $0.32 \pm 0.02$   | $0.35 \pm 0.02$   | $0.32 \pm 0.01$   |
| NMC622   | $\text{Li}_{1-x}\text{Ni}_{0.6}\text{Mn}_{0.2}\text{Co}_{0.2}\text{O}_2$    | $0.58 \pm 0.05$   | $0.21 \pm 0.02$   | $0.21 \pm 0.02$   |
| NMC811   | $\text{Li}_{1-x}\text{Ni}_{0.8}\text{Mn}_{0.1}\text{Co}_{0.1}\text{O}_2$    | $0.80 \pm 0.03$   | $0.103 \pm 0.005$ | $0.10 \pm 0.02$   |

# Part III

## **Muon Induced X-ray Emission** *Future Outlook: Tomography*



# MIXE-T(omography): Introduction

$\mu^-$



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$\mu^-$



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$\mu^-$

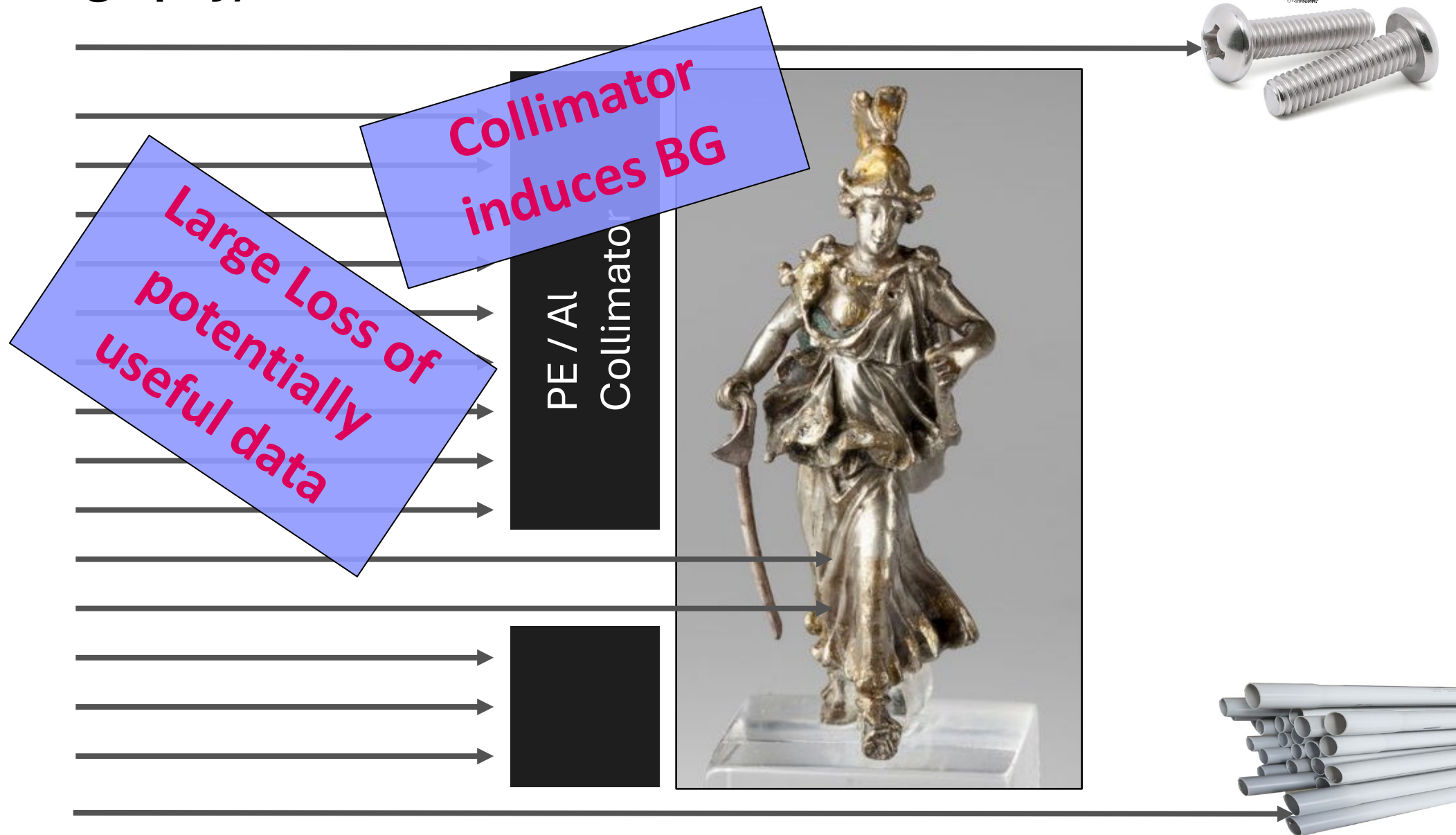
Large Loss of  
potentially  
useful data

PE / Al  
Collimator



# MIXE-T(omography): Introduction

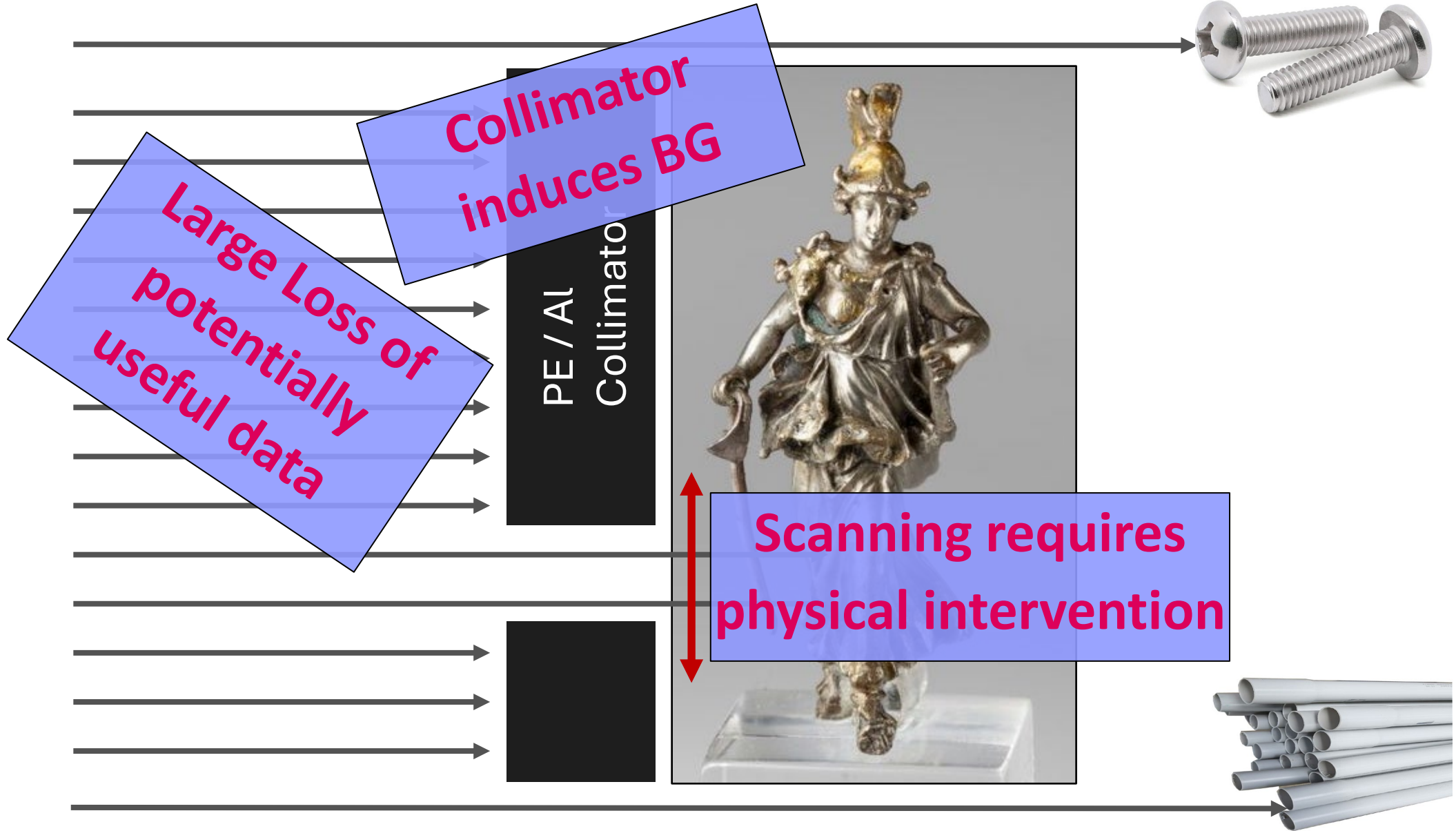
$\mu^-$





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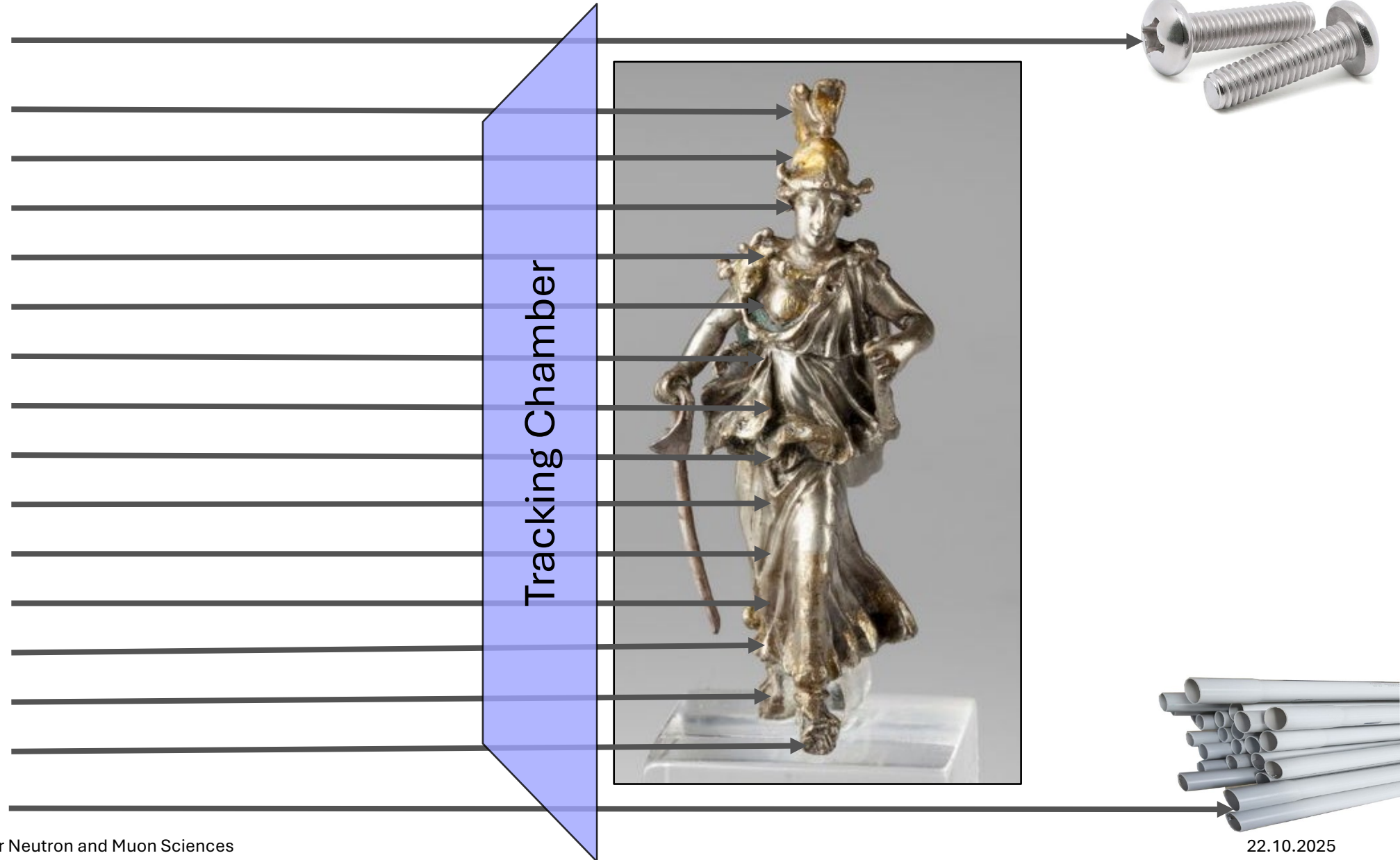
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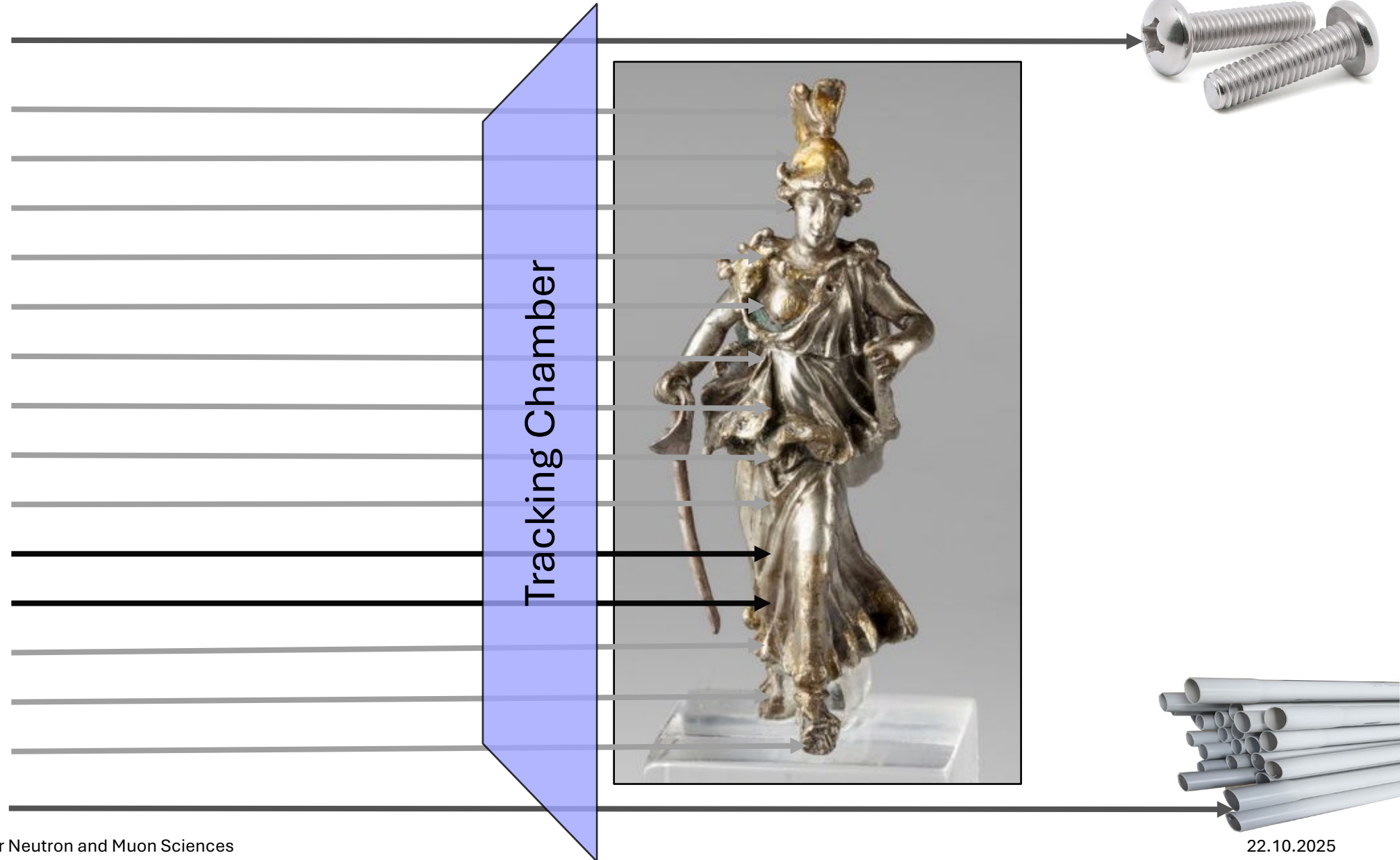
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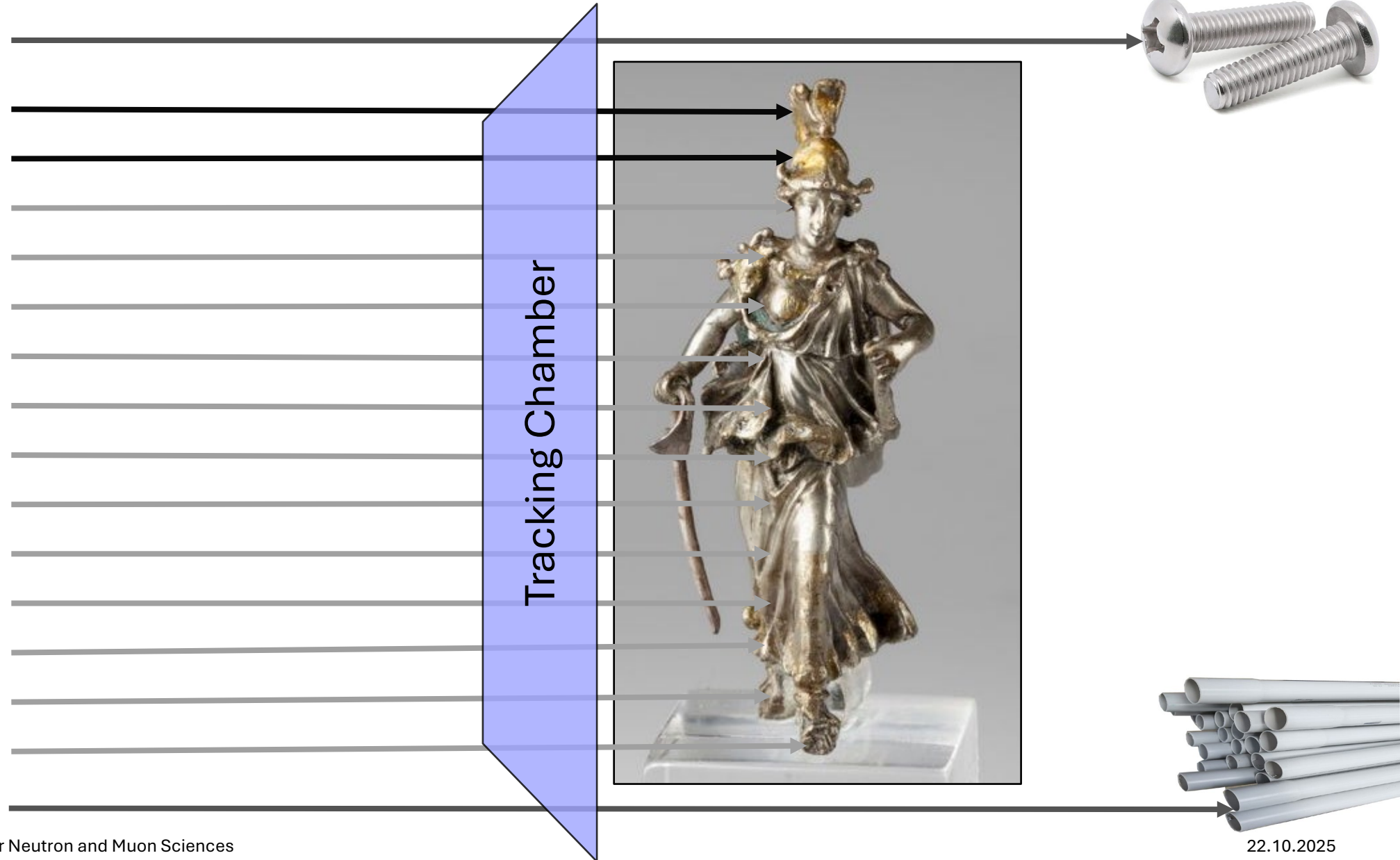
$\mu^-$





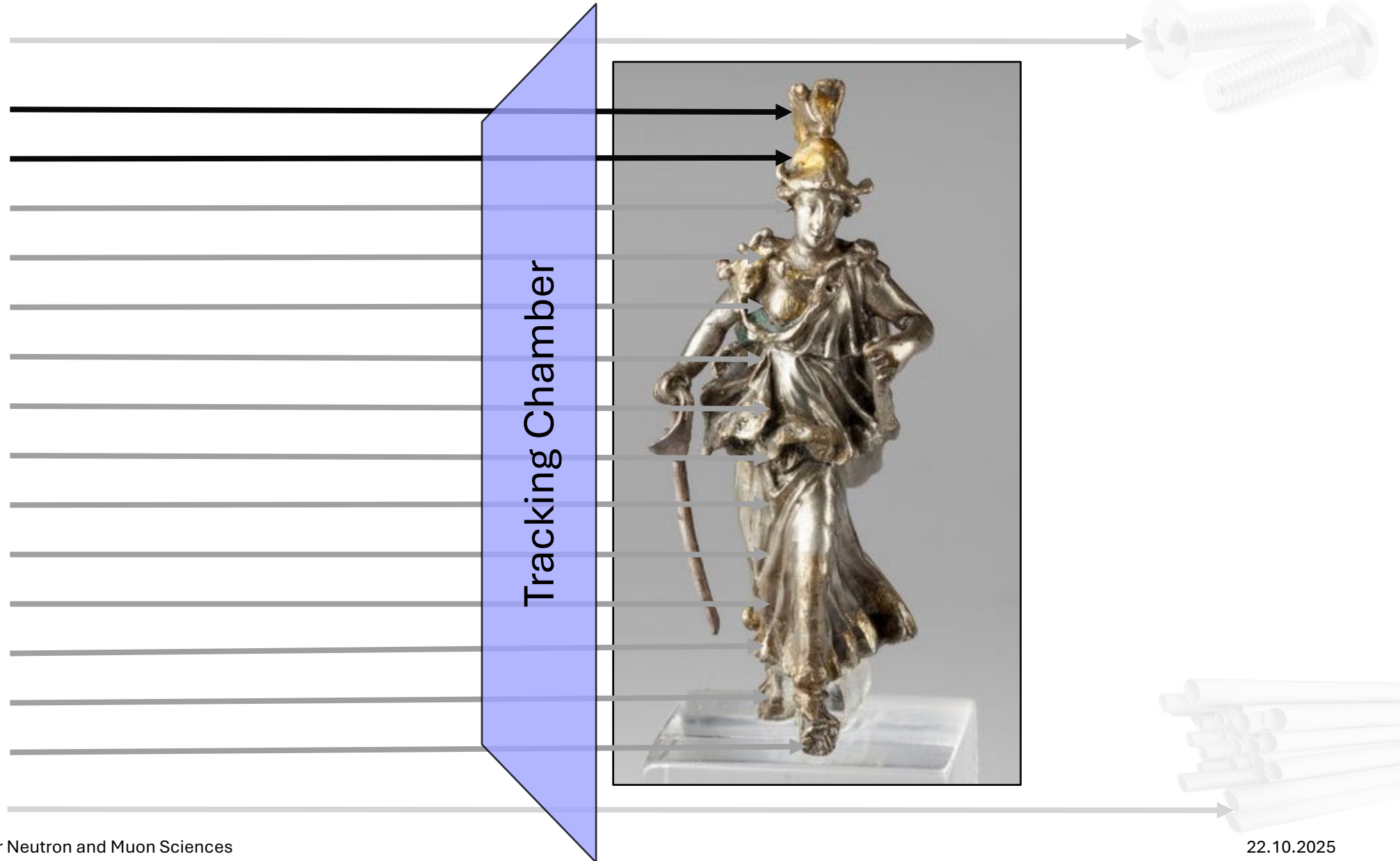
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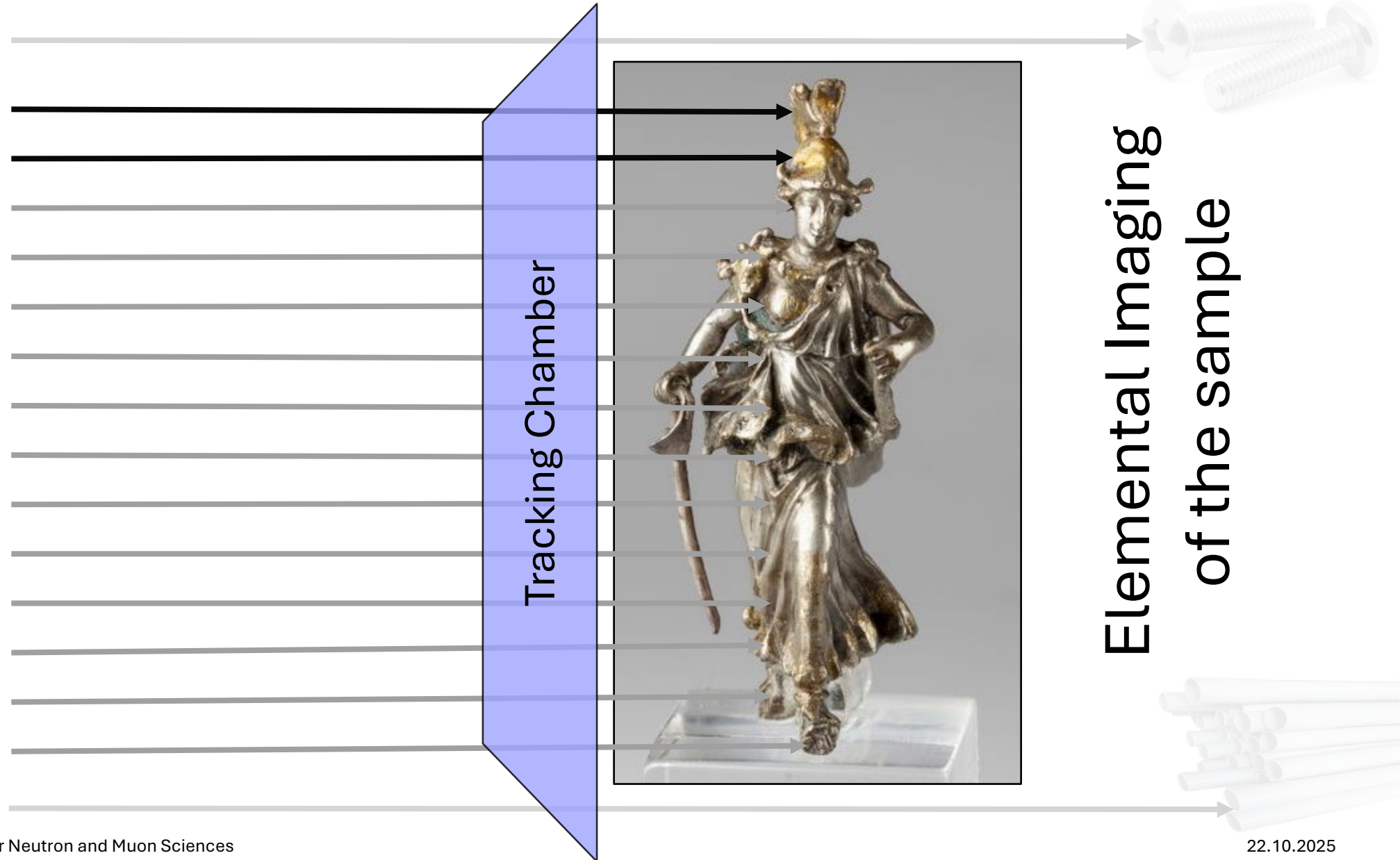
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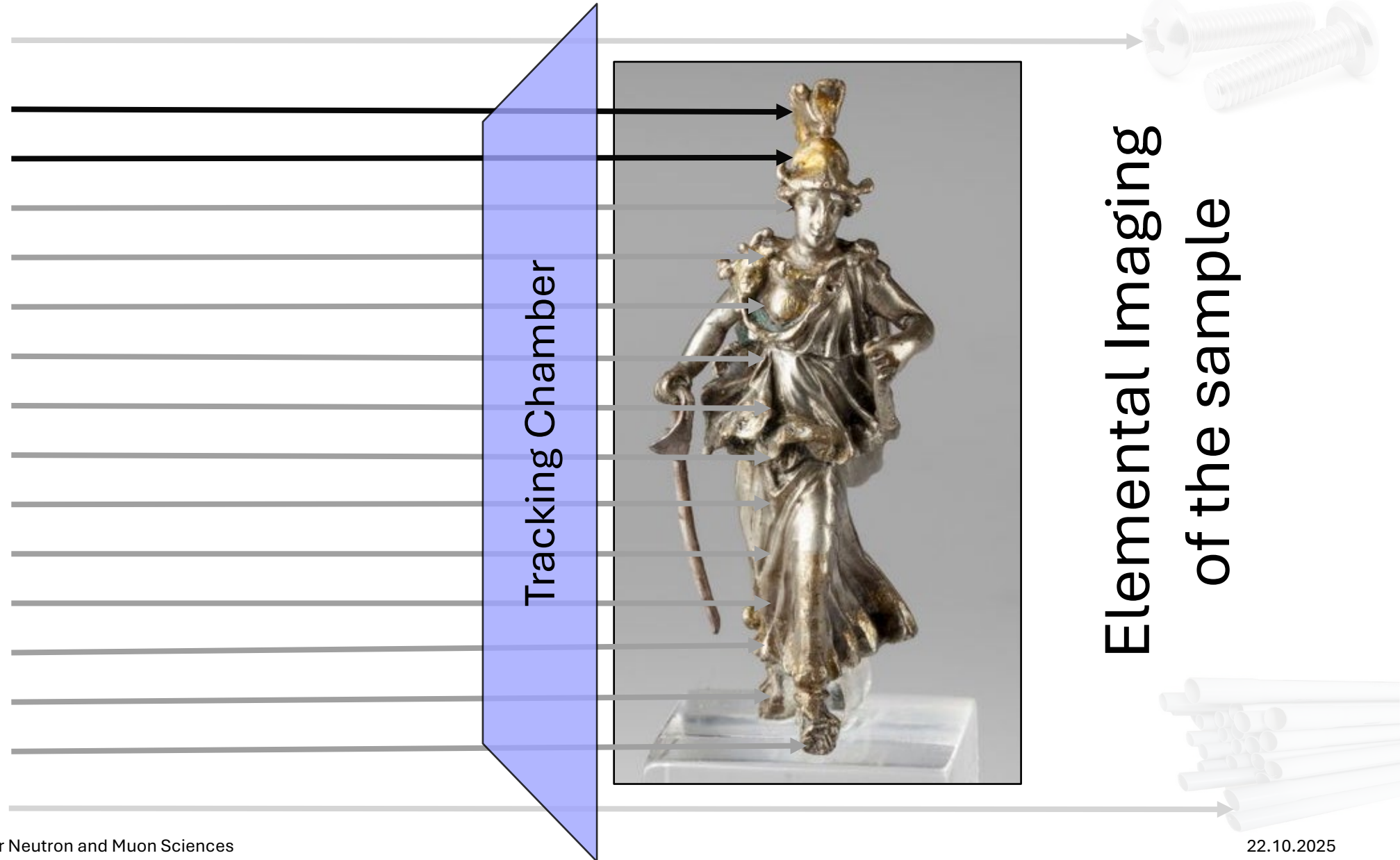
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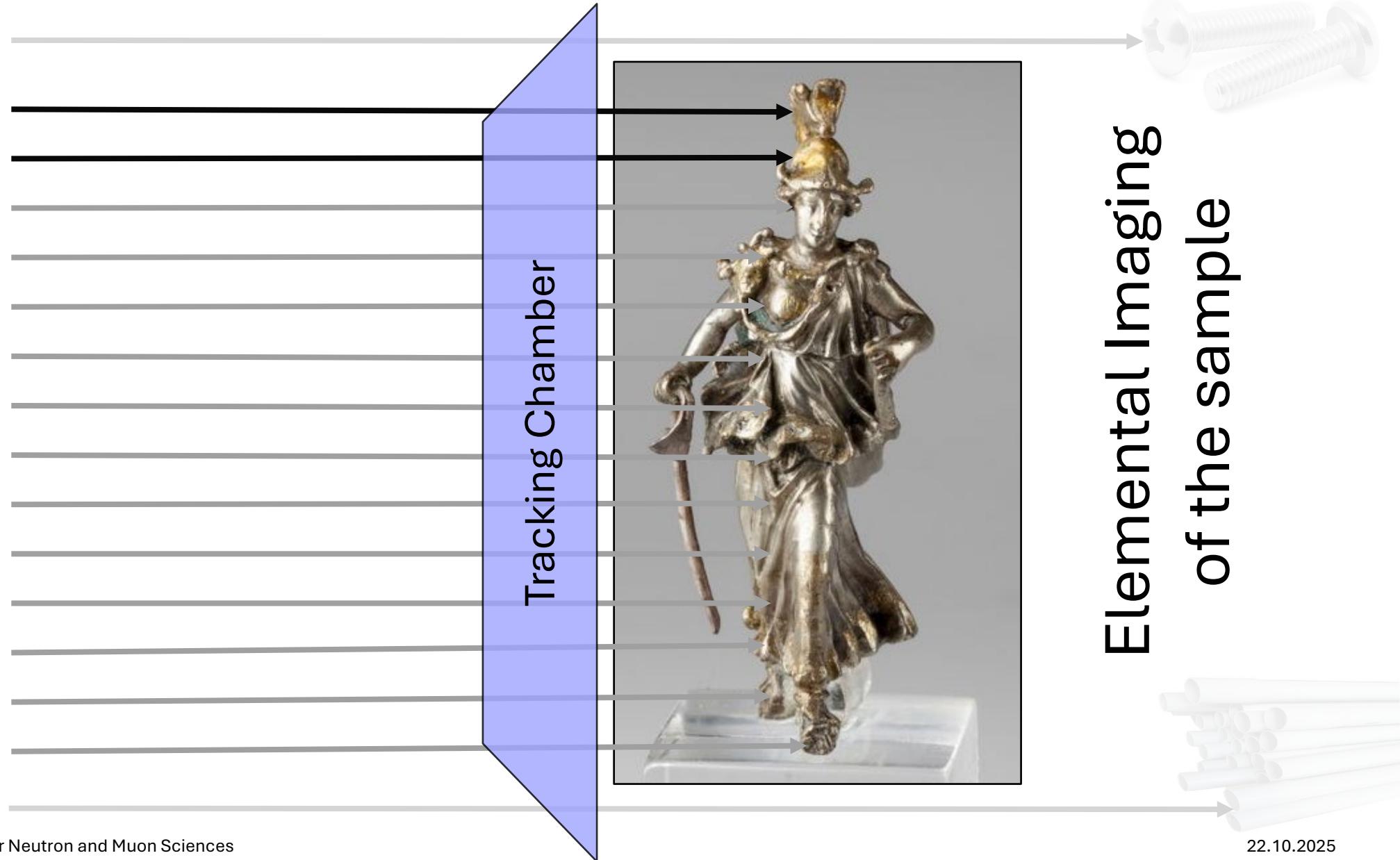
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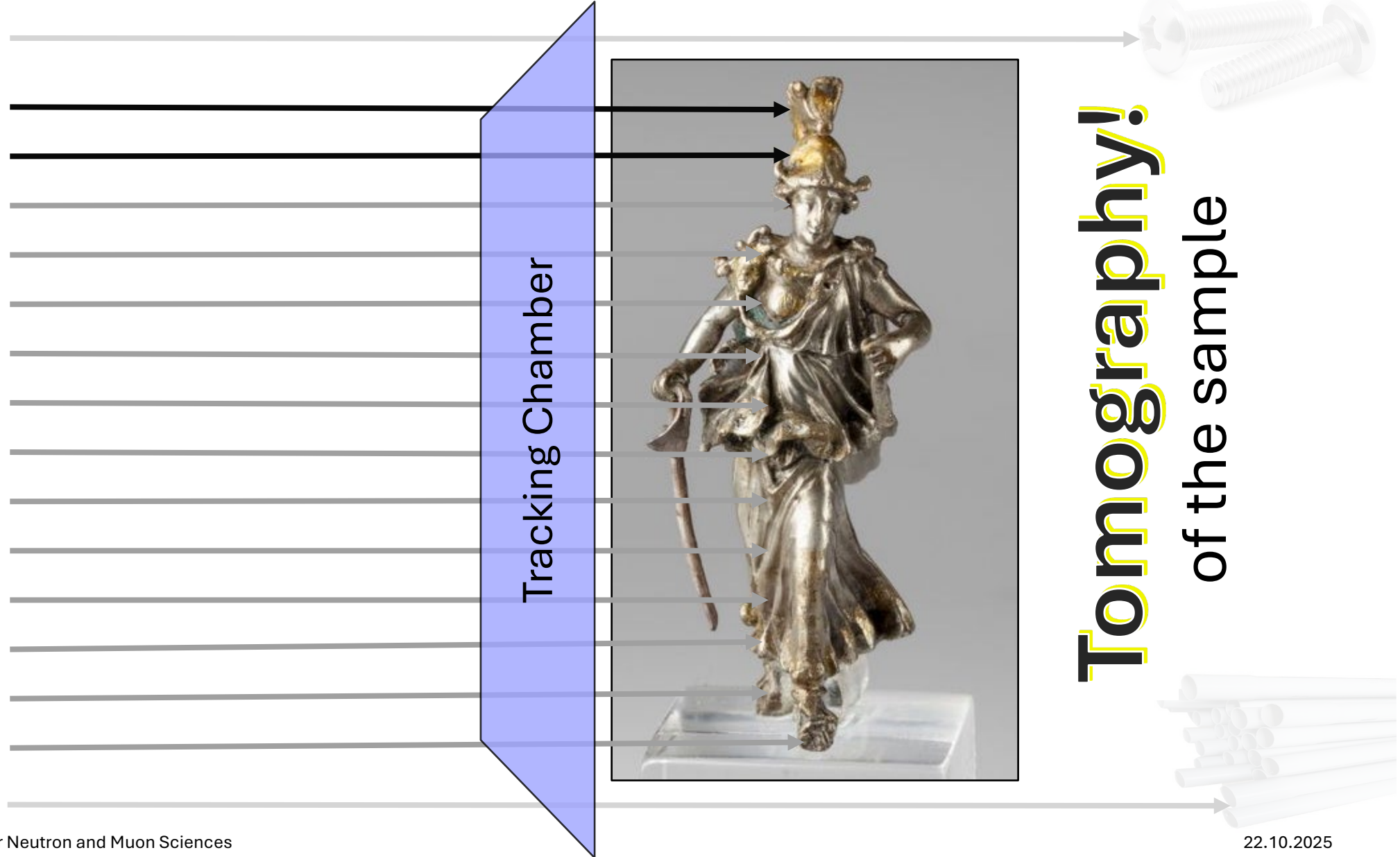
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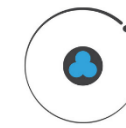


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$\mu^-$



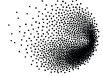
# MIXE-T(omography): Muon Tracking



HELSINKI  
INSTITUTE OF  
PHYSICS



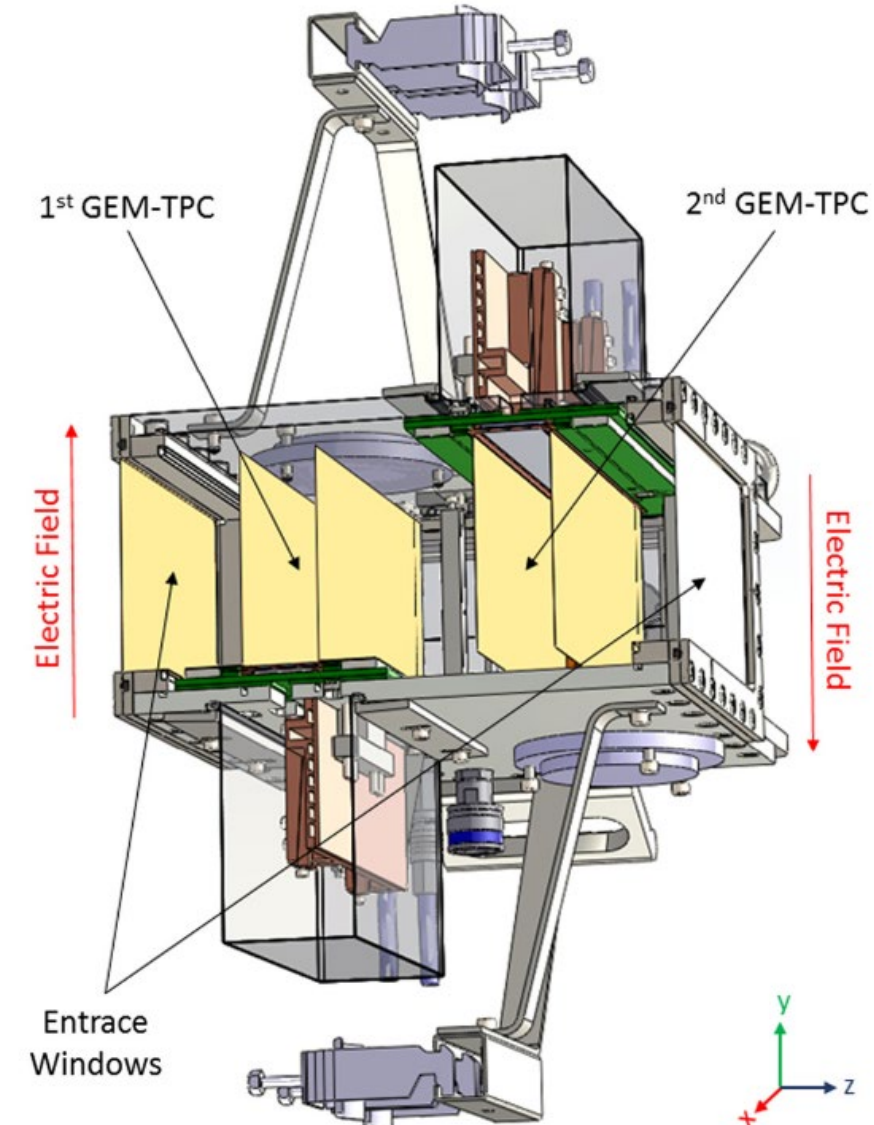
DRD1



PSI

## Adaptation of existing tracking detector prototype

- Twin **TPC** (Time-Projection-Chamber) (active area: **20x10cm<sup>2</sup>**)
- **Triple GEM** stack amplification stage
- **1D strip readout** – 0.4 mm pitch (1024 ch total)
- **Ultra-low material budget gas (He/CO<sub>2</sub>, up to 97:3)**



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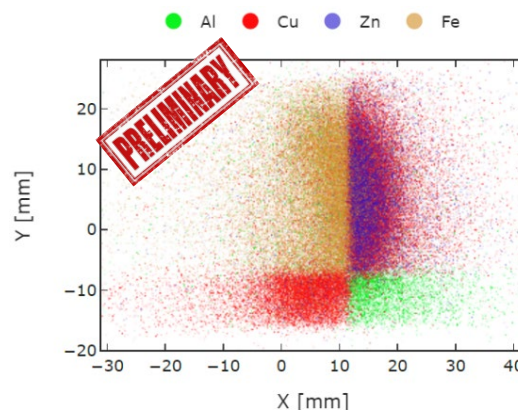
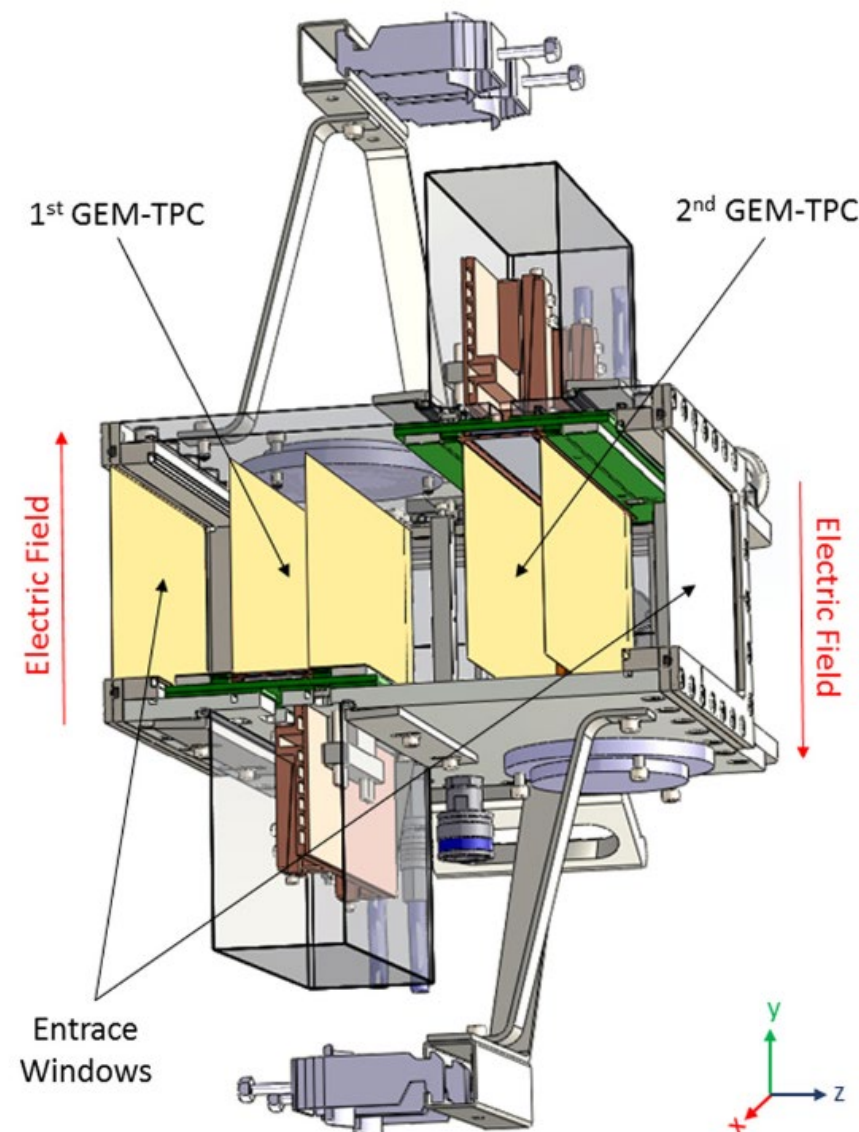
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- **Ultra-low material budget gas (He/CO<sub>2</sub>, up to 97:3)**

## Very encouraging **results**:

- Spatial Resolution >50MeV/c – X/Y: **~1 mm** ; Z: **~0.1 mm**
- Limited by large gas volume

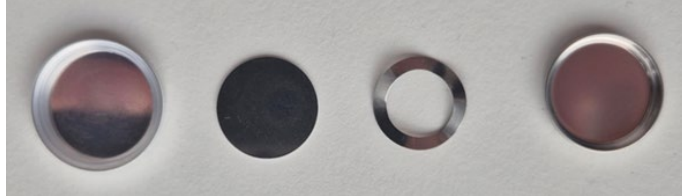
*Specialized prototype detector in development!*





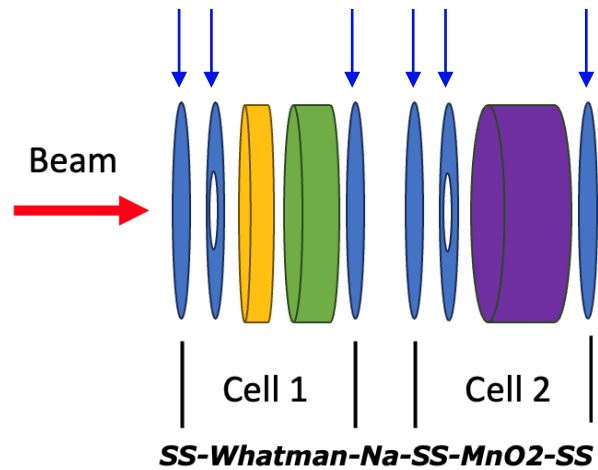
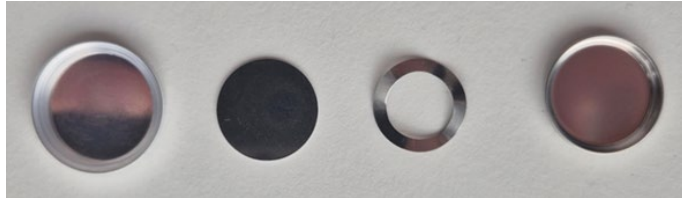
# MIXE-T(omography): Battery tomography PoC

*coin cell battery analogue*



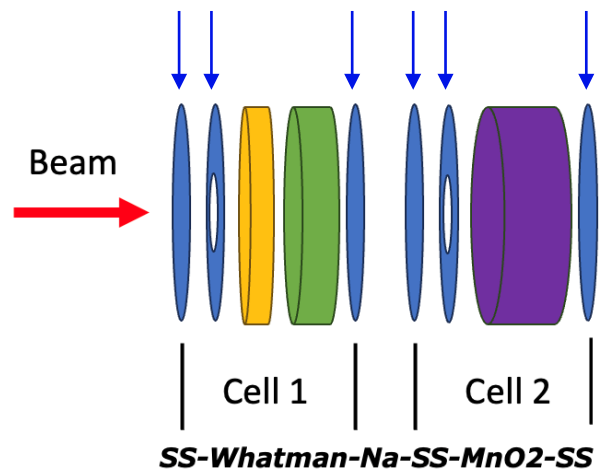
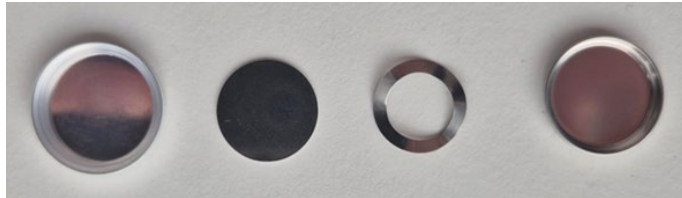
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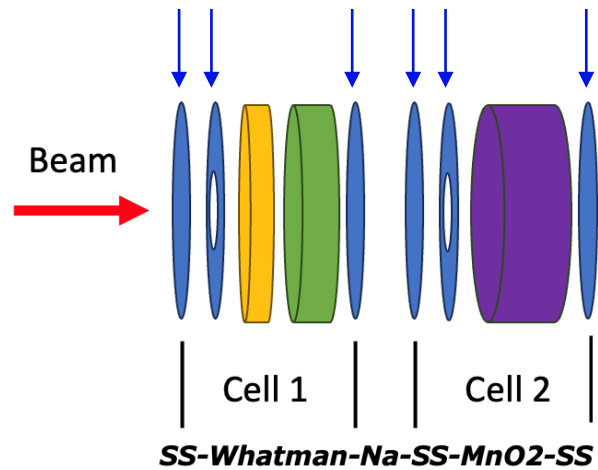
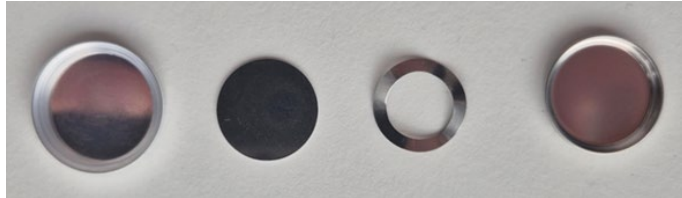
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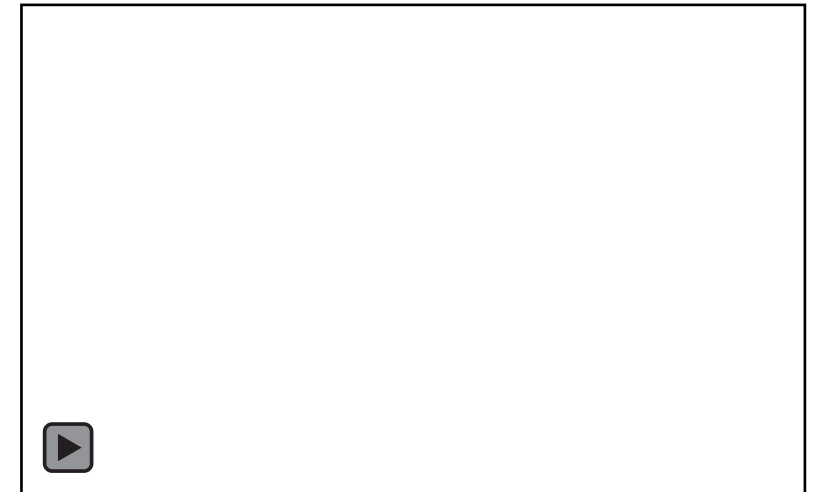
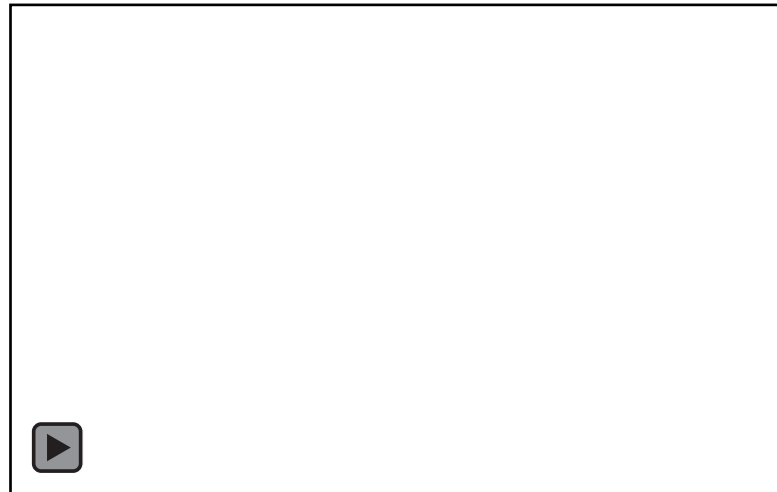
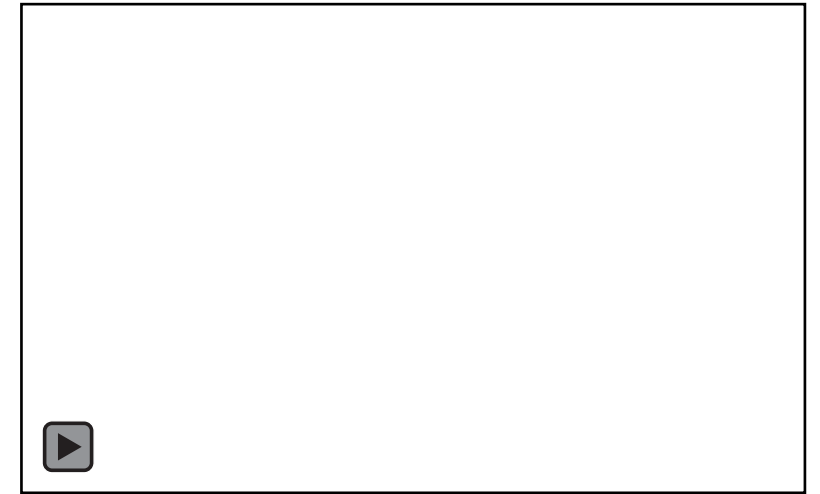
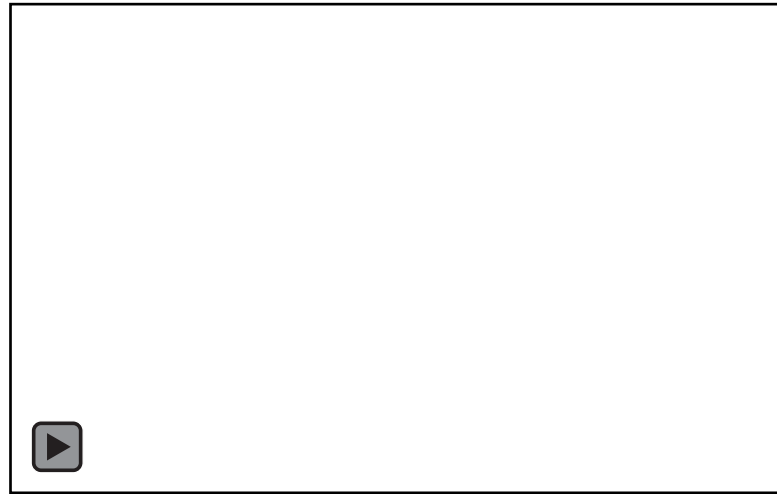
30/32/34/39/46/49/51/55/60  
MeV/c

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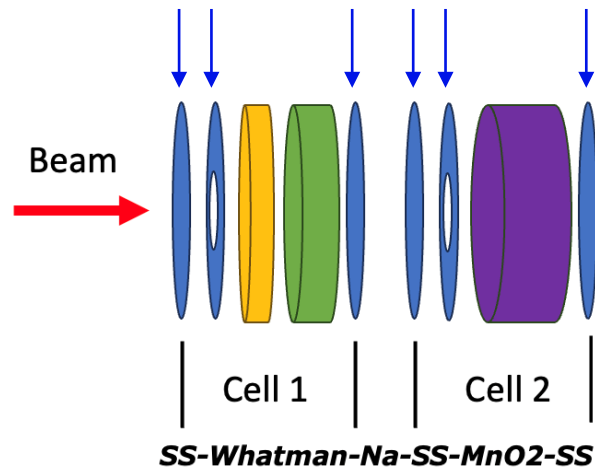
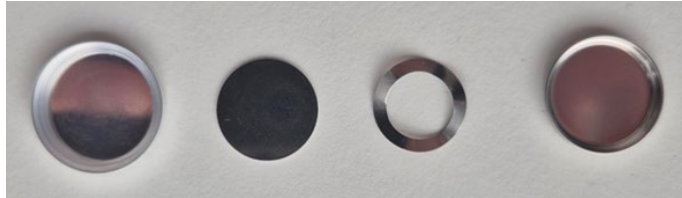
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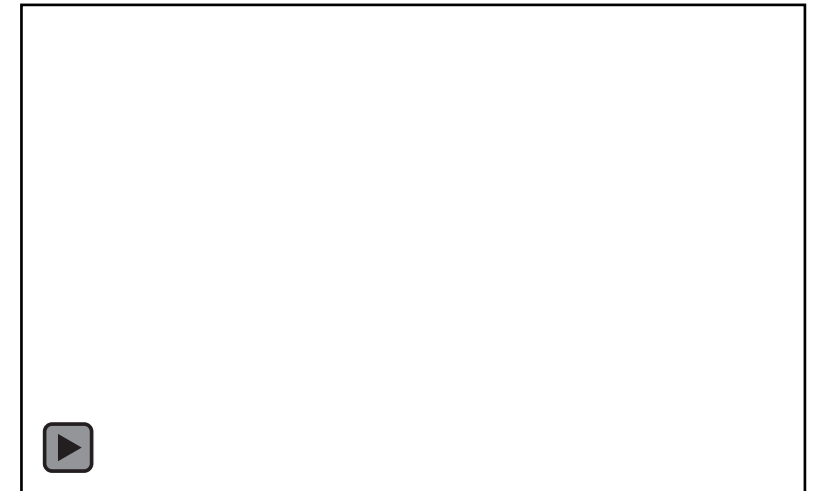
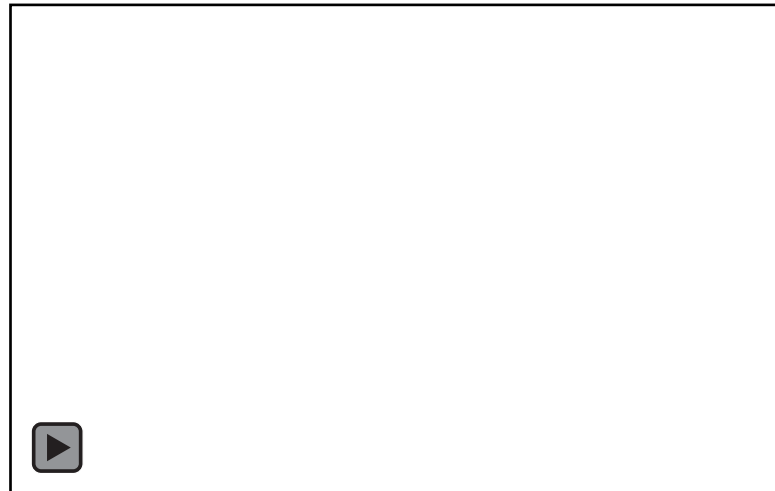
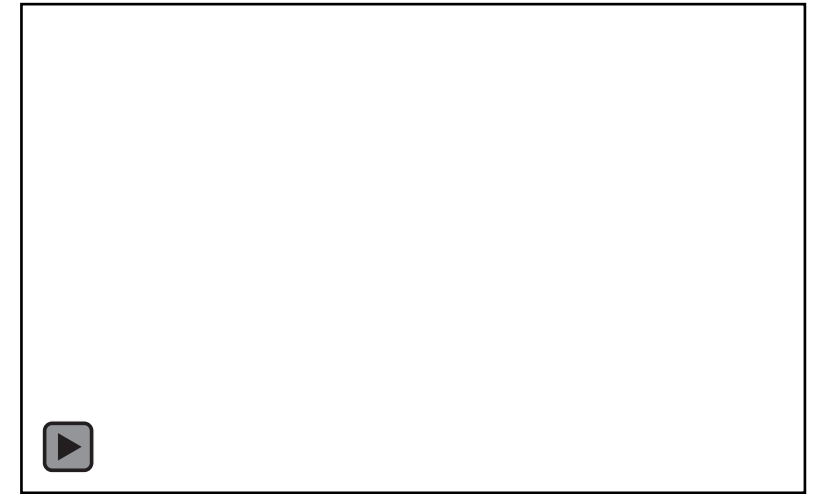
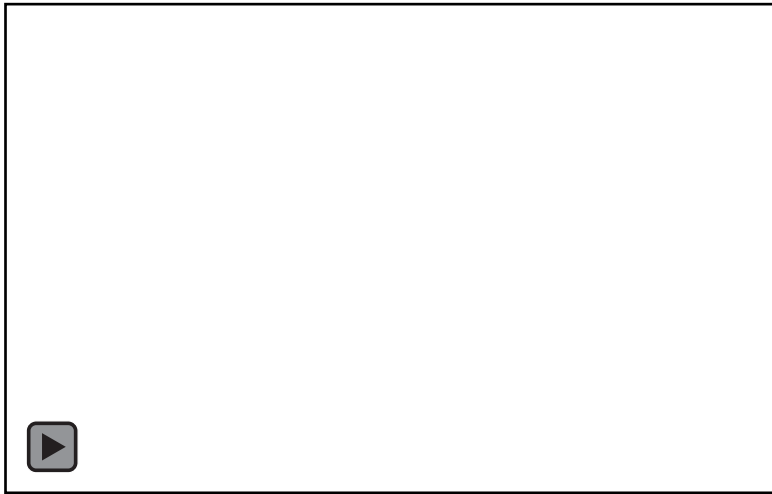


# MIXE-T(omography): Battery tomography PoC

*coin cell battery analogue*



30/32/34/39/46/49/51/55/60  
MeV/c  
+interpolation



# Thank you for your attention!



**GIANT/MIXE** is transitioning  
to user instrument!

**Open call** for user **proposals** for  
(September) 2026 measurement  
campaign will open **Nov 1!**

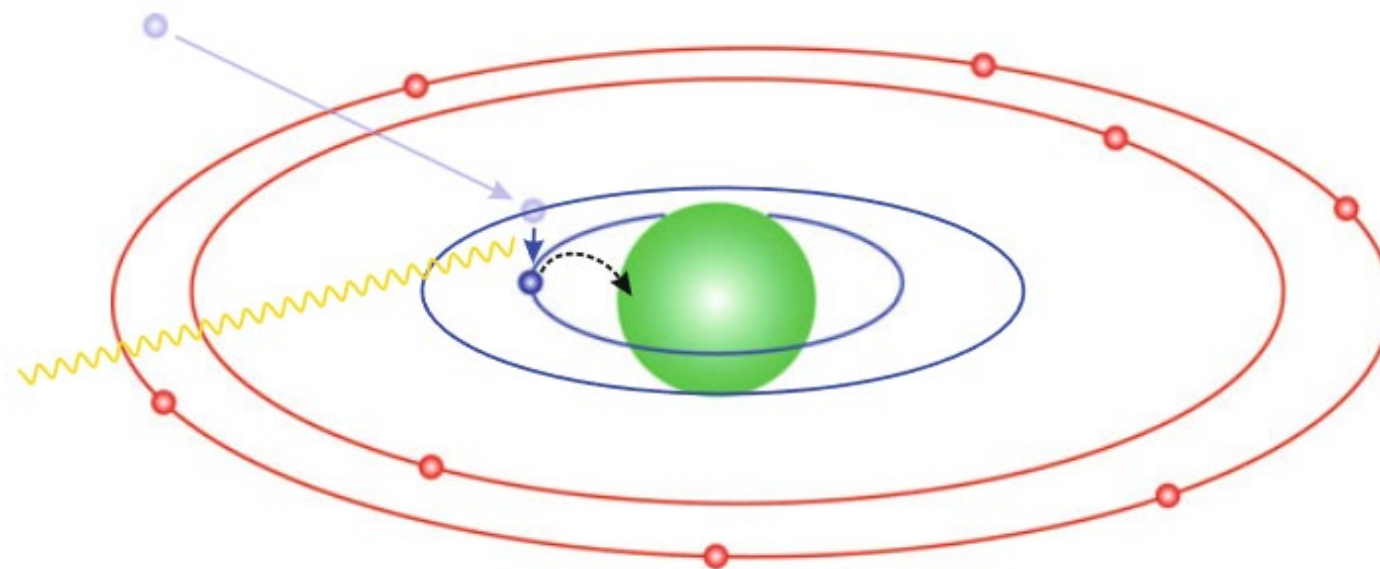
*Please don't hesitate to contact  
us if you are interested!*

[michael.heiss@psi.ch](mailto:michael.heiss@psi.ch)

<https://www.psi.ch/en/smus/calls>

# Backup

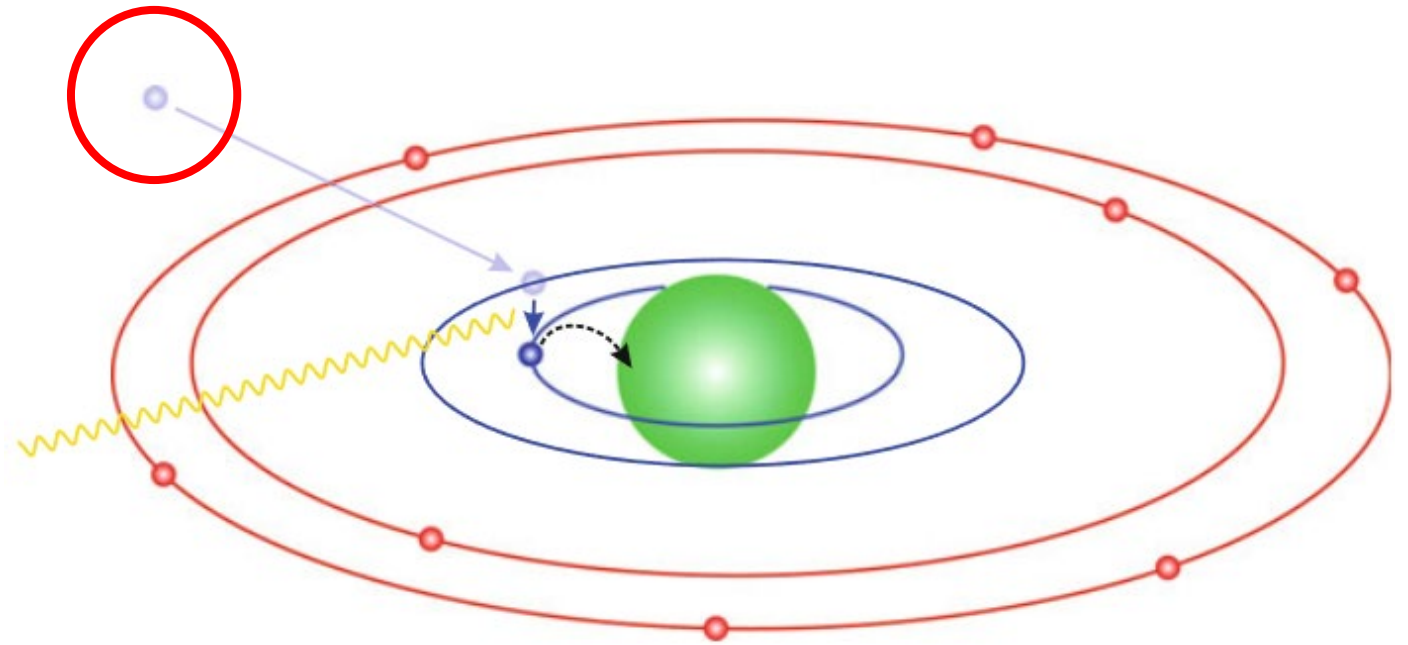
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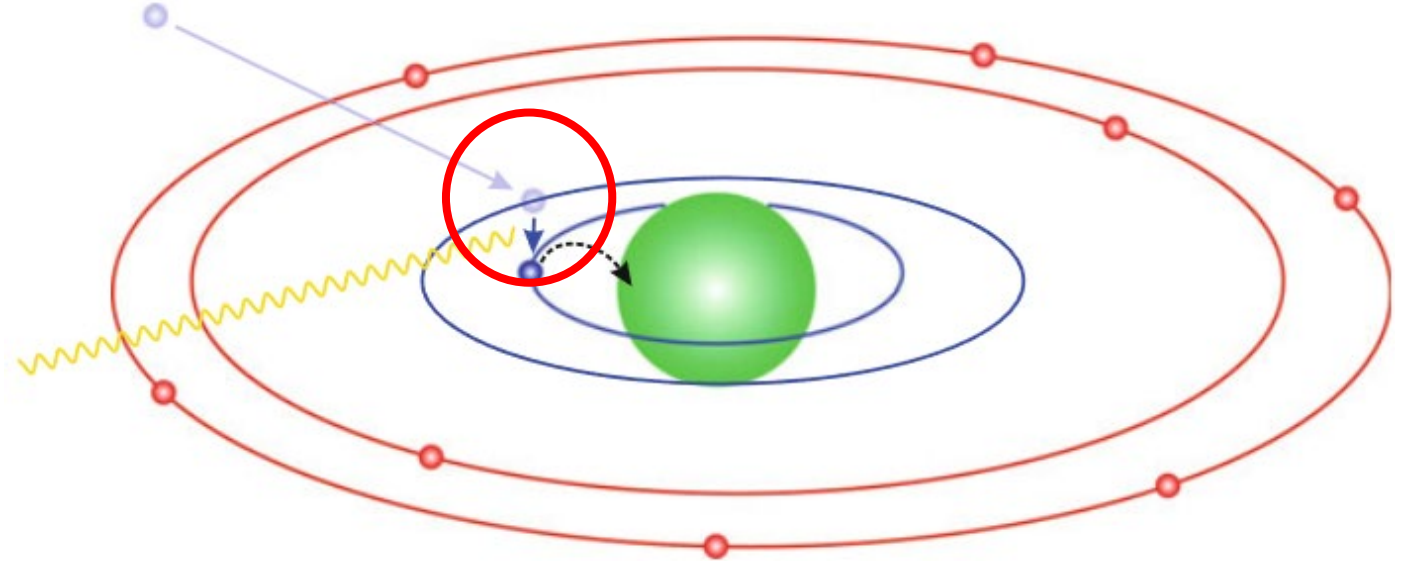
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- Muon is captured by the atom in higher excited states around:

$$n_{\mu} \approx \sqrt{\frac{m_{\mu}}{m_e}} \approx 14$$



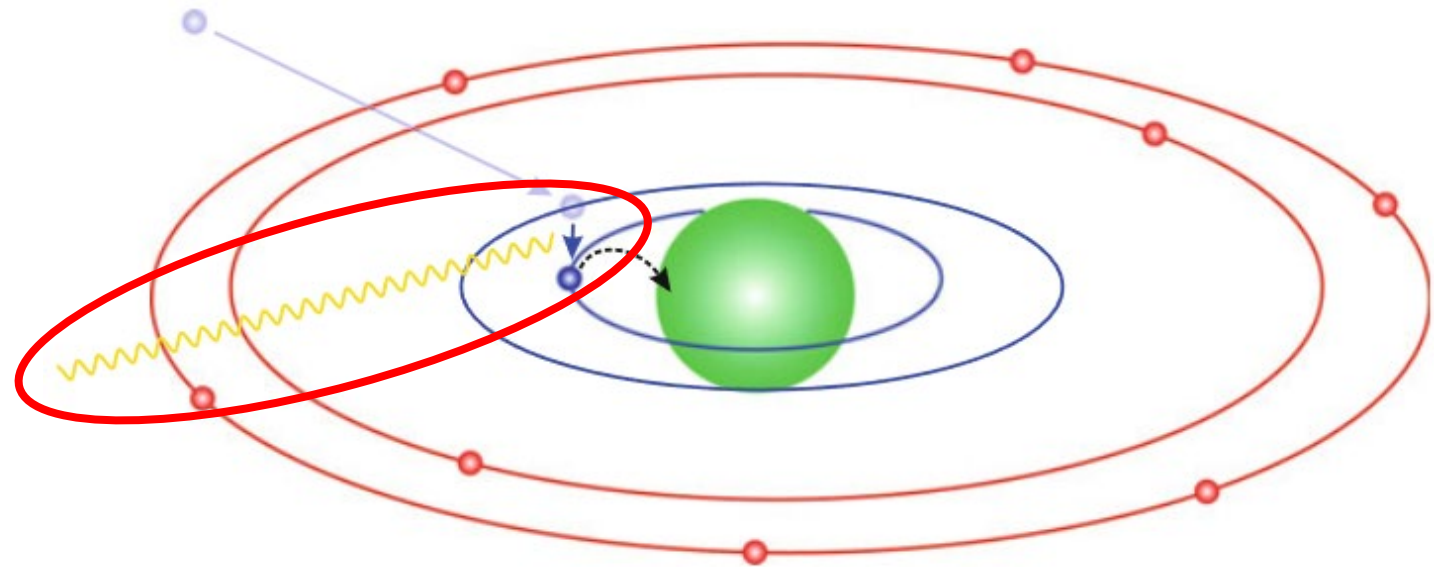
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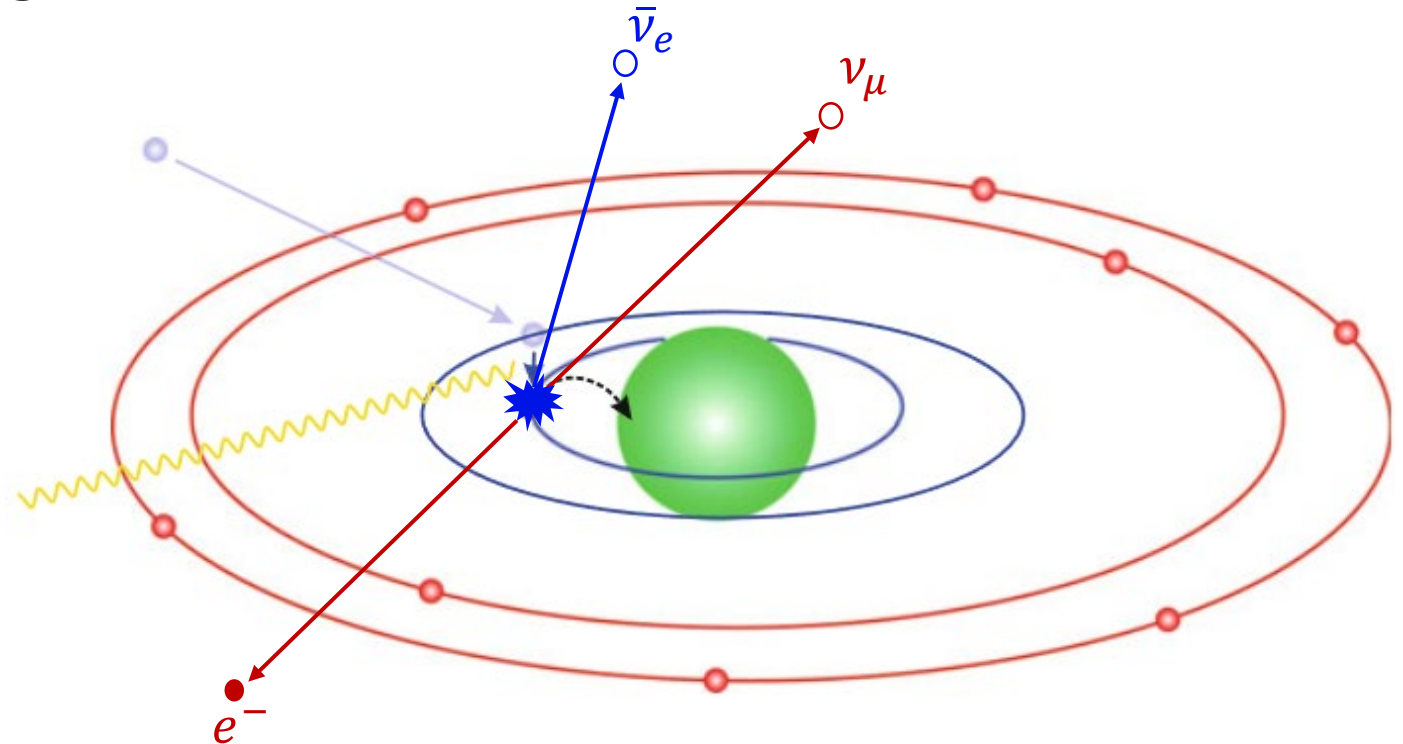
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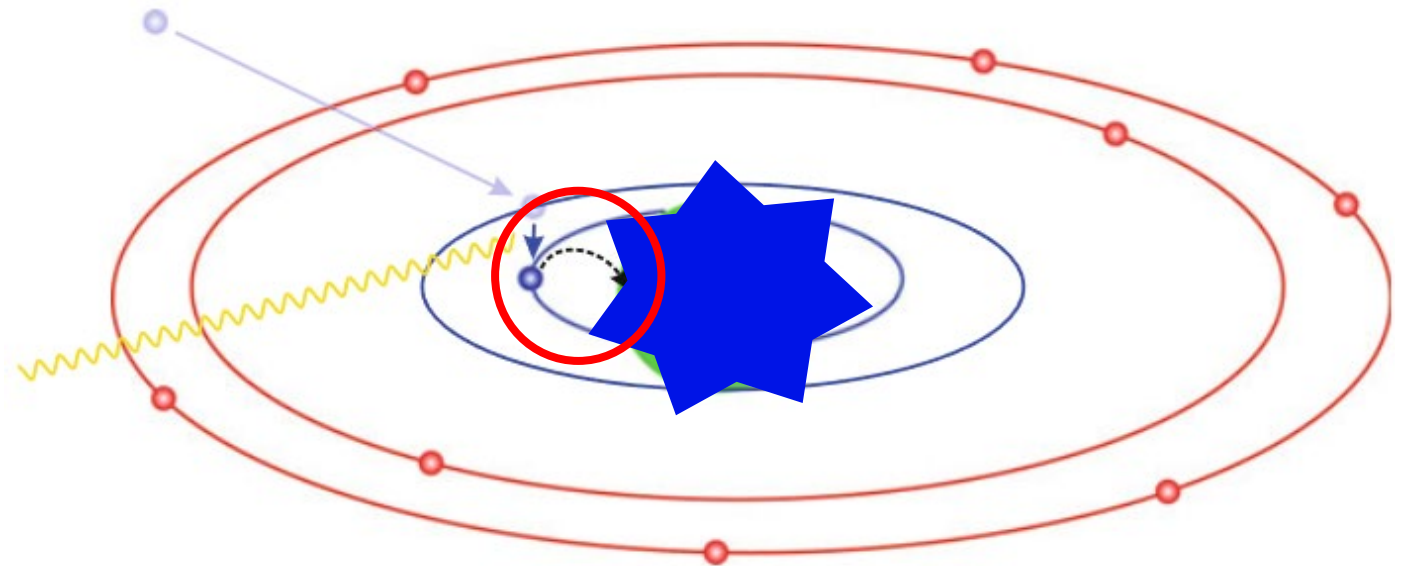
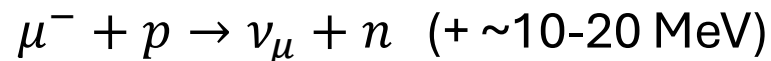
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or
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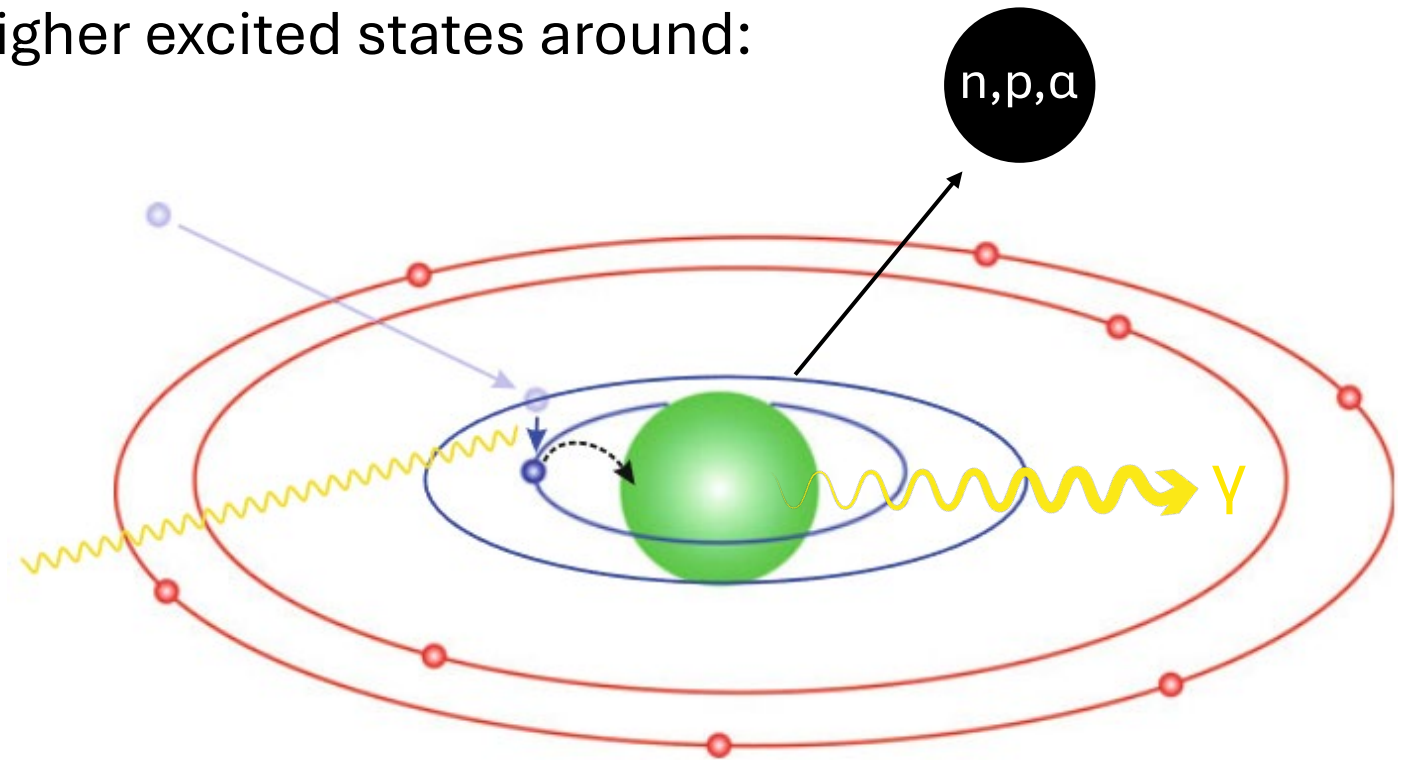
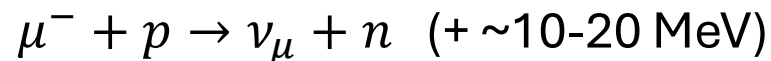
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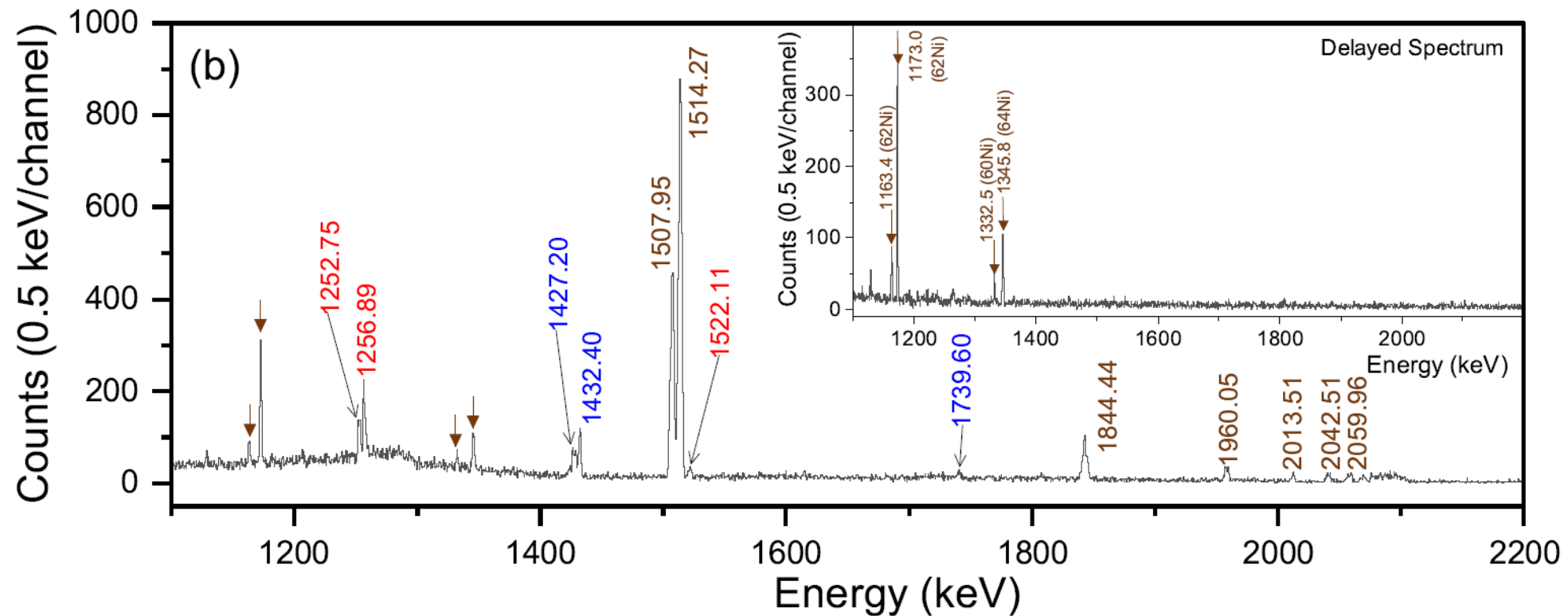
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- Nucleus loses excess energy by emitting (some combination of) n, p, α, γ

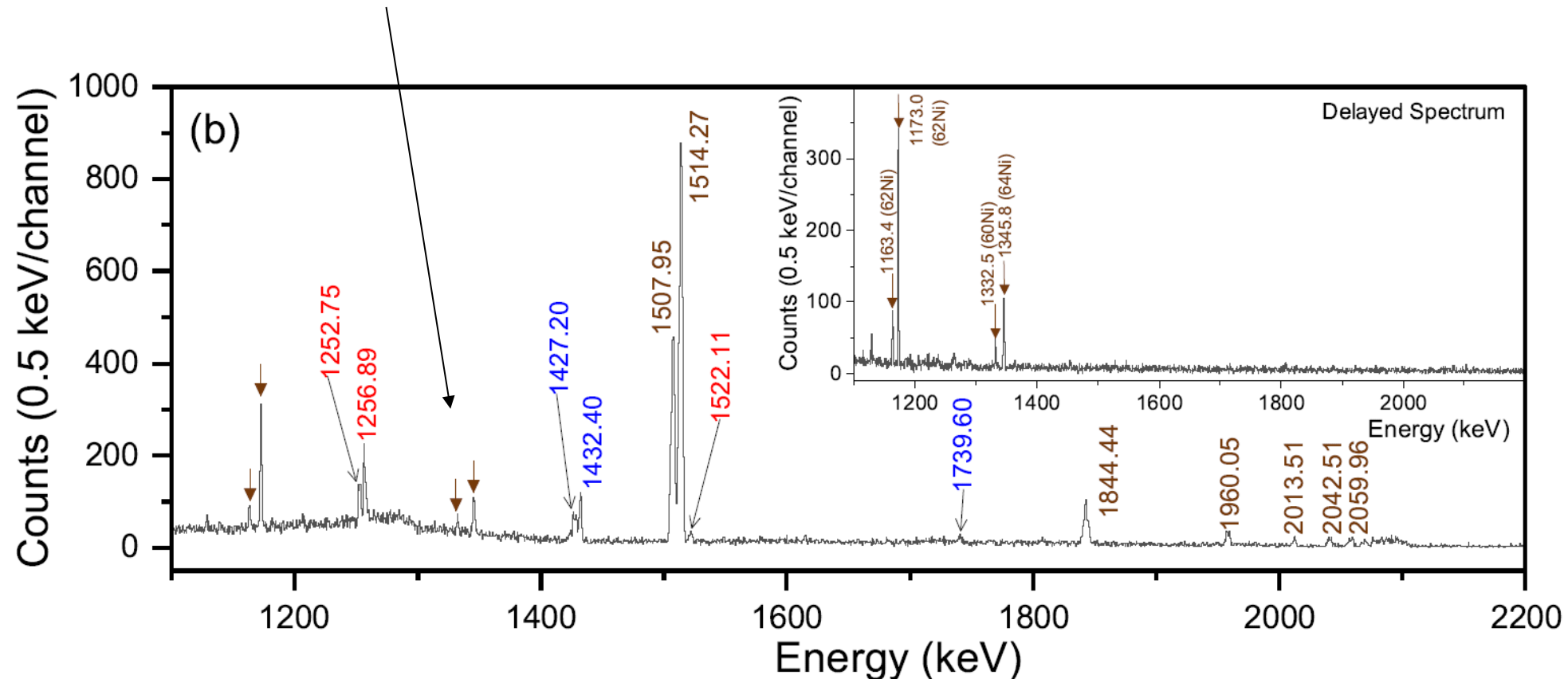
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X-ray cascade:  
prompt, ROI: <100ns

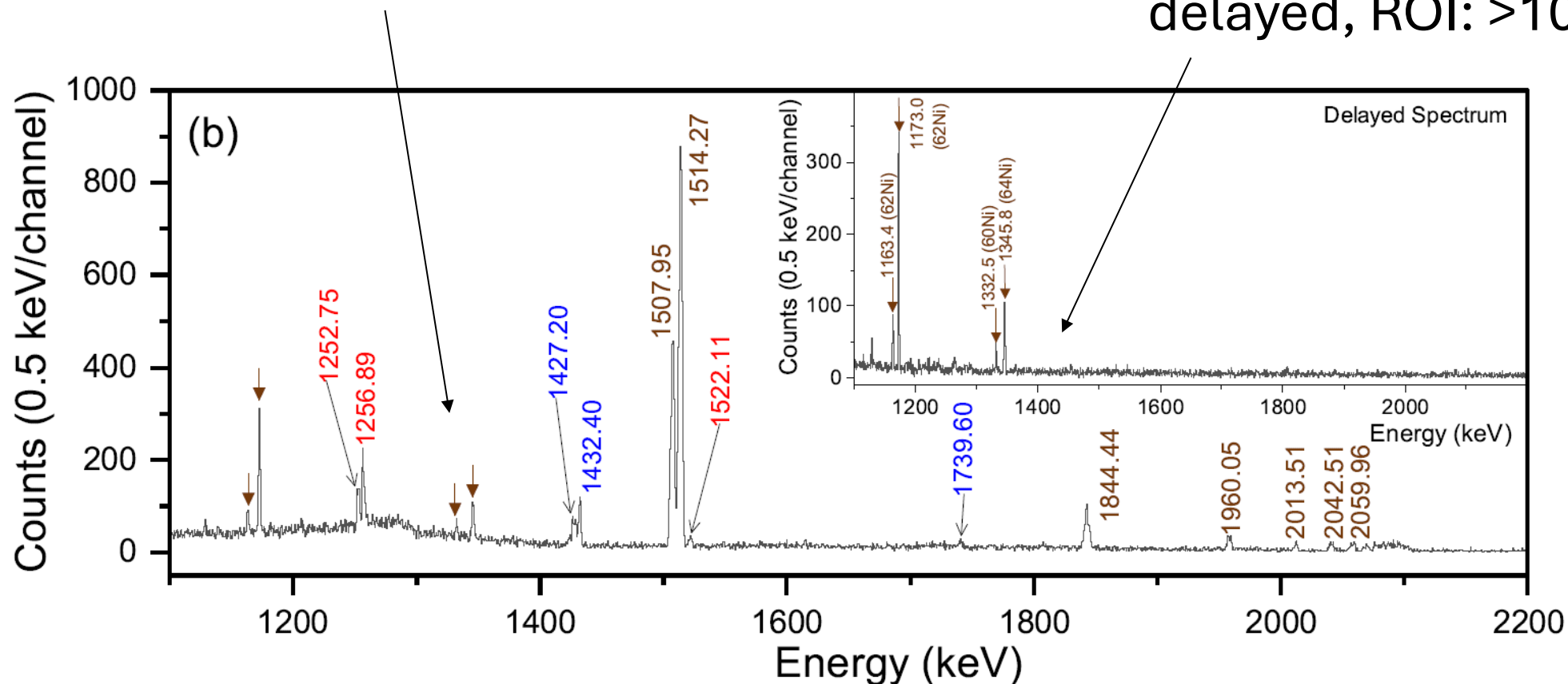


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Nuclear Capture and  
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delayed, ROI: >100ns



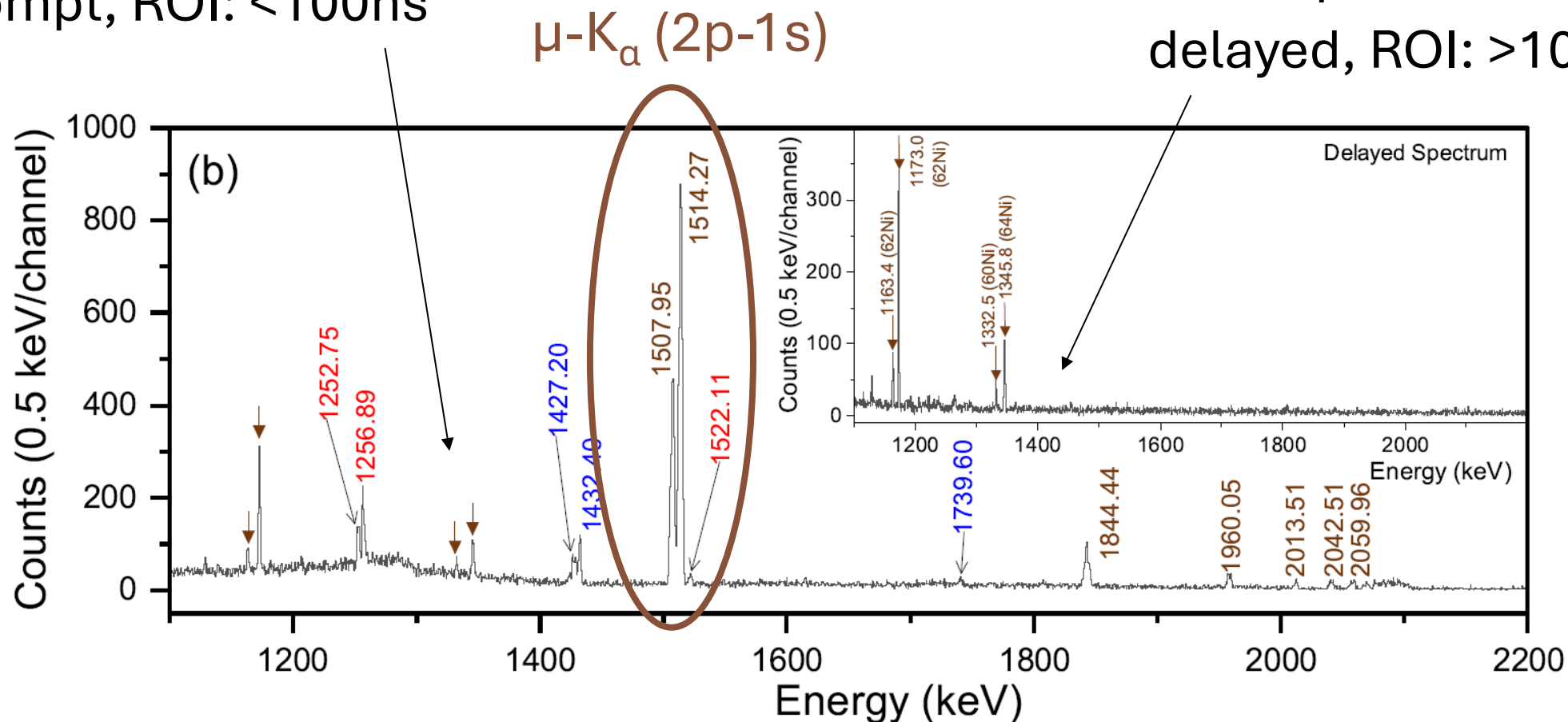


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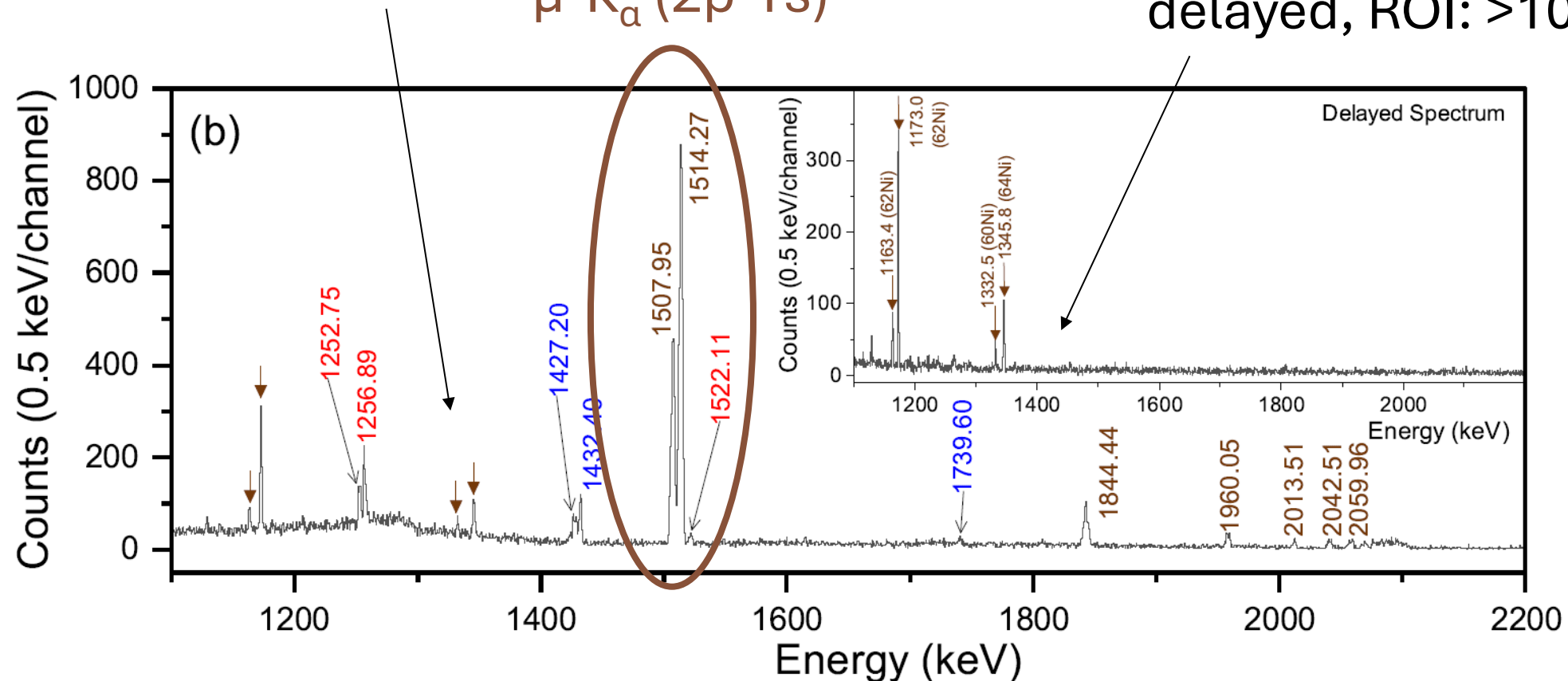
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*compare:*  
 $e-K_{\alpha} = 8.04 \text{ keV}$   
 $\mu-K_{\alpha} (2p-1s)$

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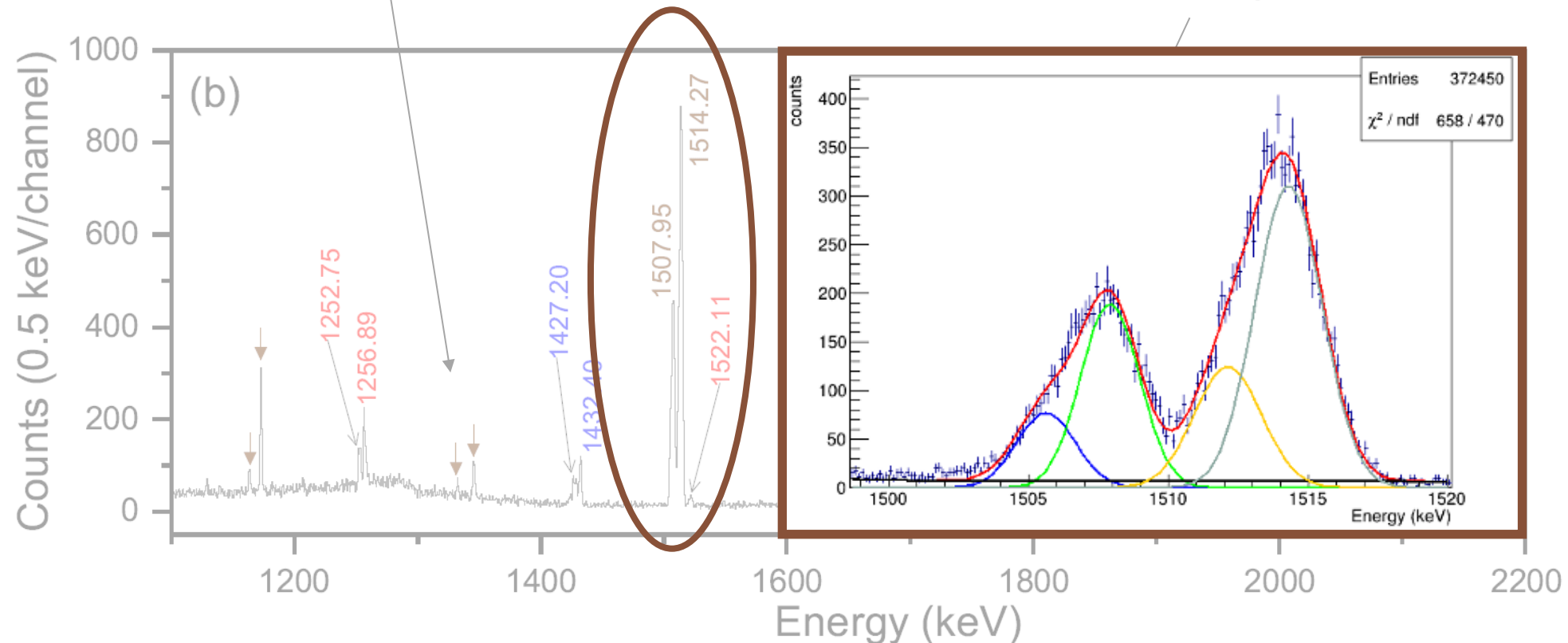
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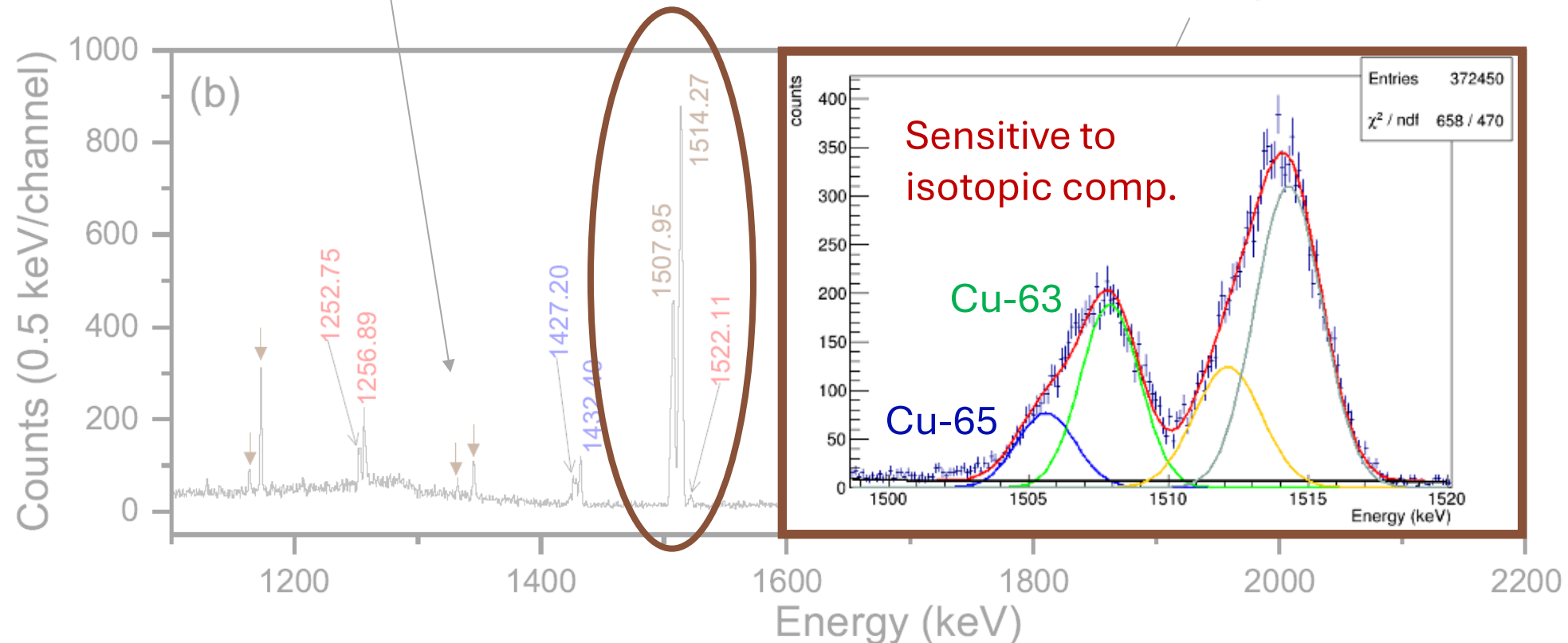
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- Swiss Spallation Neutron Source SINQ
- Swiss Muon Source SμS &  
Swiss Research Infrastructures for Particle Physics CHRISP
- Ultracold Neutron Source UCN (CHRISP)
- Proton Irradiation Facility PIF (CHRISP)
- Radionuclide Production (IP-2 and SINQ)

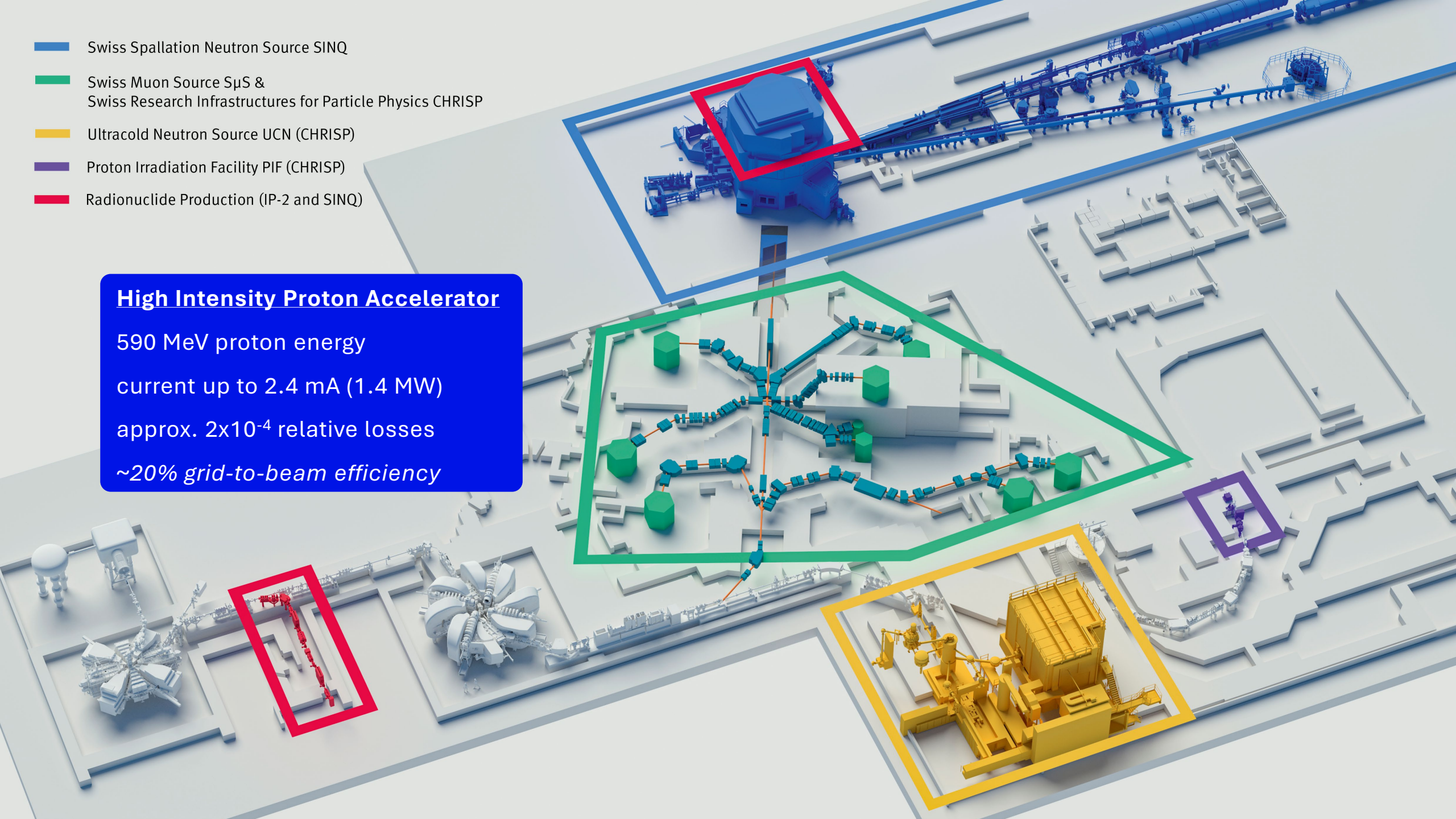
### High Intensity Proton Accelerator

590 MeV proton energy

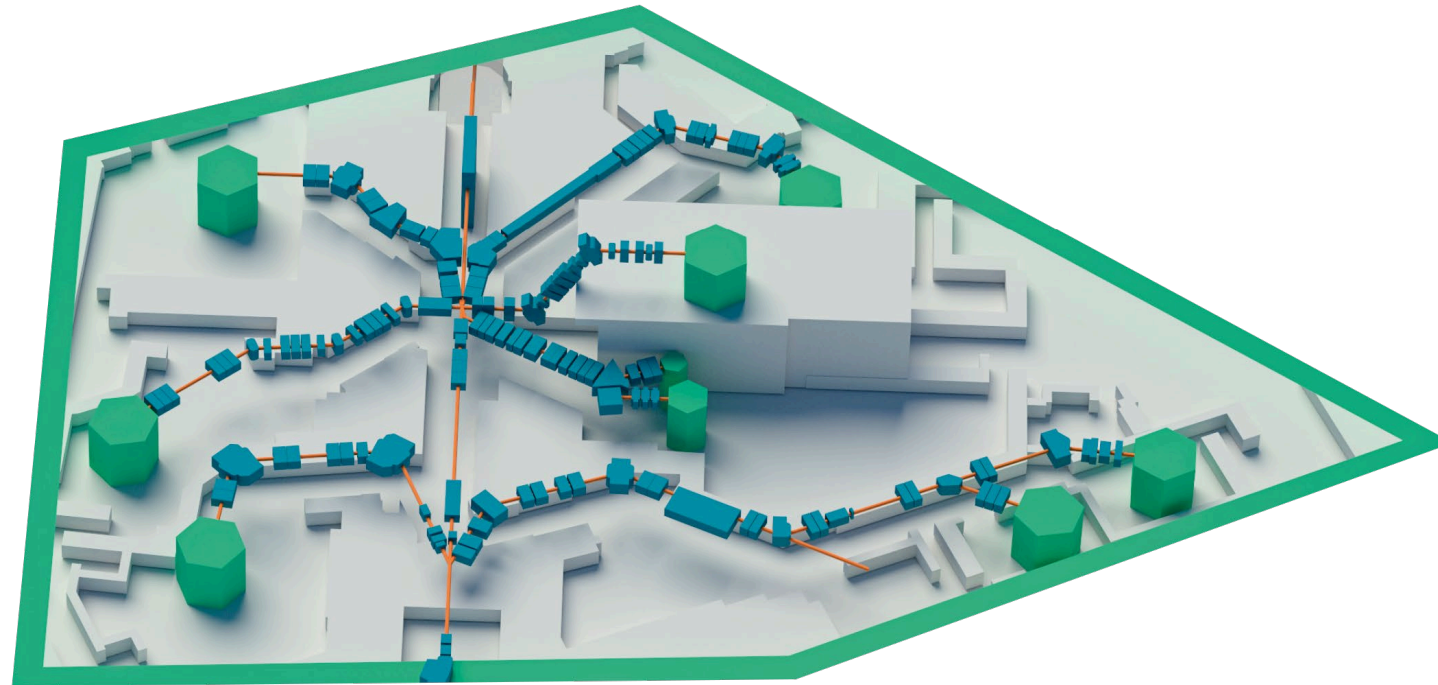
current up to 2.4 mA (1.4 MW)

approx.  $2 \times 10^{-4}$  relative losses

*~20% grid-to-beam efficiency*







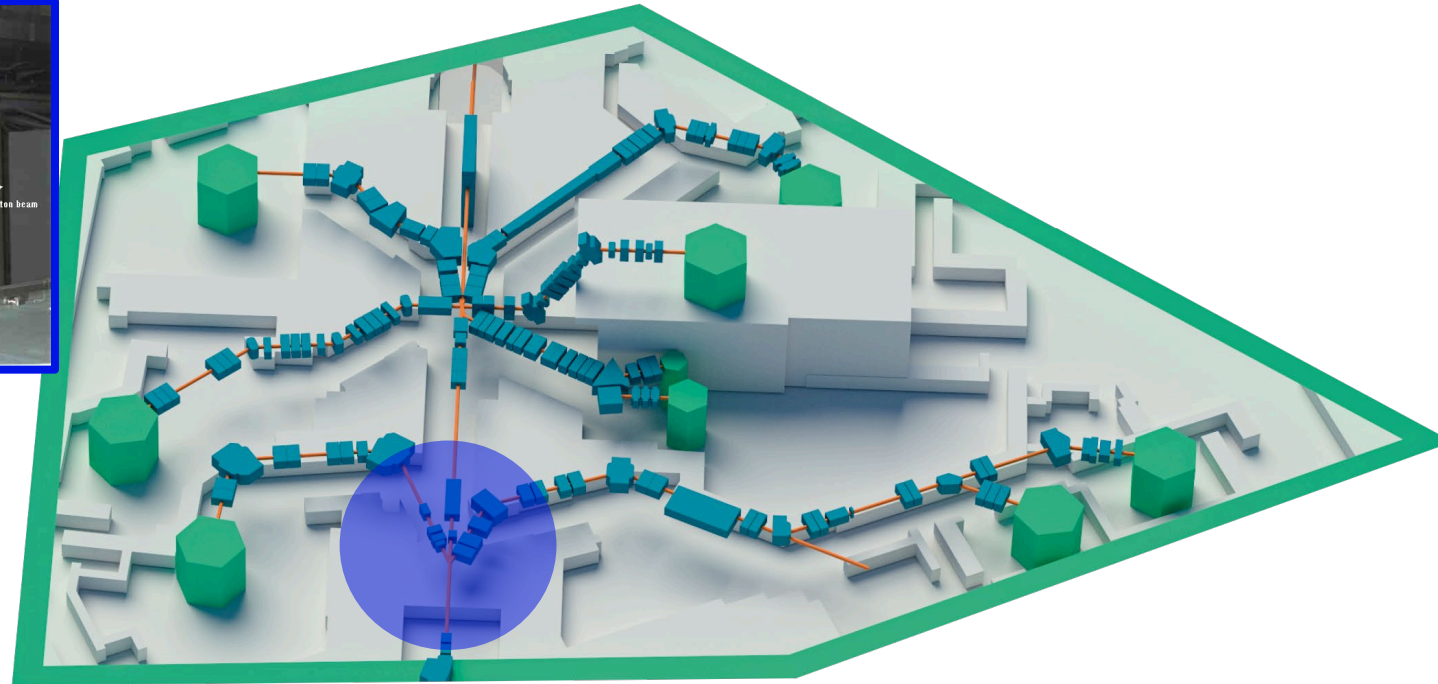
# SμS: Swiss Muon Source

**Target M** (mince) – 5mm graphite

*designed for  $\pi$  production (low rate)*

$\pi$ M3: 10-40 MeV/c (surface)  $\mu^+$  for  $\mu$ SR

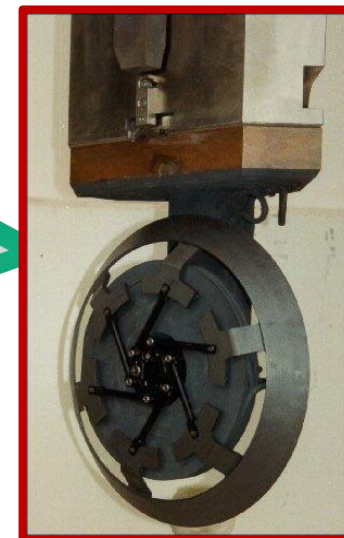
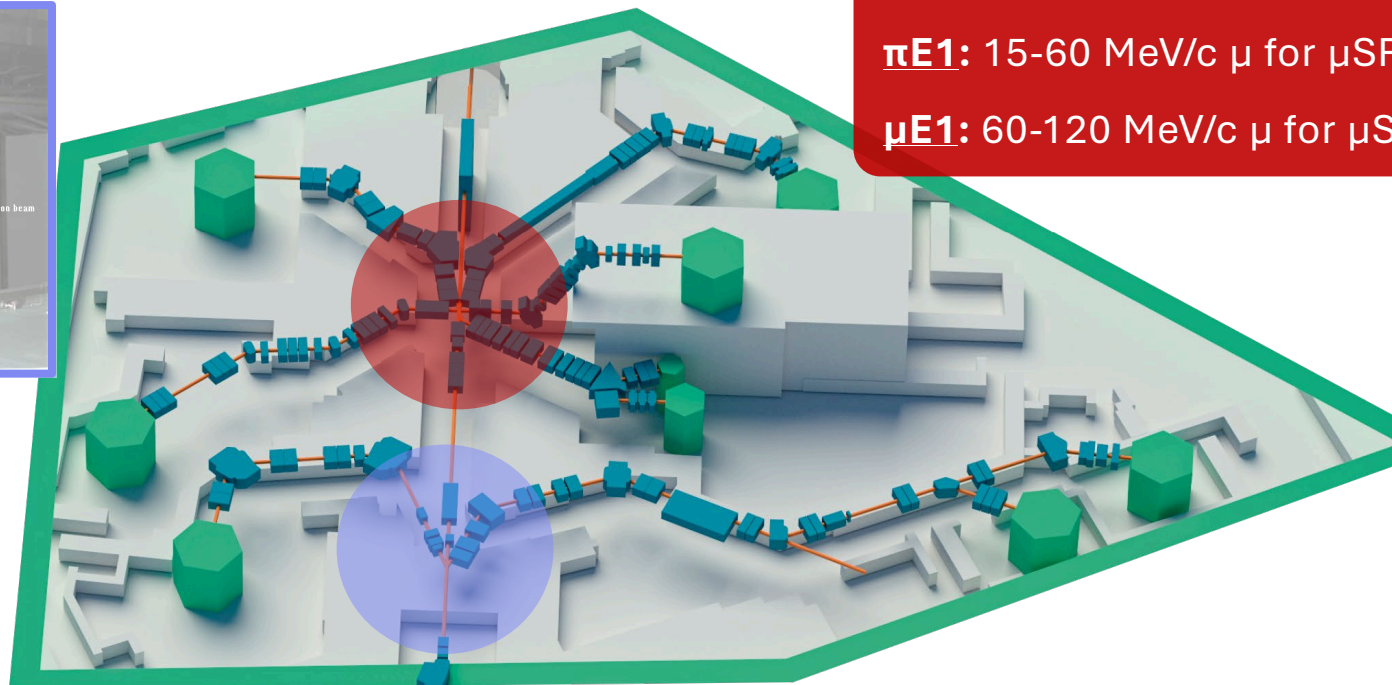
$\pi$ M1: 10-300 MeV/c  $\pi \rightarrow \mu/e$  for tests/PP



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 $\pi$ M3: 10-40 MeV/c (surface)  $\mu^+$  for  $\mu$ SR  
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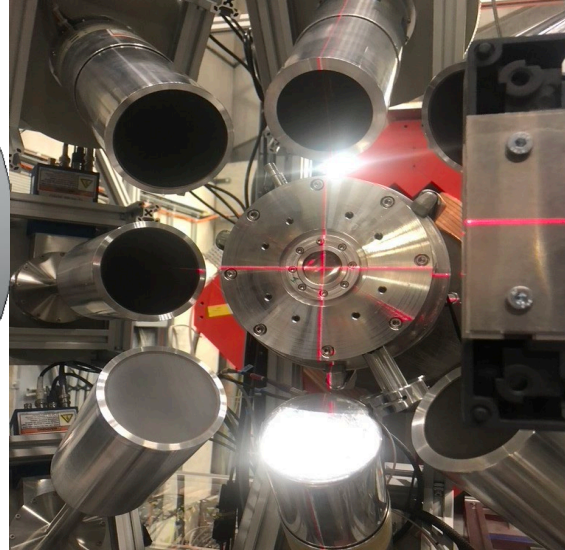
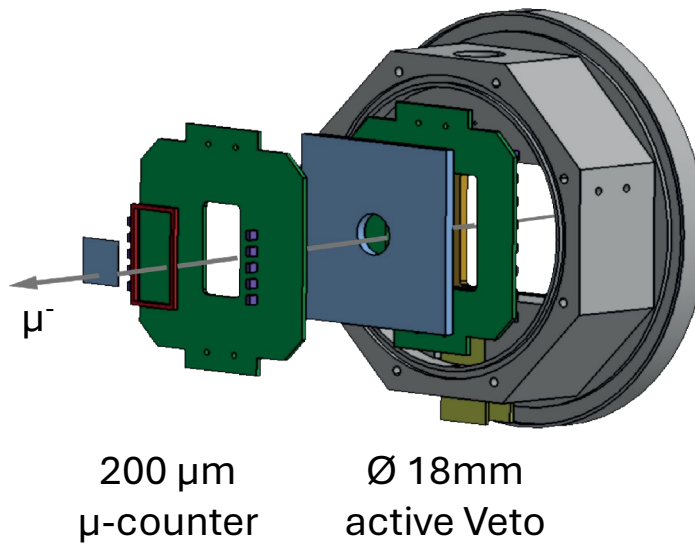
**Target E** (epaisse) – 40mm graphite  
*designed for  $\pi/\mu$  production (high rate)*  
 $\pi$ E5: 20-120 MeV/c high rate  $\mu$  for PP  
 $\mu$ E4: 10-40 MeV/c  $\mu^+$  for LEM –  $\mu$ SR and PP  
 $\pi$ E3: 10-40 MeV/c (surface)  $\mu^+$  for bulk  $\mu$ SR  
 $\pi$ E1: 15-60 MeV/c  $\mu$  for  $\mu$ SR, PP & **MIXE**  
 $\mu$ E1: 60-120 MeV/c  $\mu$  for  $\mu$ SR & **MIXE** (2028)



# GIANT: Germanium Array for Non-destructive Testing – Tagging

Tagger & Beamport (developed for muX experiment)

- BC-400 plastic scintillators (Counter and Veto)
- reduces uncorrelated background
- allows for discrimination of nuclear capture events
- 10 $\mu$ m titanium foil window to sample (~10cm air gap)

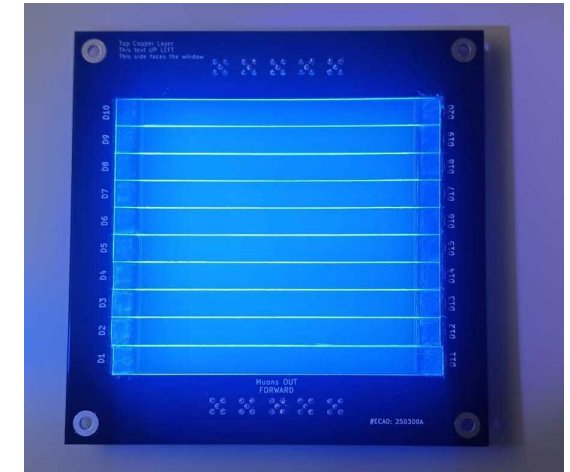
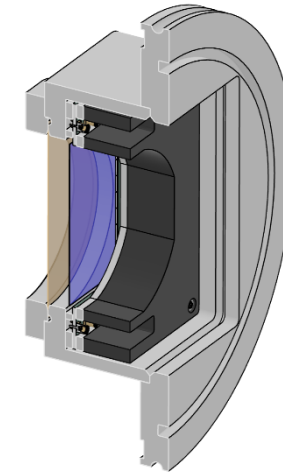
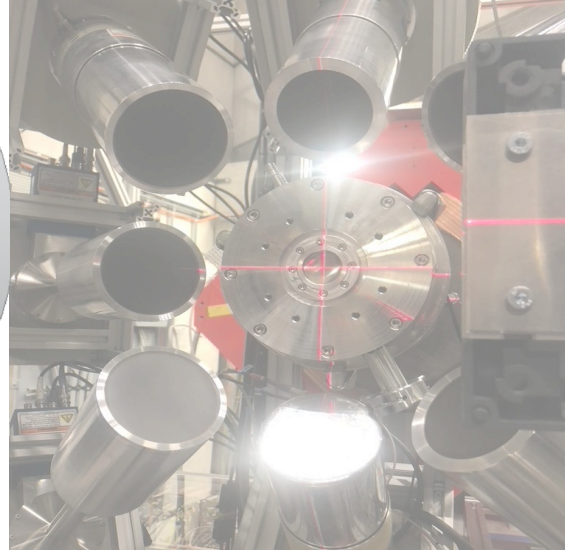
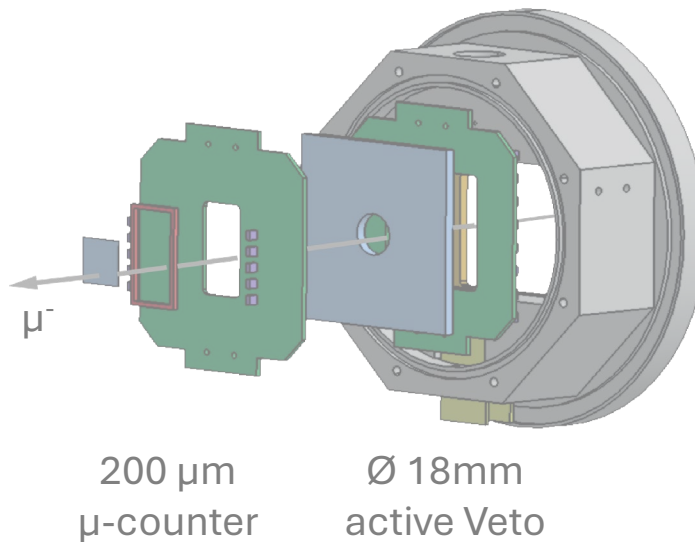




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Upgraded version (2025)

- Much larger active area ( $\sim 7 \times 7 \text{ cm}^2$ )
- Matching Window ( $\varnothing 7 \text{ cm}$ ) – 50 $\mu$ m Mylar
  - Same overall material budget!
- Optimized shielding to reduce BG
- Striped design (10 individual channels)
  - Allows higher tracker rate (see Part IV)



# MIXE 4 Batteries: Full depth profiling



## Goal:

- **In-situ** elemental **depth-profiling** of functional cells

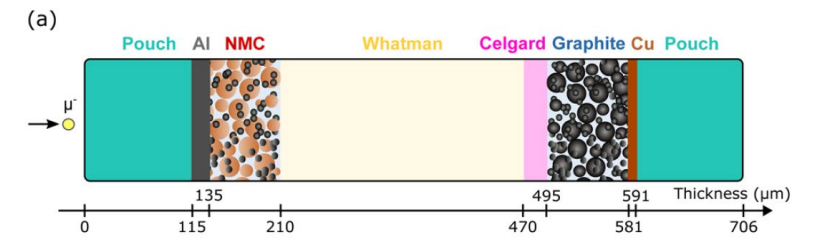
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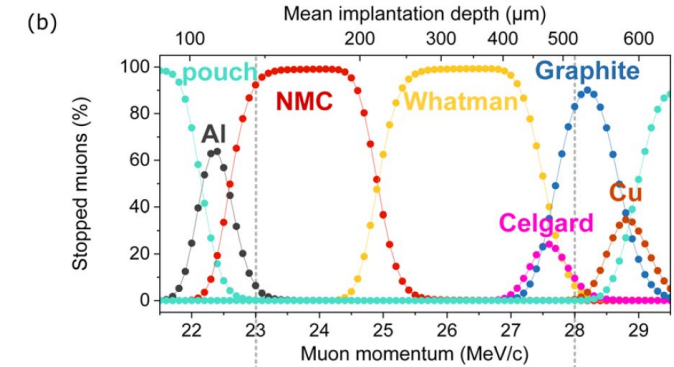
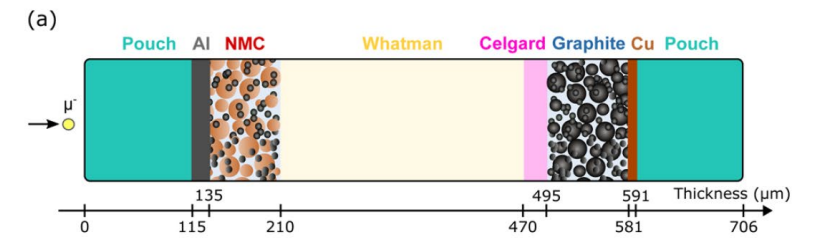
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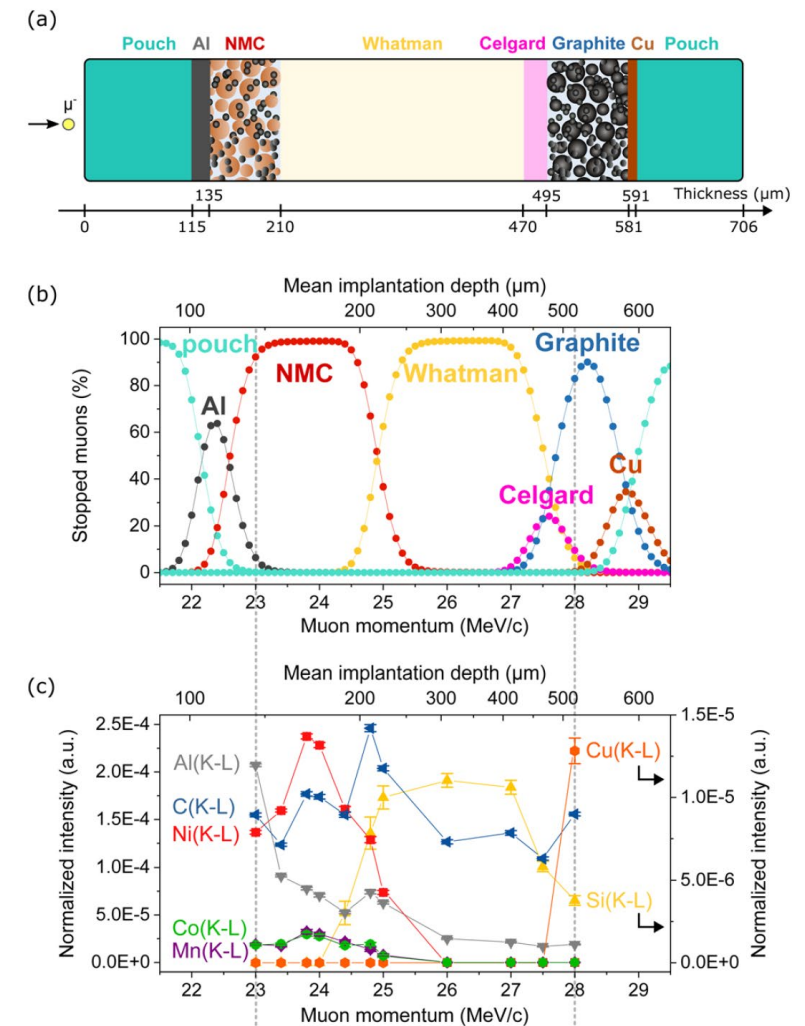
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- **Fingerprint signals** for each layer (**Al, Ni/Mn/Co, Si, Cu**) & C

*Good agreement of simulation and data*



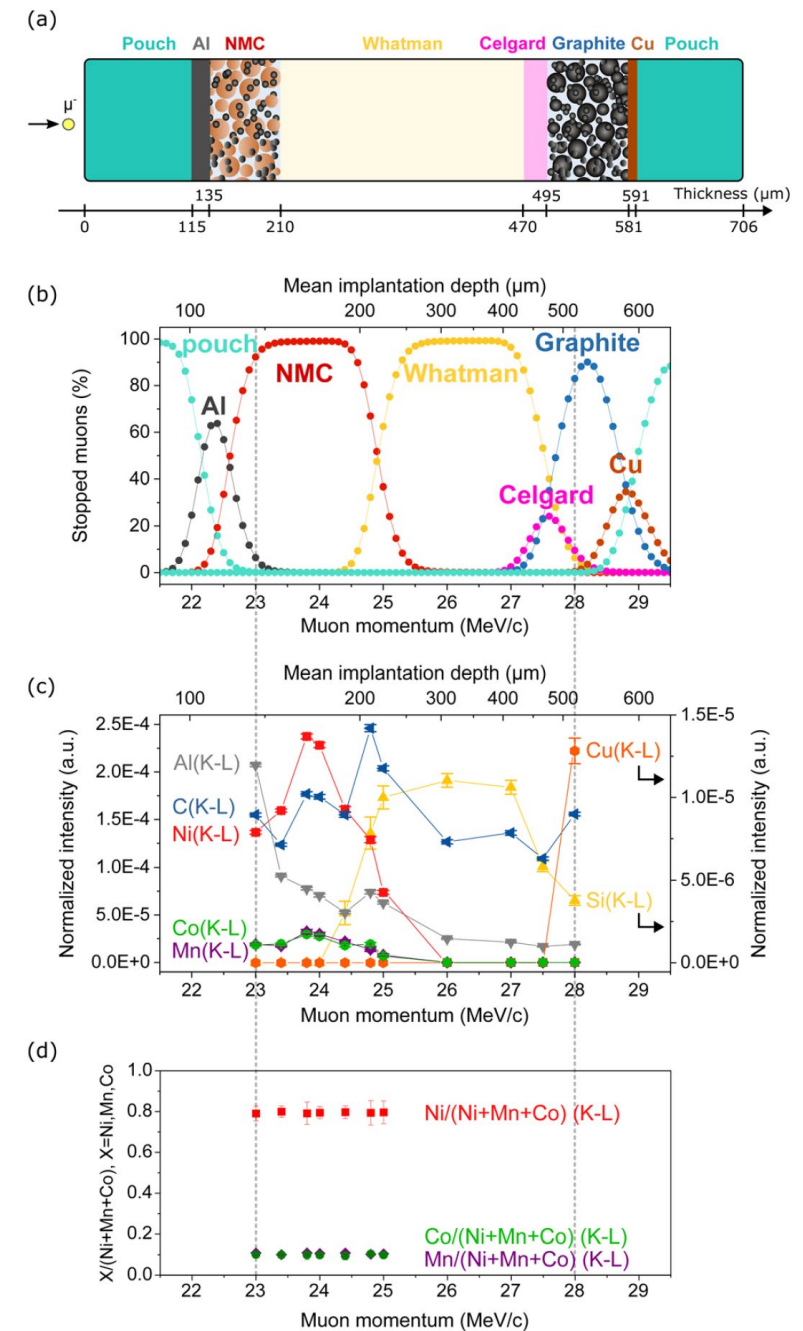
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*Good agreement of simulation and data*
- **Cross-check** of quantitative results: **NMC Stoichiometry**  
**Reproduces 8:1:1 ratio very well over full thickness**





# MIXE-T(omography): Completely New Possibilities!



a) Vincent van Gogh's Flower Still Life with Meadow Flowers and Roses, summer 1886 (Kröller-Müller Museum, Otterlo, the Netherlands), rotated for illustration purposes.

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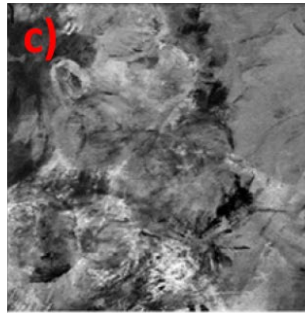
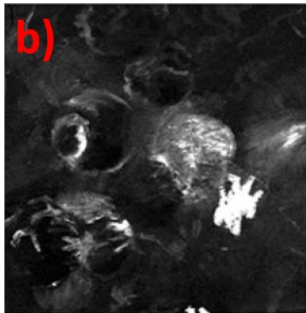
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b) Hg fluorescence signal of the area in the red box, flowers are visible.

c) Zn fluorescence signal of the same area, hints of a human face visible.

d) Zn fluorescence measured from the back of the painting with less absorption, revealing the human face as part of an overpainted wrestling scene..

**M. Alfeld and J. A. C. Broekaert**, Spectrochimica Acta Part B 88, 211-230 (2013)





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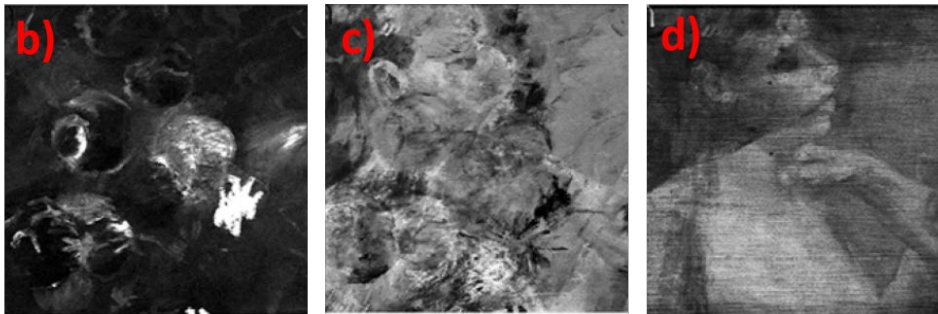
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***MIXE-T could image all elements over full canvas with much higher depth-resolution!***

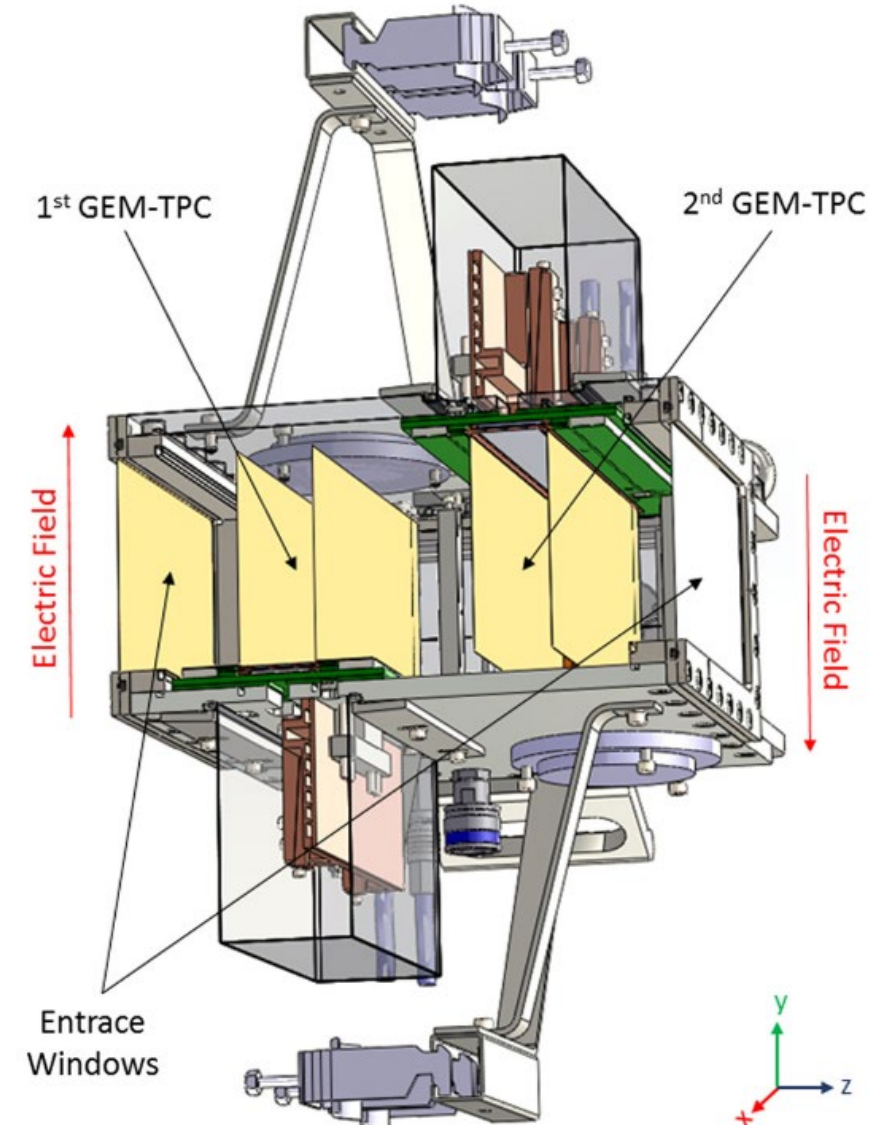
# MIXE-T(omography): Muon Tracking



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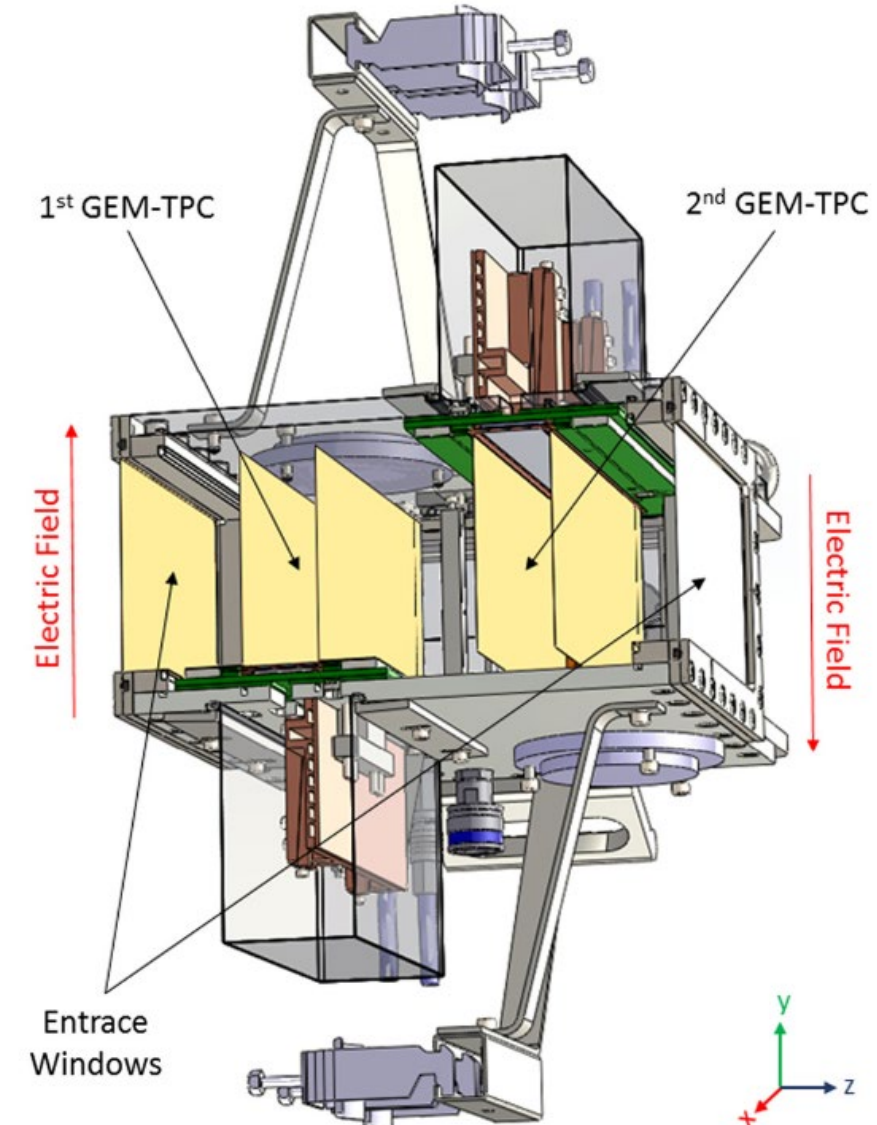
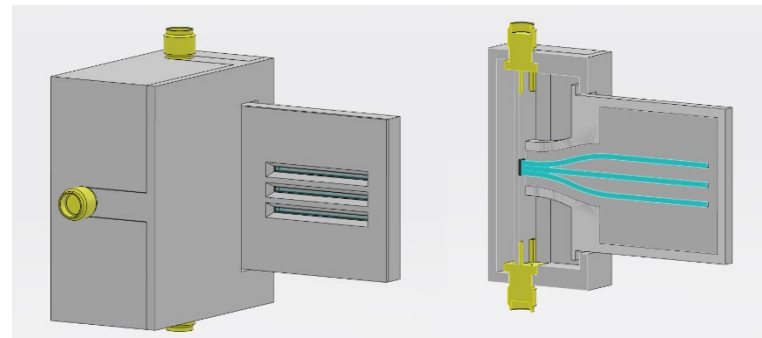
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  - 1D strip readout – 1024 ch in total – 0.4 mm pitch
  - X position given by cluster on strips
  - Y position by drift time(s) – *requires calibration*





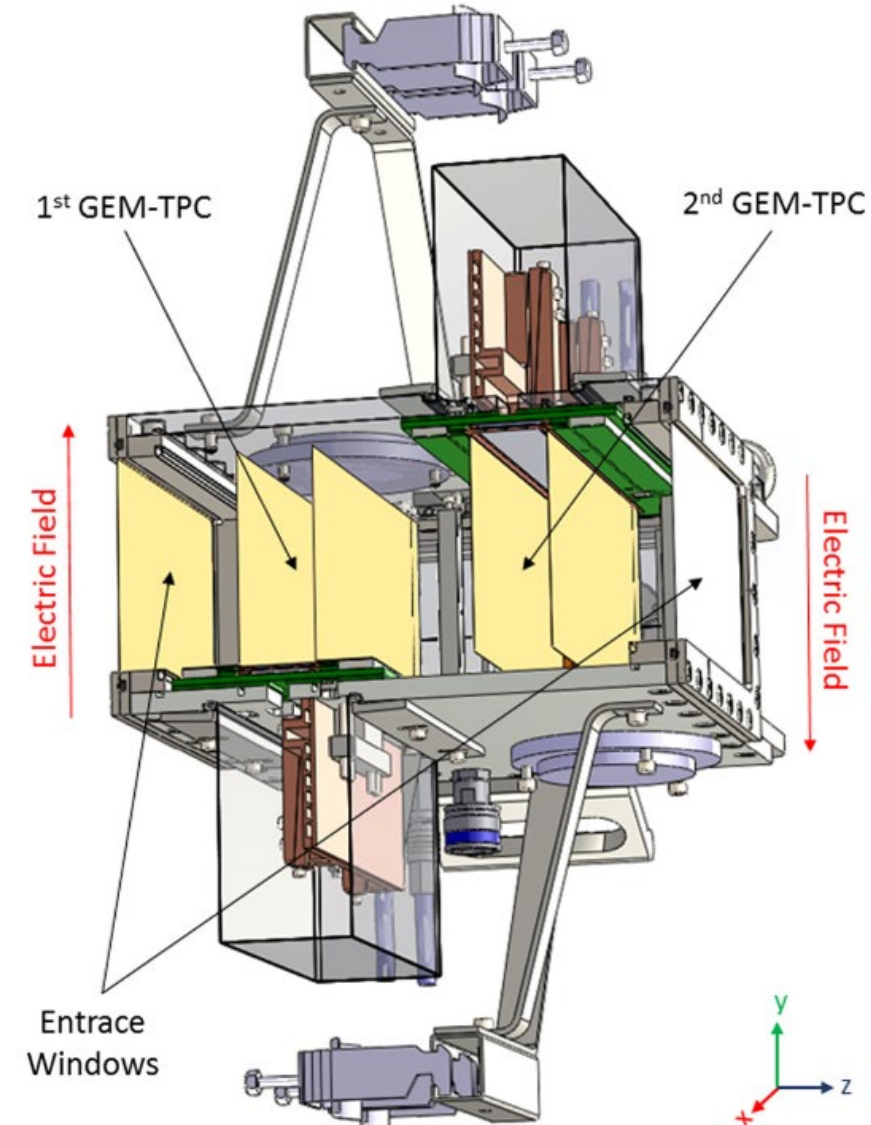
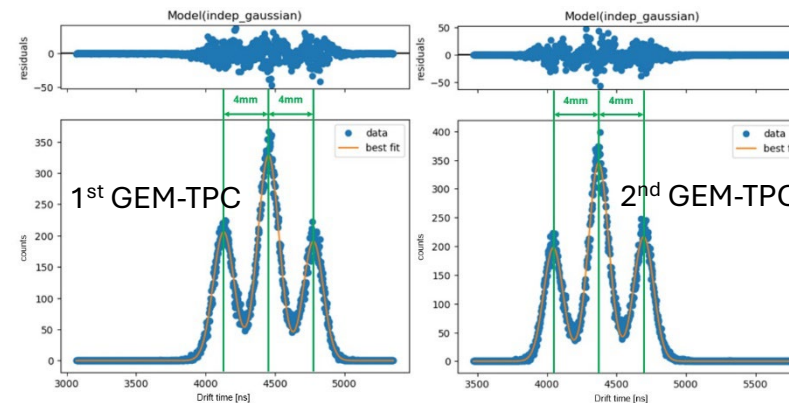
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  - In-situ calibration!



# MIXE-T(omography): First Elemental Imaging (Jun 23)

## Experimental setup

- Tracker mounted after beam port (roughly aligned)
- Standard Ar/CO<sub>2</sub> (75:25) gas mixture
- Single HPGe detector
- 60 MeV/c muon beam

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PRELIMINARY

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## Reference targets

- Four metals:
  - Brass (37% Zn)
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- Thicknesses optimized to stop downstream





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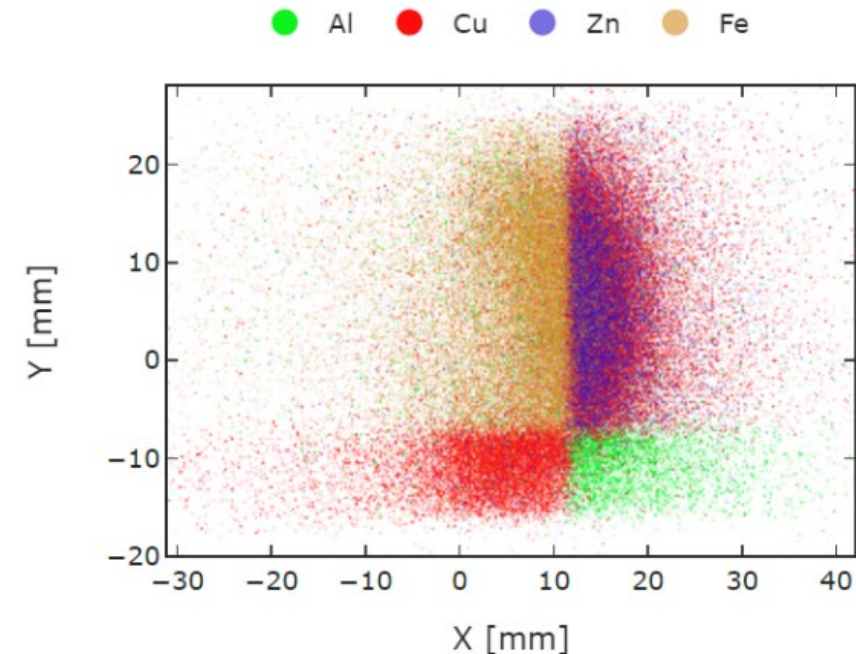
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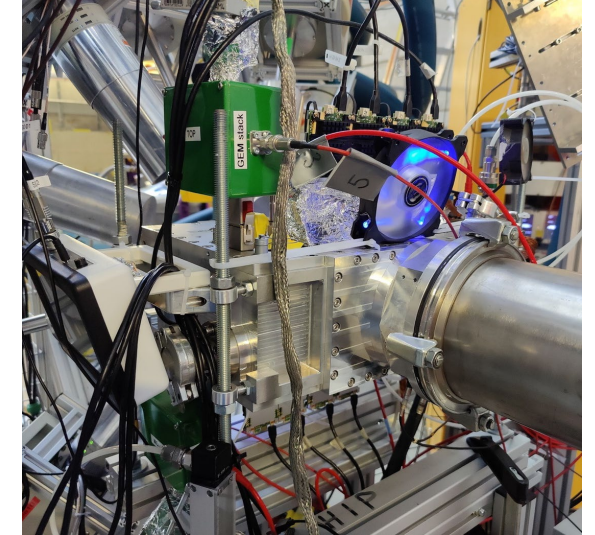
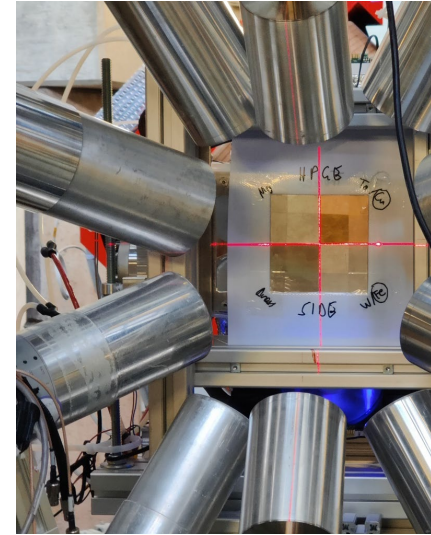


# MIXE-T(omography): Spatial Resolution for Tomography

**PRELIMINARY**

## Upgrades

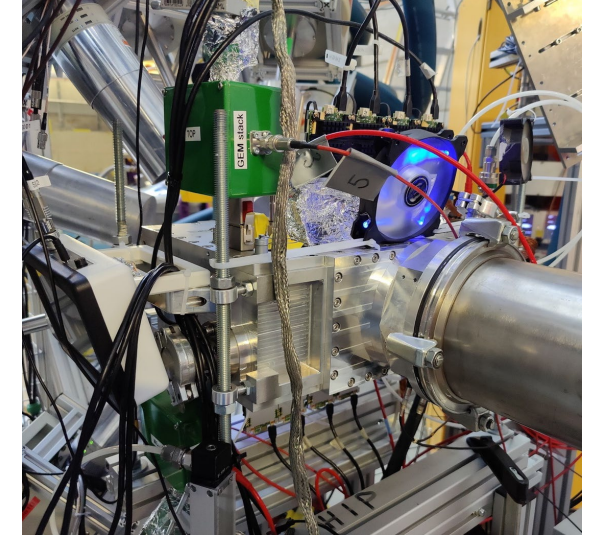
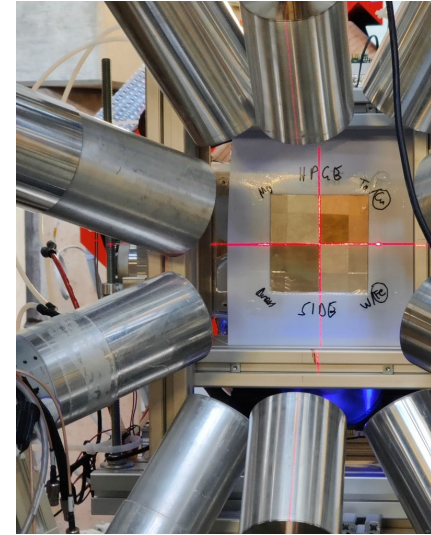
- Layered targets & Momentum Scans
- Detector flanged directly to beamport
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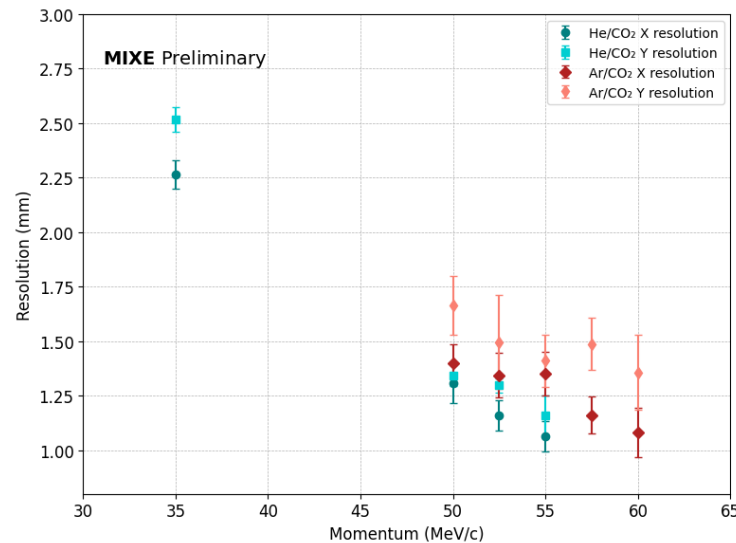
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## Results

- Spatial Resolution >50MeV/c:
  - X/Y: **~1 mm**

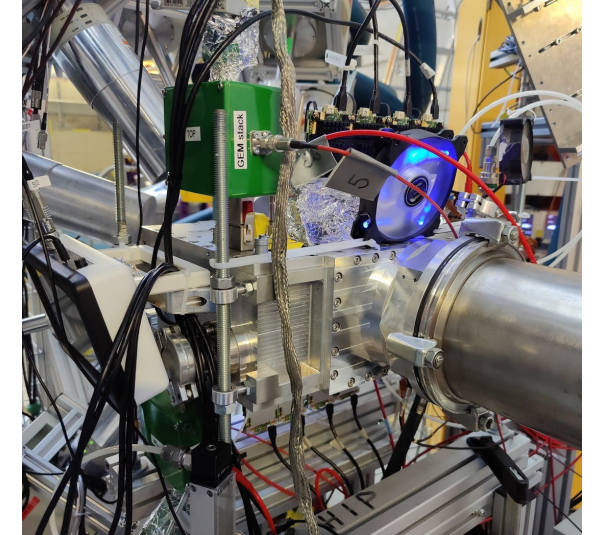
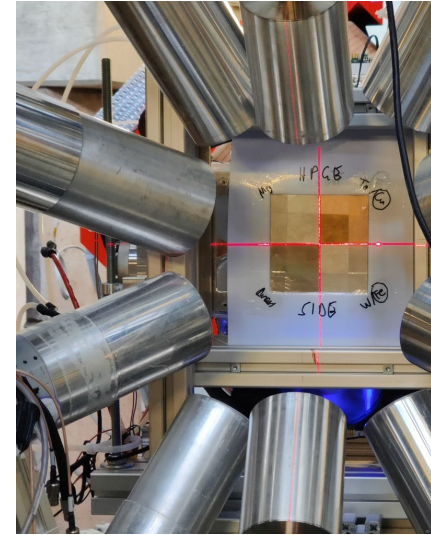


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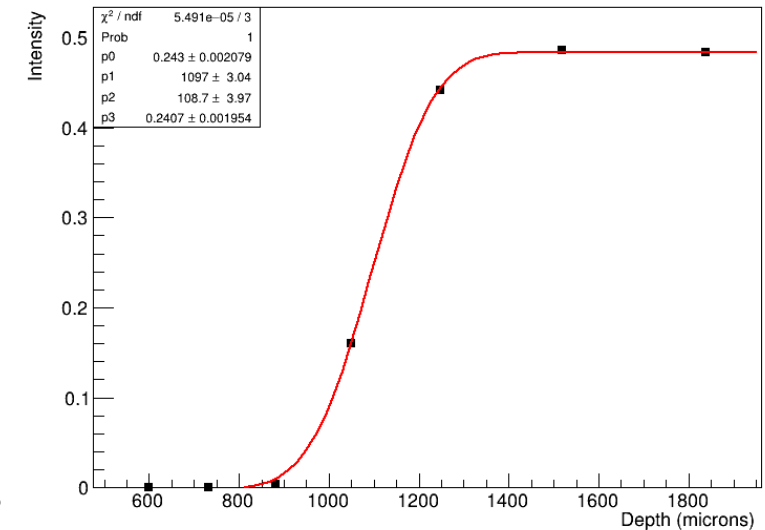
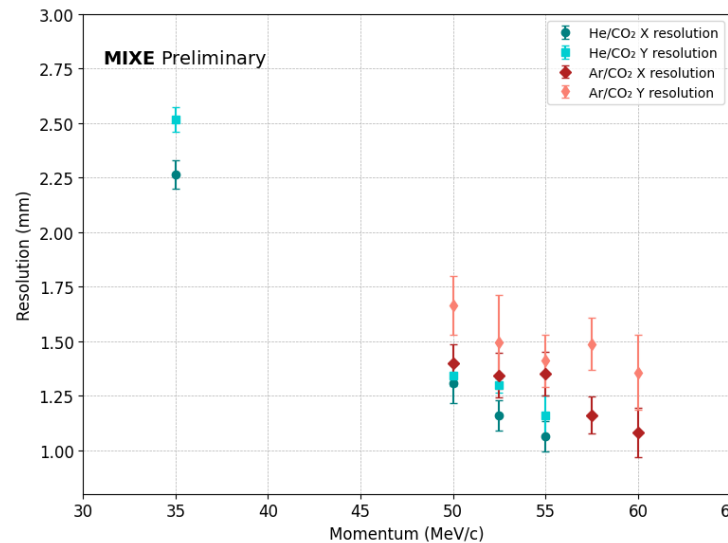
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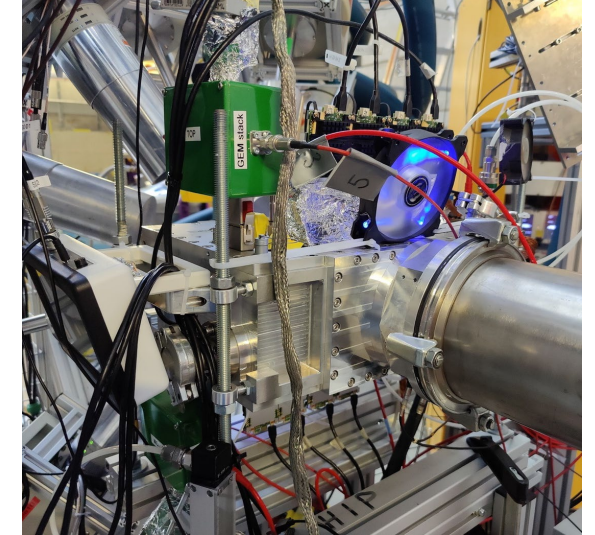
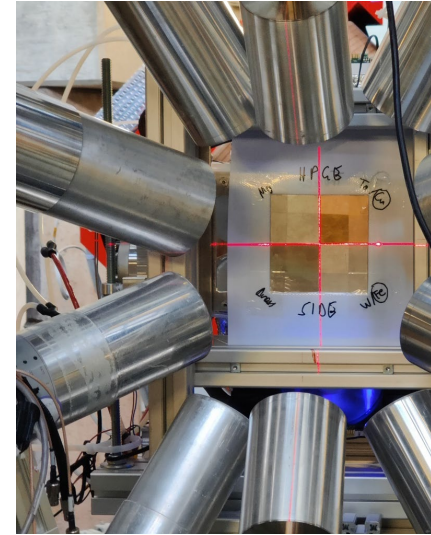


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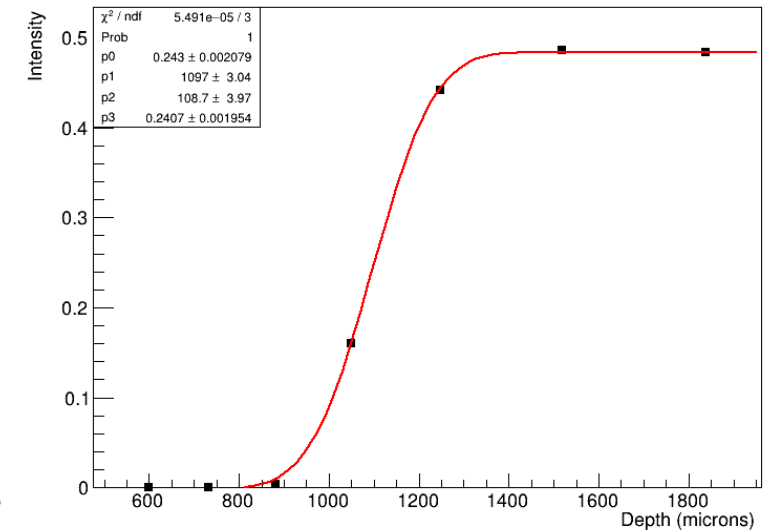
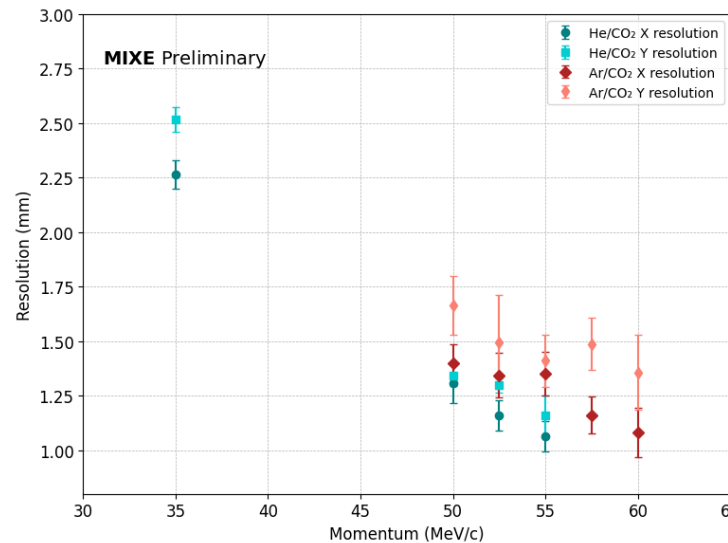


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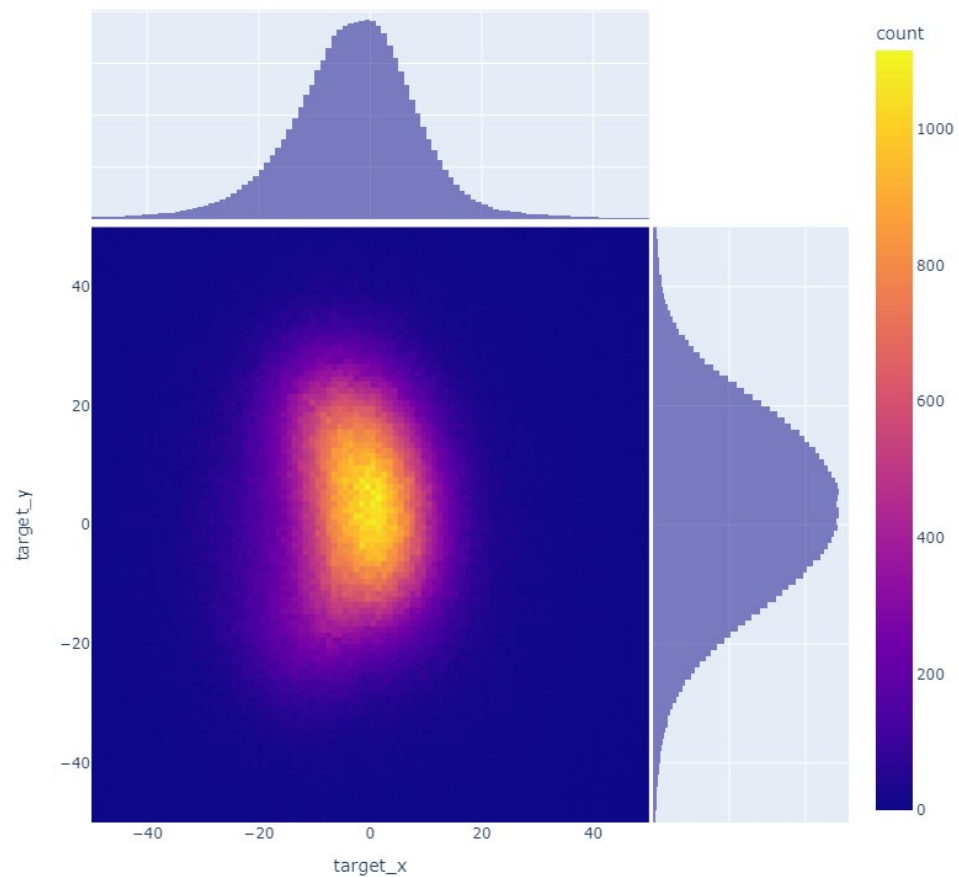
Limited by large gas volume

*Specialized prototype detector  
in development!*



# MIXE-T(omography): Determining the Resolution

**PRELIMINARY**

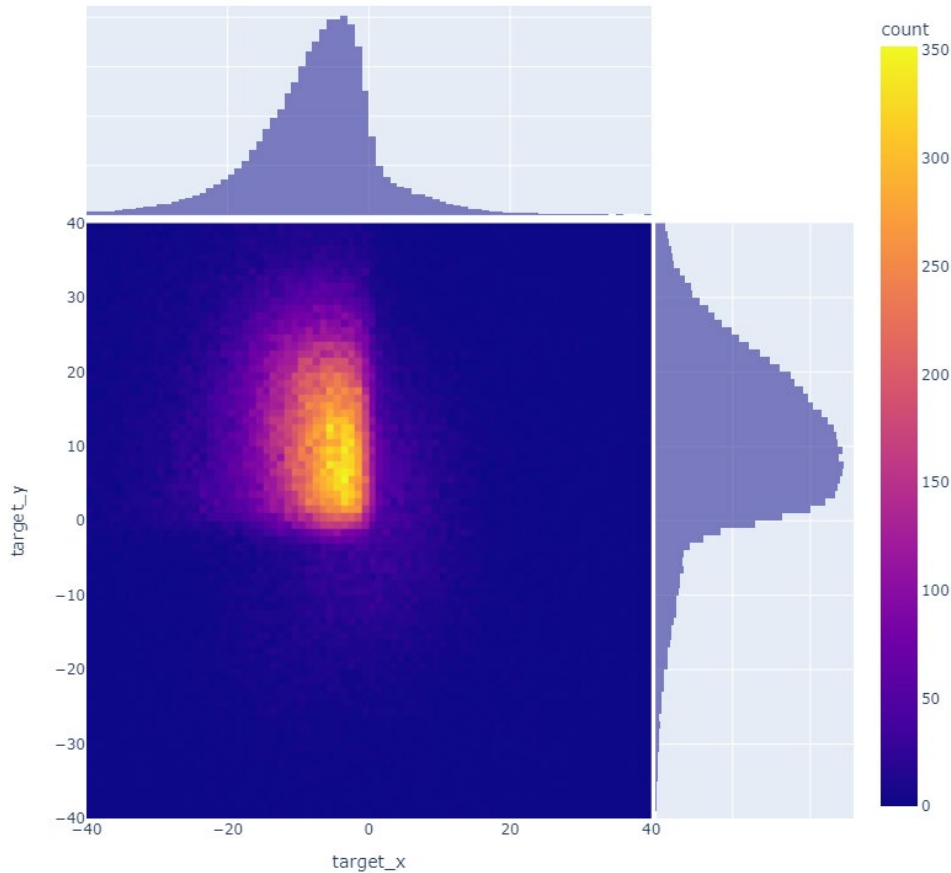




# MIXE-T(omography): Determining the Resolution

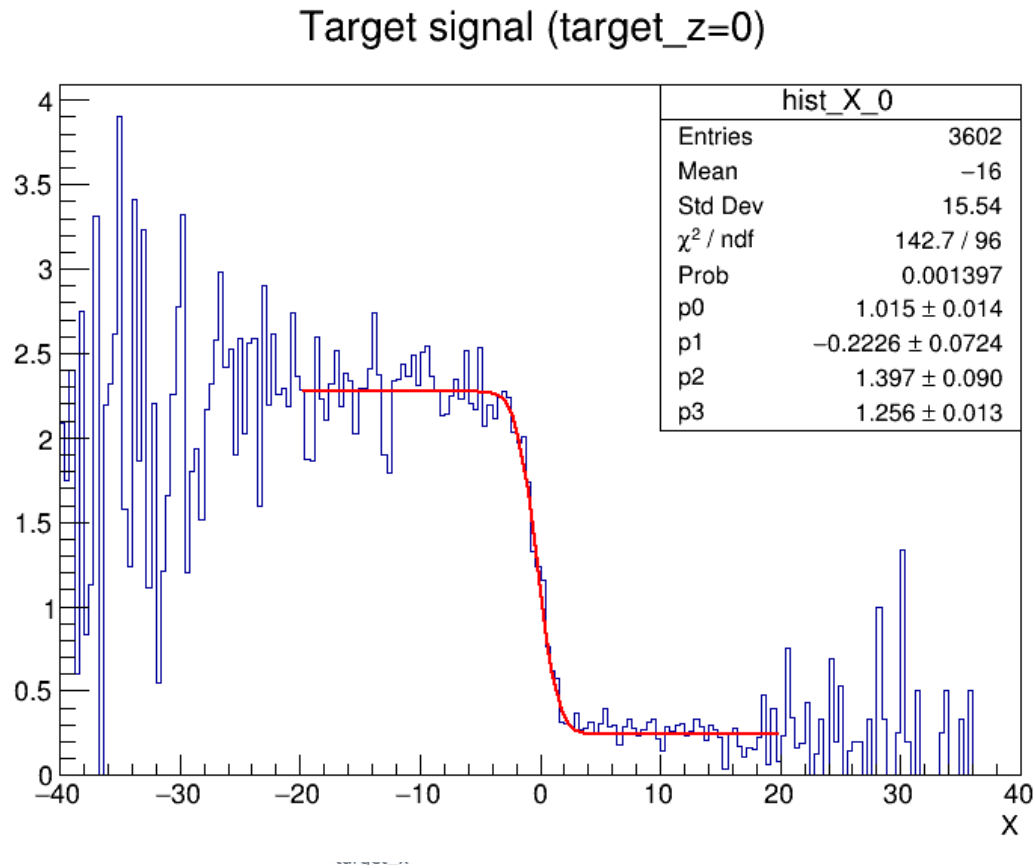
PRELIMINARY

**Step 1:** Select the desired element (Mo)



# MIXE-T(omography): Determining the Resolution

PRELIMINARY



**Step 1:** Select the desired element (Mo)

**Step 2:** Normalize the data by the beamspot

**Step 3:** Select a X/Y range to remove background

**Step 4:** Sum the data along the X/Y axis

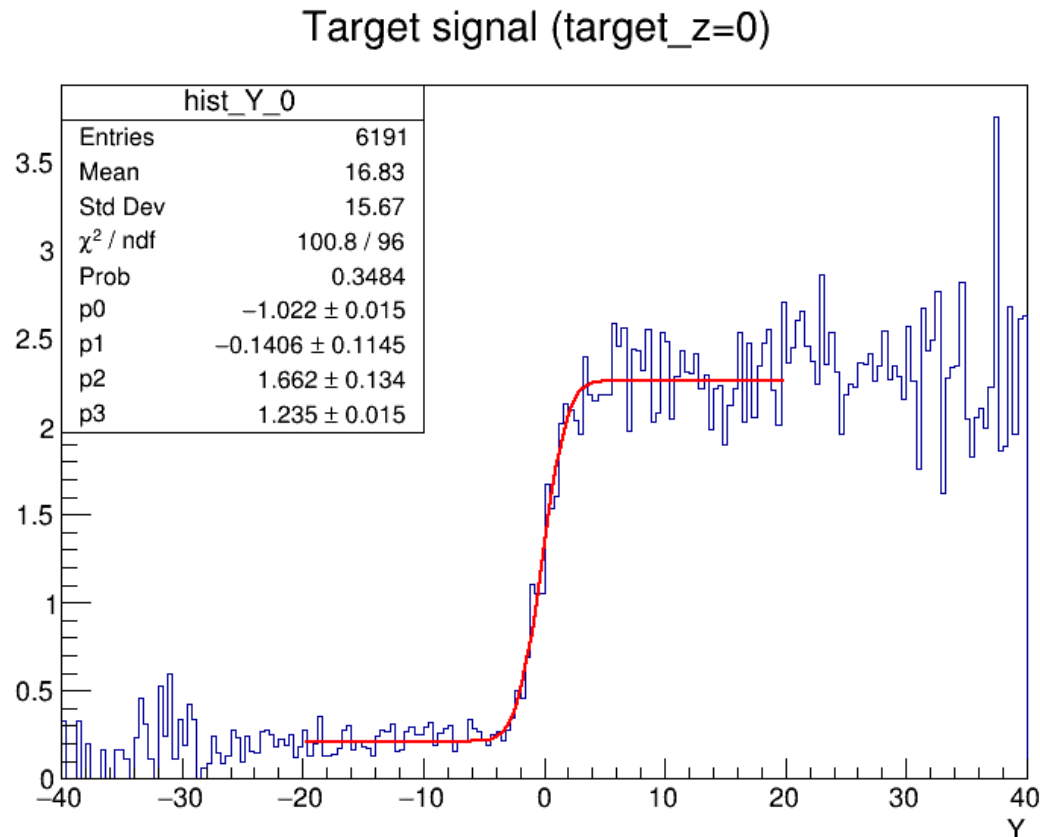
**Step 5:** Fit result using a Gauss error function

$$F(x) = P[3] + P[0]e^{\left(\frac{x-P[1]}{P[2]}\right)^2}$$

P[1]: mean    P[2]: sigma

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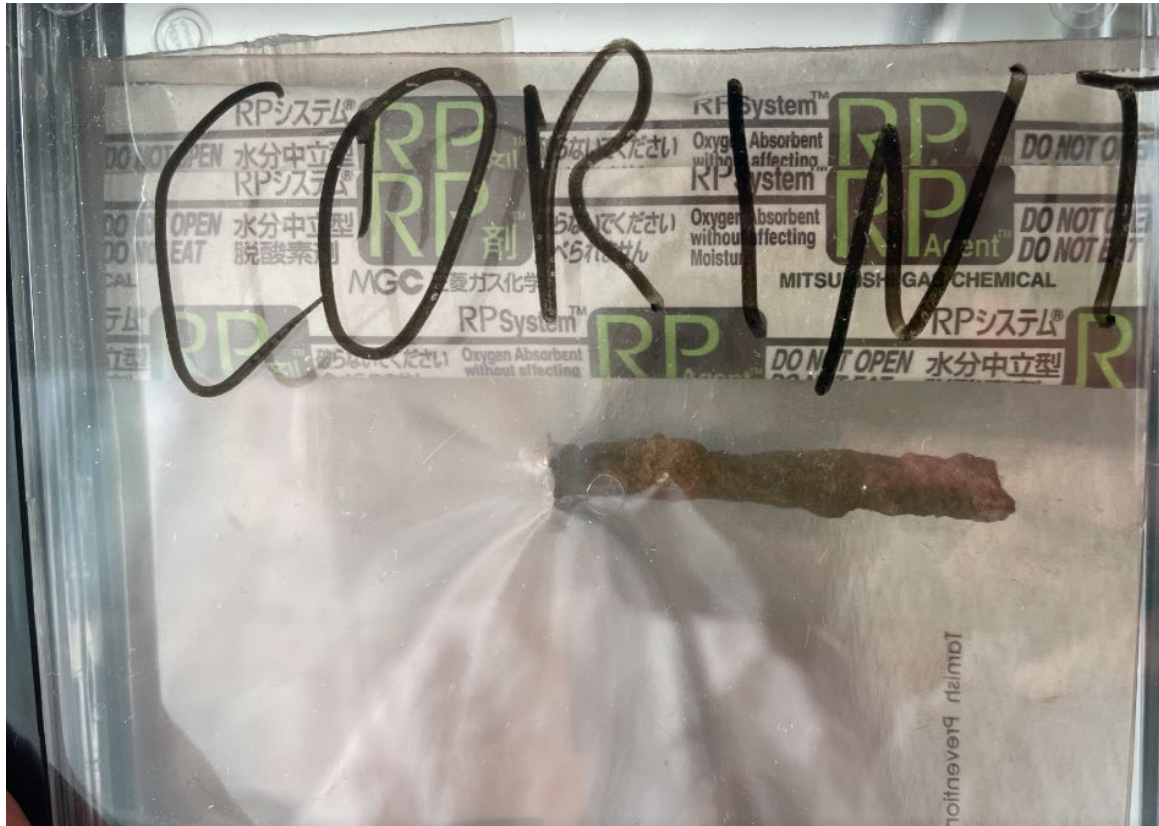
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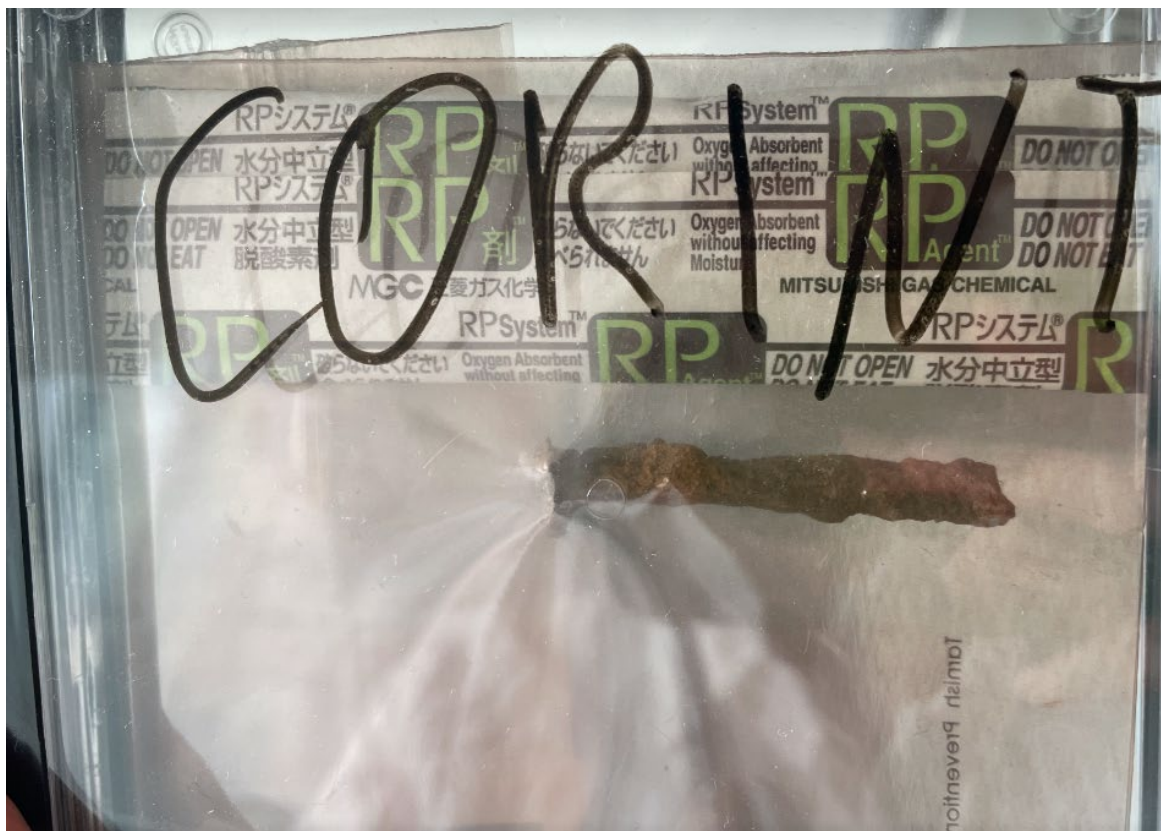
## MIXE-T(omography): “Real” Sample

- Roman iron nail (fresh find – conservation study)
- ~1.5 hours data collection with 46MeV/c muons
- Spot size covering only ~50% of the nail

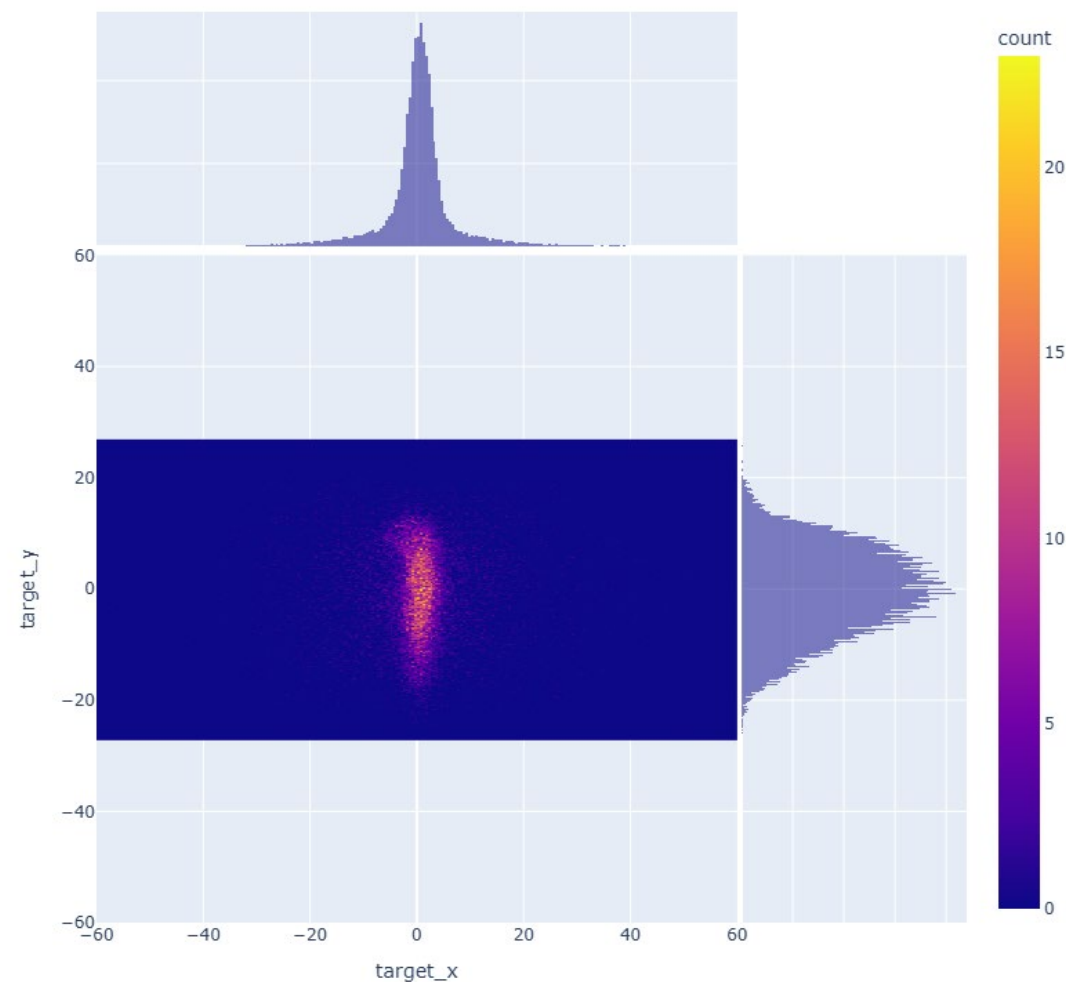


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- Tracks filtered for Fe  $K_\alpha$  and  $K_\beta$  peaks





## MIXE-T(omography): “Real” Sample

**PRELIMINARY**

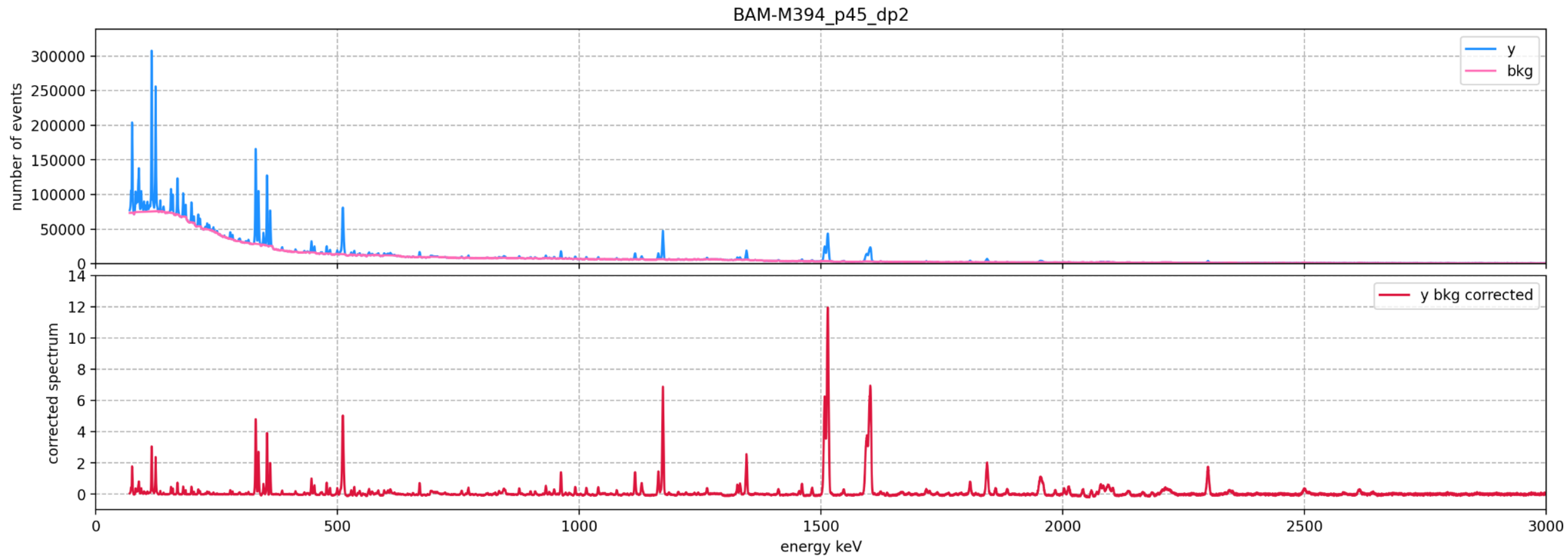


# Backup

## Smart Analysis of MUonic x-Rays with AI

- **Challenge:** “*Data analysis involves extensive domain knowledge and labor*”
  - Usually >100 (complex!) spectra taken each biannual measurement campaign
  - High degree of involvement of MIXE scientists in preparation, data-taking, and analysis
  - This leads to increasing backlog of sample analyses
- **SAMURAI:** Software development in collaboration with Swiss Data Science Center
  - Software package for fully automated analyses of MIXE spectra
  - User-friendly, no need for specialized domain knowledge or computational skills
  - Provides online analyses as immediate feedback to users
    - Allows for live changes in the experimental parameters (implantation depth, position, etc.)
  - Based on cutting-edge, efficient AI methods for rapid results (~1 minute on standard CPU)
    - Leveraging customized, problem-specific machine learning algorithm

- Step 1: Heuristic Background and Efficiency correction of raw spectra



# SAMURAI: Regression Problem

- **Datafit:** Use distance between event counts (as opposed to squared residuals): Huber distance for small  $\delta$  allows for this and for efficient optimization
- **Penalty:** use Hierarchical Sparsity, where main weight controls the K $\alpha$  lines, secondary lines are dependent on it
- **Optimization:** coordinate descent, alternating LASSO problems for  $w$  and  $v$ , fast and stable, using sparse representation of the feature (30k, 30k) matrix which saves memory and time

$$\mathbf{Huber}_\delta[a] = \begin{cases} \frac{1}{2}a^2 & \text{for } |a| \leq \delta, \\ \delta \cdot \left(|a| - \frac{1}{2}\delta\right), & \text{otherwise.} \end{cases}$$

$$\mathbf{Huber}_\delta \left[ \mathbf{y} - \sum_{z=1}^Z w_z \left( \mathbf{x}_0 + \sum_{t=2}^{T_z} v_t \mathbf{x}_t \right) \right]$$

Diagram illustrating the regression model structure with labels:

- Measured spectrum**: points to  $\mathbf{y}$
- Main amplitudes**: points to  $w_z$
- K $\alpha$  template**: points to  $\mathbf{x}_0$
- Secondary amplitudes**: points to  $v_t$
- Secondary template**: points to  $\mathbf{x}_t$
- Main penalty**: points to the  $w_z$  term
- Secondary penalty**: points to the  $v_t$  term



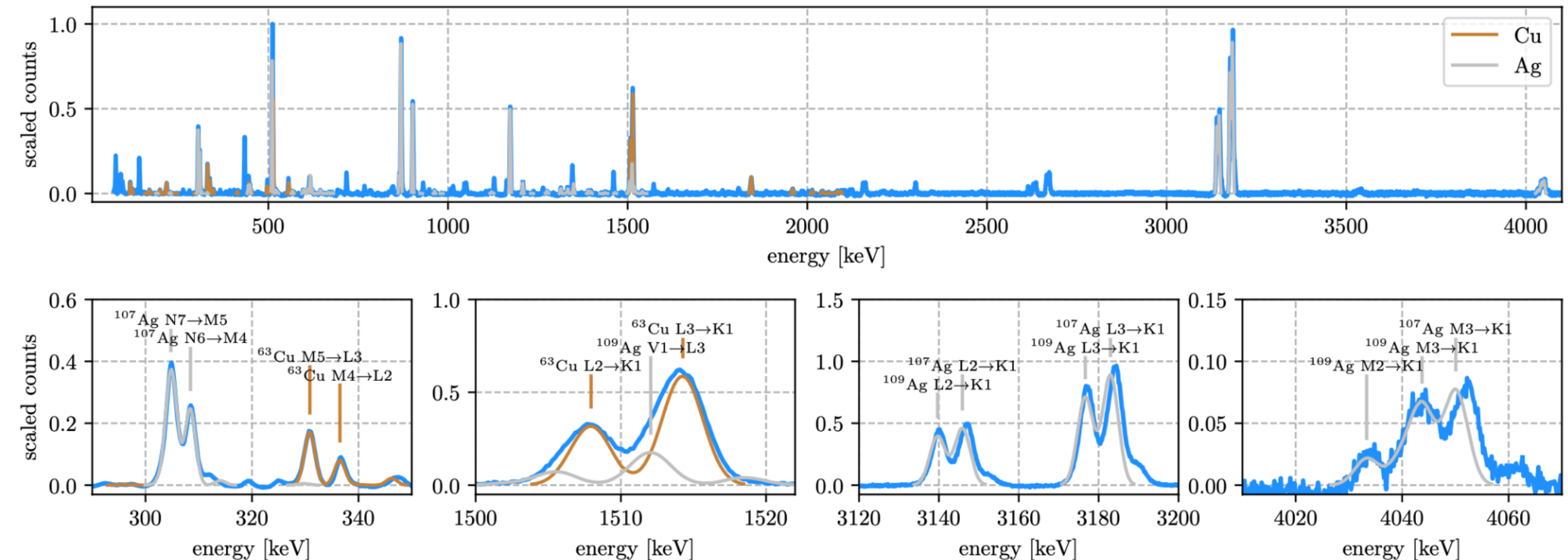
# SAMURAI: Demo II

PRELIMINARY

Sturniolo, S, Hillier, A. Mudirac: A Dirac equation solver for elemental analysis with muonic X-rays. *X-Ray Spectrom.* **2020**

- Step 2: Simultaneous fitting of all theory (MuDirac 1.0) peaks, using hierarchical sparsity

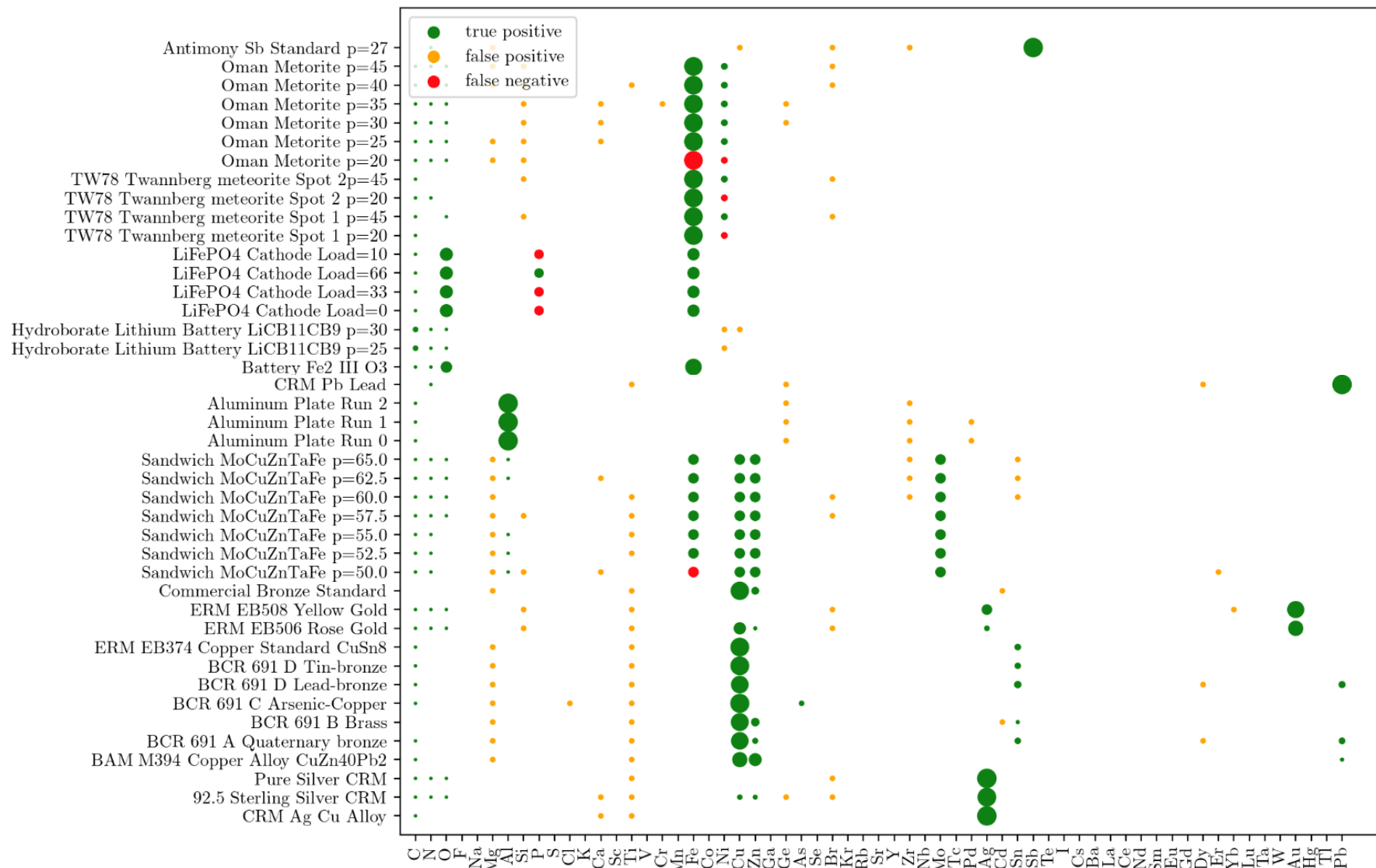
CRM Ag Cu Alloy



# SAMURAI: Qualitative Results

## Confusion matrix

- Almost all large elements are detected
- Very few false negatives
  - *manual check pending*
- Few false positives
  - Usually very small proportion
- Detection threshold can be tuned by user
- Additional “confidence score” in development



# SAMURAI: Quantitative Results

PRELIMINARY

## Composition table

- Benchmarked on CRMs
- Composition calculated (no references)
  - generally fair agreement
    - *manual check pending*
- overall precision ~ 5-20 %
  - main limitation: knowledge of muon capture probabilities
  - to a lesser degree: self-absorption in sample, efficiency estimate

***open-source software  
release in preparation***

