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SHERPA: a Spectrometer for High Energy Resolution Polarization Analysis

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Overview

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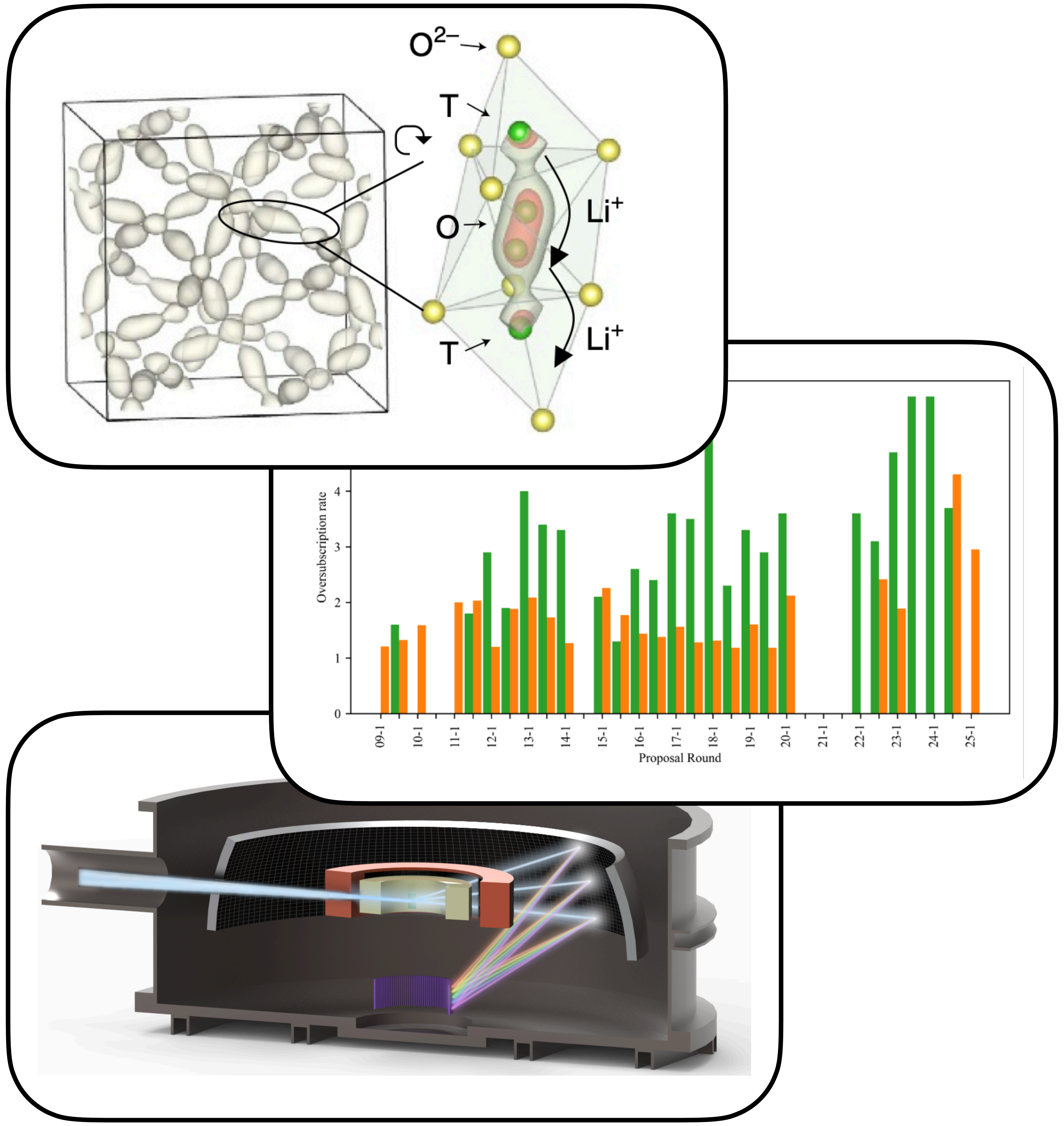
1. SHERPA is an indirect geometry spectrometer concept that combines a **novel secondary spectrometer design** with **routine polarization analysis**. This will enable it to probe small samples with the ability to separate collective and self dynamics.

2. SHERPA will **extend the capabilities** of the cold spectroscopy instrument suite and **increase capacity** - cold spectrometers at ISIS are currently highly oversubscribed.

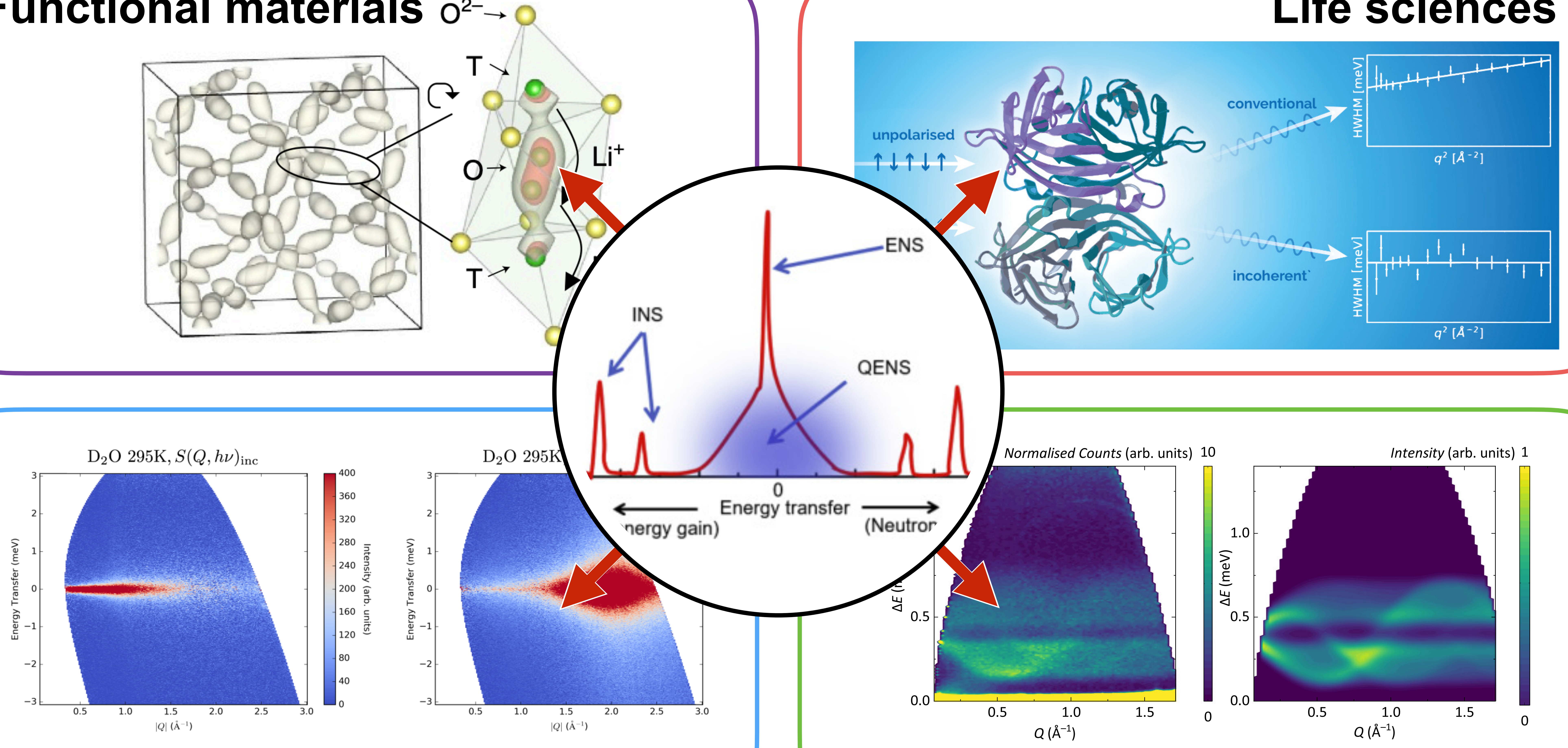
3. The performance of SHERPA will exceed the current IRIS instrument (which it replaces) **by a factor >100 unpolarized and >10 polarized**.



Science case: dynamics and functionality

Functional materials

Life sciences



Soft matter and liquids

Quantum materials

Science case: the need for polarization

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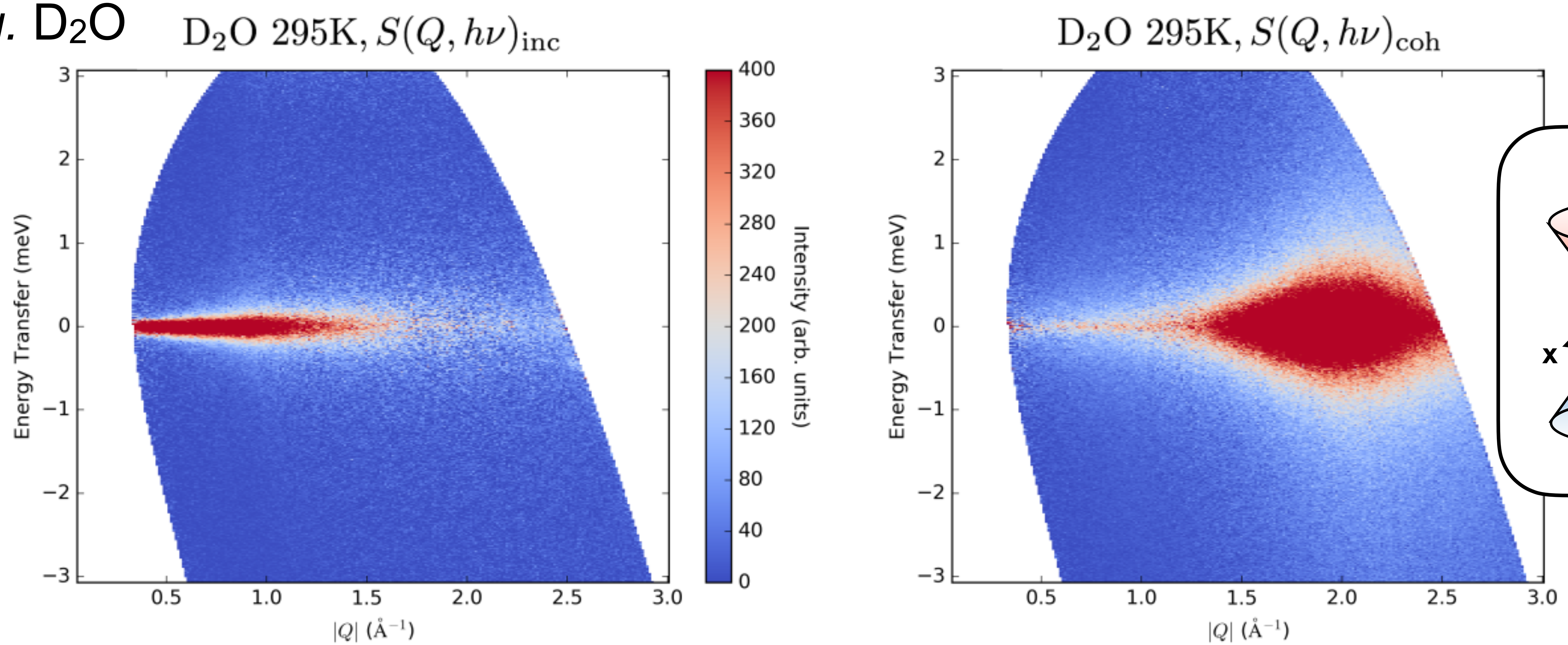
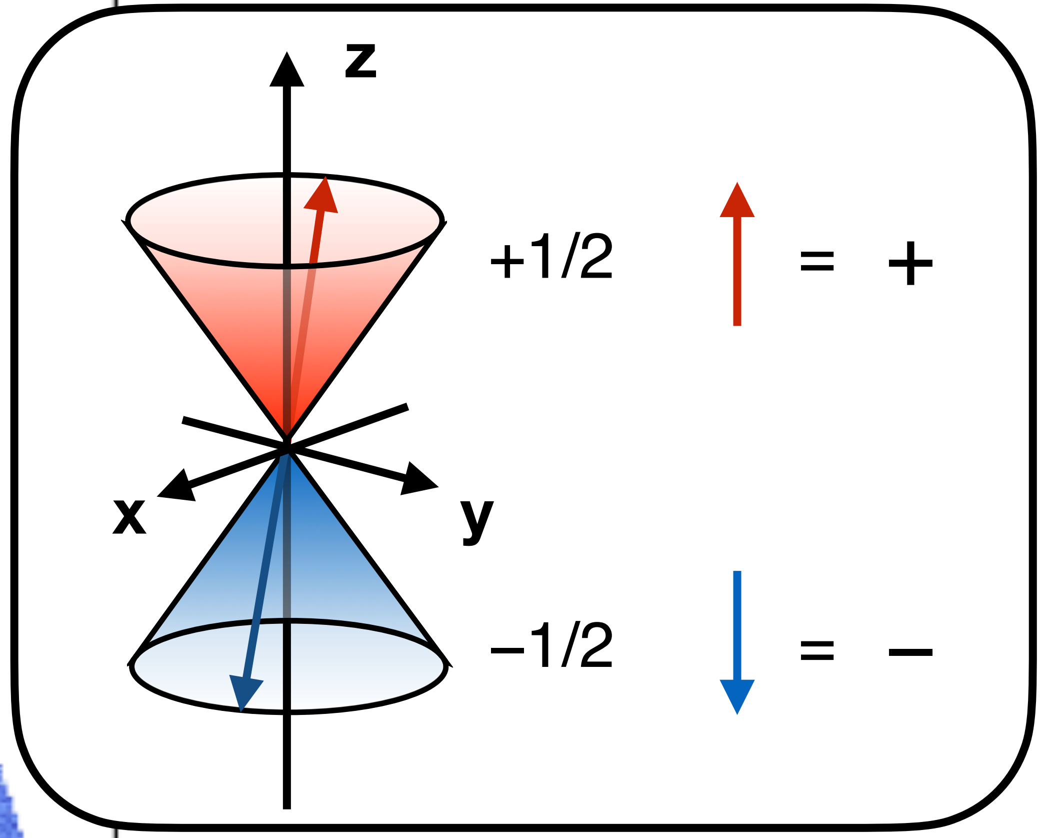
- Many cases benefit significantly from polarization analysis, which grants the ability to separate coherent (corresponding to collective) and incoherent (self) dynamics:

e.g. D_2O





Arbe et. al., Phys. Rev. Research **2**, 022015(R) (2020)

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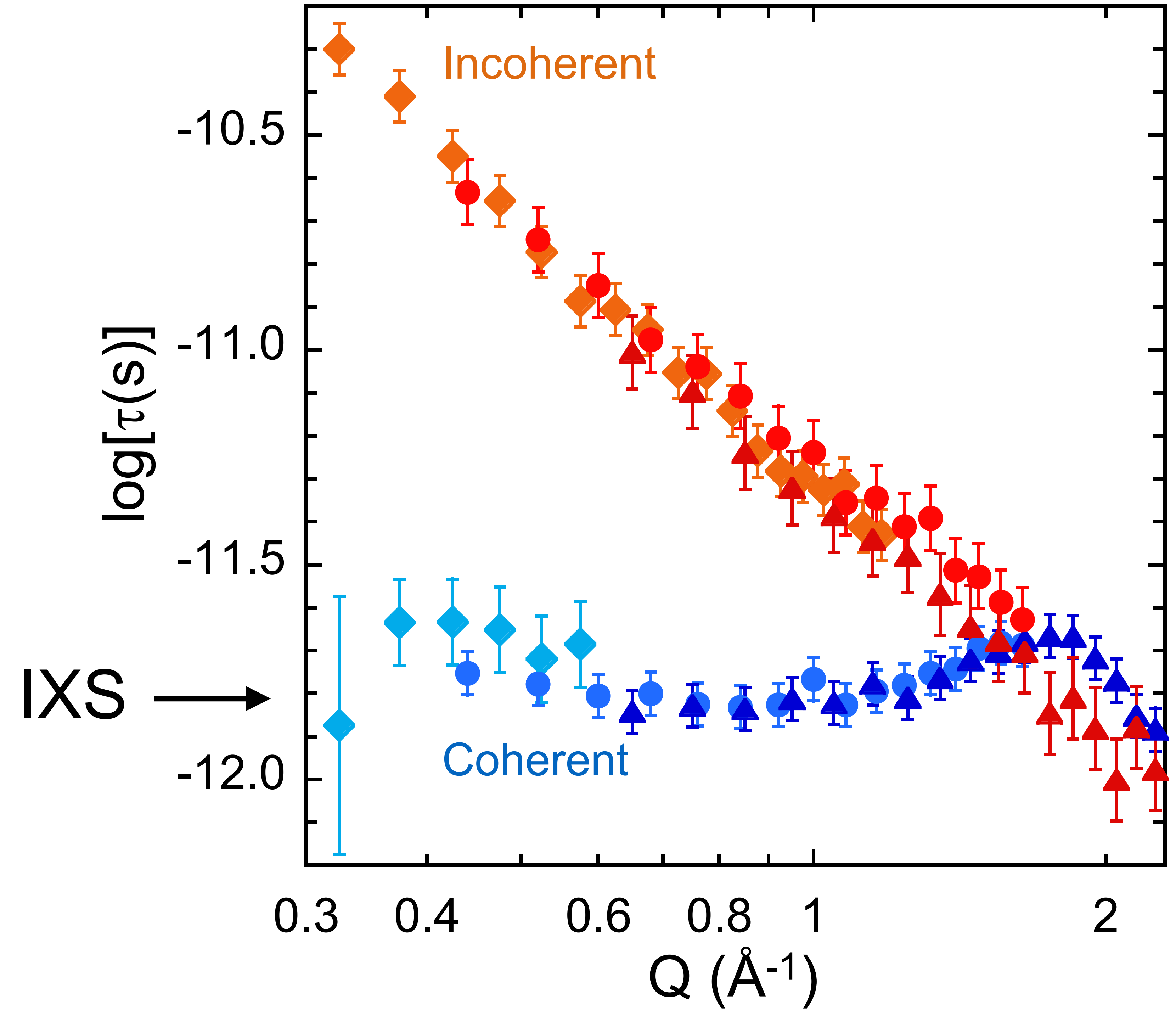
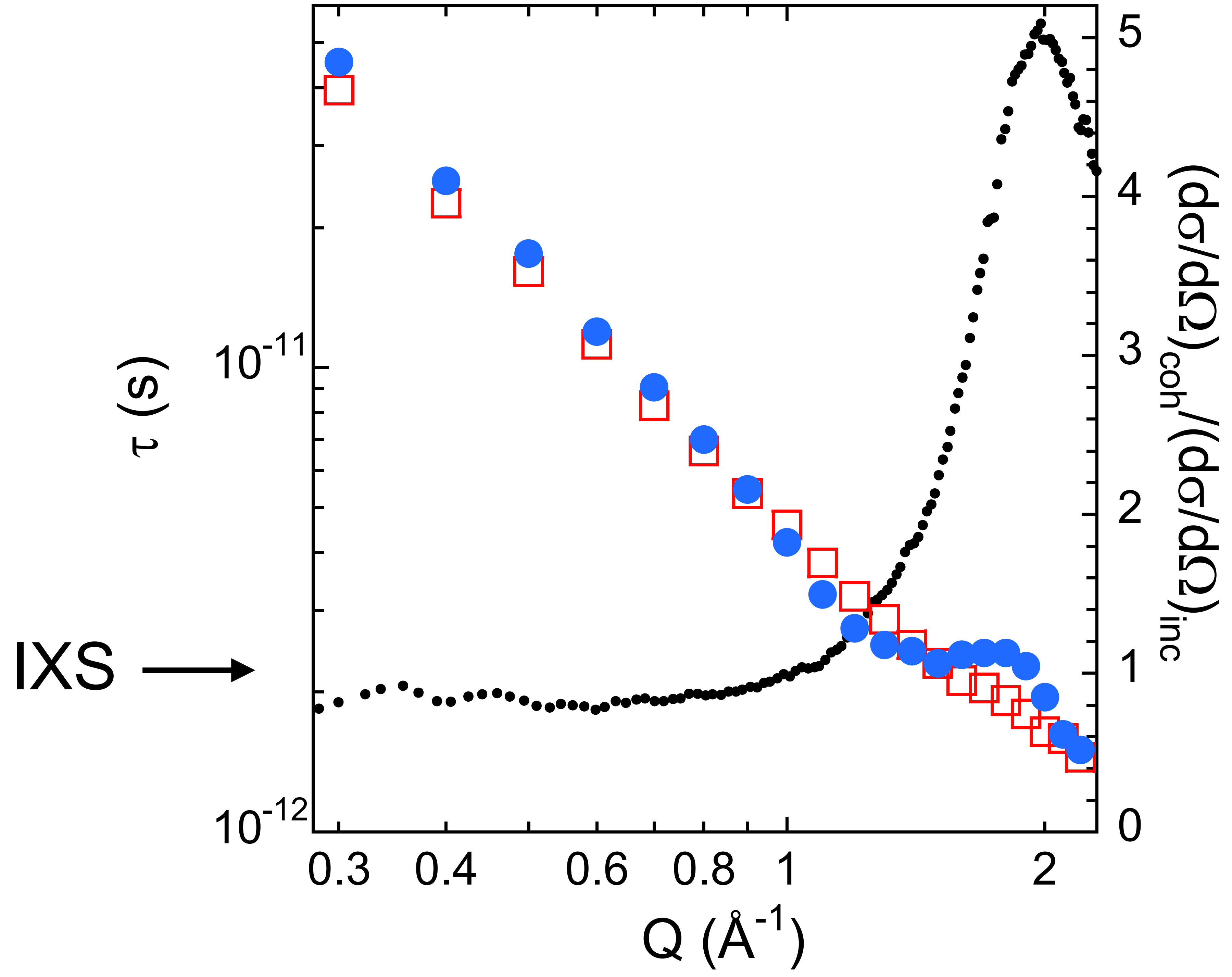
Polarized



Arbe et. al., Phys. Rev. Research **2**, 022015(R) (2020)

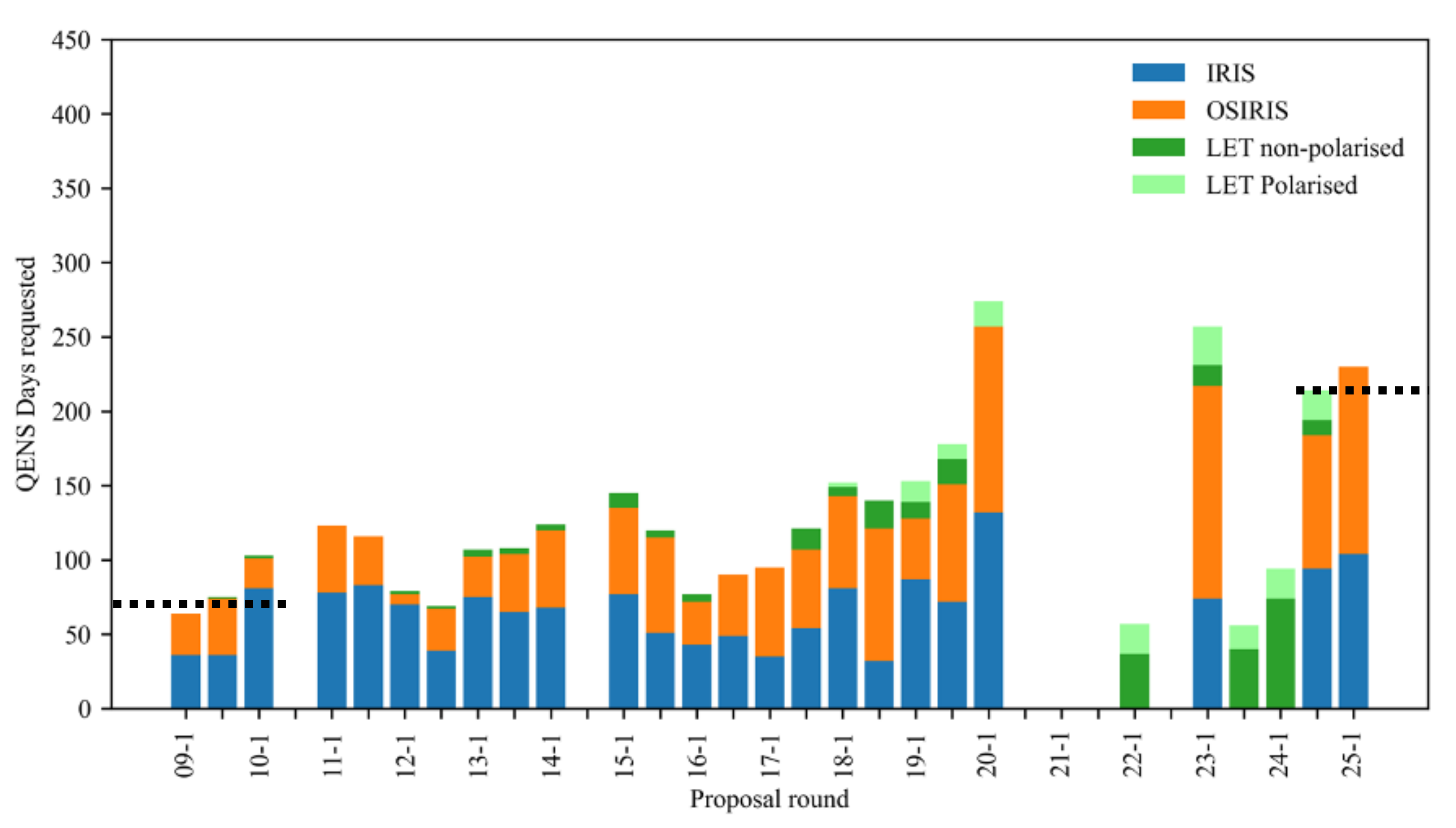
Unpolarized

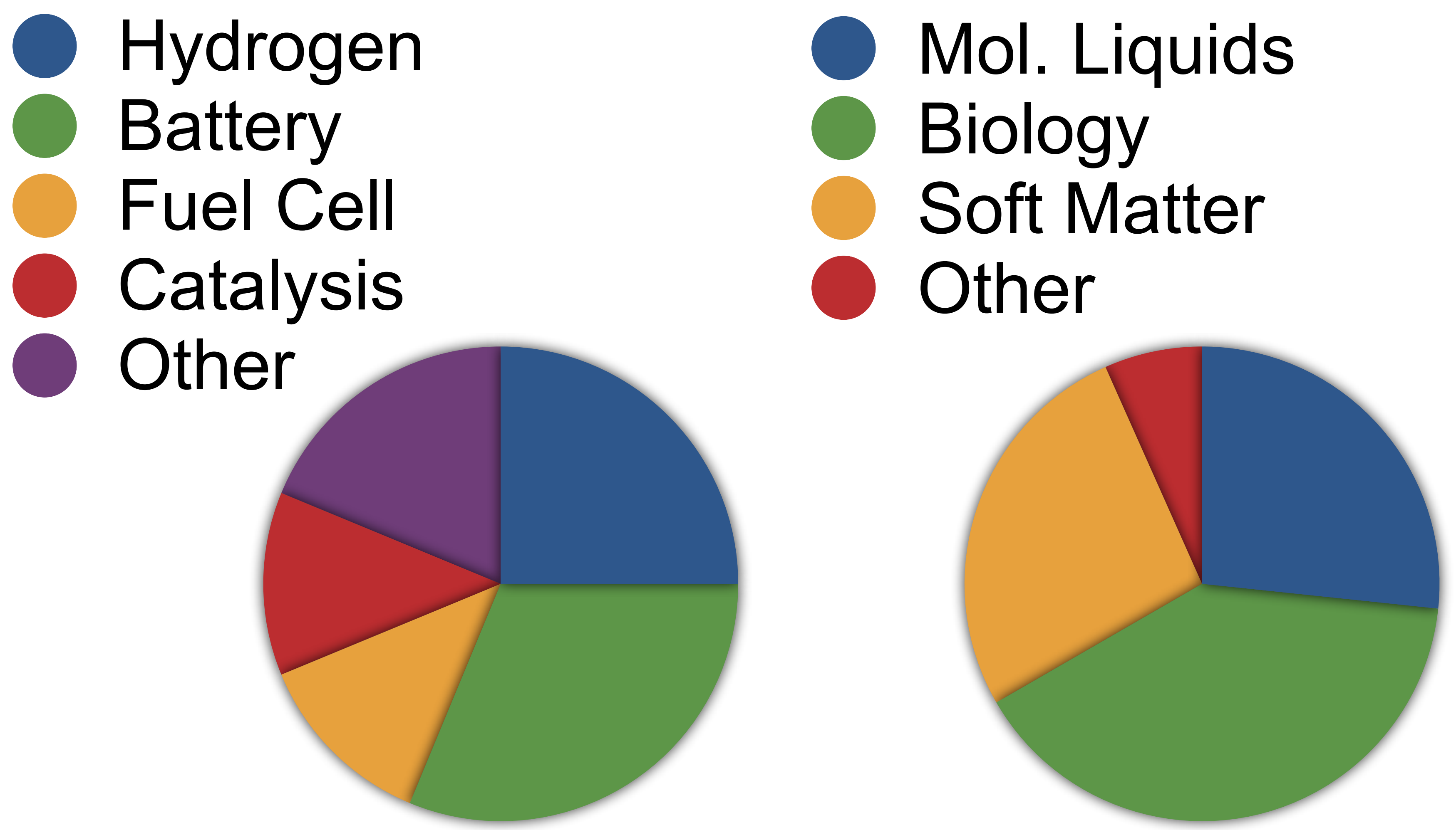


Arbe et. al. Phys. Rev. Lett. **117** 185501

Business case

- Cold spectroscopy capabilities at ISIS provided by three instruments: OSIRIS, IRIS (indirect), LET (direct)
- Major increase (factor ~3) in days requested over the last 15 years. Supply is not keeping up with demand: after 2022, **average oversubscription ~ 3**
- Similar increases observed at other European institutions *e.g.* ILL
- Considerable recent interest in polarized experiments: **>50% of accepted QENS proposals on LET across a broad range of fields**





Science case: high count rate and resolution

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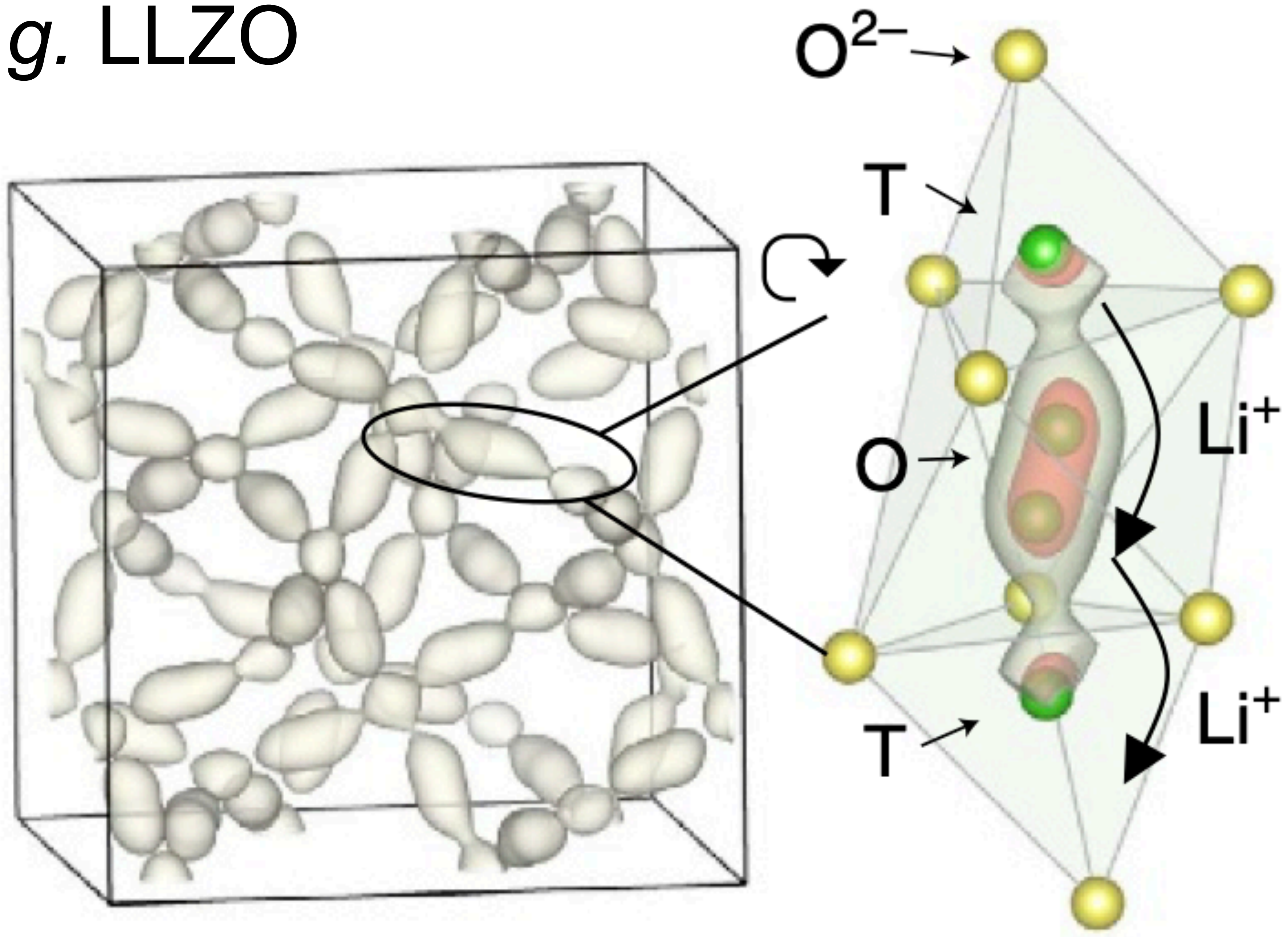
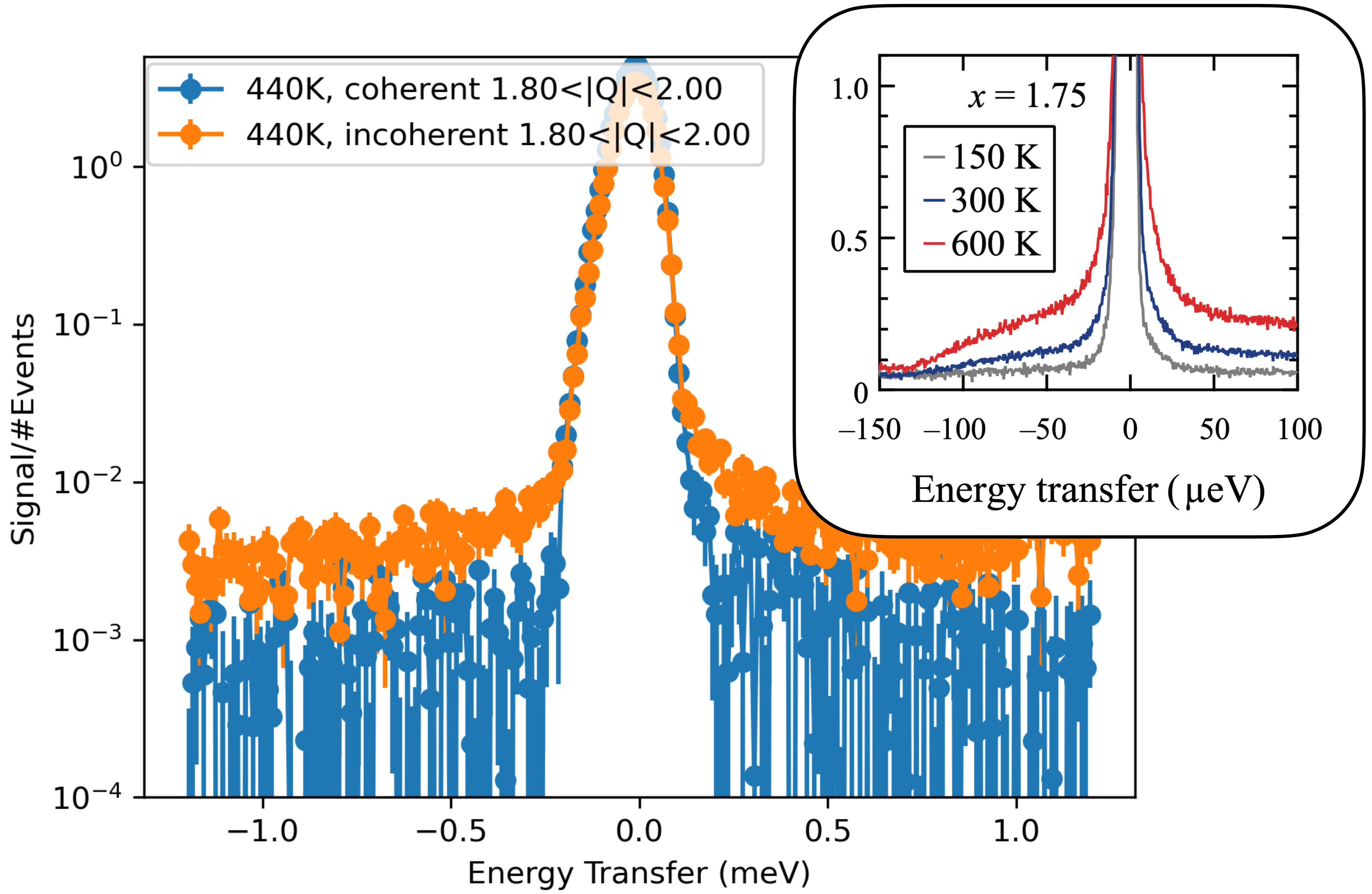
- But, in some other cases, the flux/resolution on LET are insufficient to resolve spectral components:

e.g. LLZO





C. Wang *et al.*, Chem. Rev. **120**, 4257 (2020)

G. J. Nilsen *et al.*, unpublished; H. Nozaki Toyota **46**, 37 (2015)

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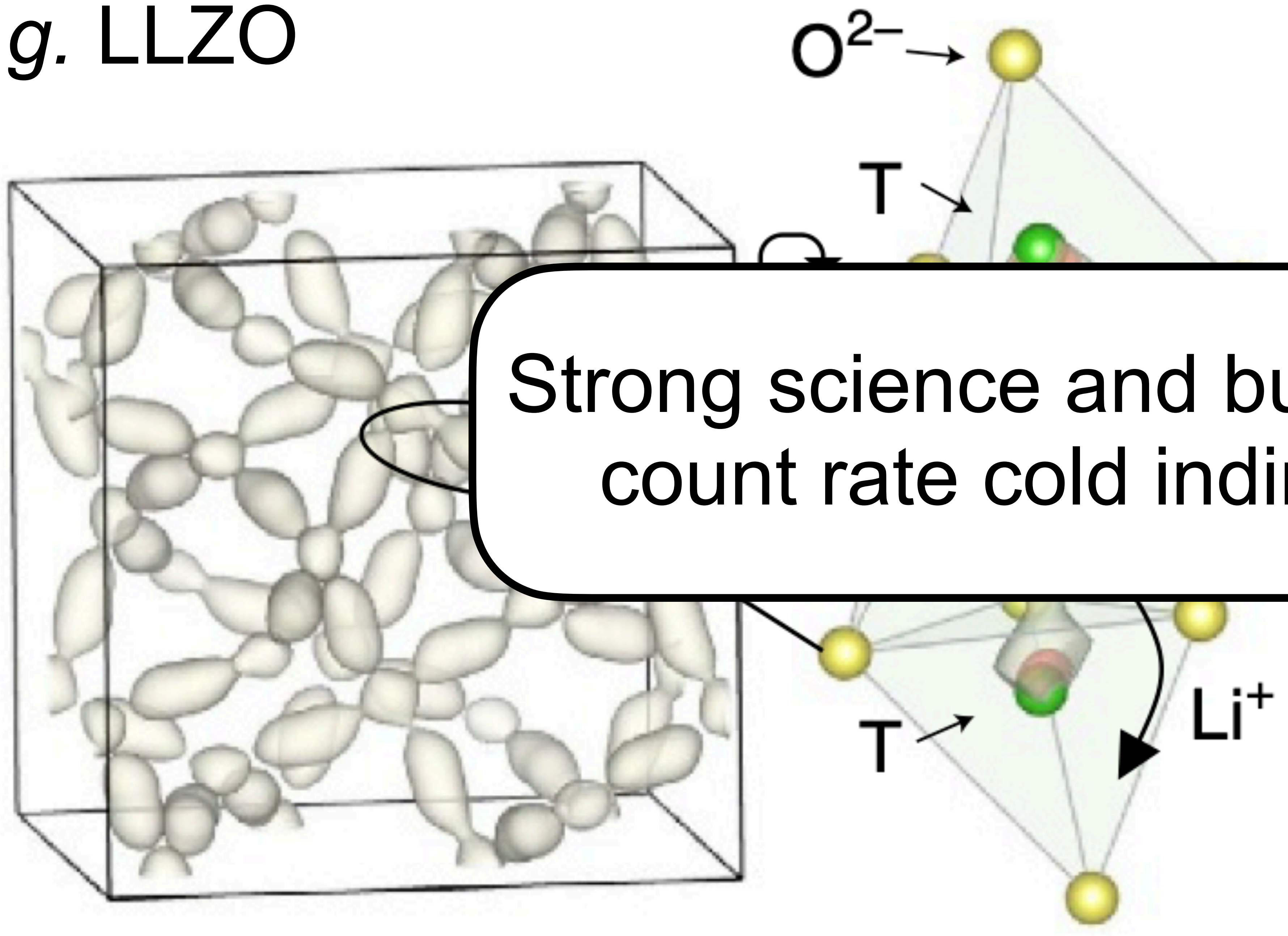
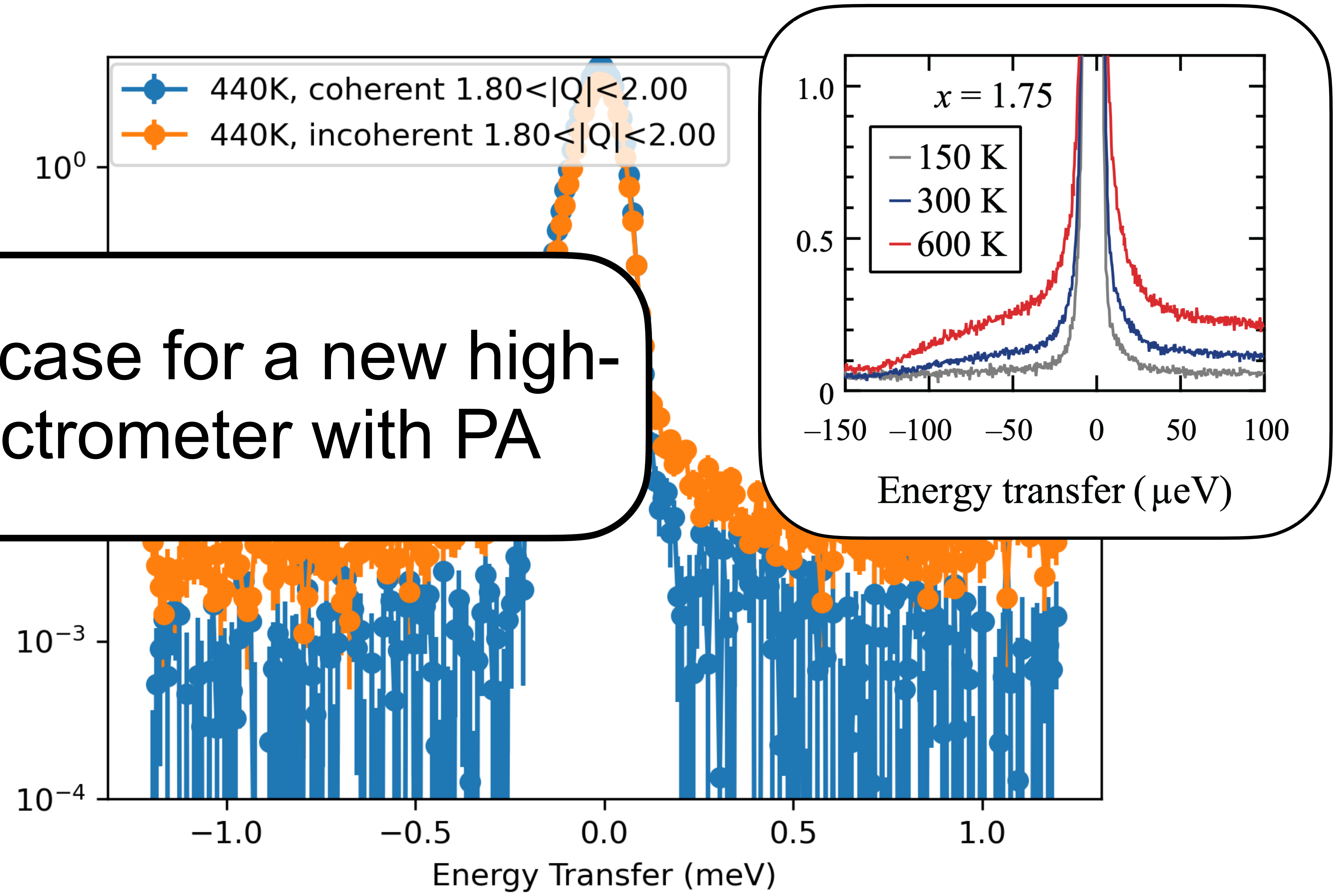




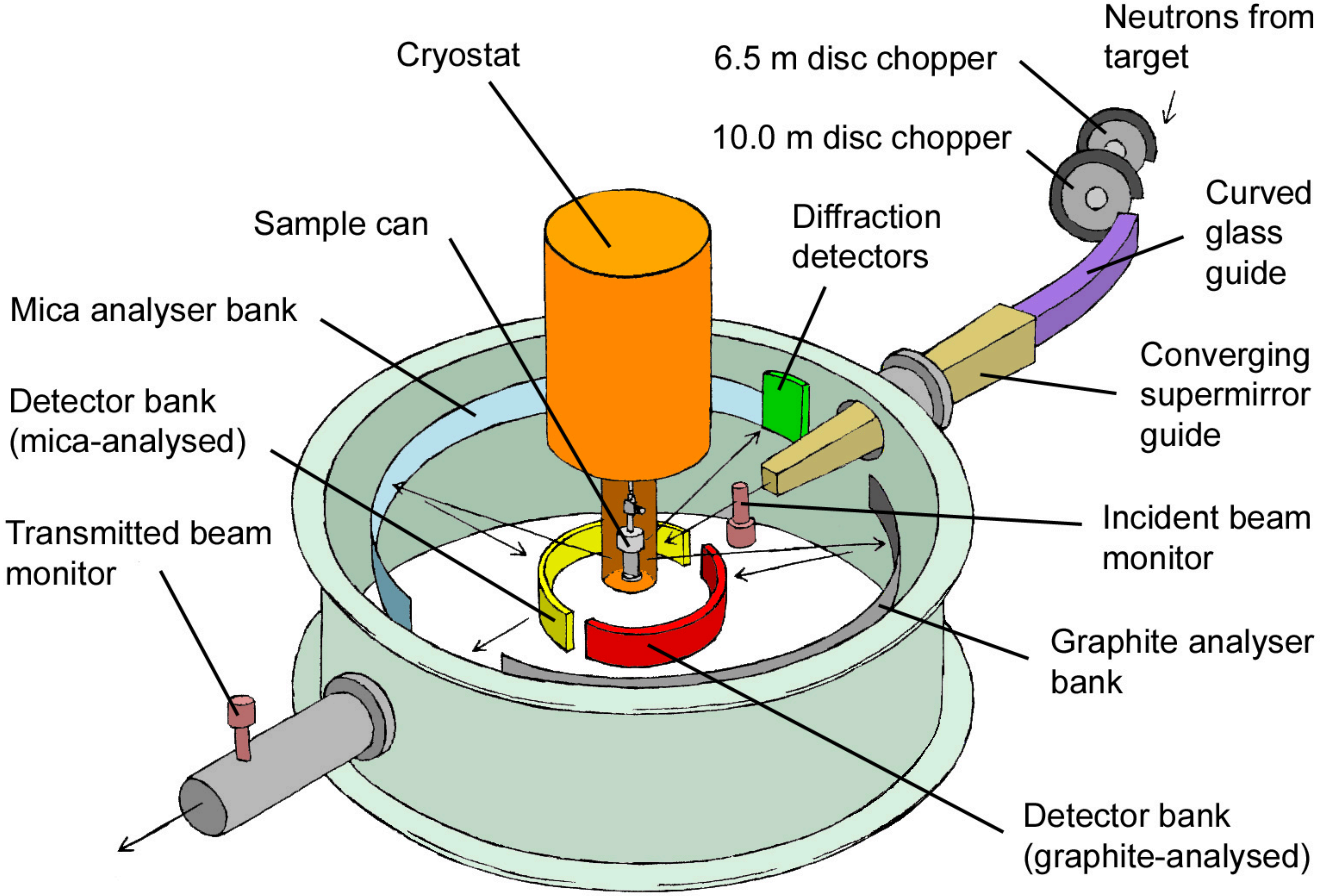
Strong science and business case for a new high-count rate cold indirect spectrometer with PA

C. Wang *et al.*, Chem. Rev. **120**, 4257 (2020)

G. J. Nilsen *et al.*, unpublished; H. Nozaki Toyota **46**, 37 (2015)

From IRIS to SHERPA

- IRIS: indirect geometry time-of-flight spectrometer
  - Part of original instrument suite (1988)
  - Workhorse instrument
    - *m* = 1 curved guide
    - *m* = 2 focusing nose
    - L_1 = 36.5 m
    - PG(002) analyzer
    - Resolution ΔE=17.5μeV



Carlile and Adams, Physica B **182**, 431 (1992)

Requirements

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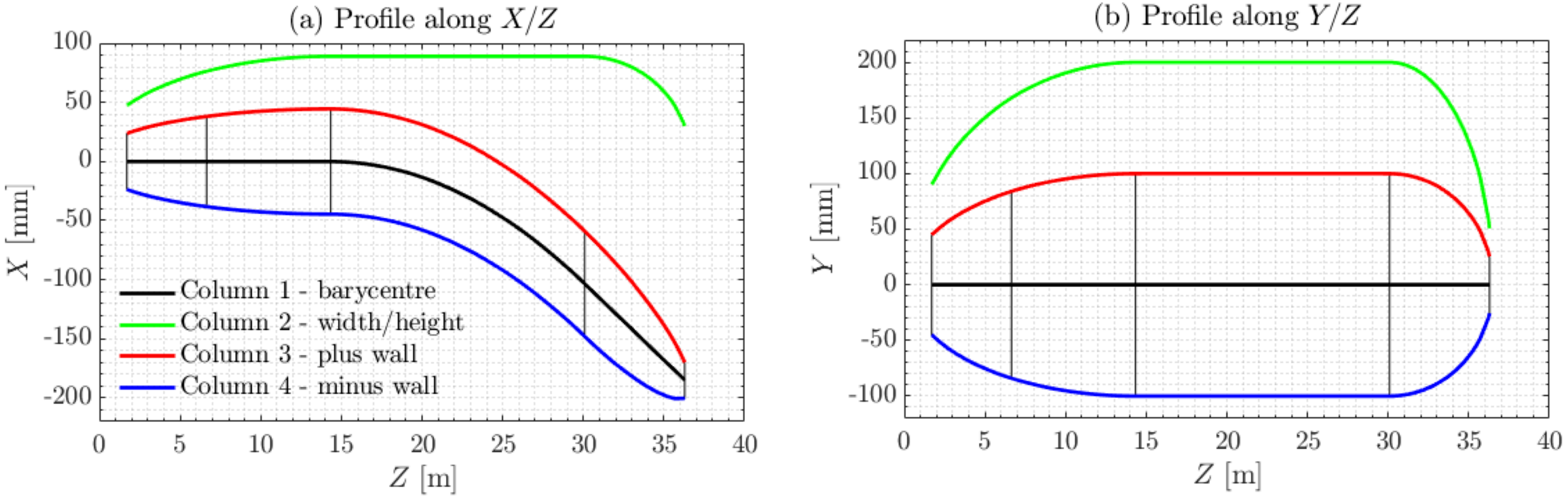
- **At least 100× IRIS count rate**
- **Rapid changeover to polarization analysis mode**
- **17.5 μeV resolution (ΔE FWHM) for a 3 cm tall sample**
- Similar Q range to the OSIRIS spectrometer $0.2 < Q < 1.8 Å^{-1}$
- Maximum Q resolution $\Delta Q = 0.3° Å^{-1}$ at minimum accessible scattering angle ($2\theta_{min}$ ~10°) without collimation
- Controllable Q-resolution down to $\Delta Q = 0.1° Å^{-1}$
- Polarization analyzer that accommodates a sample width of 20 mm and allows full view of the energy analyzer
- Suppression of the PG(004) reflection to the level of 10^{-4}

SHERPA concept: primary spectrometer

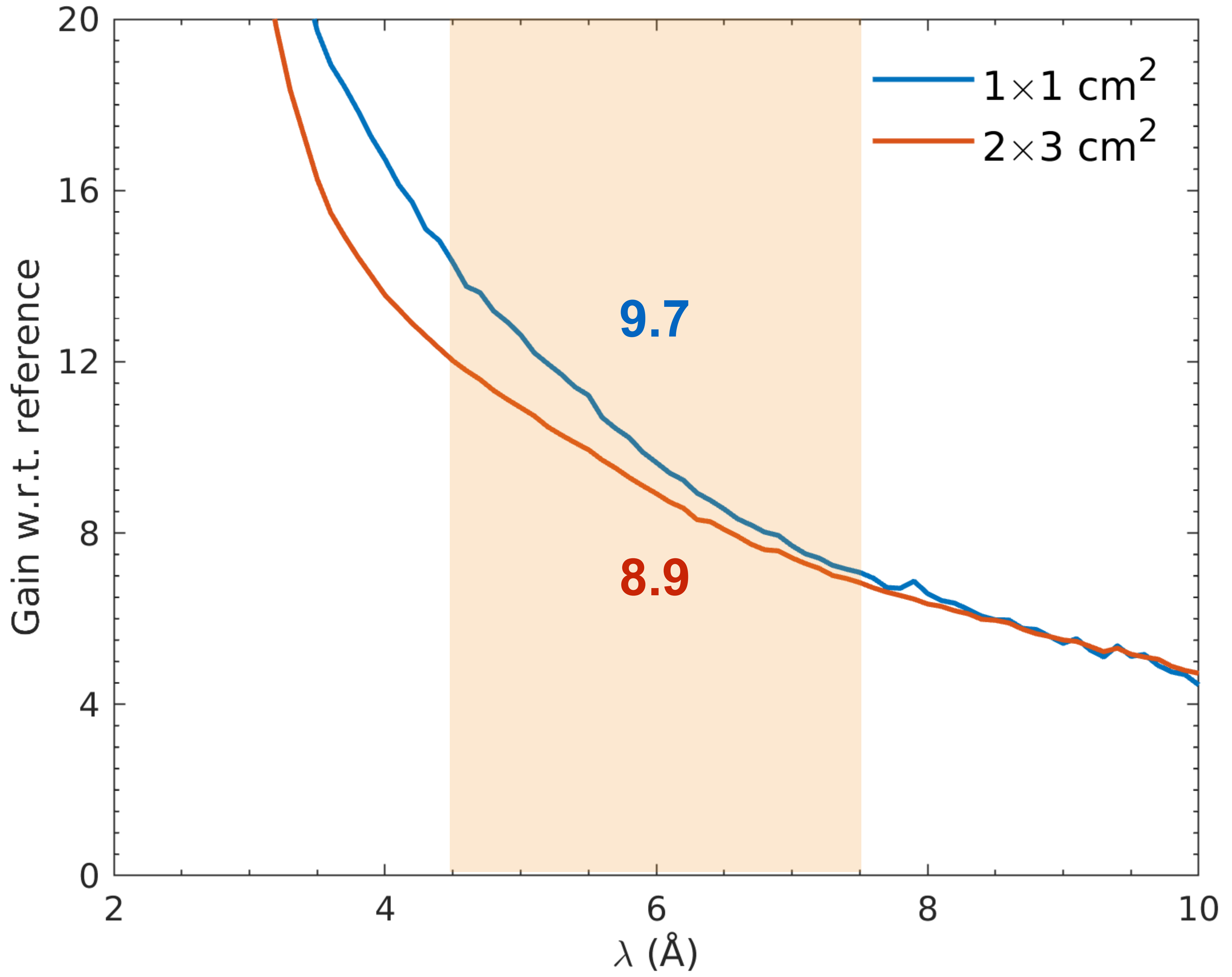
- Modern double-elliptical supermirror guide (like OSIRIS)
- Optimize using OSIRIS guide as starting point - result nearly identical:



A. Perrichon and F. Demmel, NIMA **1039**, 167014 (2022)

Gain factor: guide

- Gain factor over expected wavelength band of instrument around a **factor 10**:



FARO concept: secondary spectrometer

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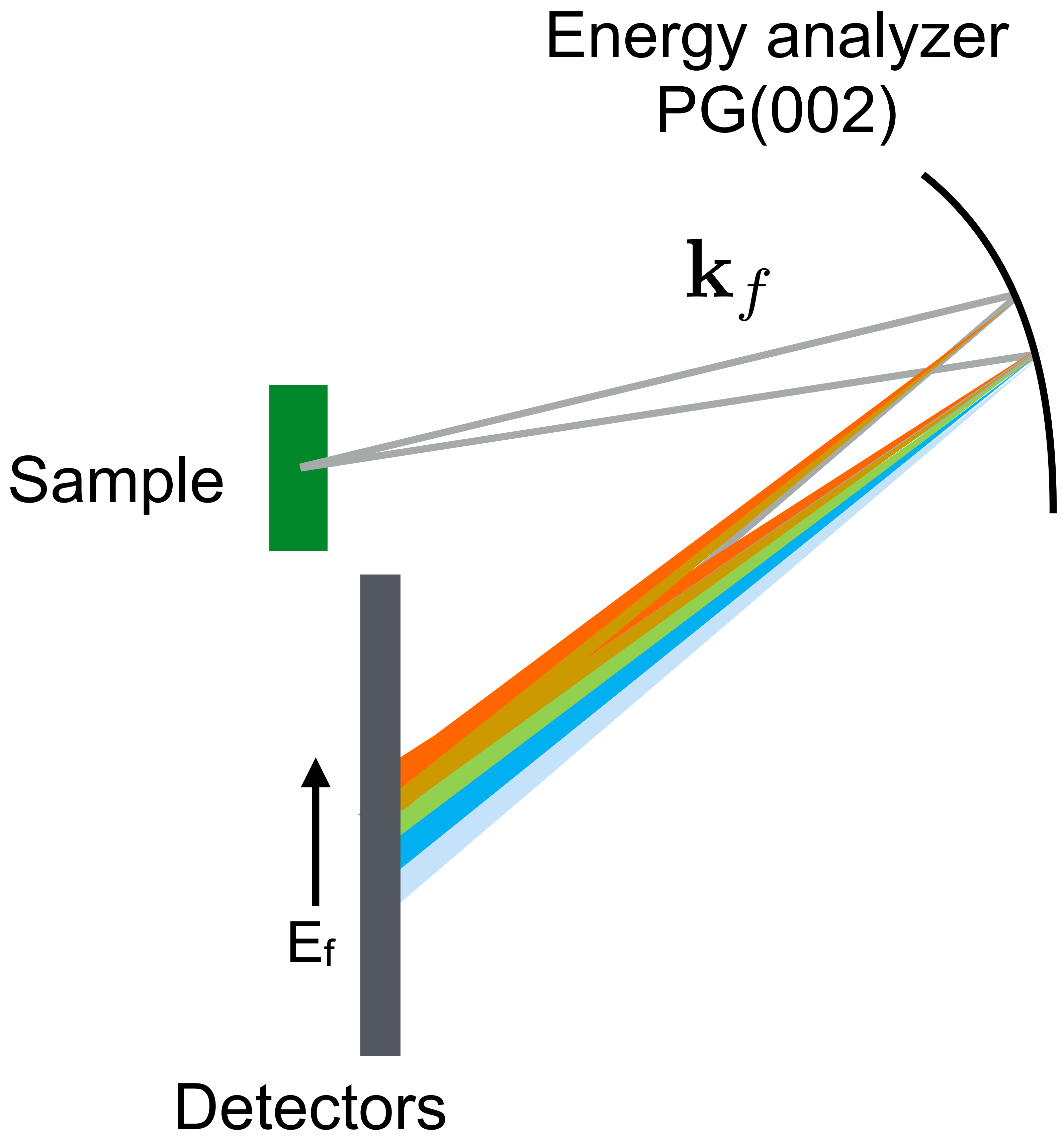
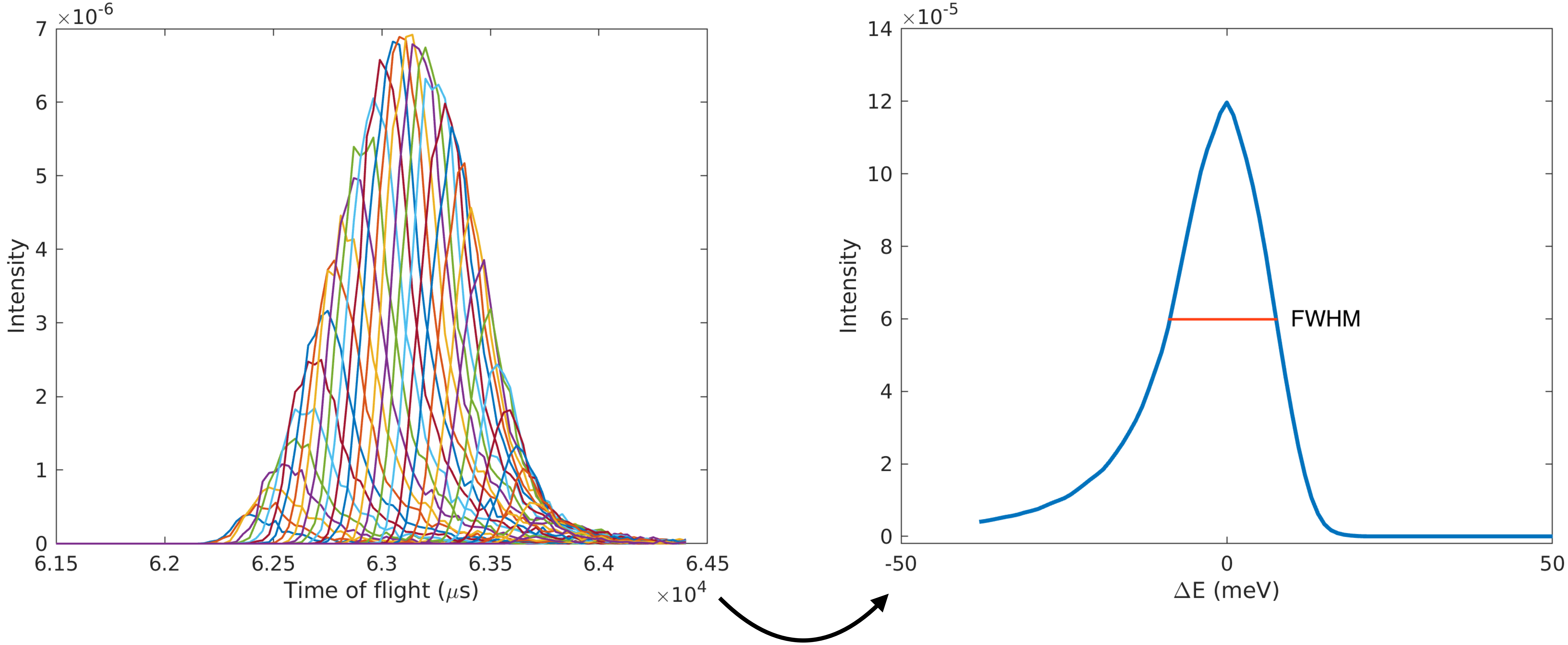


$$I \propto \Phi d\Omega \Delta\lambda$$
$$\Delta\lambda = \mu\lambda \cot\theta$$

	λ (Å)	μ(°)	cot θ	dΩ	Φ	**Gain**
IRIS	6.64	0.8	0.0437	0.2	1E+07	**1**
SHERPA	6.47	1.5	0.2586	0.6	1E+08	**330***

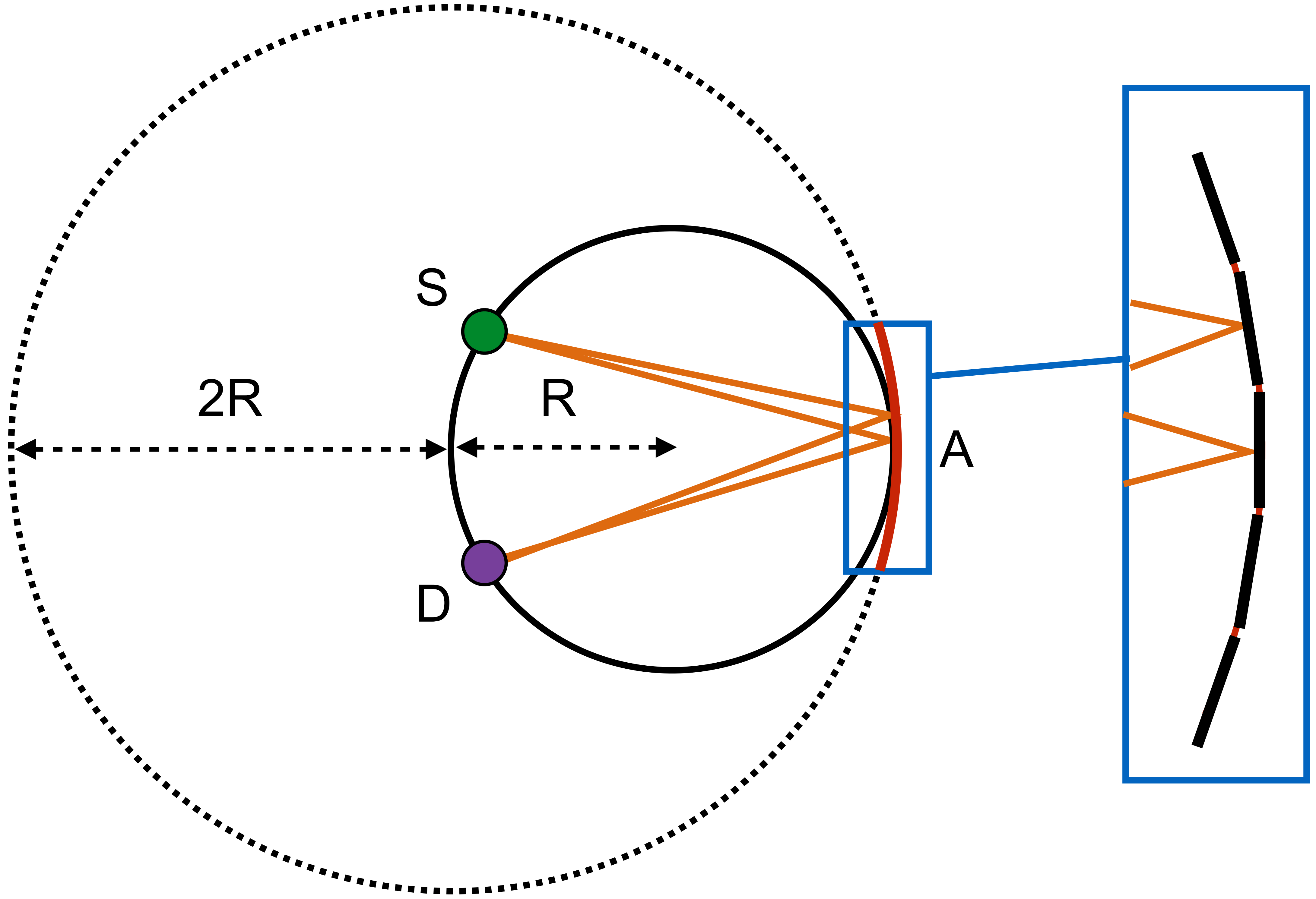
Energy resolution

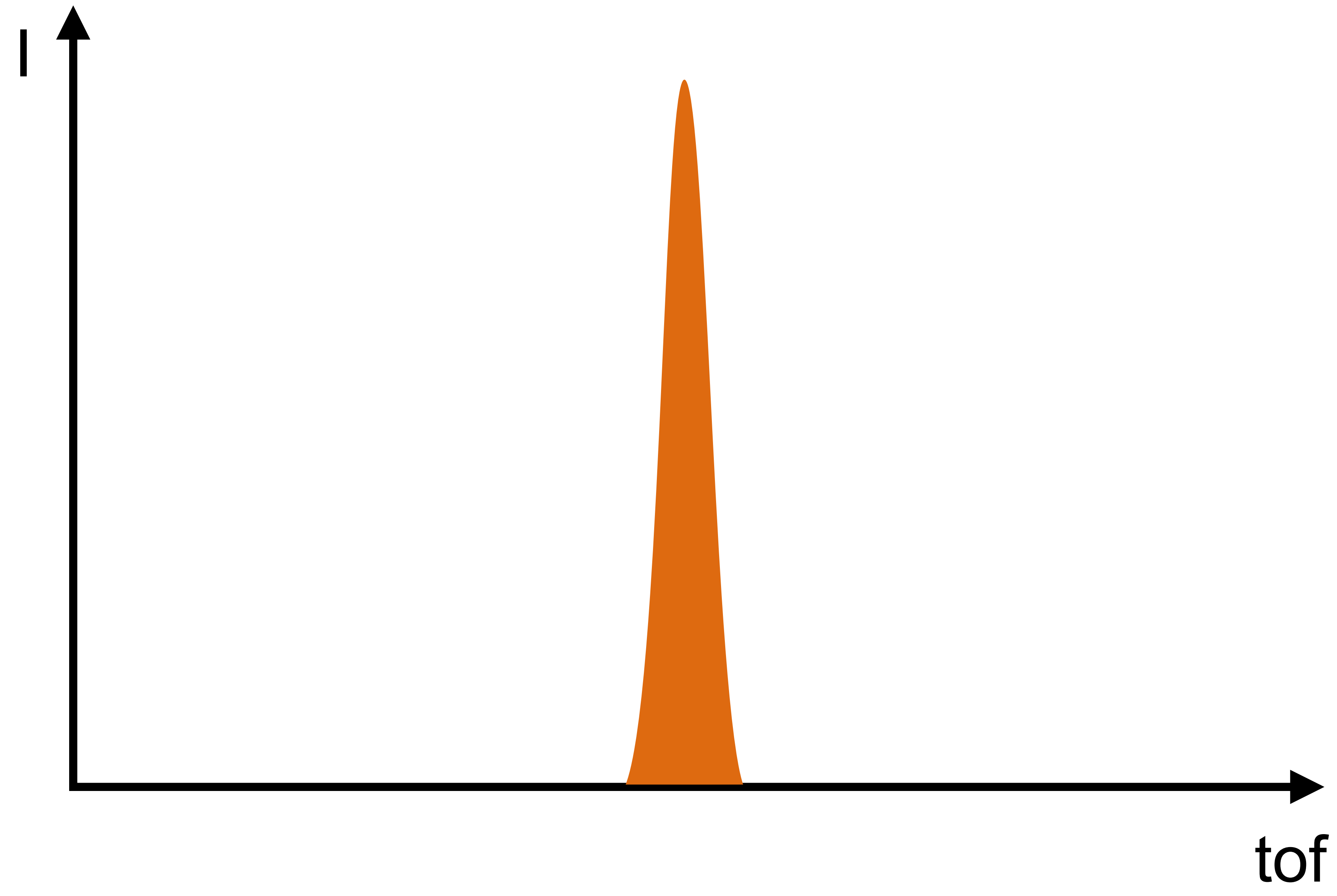
- The data can be analyzed pixel by pixel, then recombined. There is thus a decoupling of the crystal mosaic and resolution that allows larger cot(θ)



Geometry

- Starting point: Rowland circle, each crystal placed on a circle such that final energy and path length, and hence TOF (close to) the same for all paths between S and D:

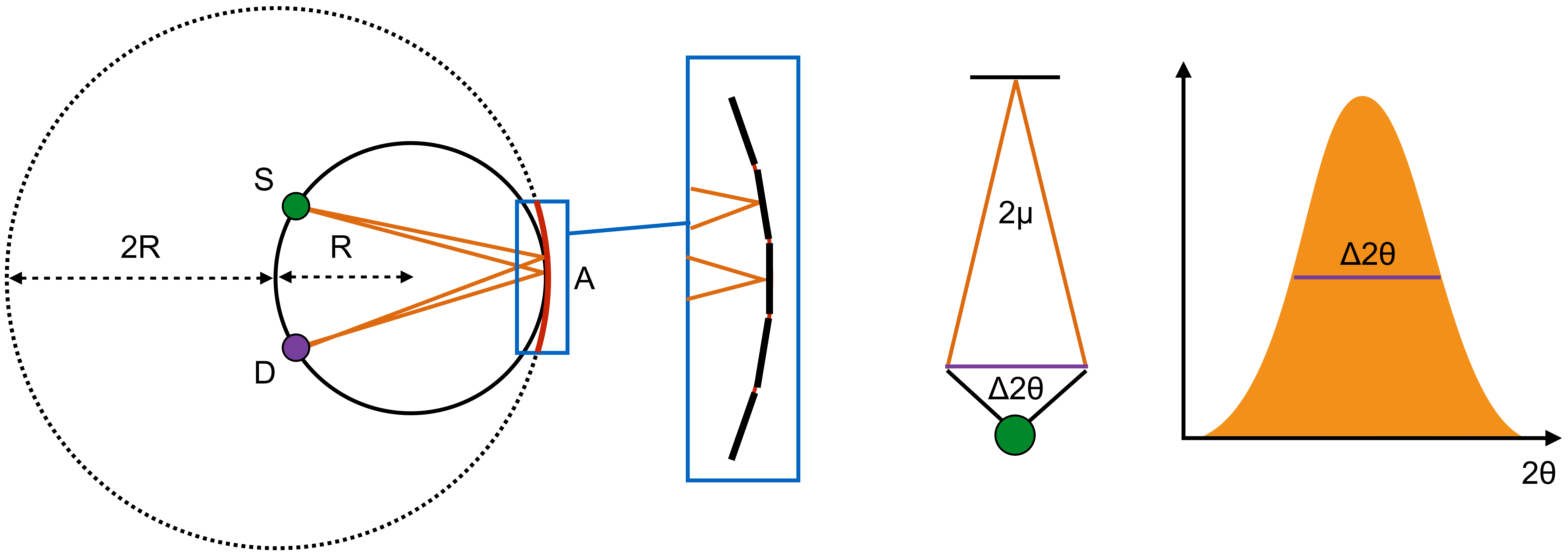




Decouple

Geometry

- Near backscattering, this places the detector close to the sample, which is both impractical and leads to a degradation of Q-resolution due to the analyser mosaic:



Technical case:prismatic effect

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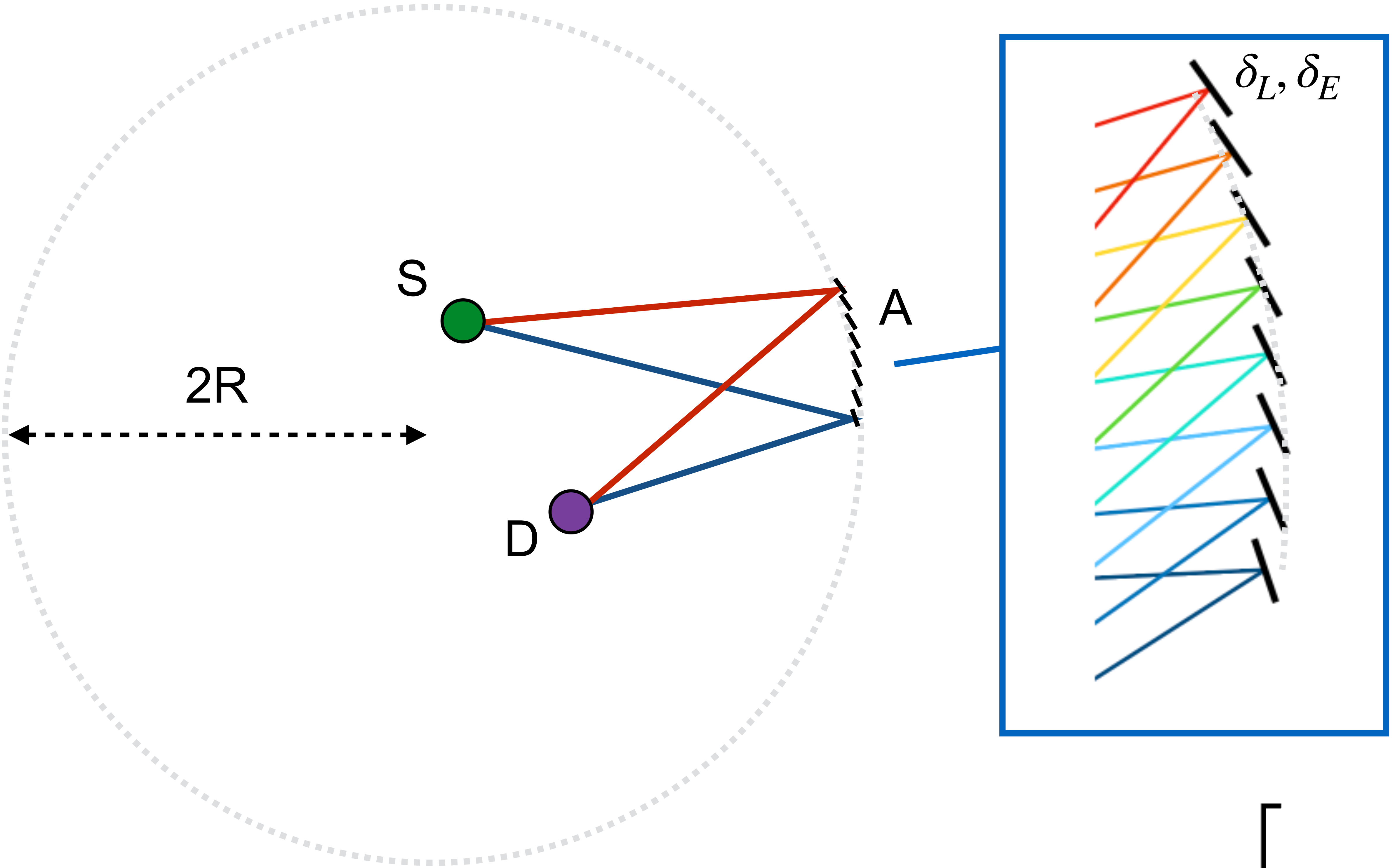
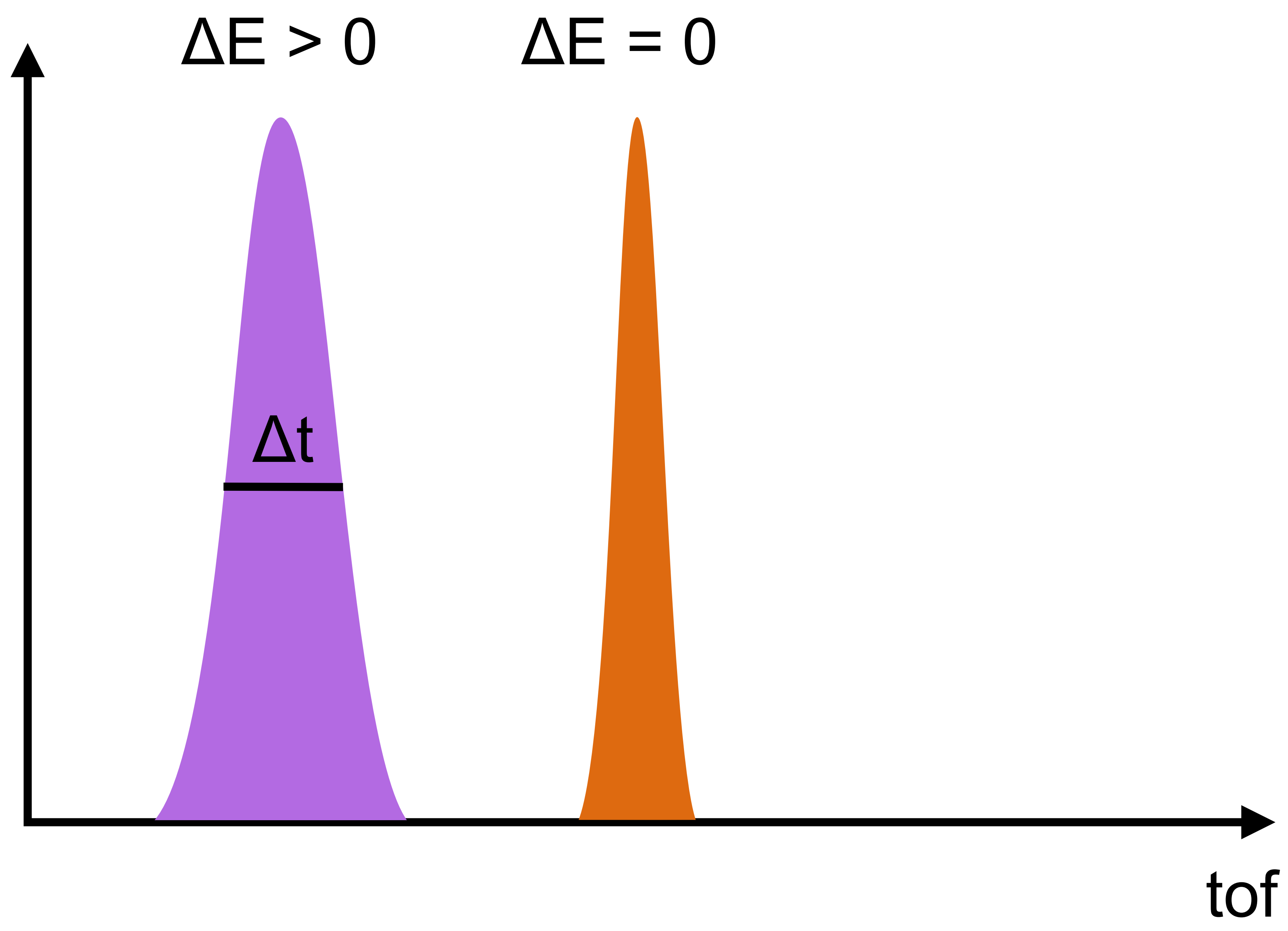
- SHERPA uses a novel time-focusing geometry to achieve improve the Q-resolution at a small price to the ΔE resolution away from the elastic line:





$$\Delta t = C\left[\delta_L\sqrt{E_f} + \delta_E\left(\frac{L_{ms}}{2\sqrt{E_f - \Delta E}} + \frac{L_{sd}}{2\sqrt{E_f}}\right)\right]$$

Q and ΔE resolution

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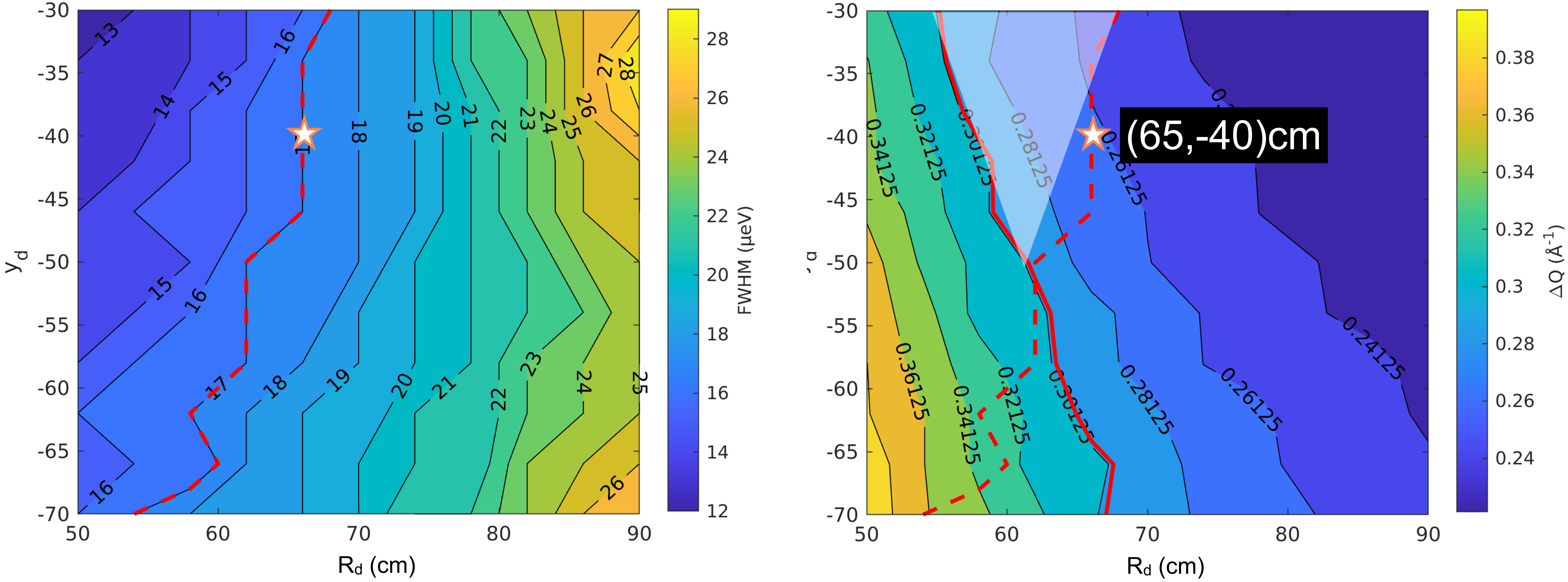
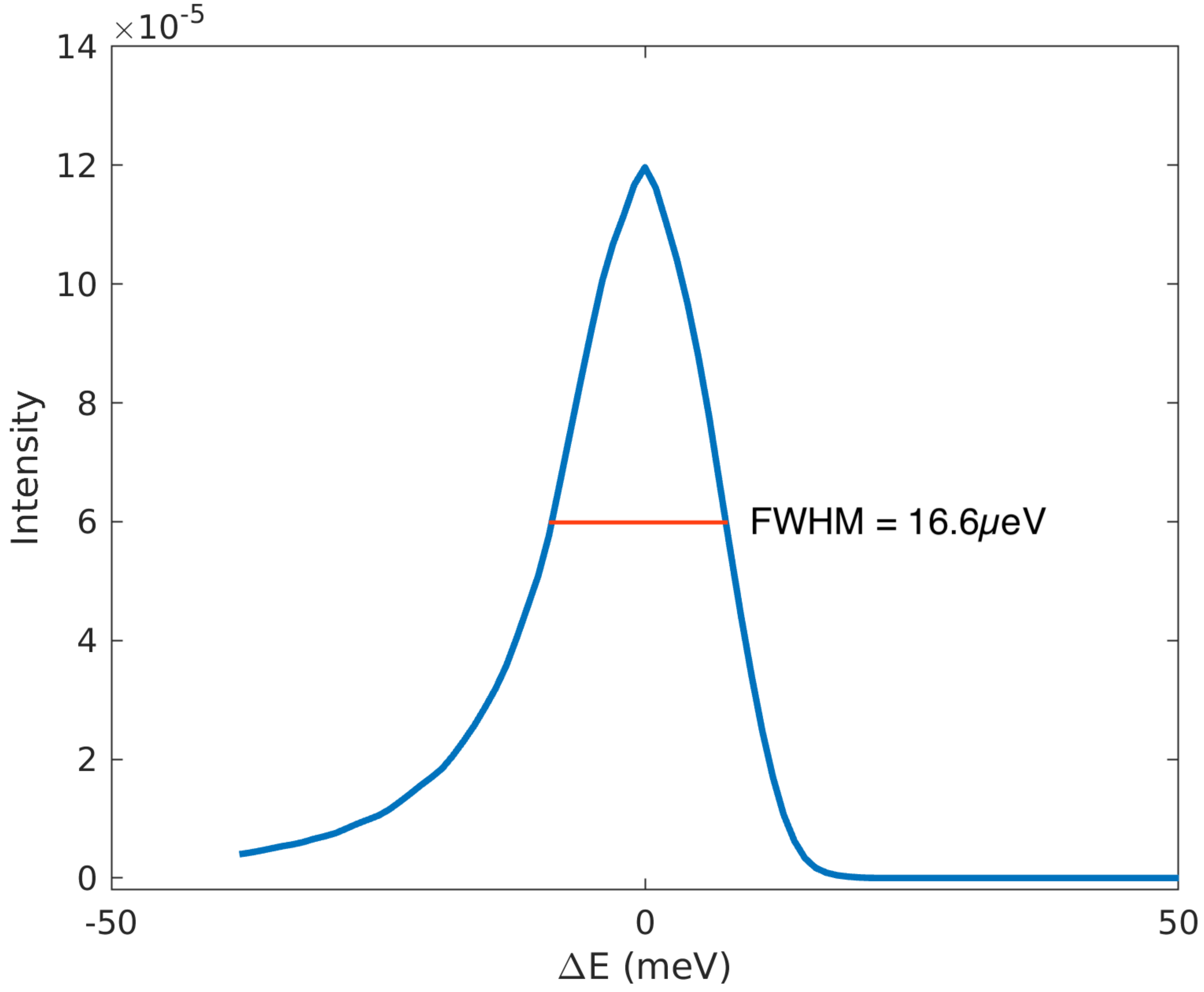
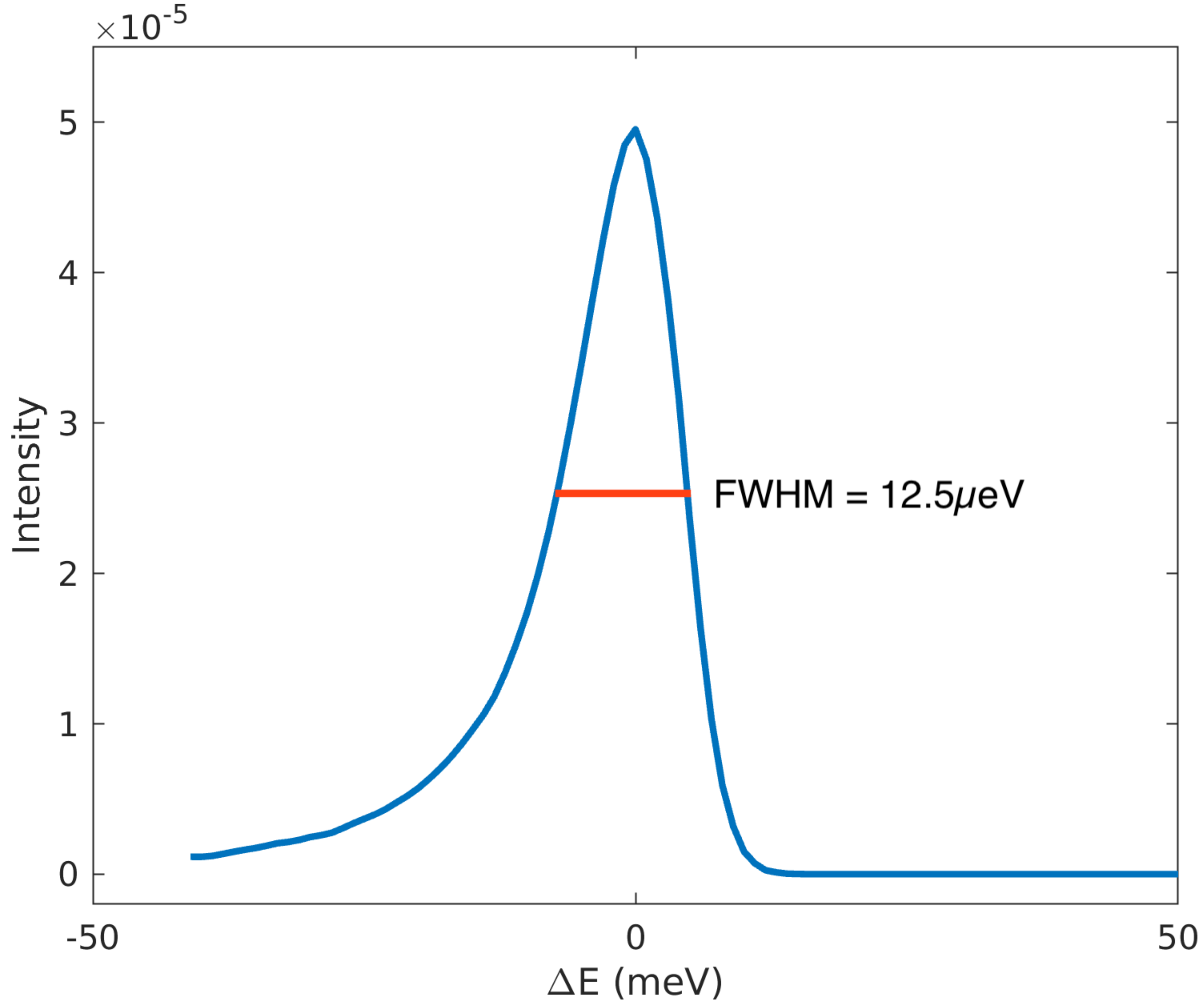
- Optimal solution for Lsd = 140cm, central pixel of detector at (65,-40)cm



Energy resolution sample size

- Resolution shows some size-dependence:





Overall gains:

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- **Gain from new guide ~8.9**
- Increased solid angle of analyser:
  - Old analyser ~3% of 4π
  - New analyser ~4.3% of 4π
  - **Gain ~1.3**
- Moving further from backscattering and increasing crystal mosaic:
  - Old cot(87.5) = 0.04366, new cot(72.5) = 0.31530 (L_2 = 140cm) → **Gain ~7.0**
  - Old μ = 0.8°, new μ = 1.7° → **Gain ~2.1**
- **Total gain: ~200 at L_{sa} = 1.4m**

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SHERPA secondary spectrometer

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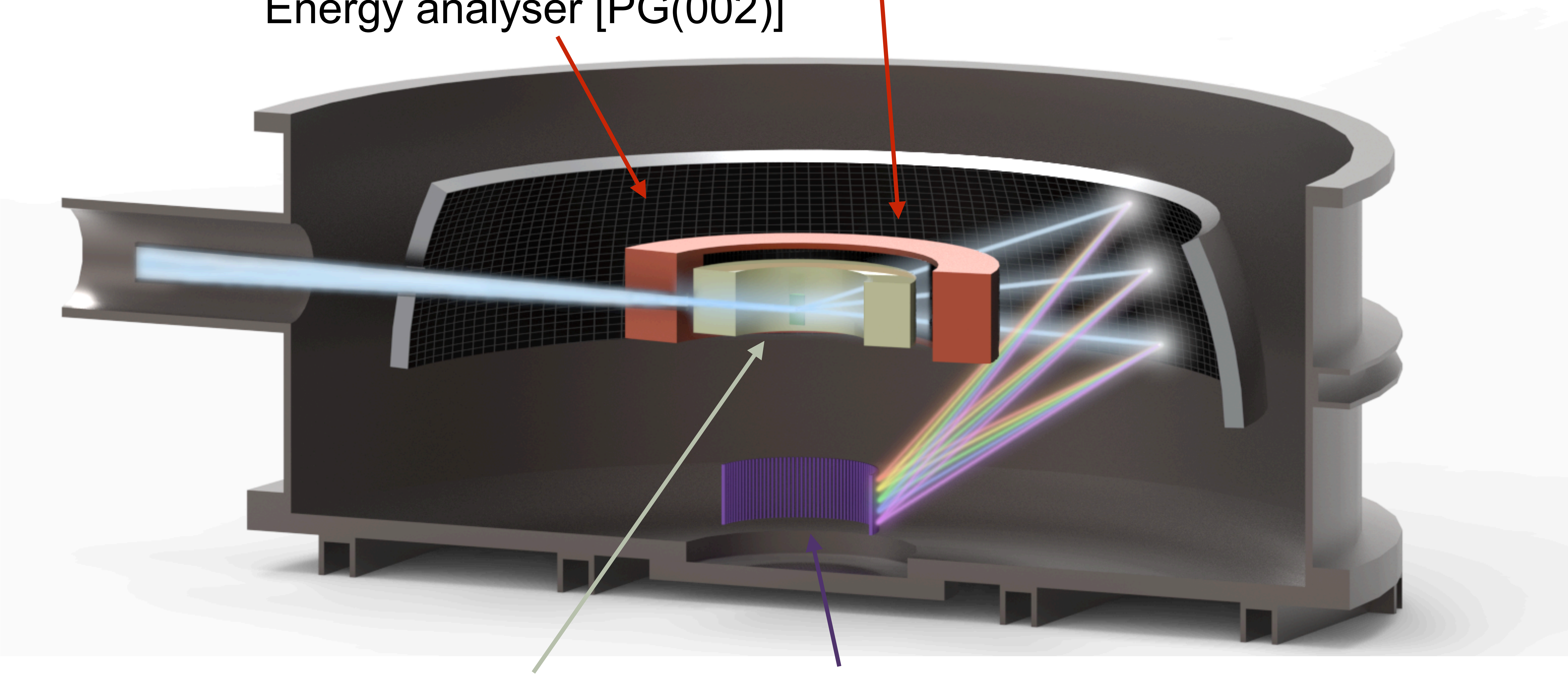
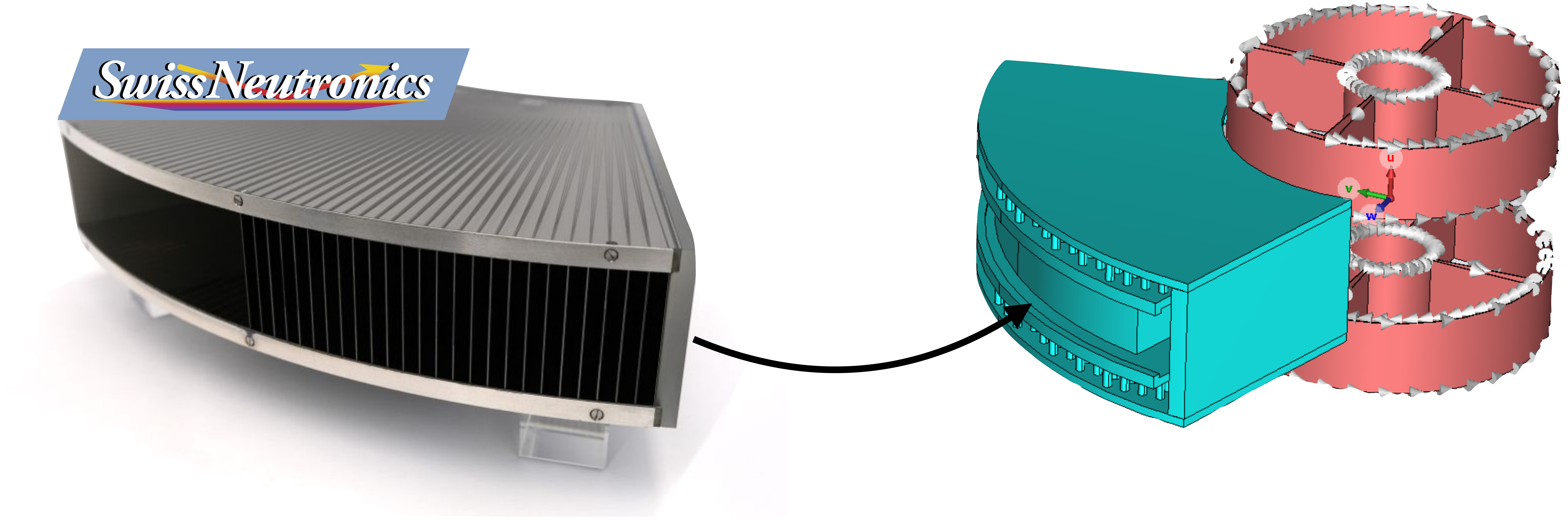


Polarization

- SHERPA aims to offer offer push-button access to polarization analysis by taking advantage of recent developments in polarized neutron optical devices:

  e.g. WISH polarization analyzer



Summary

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- At least 100× IRIS count rate - **200× (~100×LET)** ✓
- Push-button polarization analysis mode - **all-supermirror** ✓
- 17.5 μeV resolution (ΔE FWHM) for a 3 cm tall sample - **16.6μeV (12.5μeV 1cm)** ✓
- Similar Q range to the OSIRIS spectrometer $0.2 < Q < 1.8Å^{-1}$ - ✓
- Maximum Q resolution $\Delta Q = 0.3Å^{-1}$ at minimum accessible scattering angle ($2\theta_{min}$ ~10°) without collimation - **$0.27Å^{-1}$** ✓
- Controllable Q-resolution down to $\Delta Q = 0.1Å^{-1}$ ✓
- Polarization analyzer that accommodates a sample width of 20 mm and allows full view of the energy analyzer - (**nearly**) ✓
- Suppression of the PG(004) reflection to the level of 10^{-4} ✓

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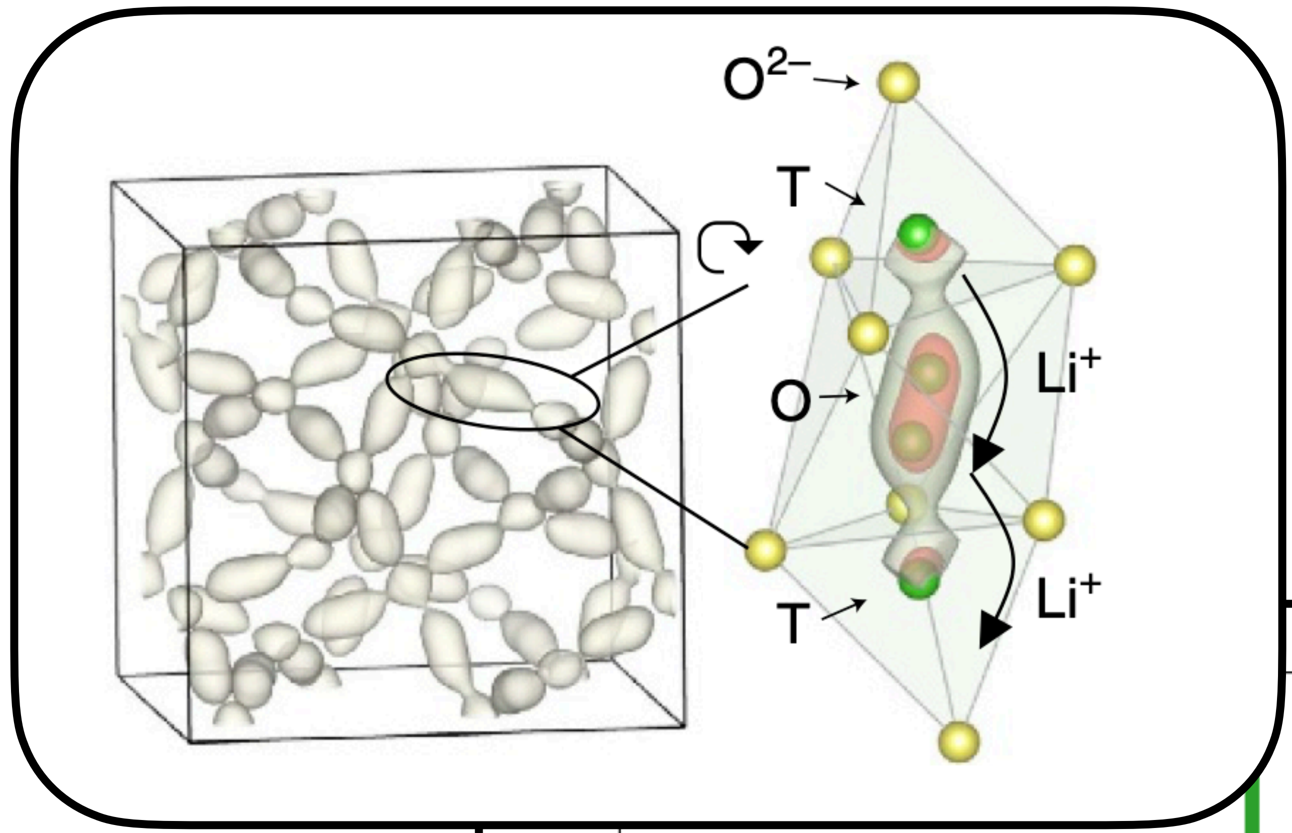

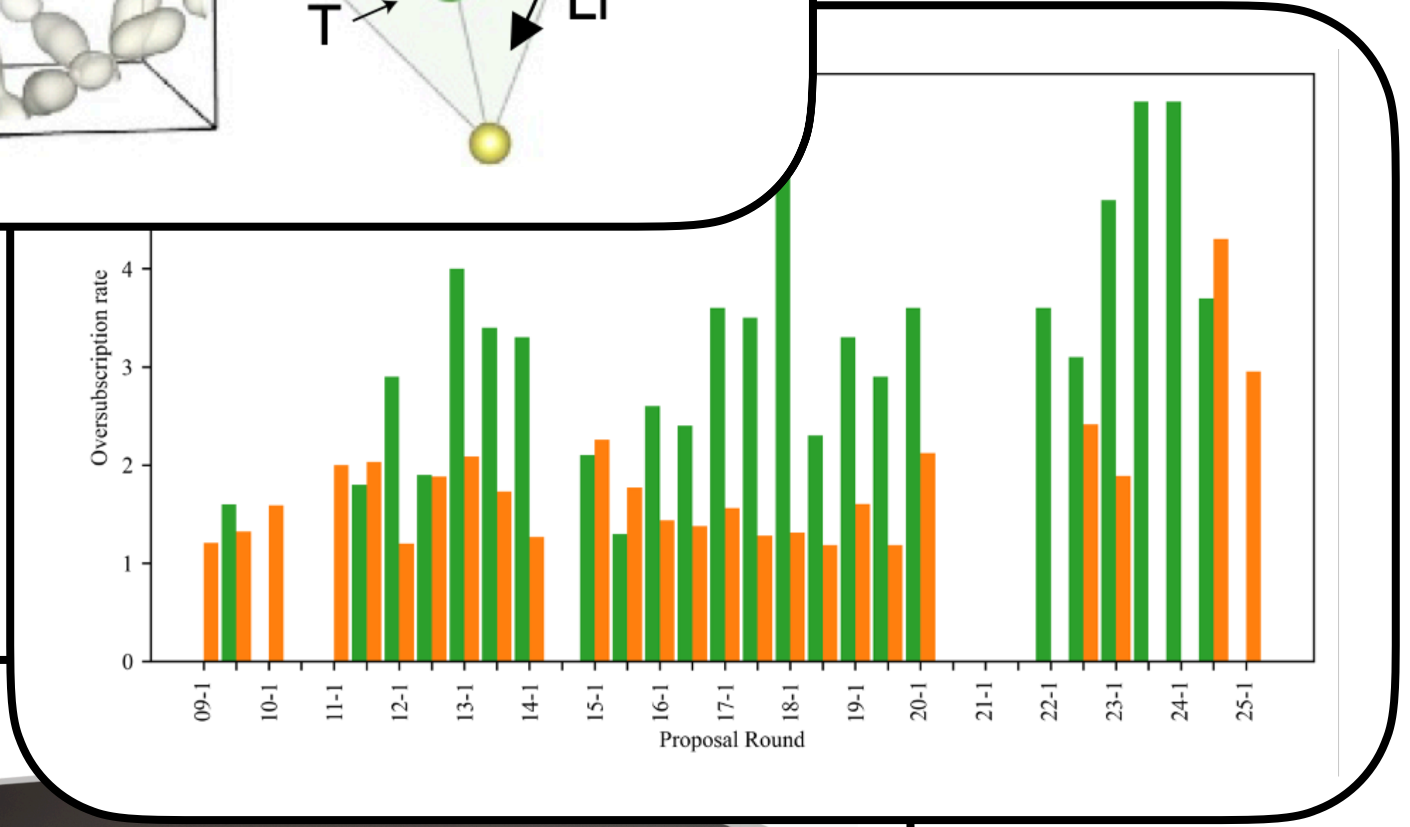

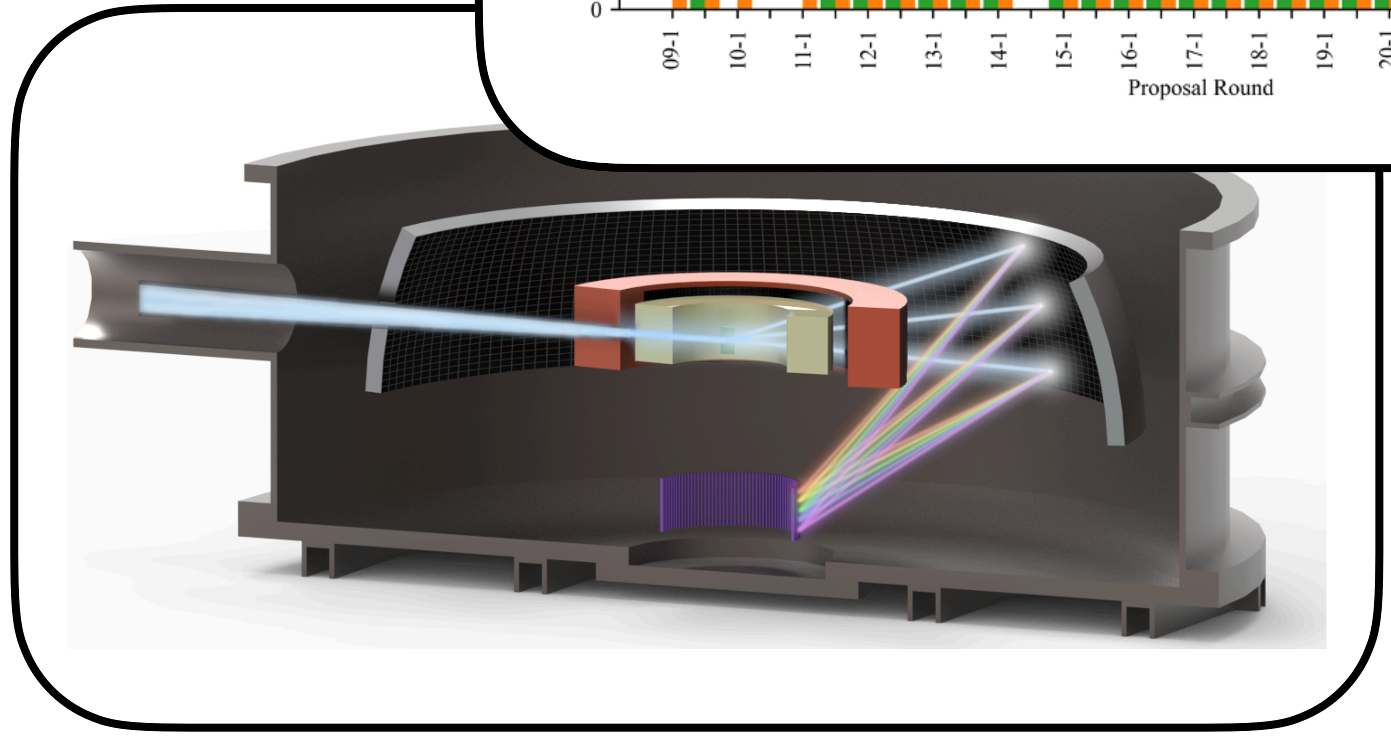

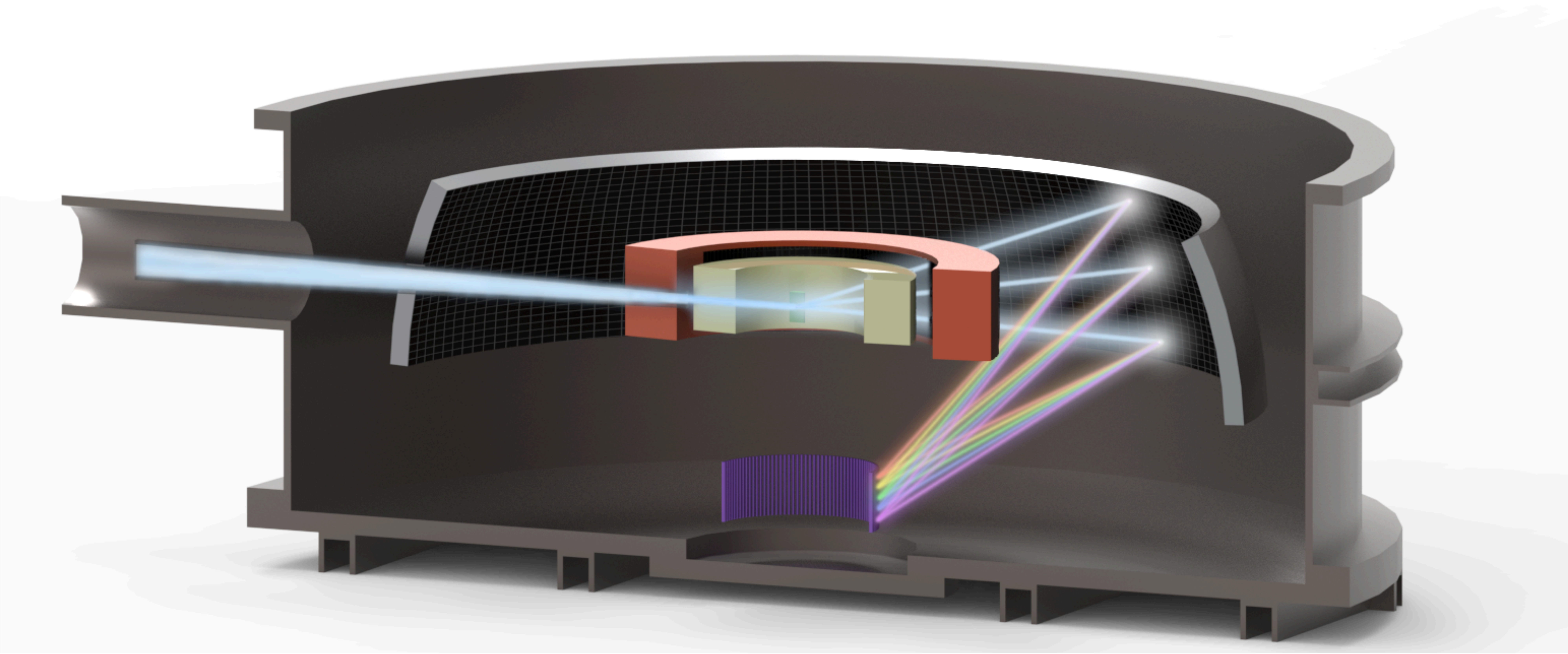

Now part of Endeavour Phase 3