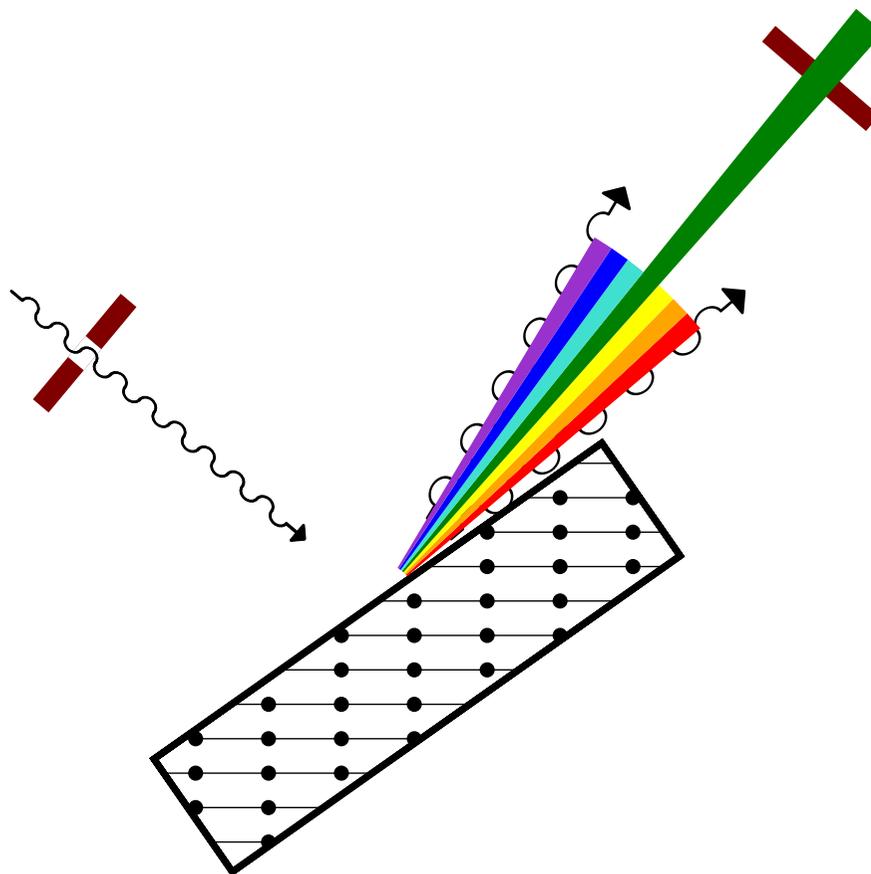




... for a brighter future

Advances in X-Ray Optics for IXS Spectroscopies

Yuri Shvyd'ko



U.S. Department
of Energy

UChicago ►
Argonne_{LLC}



A U.S. Department of Energy laboratory
managed by UChicago Argonne, LLC

Content

**New ideas in high-energy-resolution x-ray optics
and their potential impact on the IXS spectroscopies**

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New ideas in high-energy-resolution x-ray optics and their potential impact on the IXS spectroscopies

- **Position sensitive detectors:**

overcoming problems of the geometrical broadening.

*A path to high-resolution, compact,
high throuput multianalyzer IXS spectrometers*

- **Effect of angular dispersion:**

overcoming limitations in energy resolution set by the Darwin width.

A path to ultra-high resolution IXS spectrometers

Content

New ideas in high-energy-resolution x-ray optics and their potential impact on the IXS spectroscopies

- **Position sensitive detectors:**

overcoming problems of the geometrical broadening.

- Basic concepts
- Experience with MERIX@APS
- A next generation high-resolution IXS spectrometer.

- **Effect of angular dispersion:**

overcoming limitations in energy resolution set by the Darwin width.

- Principles.
- Concept of a sub-meV IXS spectrometer.
- First experiments and technical challenges.

Analyzer Resolution & Geometrical Broadening

$$\Delta E_{\text{tot}} = \sqrt{\Delta E_i^2 + \Delta E_g^2}$$

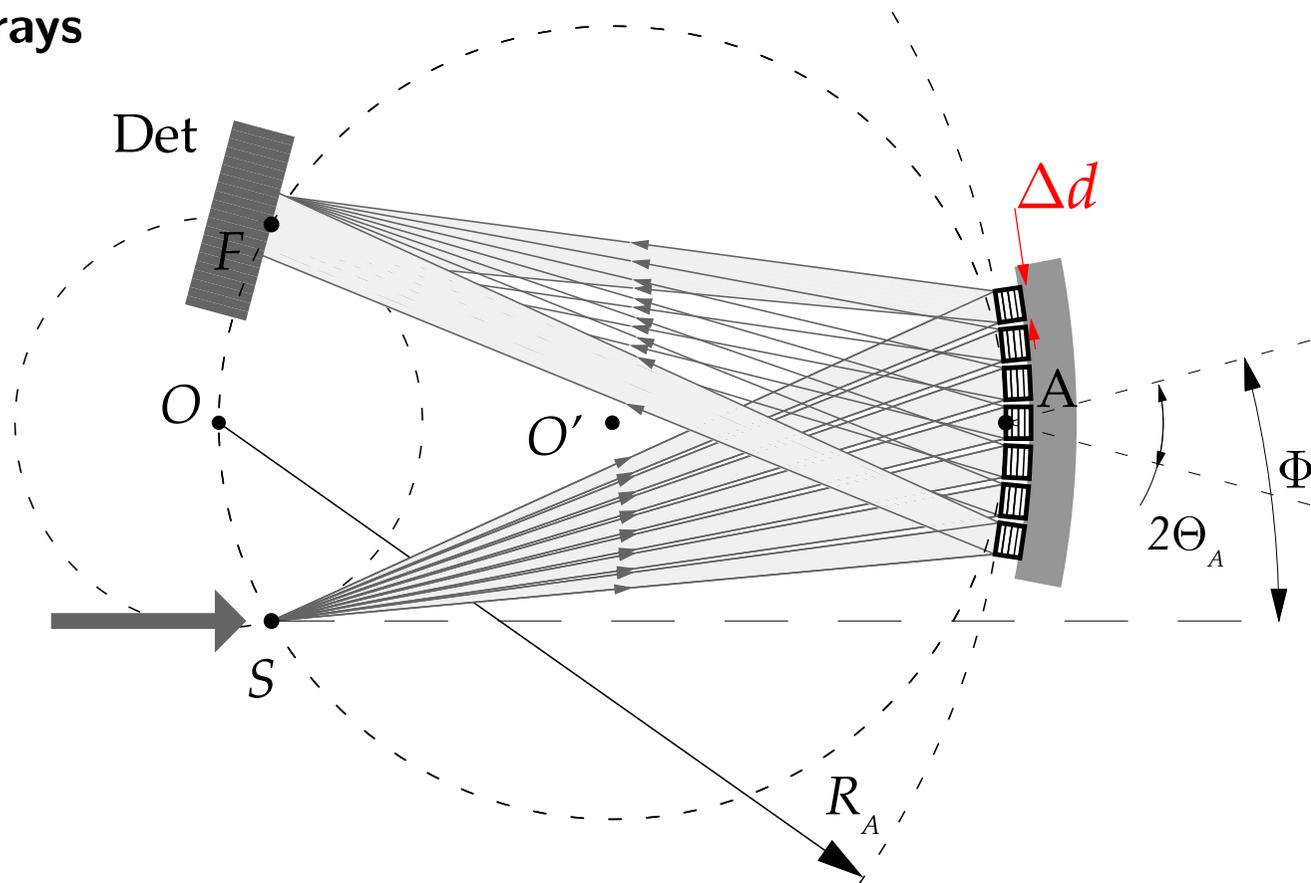
ΔE_i = intrinsic (Darwin) width of the Bragg reflection

ΔE_g = “geometrical” broadening

due to angular spread of x-rays

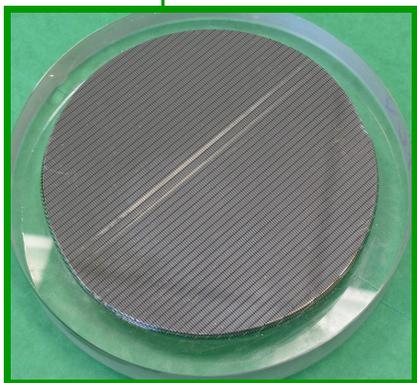
$$\frac{\Delta E_g}{E} = \frac{\Delta\theta}{\tan\theta_B} \simeq \frac{\Delta d/R_A}{\tan\theta_B}$$

Δd = crystal segment

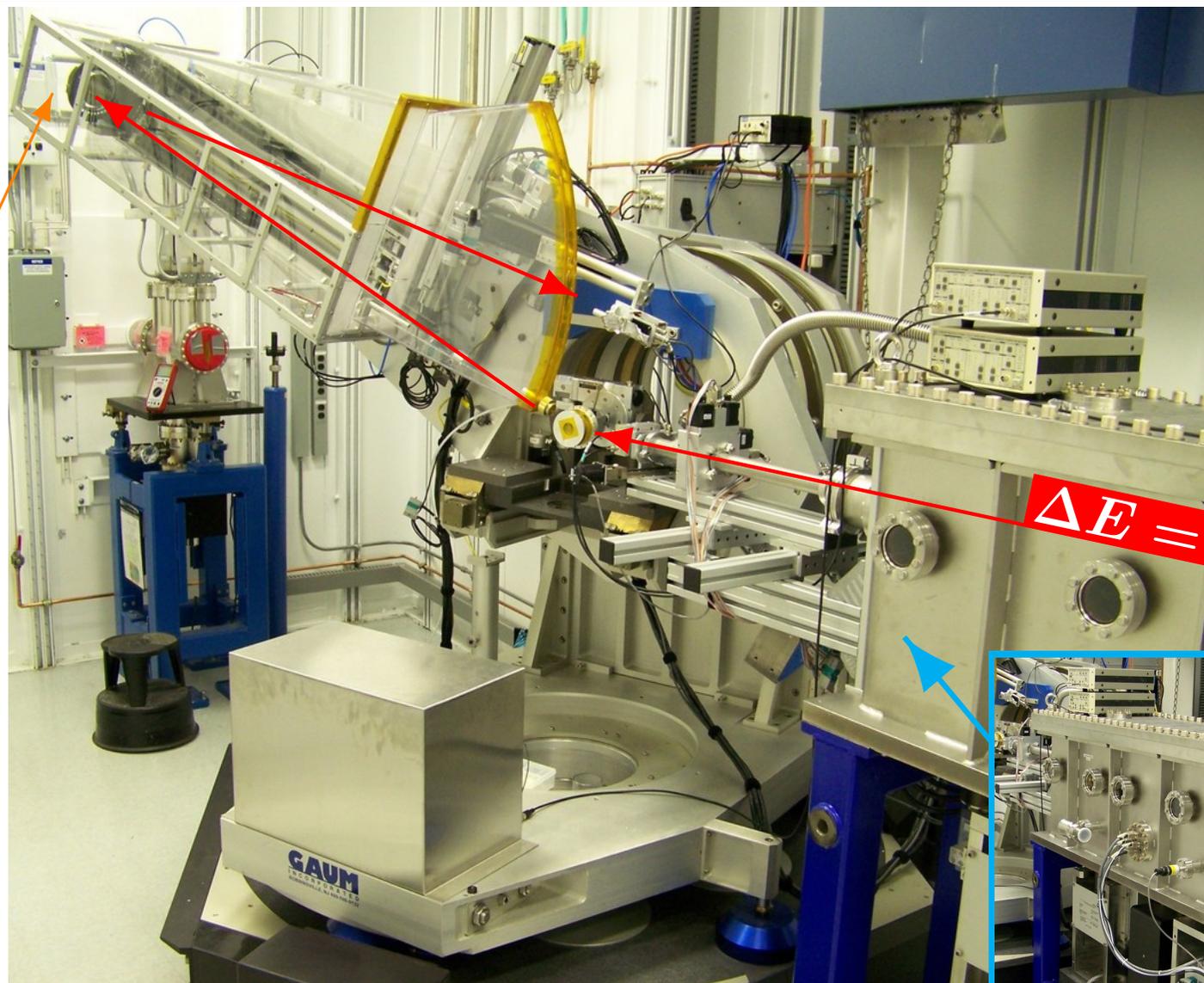


MERIX Spectrometer@30-ID.APS

Analyzer gimbal



Ge(337)
diced analyzer:
 $\Delta E_i = 42 \text{ meV}$



$\Delta E = 72 \text{ meV}$

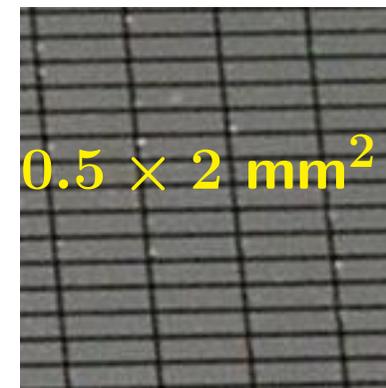
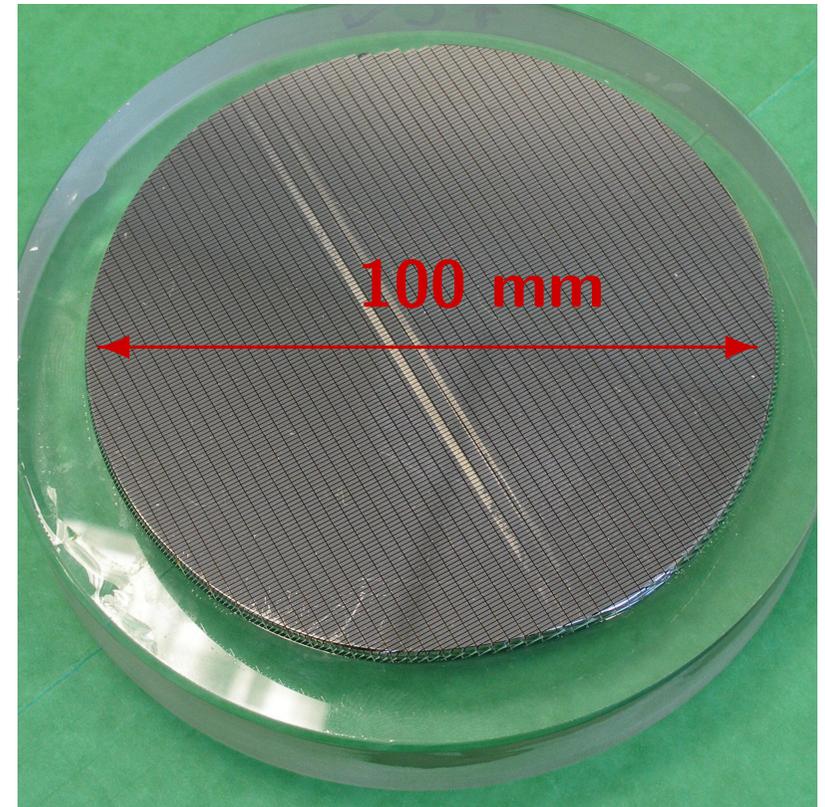
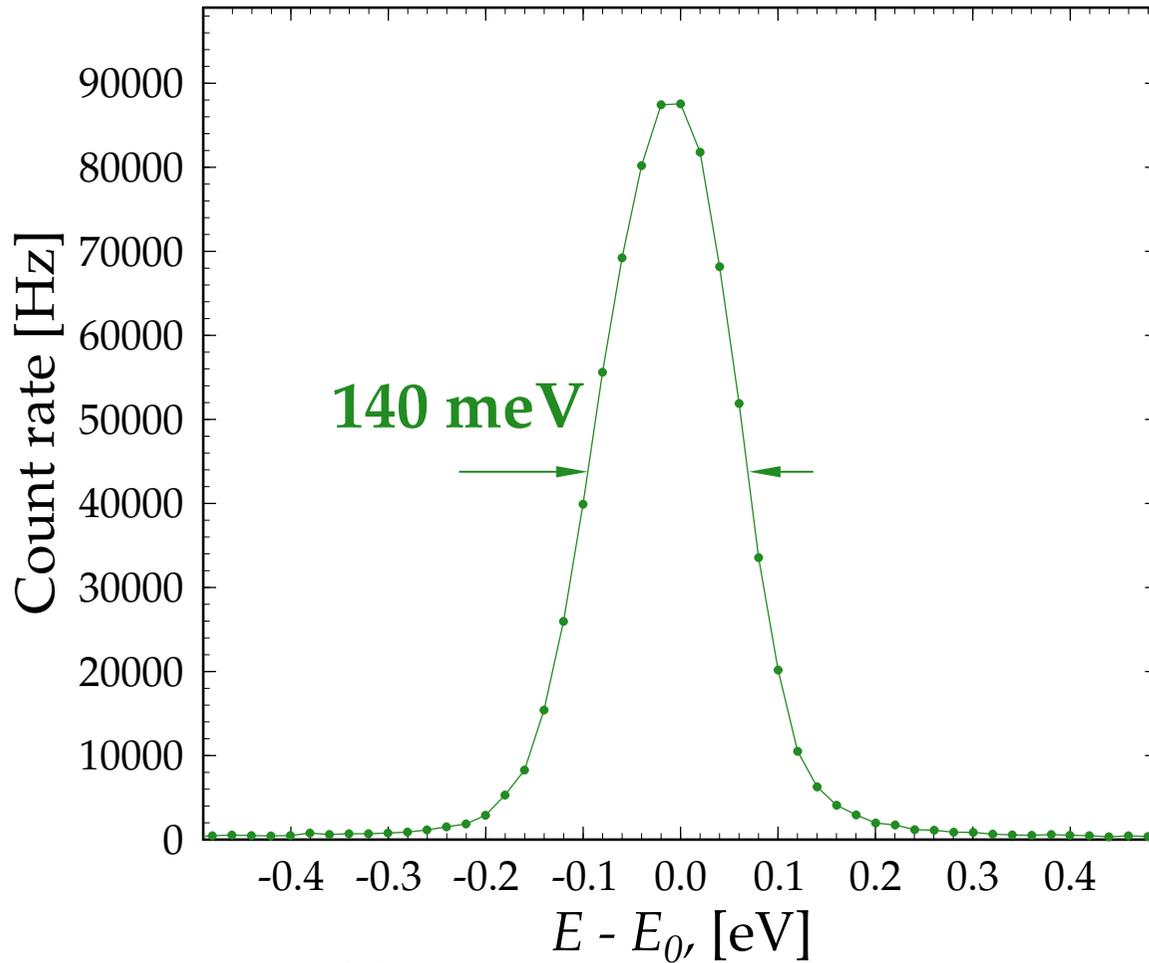
MERIX mirror.
Focus: $5 \mu\text{m (V)} \times 40 \mu\text{m (H)}$

J. Hill
C. Burns
S. Coburn
E. Alp
A. Said
T. Toellner
Yu. Shvyd'ko
and many others



Cu K-edge RIXS Analyzer

Ge(3 3 7) analyzer
 $R_A = 2$ m & conventional detector

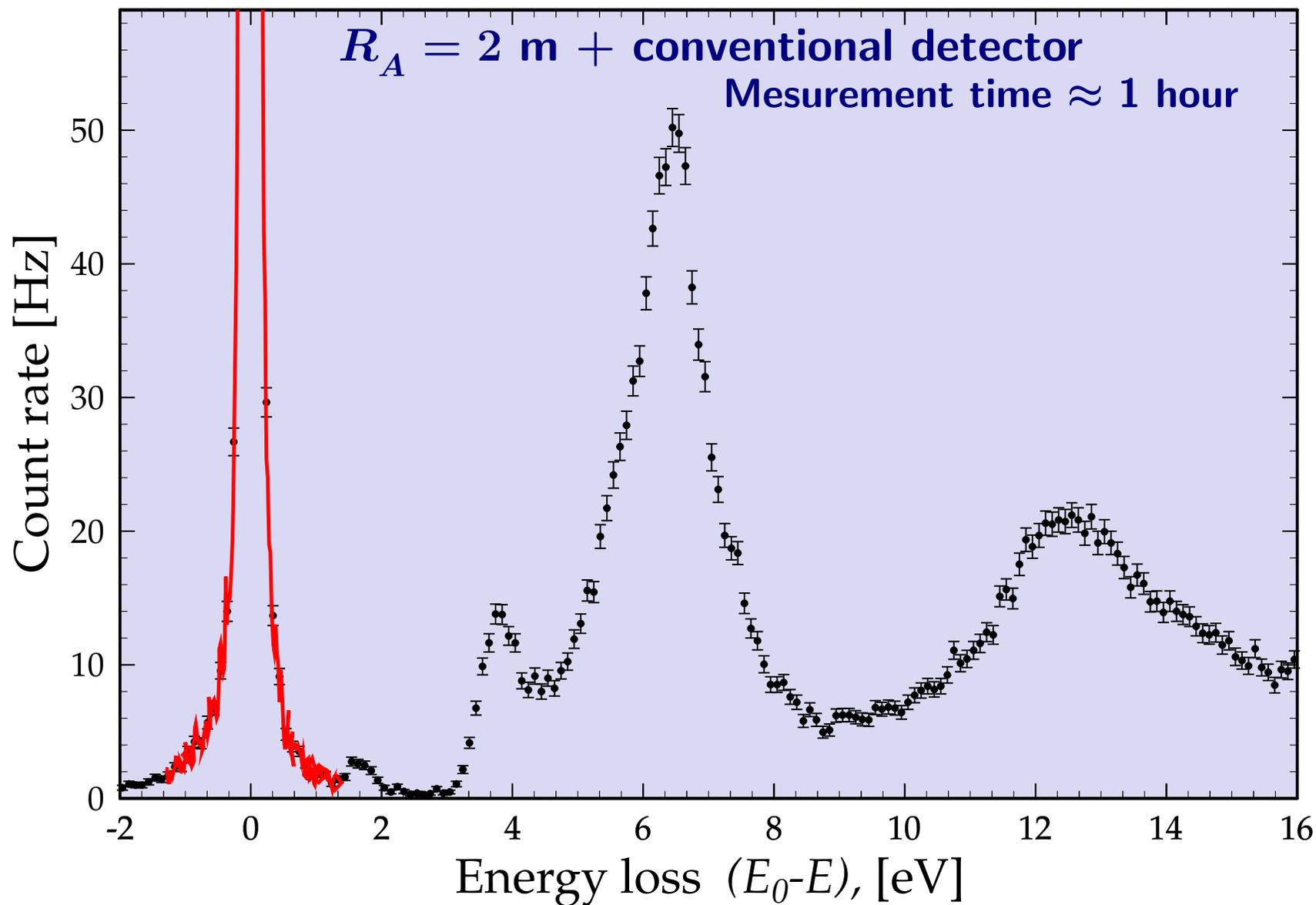


Expected: **115 eV**

Deconvoluted width : **120 meV**

RIXS Spectroscopy with MERIX

CuGeO_3 ; $Q = (1.5\ 0\ 0)$, $E_0 = 8.990$ keV



Analyzer Resolution & Geometrical Broadening

$$\Delta E_{\text{tot}} = \sqrt{\Delta E_i^2 + \Delta E_g^2}$$

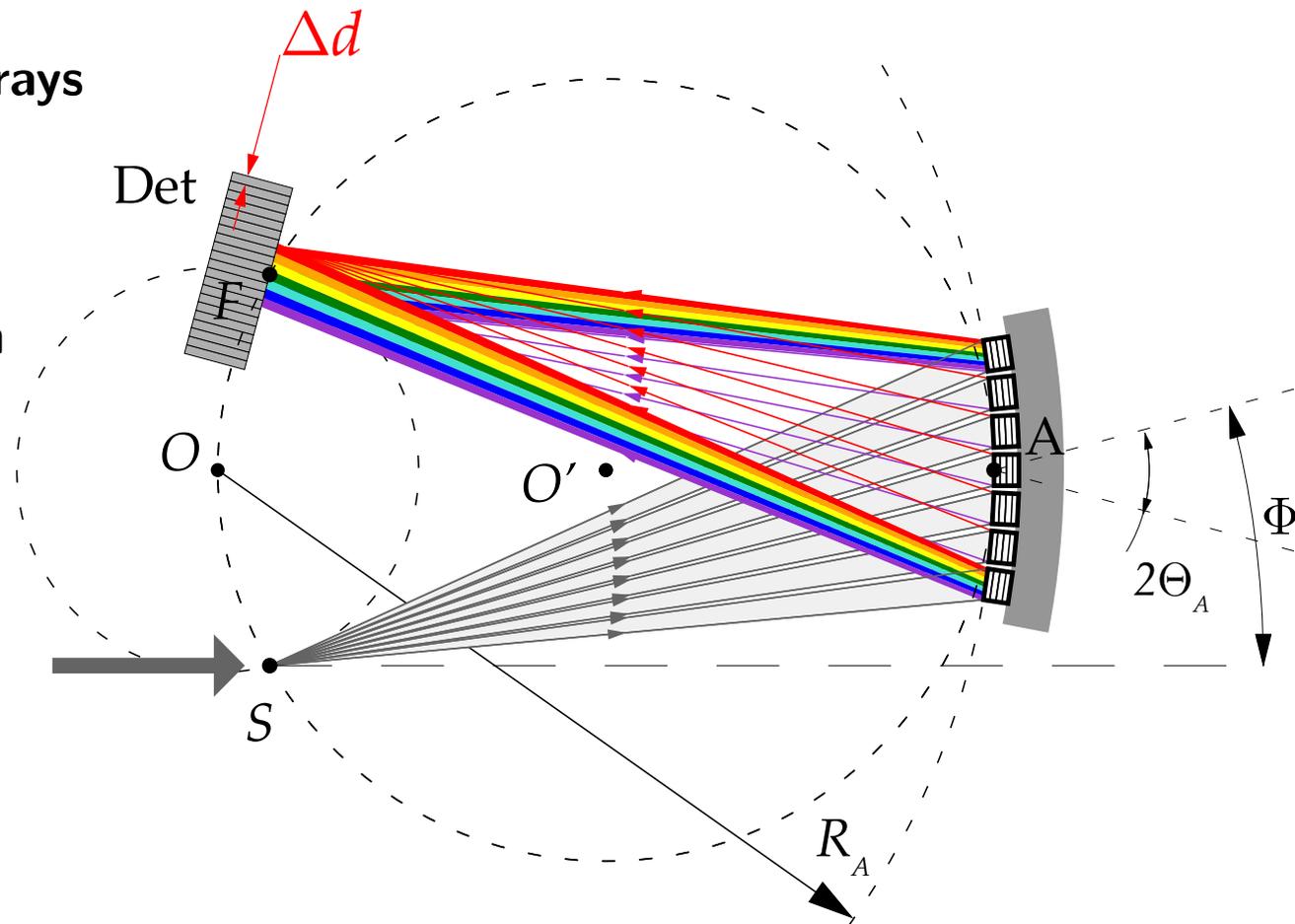
ΔE_i = intrinsic (Darwin) width of the Bragg reflection

ΔE_g = “geometrical” broadening

due to angular spread of x-rays

$$\frac{\Delta E_g}{E} = \frac{\Delta\theta}{\tan\theta_B} \simeq \frac{\Delta d/2R_A}{\tan\theta_B}$$

Δd = detector’s spatial resolution



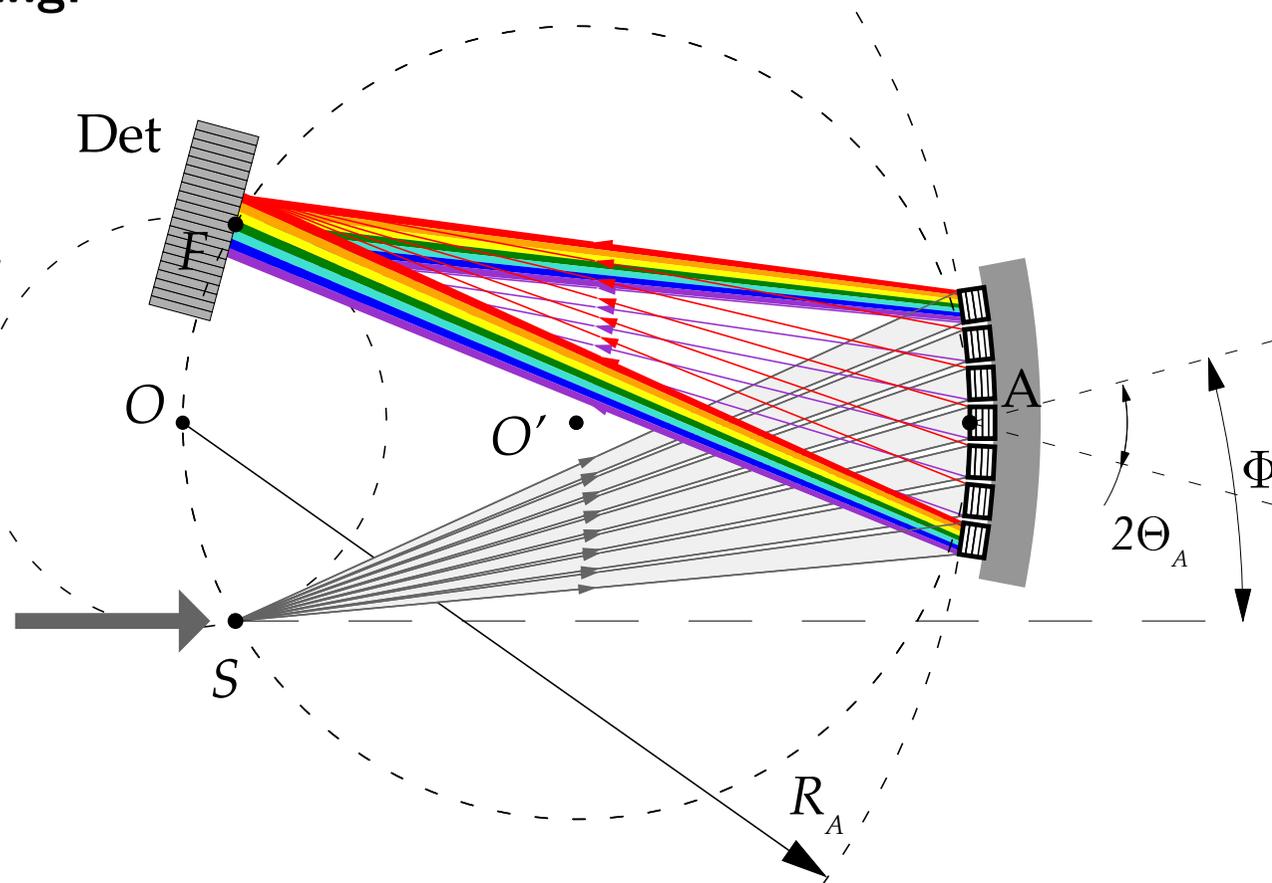
Next generation IXS spectrometer

S. Huotari, Gy. Vanko, F. Albergamo, C. Ponchut, H. Graafsma,
C. Henriquet, R. Verbeni, and G. Monaco, *Synchrotron Rad.* (2005) 12, 467 :

Use position sensitive detector
to detect IXS signal differentially
in space and thus in photon energy,
and overcome geometrical broadening.

Implications:

1. Energy resolution determined by detector's spatial resolution.
2. Energy resolution independent of crystal segment size.
3. Better energy resolution even with smaller R_A .
4. Higher countrates $\propto 1/R_A^2$
5. Less demanding analyzer fabrication.

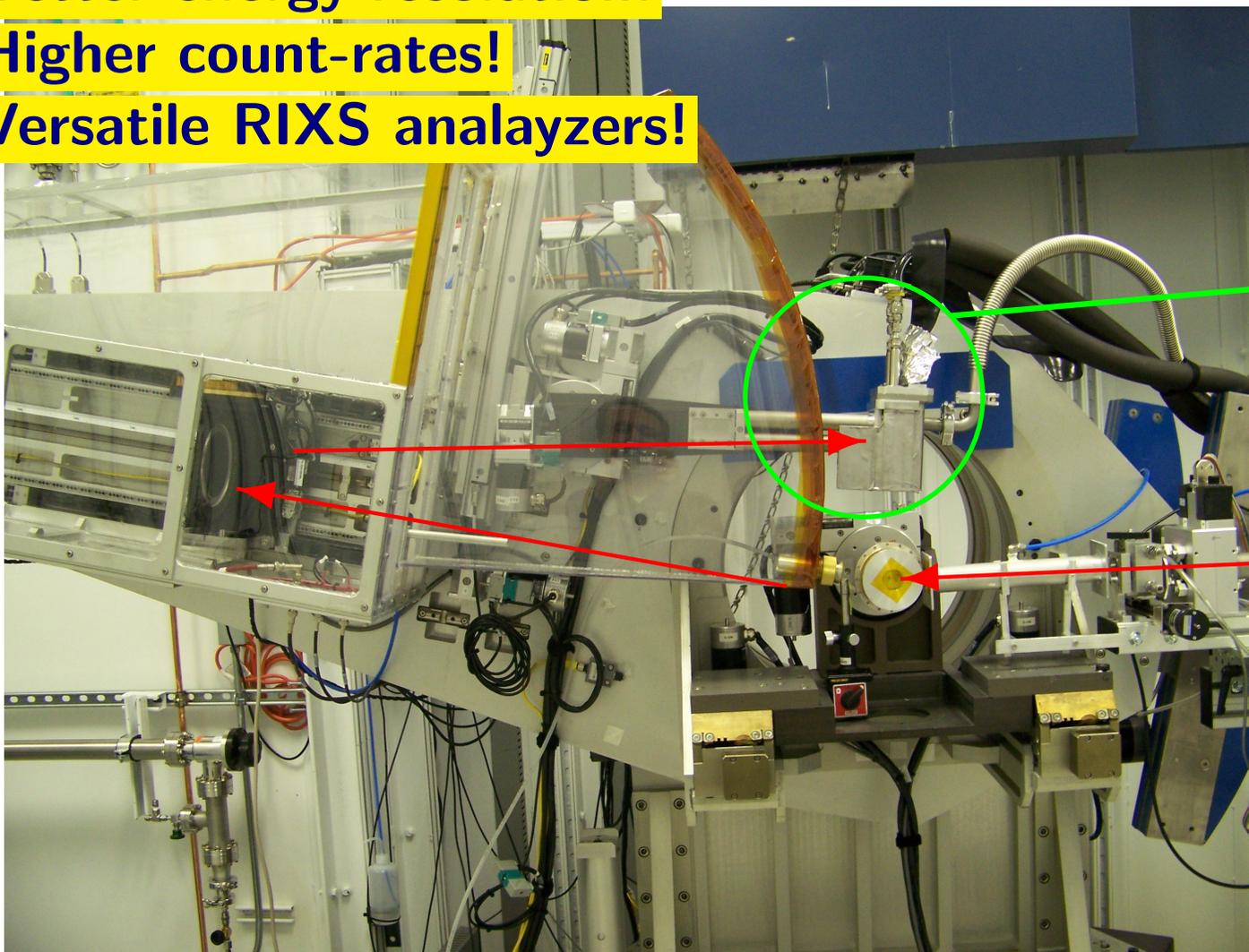


MERIX Upgrade with Strip Detector

Better energy resolution!

Higher count-rates!

Versatile RIXS analyzers!



**Photon-Counting
Si Microstrip detector:**

Built by D. Peter Siddons (BNL)

640 strips

1 strip = 125 μm

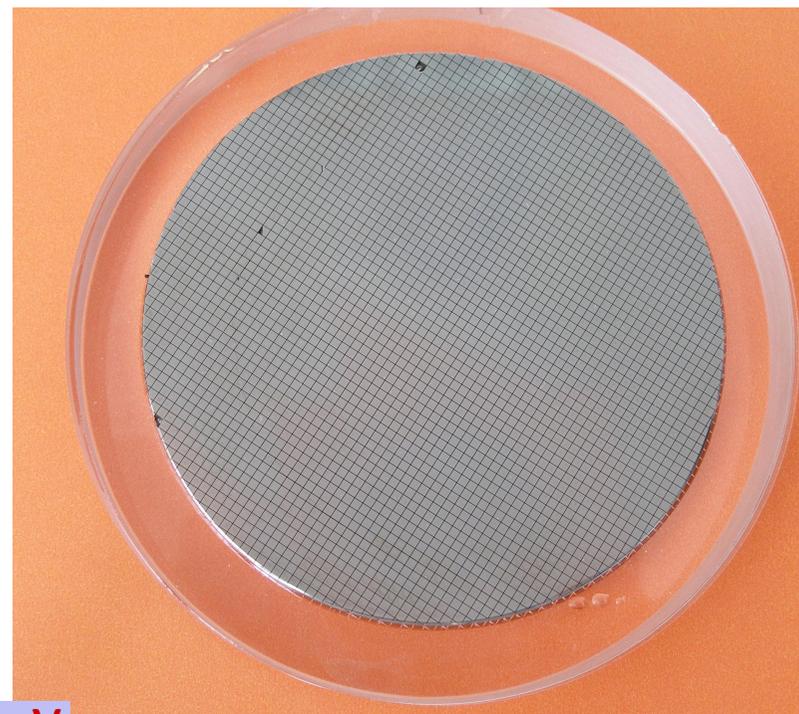
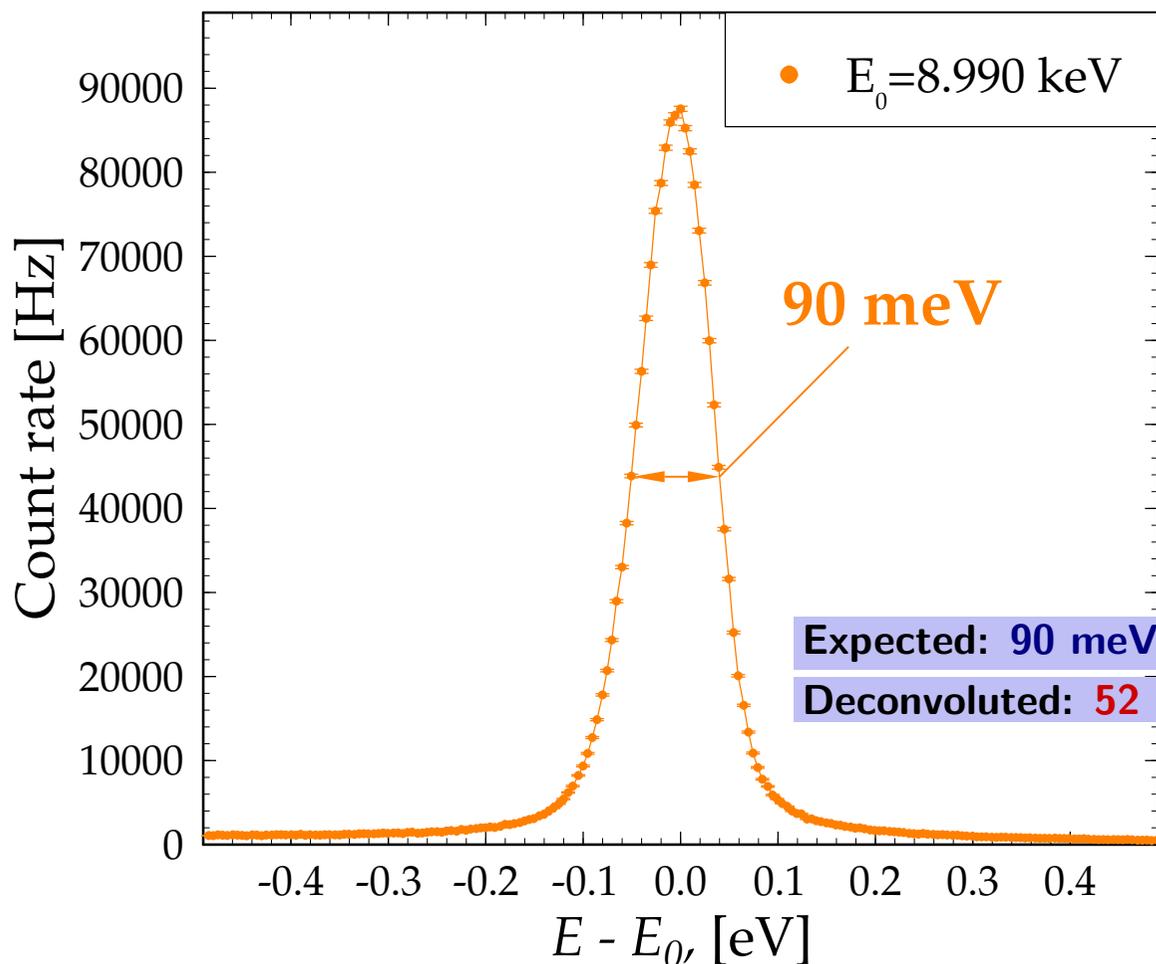
1 strip = 40 meV

640 strip = 25 eV

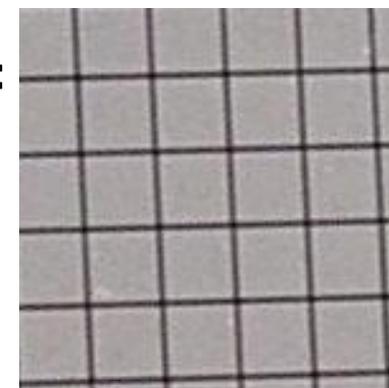
Donated to IXS-CDT
by Steve Cramer, UC Davis

Cu K-edge RIXS Analyzer: Improved Resolution

Ge(3 3 7) analyzer
 $R_A = 1$ m & strip detector



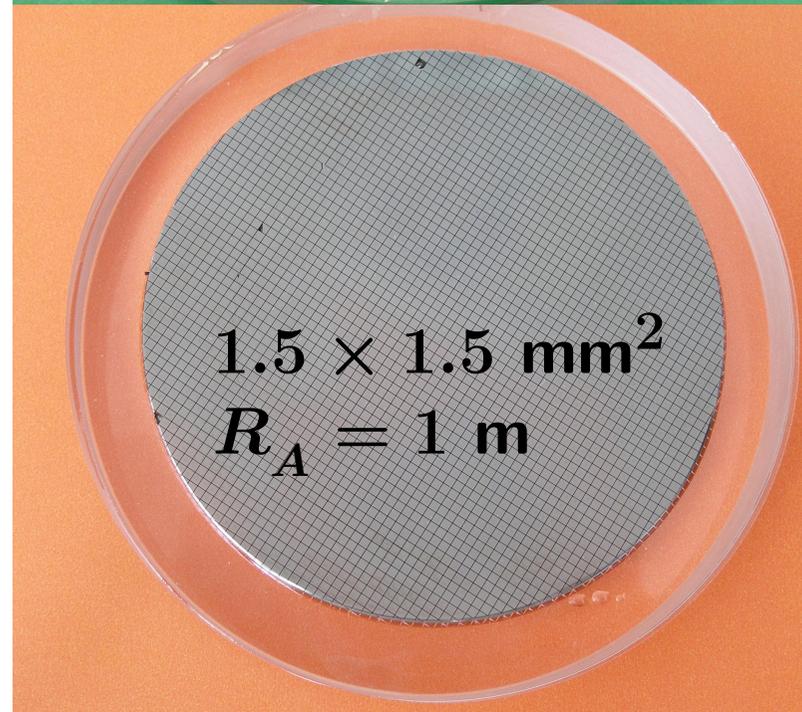
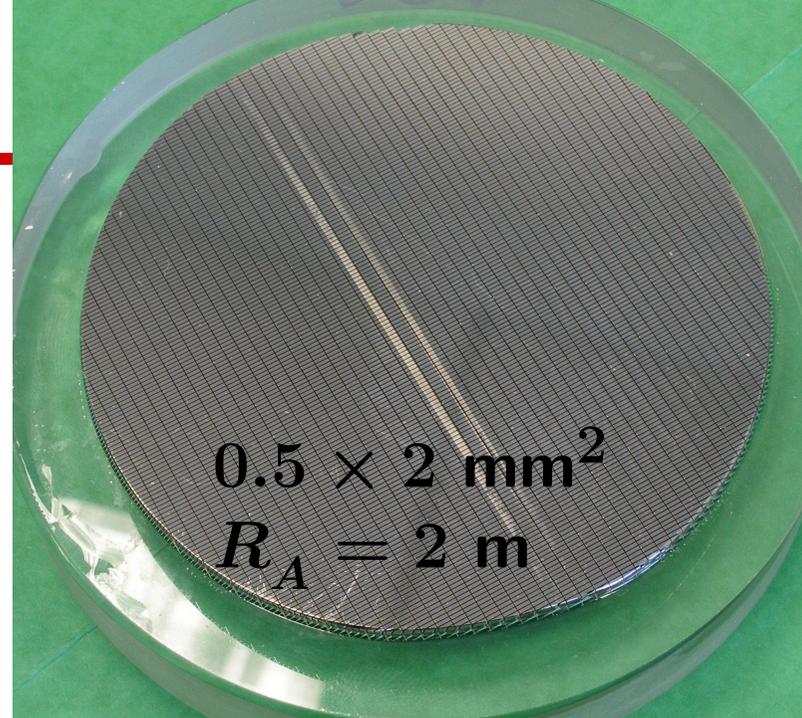
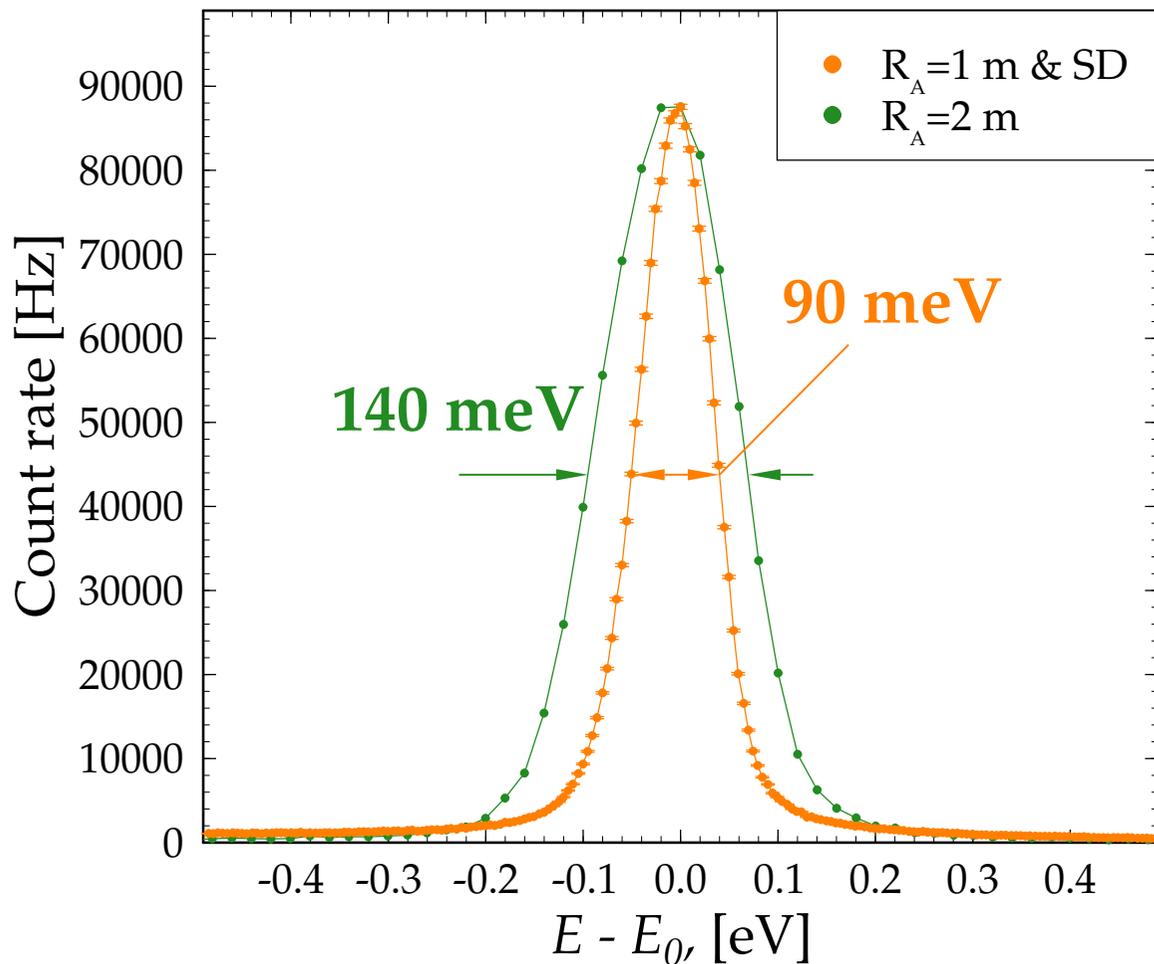
Crystal segments:
 1.5×1.5 mm²



- Better energy resolution.
- Less demanding analyzer fabrication.

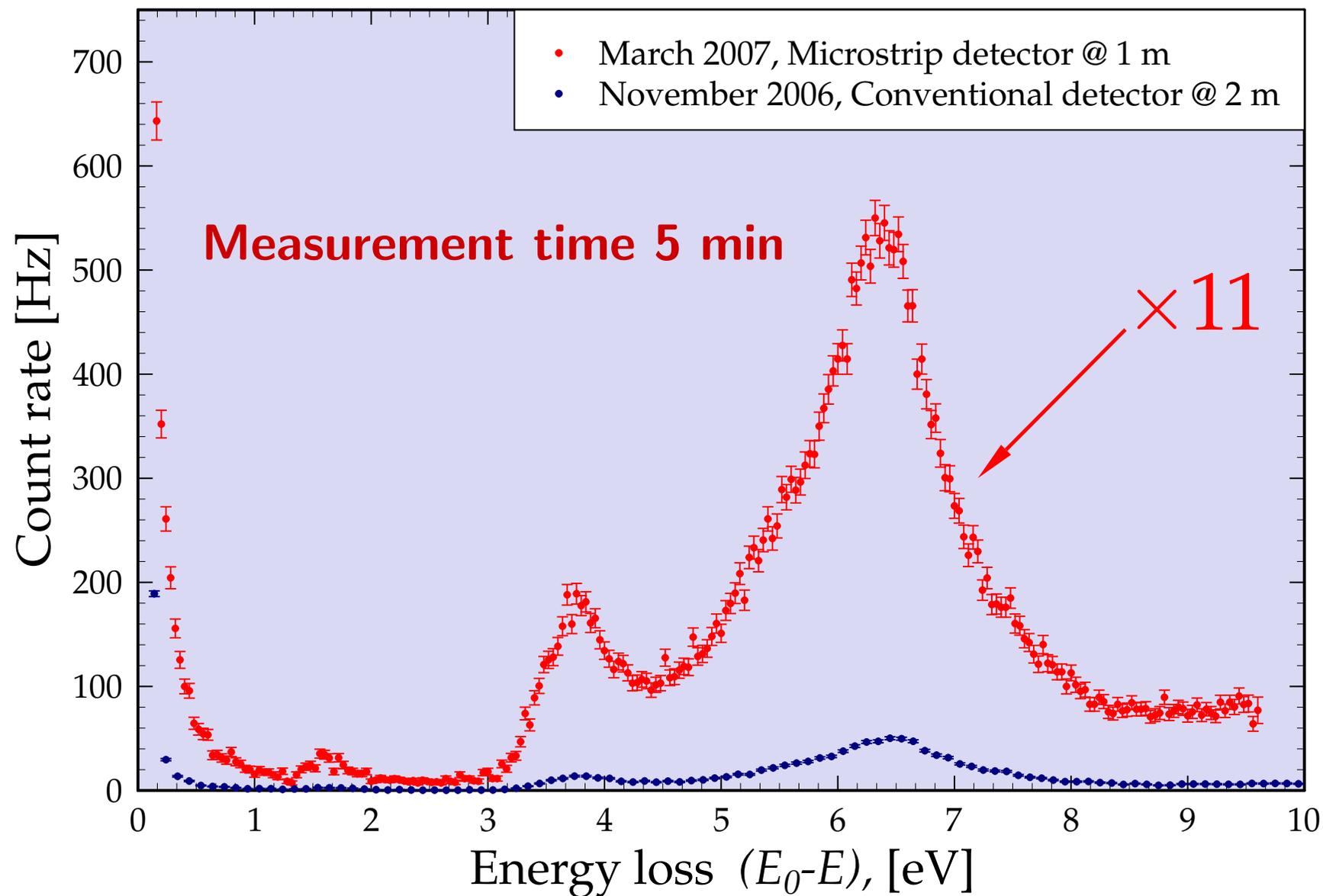
Cu K-edge RIXS Analyzers

Ge(3 3 7) analyzer



Dramatic Increase in Count Rate

CuGeO_3 ; $Q = (1.5\ 0\ 0)$, $E_0 = 8.990\ \text{keV}$



Unique Set of RIXS Analyzers

tested

exist

Element	E [keV]	Crystal	Reflec- tion	ΔE_i intr. [meV]	ΔE_g geom. [meV]	ΔE_{tot} total [meV]
V(O)	5.480	LiNbO ₃	(0 0 $\bar{0}$ 12)	109	71	130
Cr(O)	6.009	Si	(5 1 1)	52.2	61	81
Mn(O)	6.555	Si	(0 4 4)	62	72	95
Fe(O)	7.130	Ge	(6 2 0)	115	108	158
Co(O)	7.720	LiNbO ₃	(3 3 $\bar{6}$ 6)	49	36	60
Ni(O)	8.345	LiNbO ₃	(0 6 $\bar{6}$ 0)	50	19	54
		Ge	(2 4 6)	76	99	123
Cu(O)	8.990	Ge	(3 3 7)	42	41	59
Eu	6.977	Ge	(6 2 0)	112	51	123
Yb	8.944	Ge	(0 0 8)	64	131	145

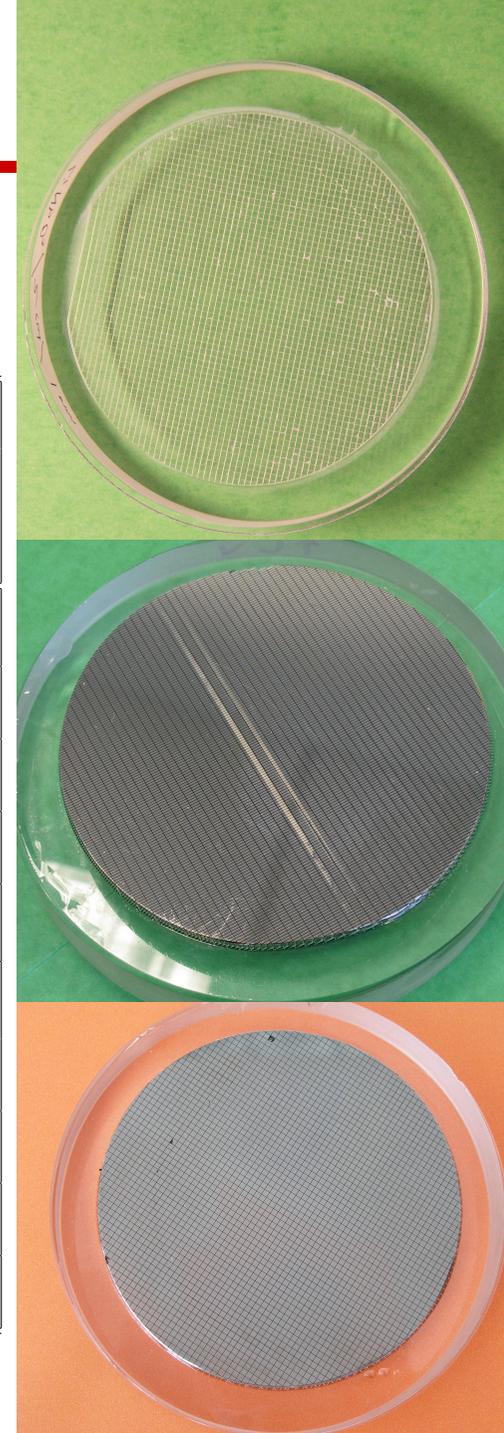
Yu. Shvyd'ko

A. Said

R. Khachatryan

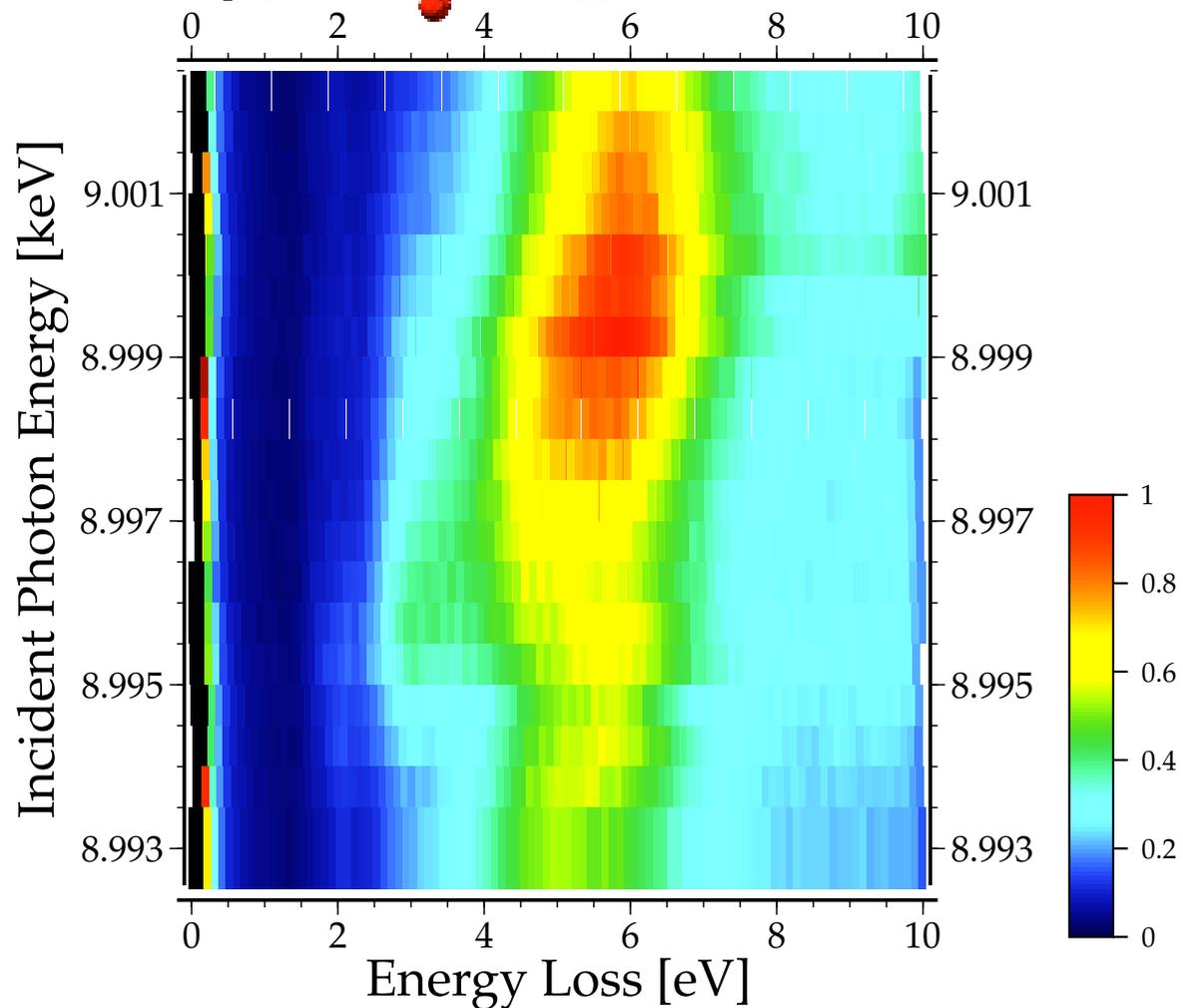
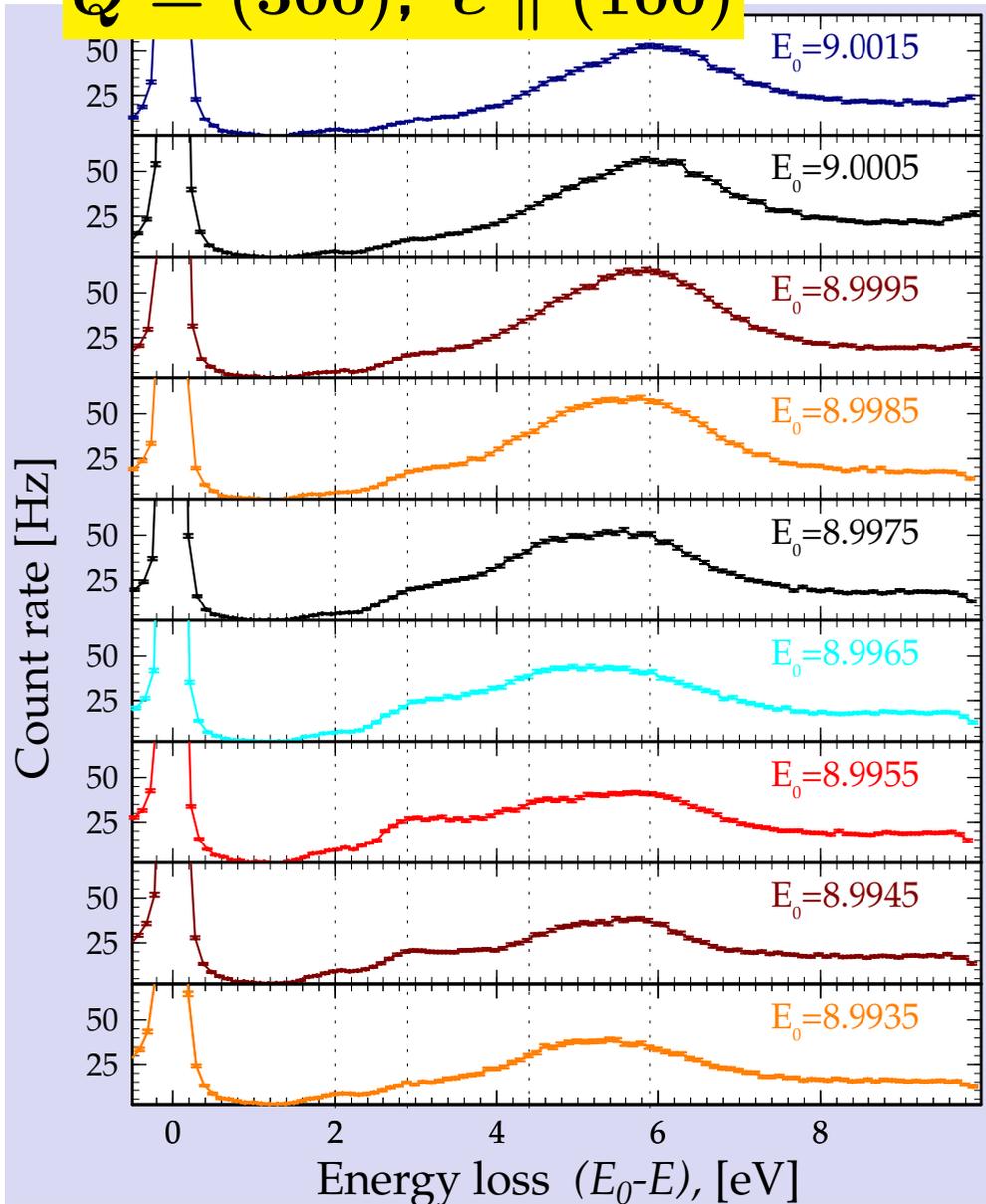
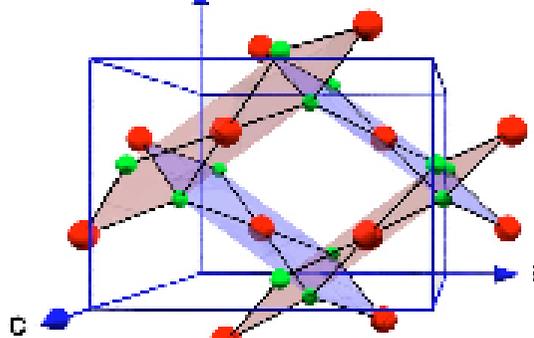
M. Wiczorek

D. Casa



Cu K-edge RIXS in CuO

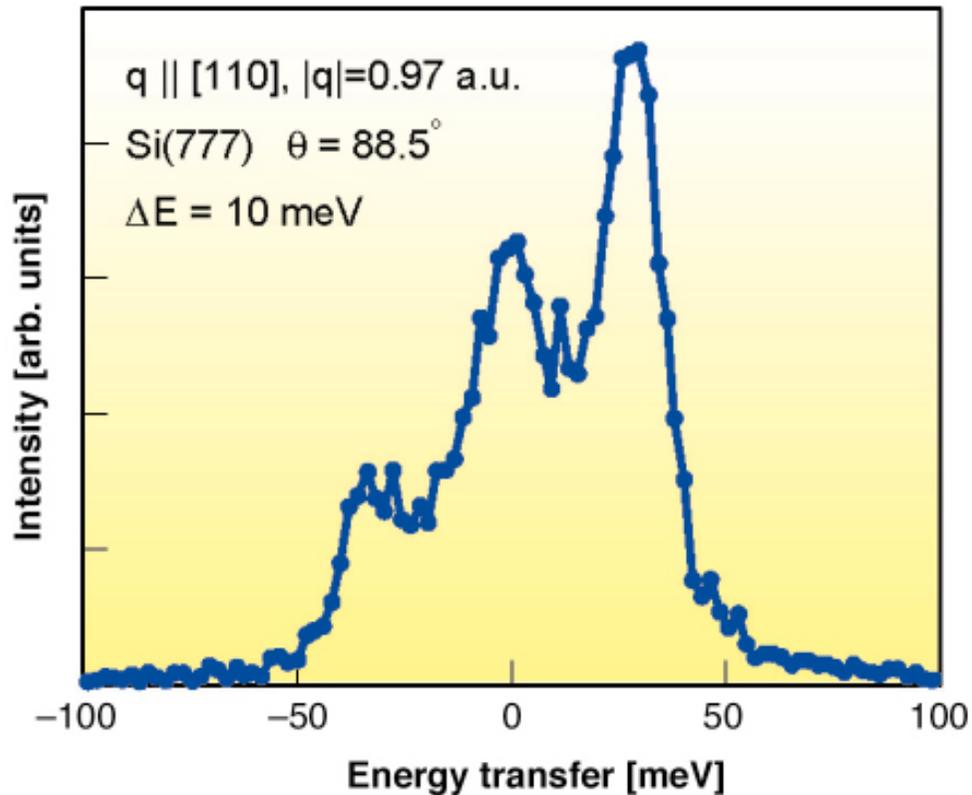
$$\vec{Q} = (300), \vec{e} \parallel (100)$$



Yu. Shvyd'ko, H. Yavas, E. Alp, D. Casa, A. Said (2007)

Coming next:

- How Simo Huotari's idea has been applied to MERIX?
- **How Simo Huotari's idea could be applied to high-resolution IXS?**
10 meV IXS spectroscopy with 1 m arm spectrometer.

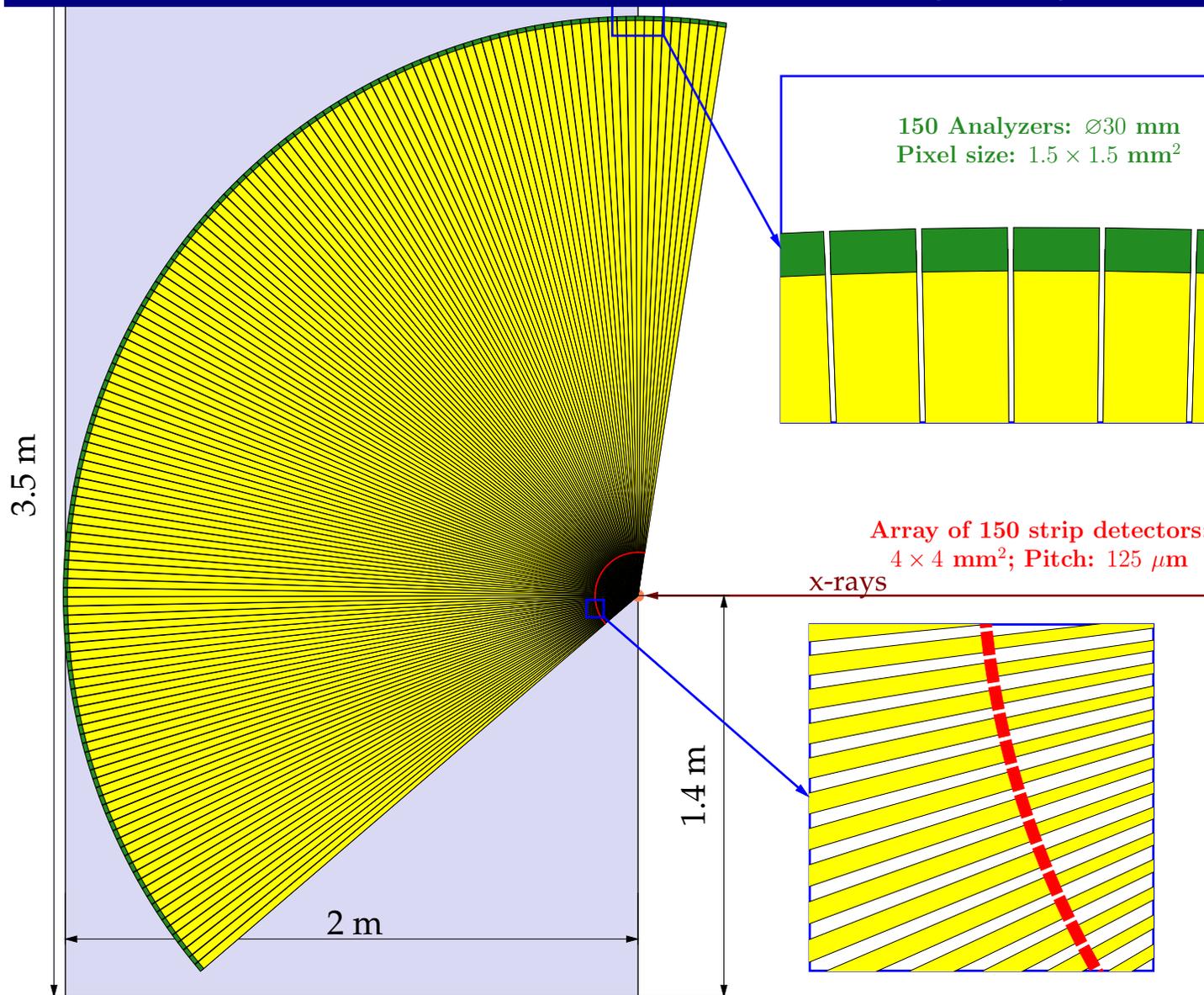


S. Huotari et al (2005)

Compact, high-resolution

ANGIX: A Next Generation IXS Spectrometer

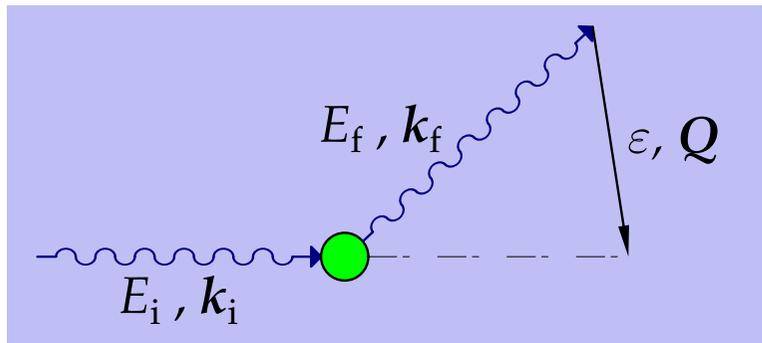
Upgrade concept for the IXS beamline (30ID) at the APS



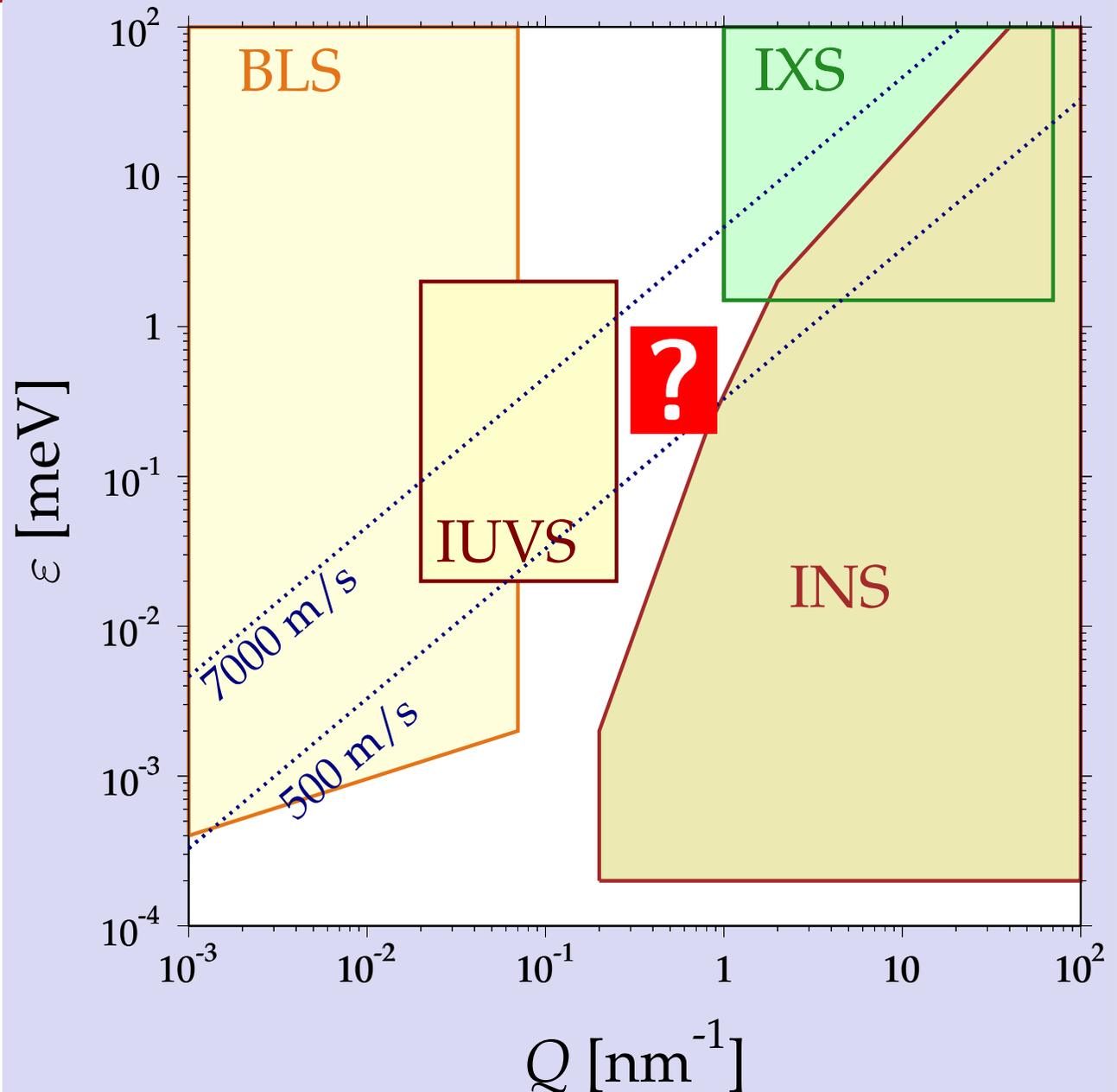
- High-resolution:
 $\approx 1.5 - 5$ meV
- Multi-analyzer
- Compact

Key element:
Array of strip detectors.

Probes for Vibrational Dynamics



Better ϵ resolution
demands!
better Q resolution!



Content

New ideas in high-energy-resolution x-ray optics and their potential impact on the IXS spectroscopies

● Position sensitive detectors:

overcoming problems of the geometrical broadening.

- Basic concepts
- Experience with MERIX@APS
- A next generation high-resolution IXS spectrometer.

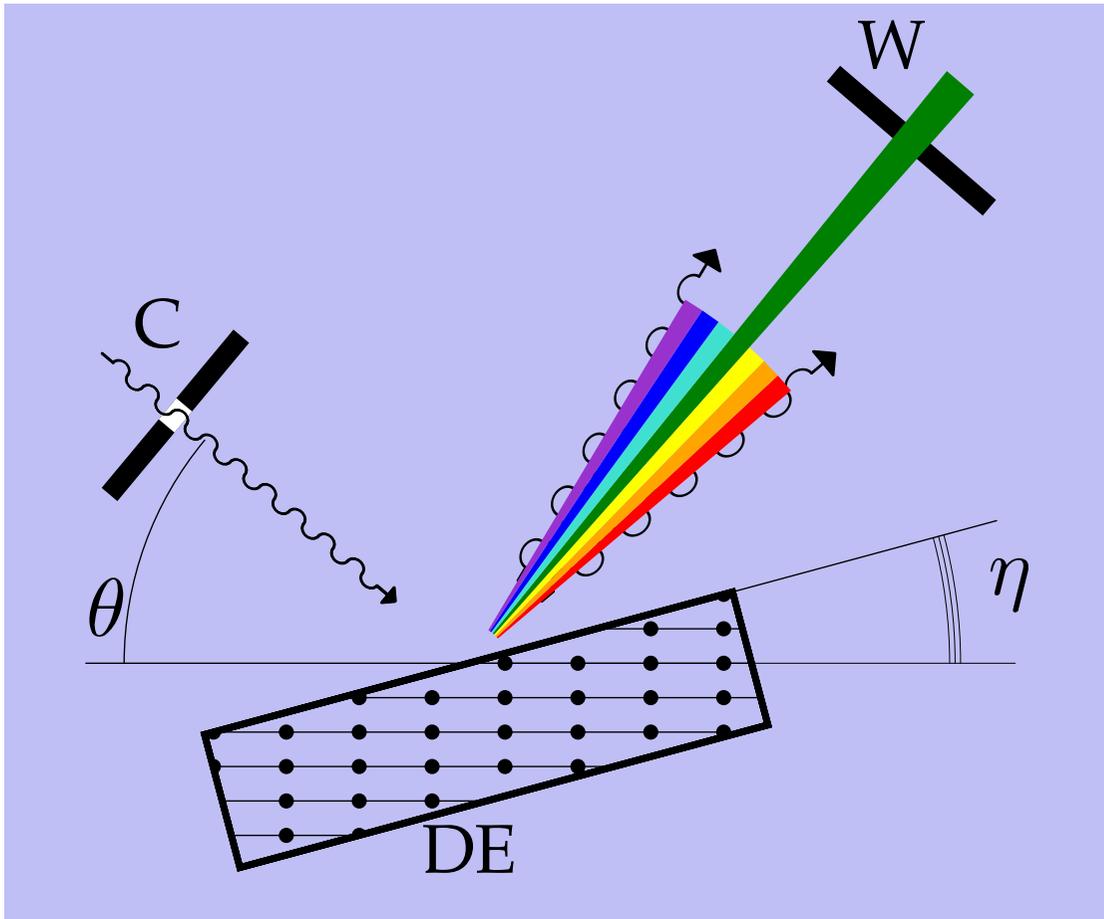
● Effect of angular dispersion:

overcoming limitations in energy resolution set by the Darwin width.

- Principles.
- Concept of a sub-meV IXS spectrometer.
- First experiments and technical challenges.

Angular Dispersion

An asymmetrically cut crystal behaves like an optical prism dispersing the photons with different photon energies: **effect of angular dispersion.**



C - collimator

DE - dispersing element

W - wavelength selector

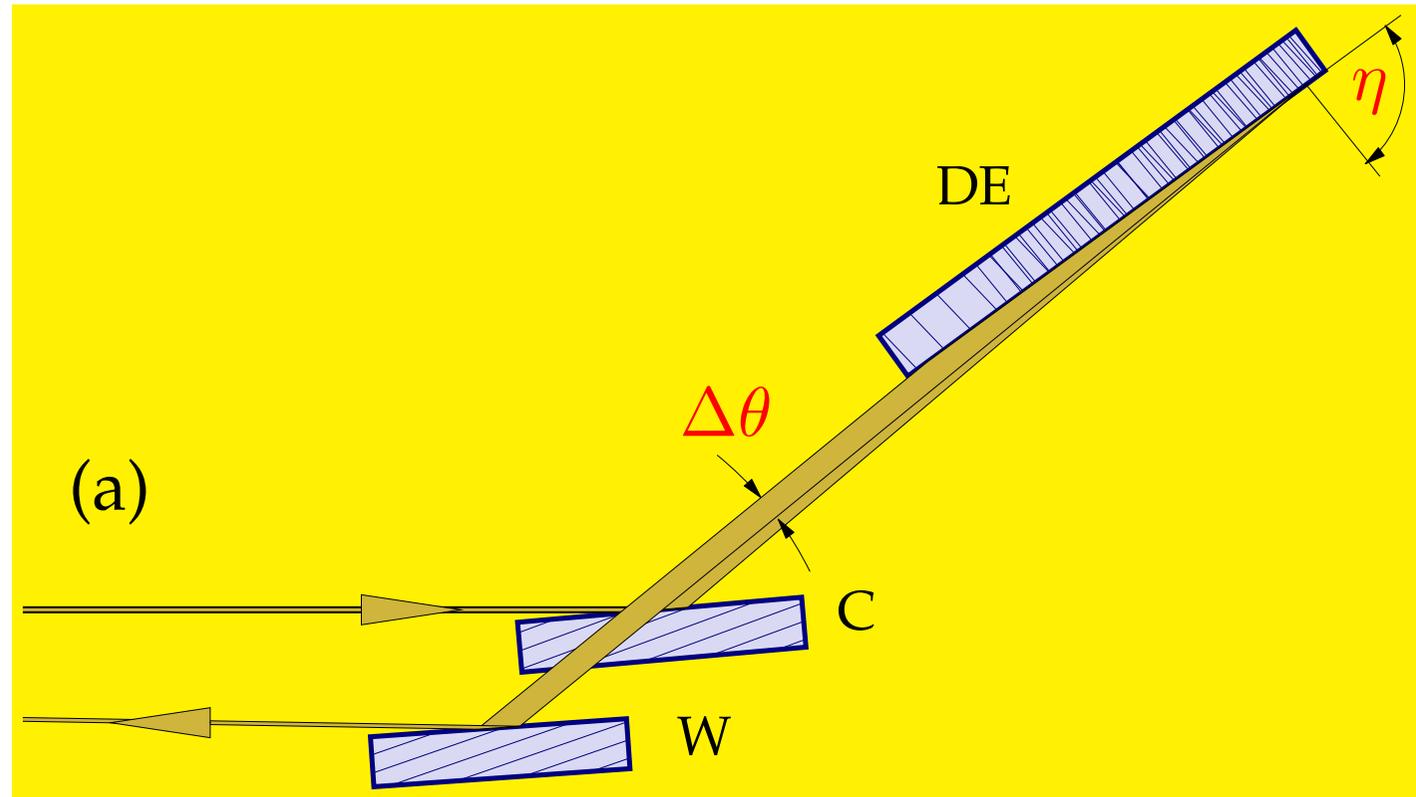
Angular dispersion is biggest for $\eta \rightarrow 90^\circ$ and thus $\theta \rightarrow 90^\circ$

CDW-Monochromator and its Spectral Resolution

$$\frac{\Delta E}{E} = \frac{\Delta \theta}{\tan \eta}$$

Yu. Shvyd'ko

X-Ray Optics, Springer-Verlag (2004)



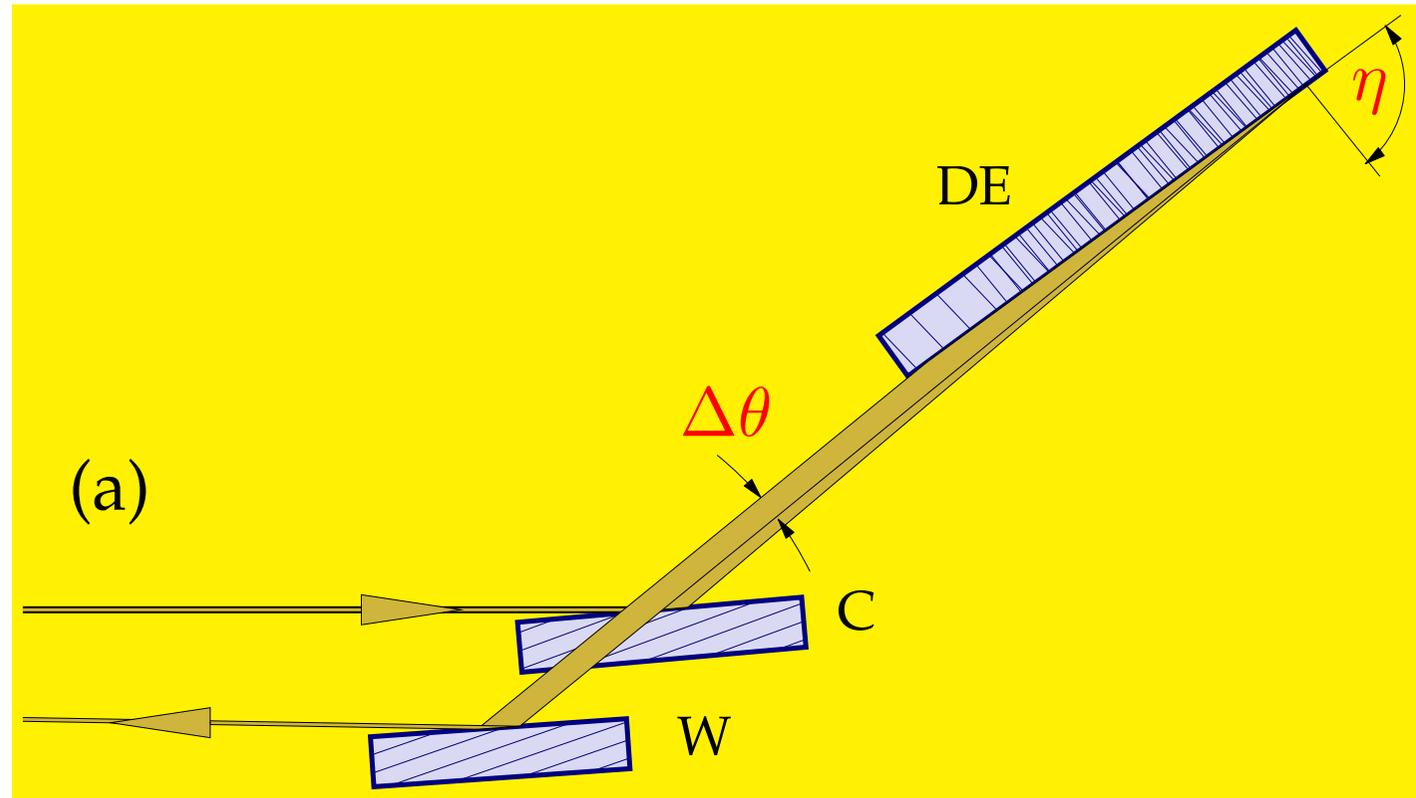
- The smaller the photon energy E , the smaller is the energy bandwidth ΔE (fortunately!).
- Bandwidth ΔE is controlled by asymmetry angle η ,

Spectral Resolution of the CDW-Monochromator

$$\frac{\Delta E}{E} = \frac{\Delta \theta}{\tan \eta}$$

$$\frac{\Delta E}{E} = 10^{-6} - 10^{-8}$$

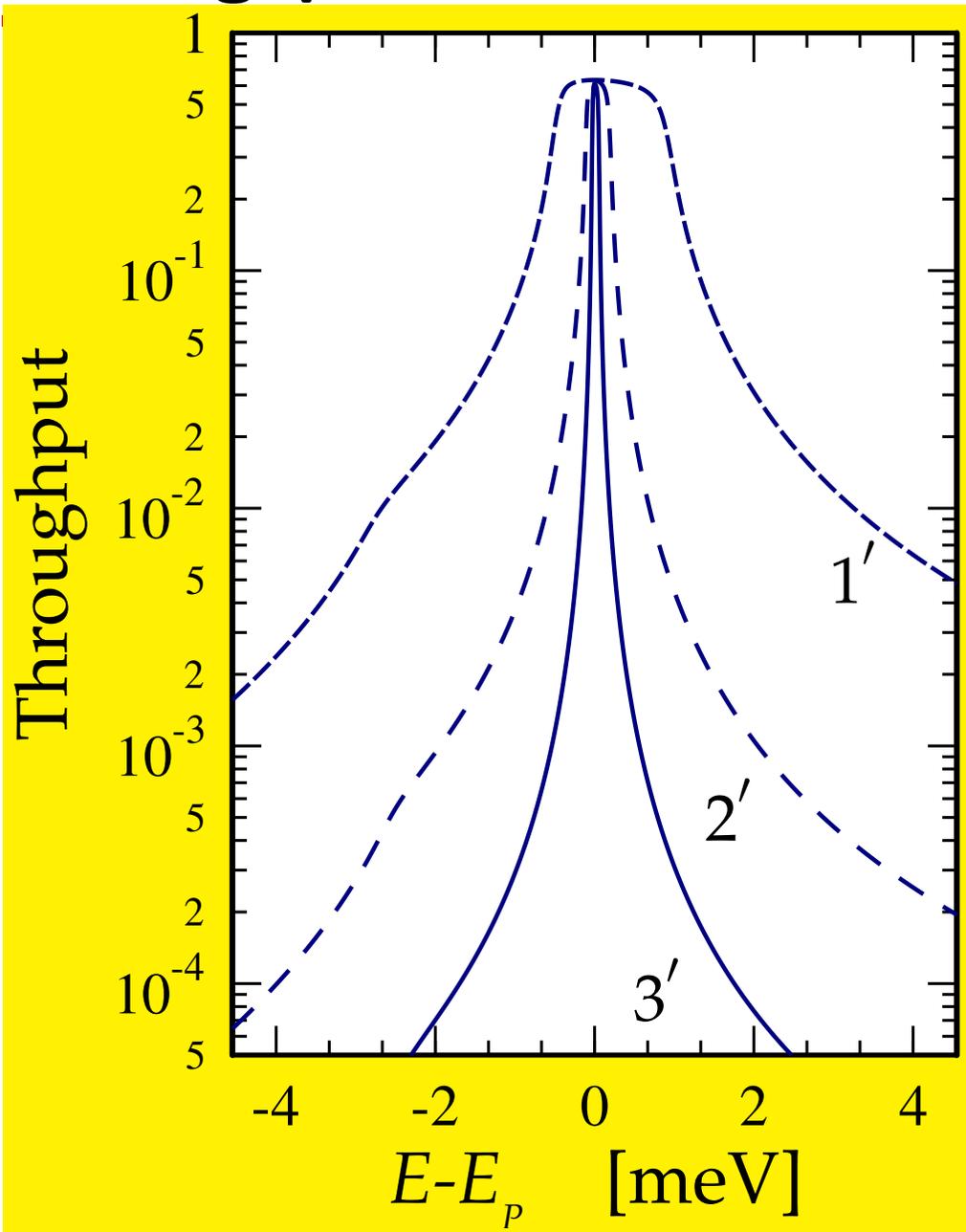
is feasible



$$E = 10 \text{ keV} \Rightarrow \Delta E = 10 - 0.1 \text{ meV}$$

$$E = 5 \text{ keV} \Rightarrow \Delta E = 5 - 0.05 \text{ meV}$$

Throughput of the CDW-Monochromator

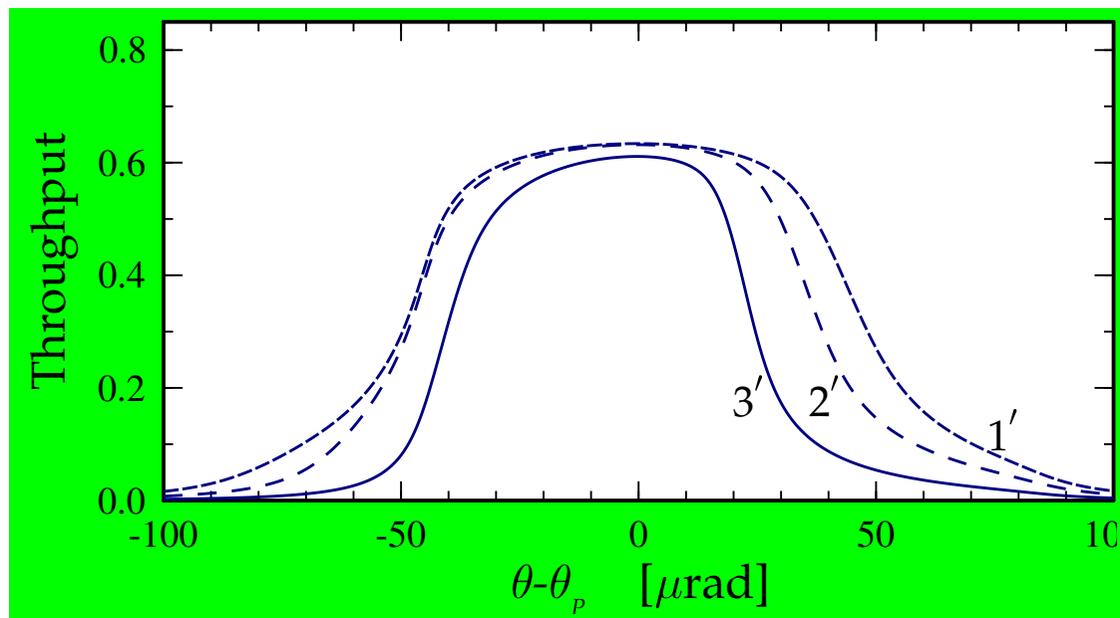
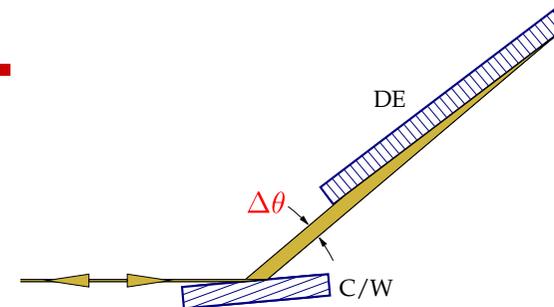


$$E = 9.1 \text{ keV}$$

$$1' : \Delta E = 1.5 \text{ meV } (\eta = 85^\circ)$$

$$2' : \Delta E = 0.3 \text{ meV } (\eta = 89^\circ)$$

$$3' : \Delta E = 0.09 \text{ meV } (\eta = 89.6^\circ)$$

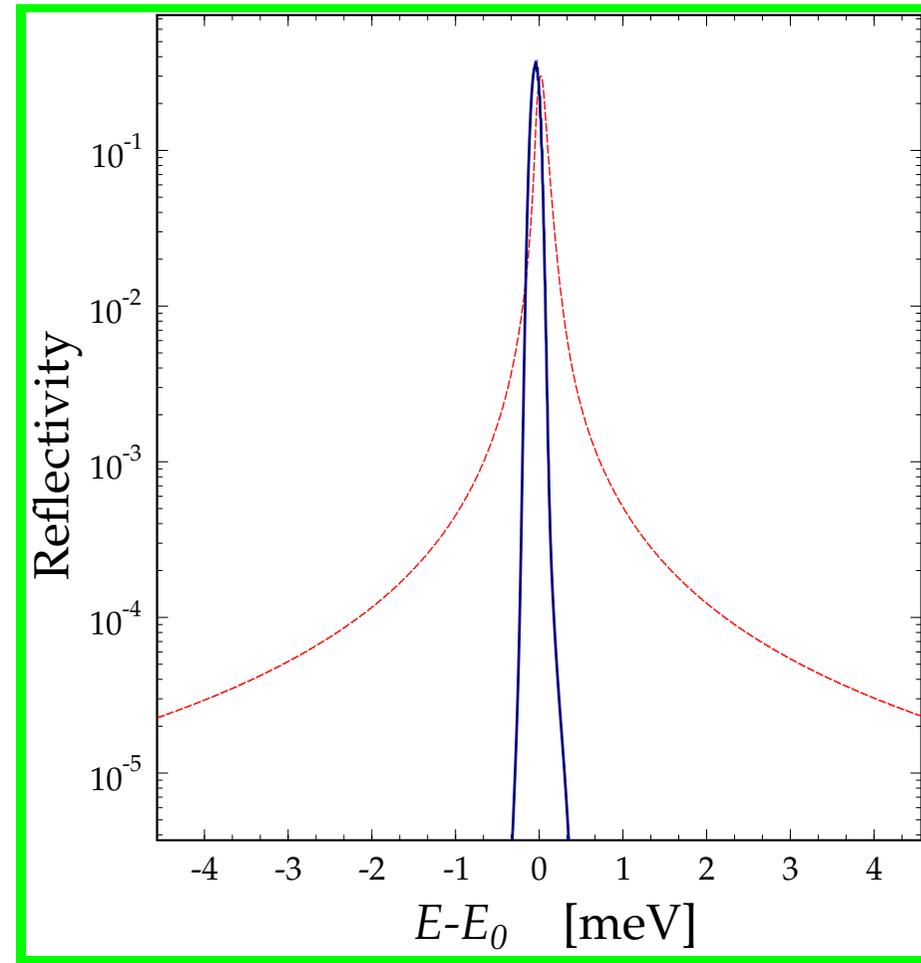
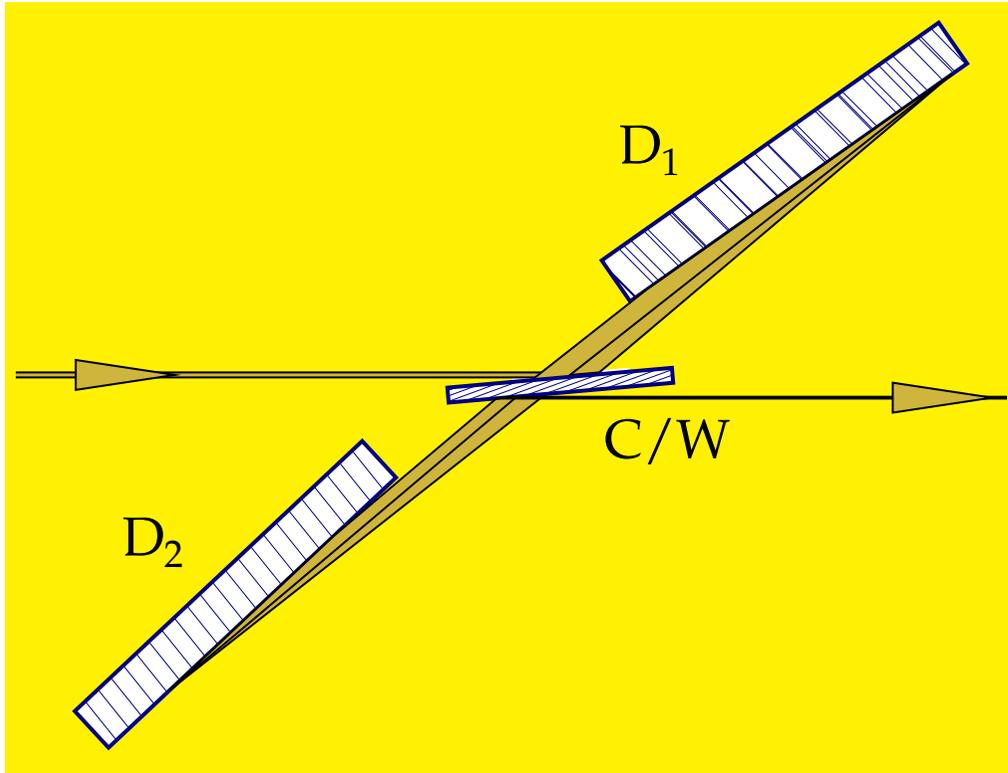


Angular-Dispersive In-line CDDW-monochromator

The angular dispersion is enhanced by a factor of 2:

Smaller asymmetry angle!

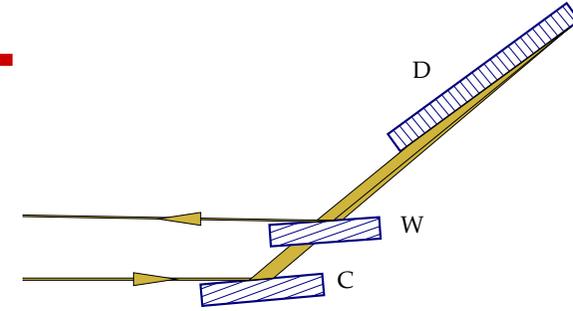
Shorter dispersing elements D_1 , D_2 !



Angular-dispersive CDDW monochromator:
 $E = 9.1315$ keV, $\Delta E = 0.1$ meV, D=Si(008)

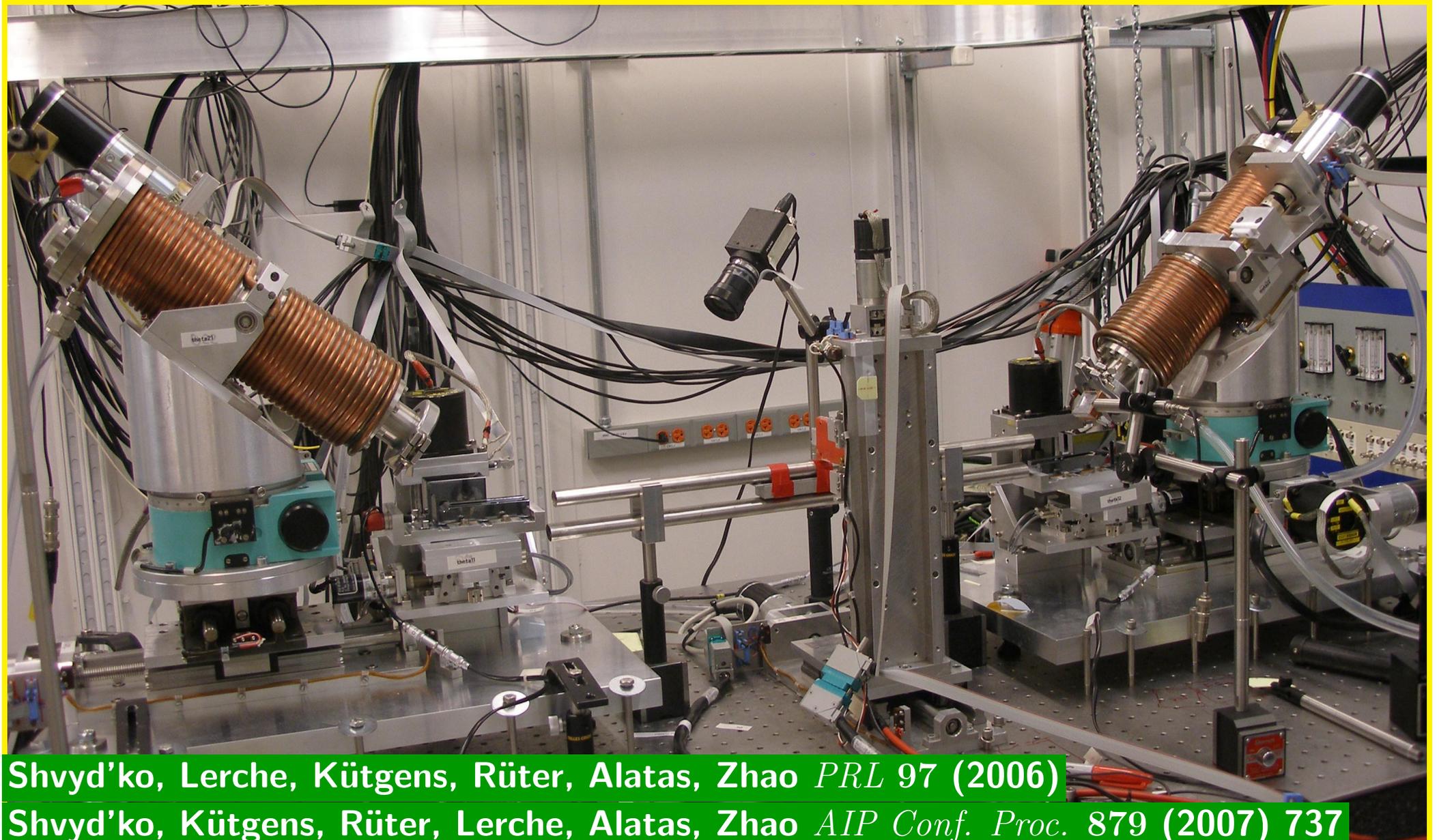
Single-bounce backscattering monochromator:
 $E = 31.02$ keV, $\Delta E = 0.1$ meV, Si(1 3 27).

Features of the CDW-Monochromators



1. $\Delta E/E$ is independent of E or of Bragg reflection.
2. The smaller the photon energy E the smaller is the bandpass ΔE .
3. ΔE can be varied by changing η (E is fixed).
4. The peak throughput T and the angular acceptance $\Delta\theta$
are almost constant (while changing η).
5. Steep wings in the spectral function.
6. The temperature control and energy tuning is technically not demanding
(for x-ray photons in the low-energy region 5 – 10 keV).

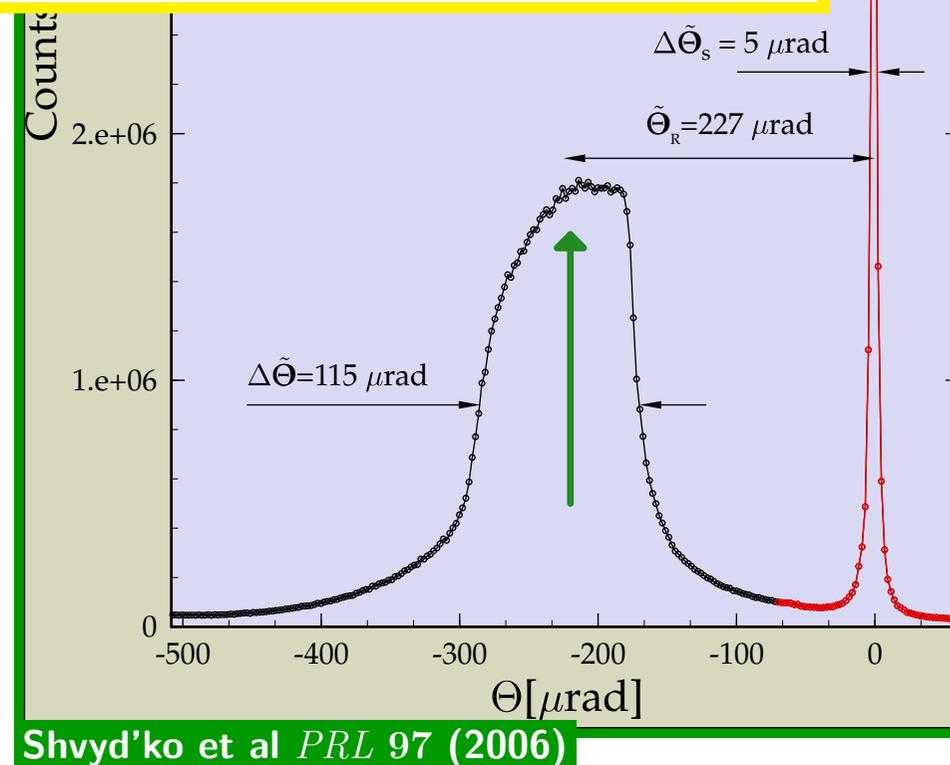
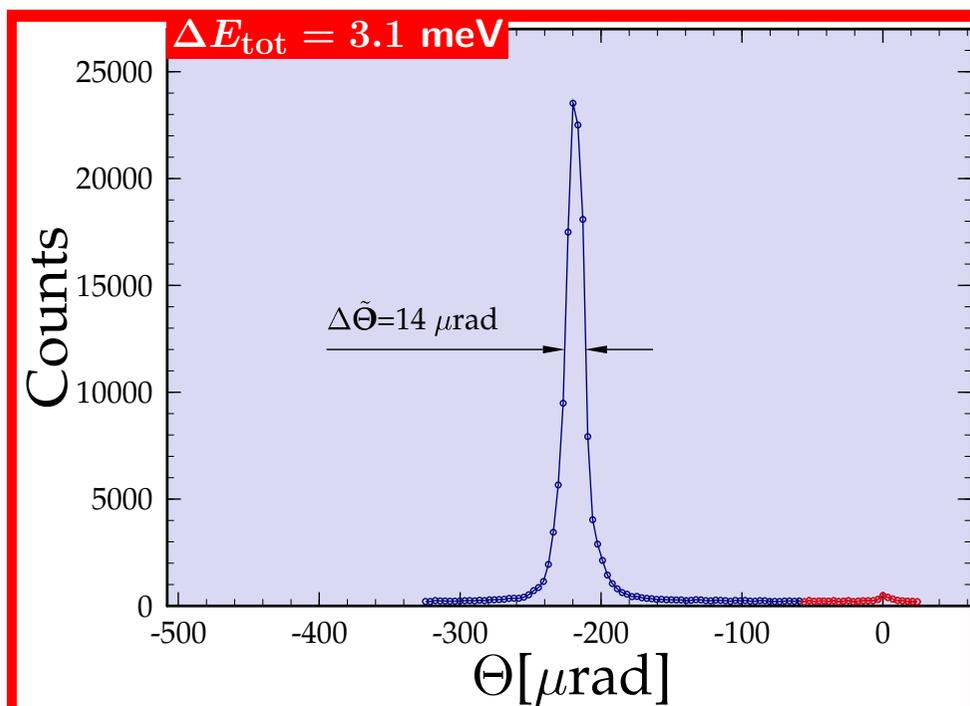
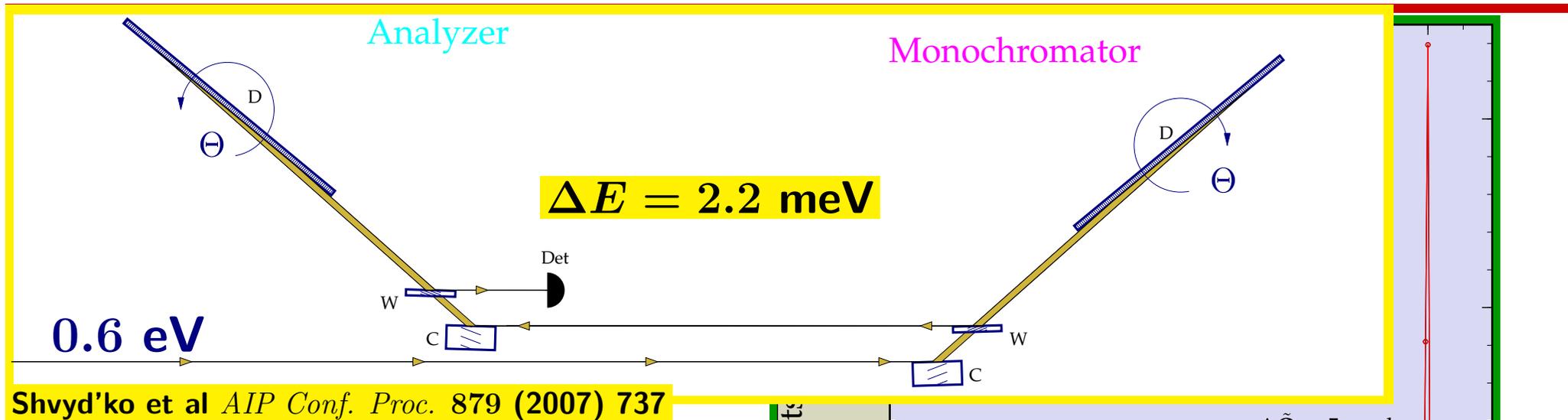
Experimental Set-up: @APS



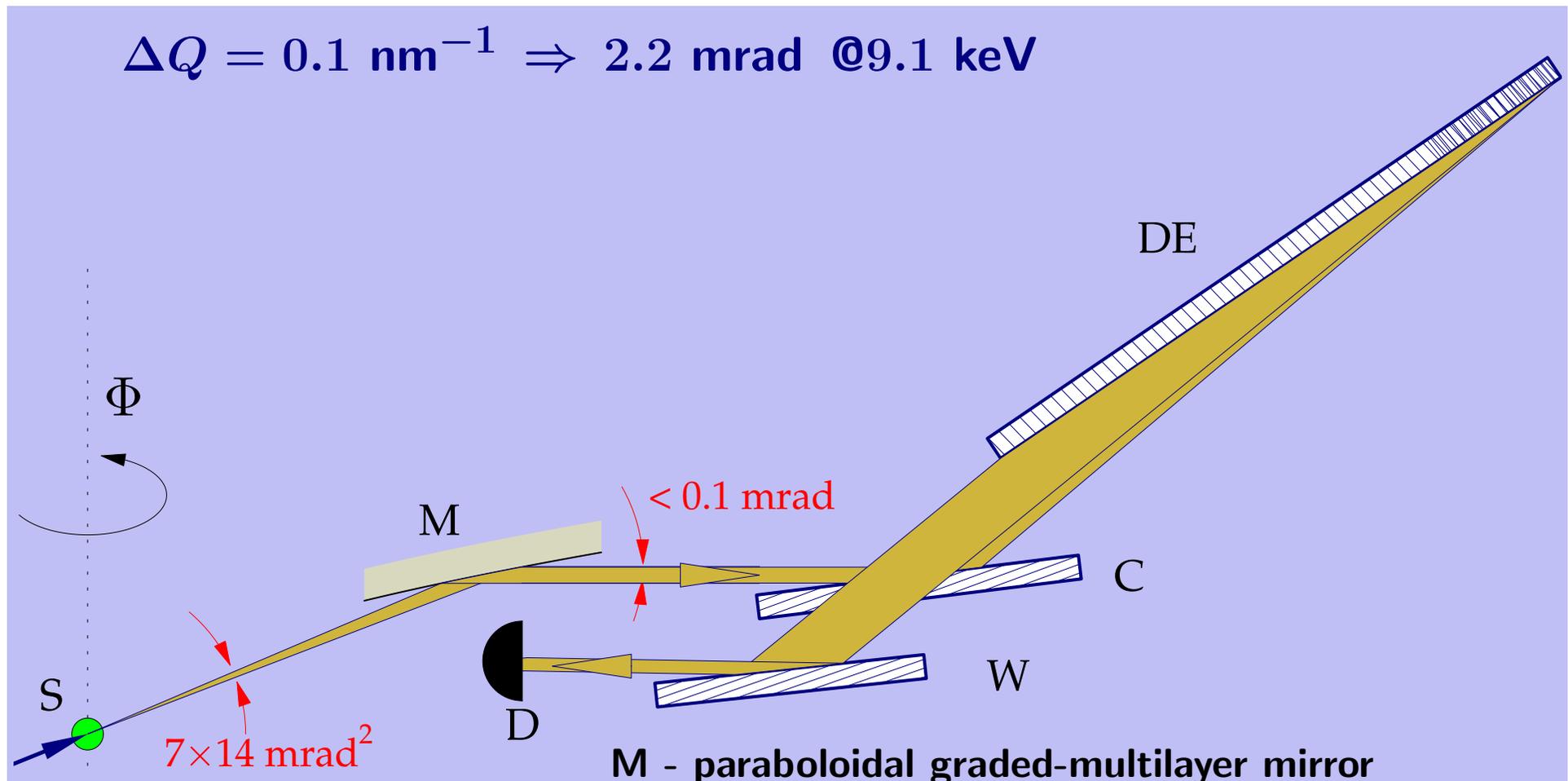
Shvyd'ko, Lerche, Kütgens, Rüter, Alatas, Zhao *PRL* 97 (2006)

Shvyd'ko, Kütgens, Rüter, Lerche, Alatas, Zhao *AIP Conf. Proc.* 879 (2007) 737

Energy Resolution - Direct Measurements



CDW-Analyzer



M - paraboloidal graded-multilayer mirror
development in progress @ APS

S - sample

D - detector

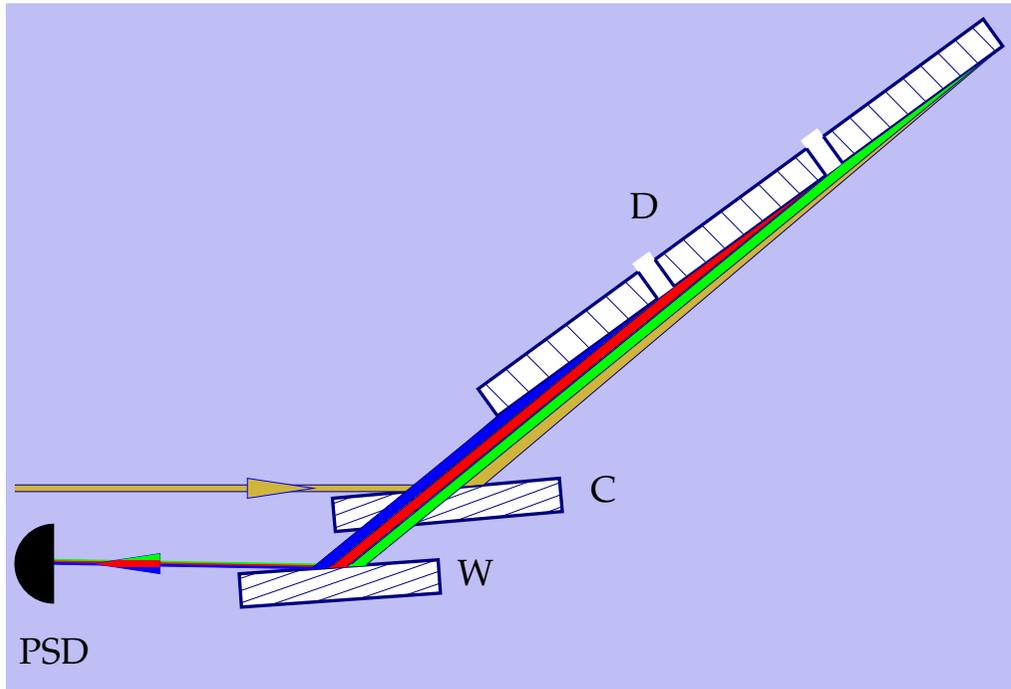
W - wavelength selector

DE - dispersing element

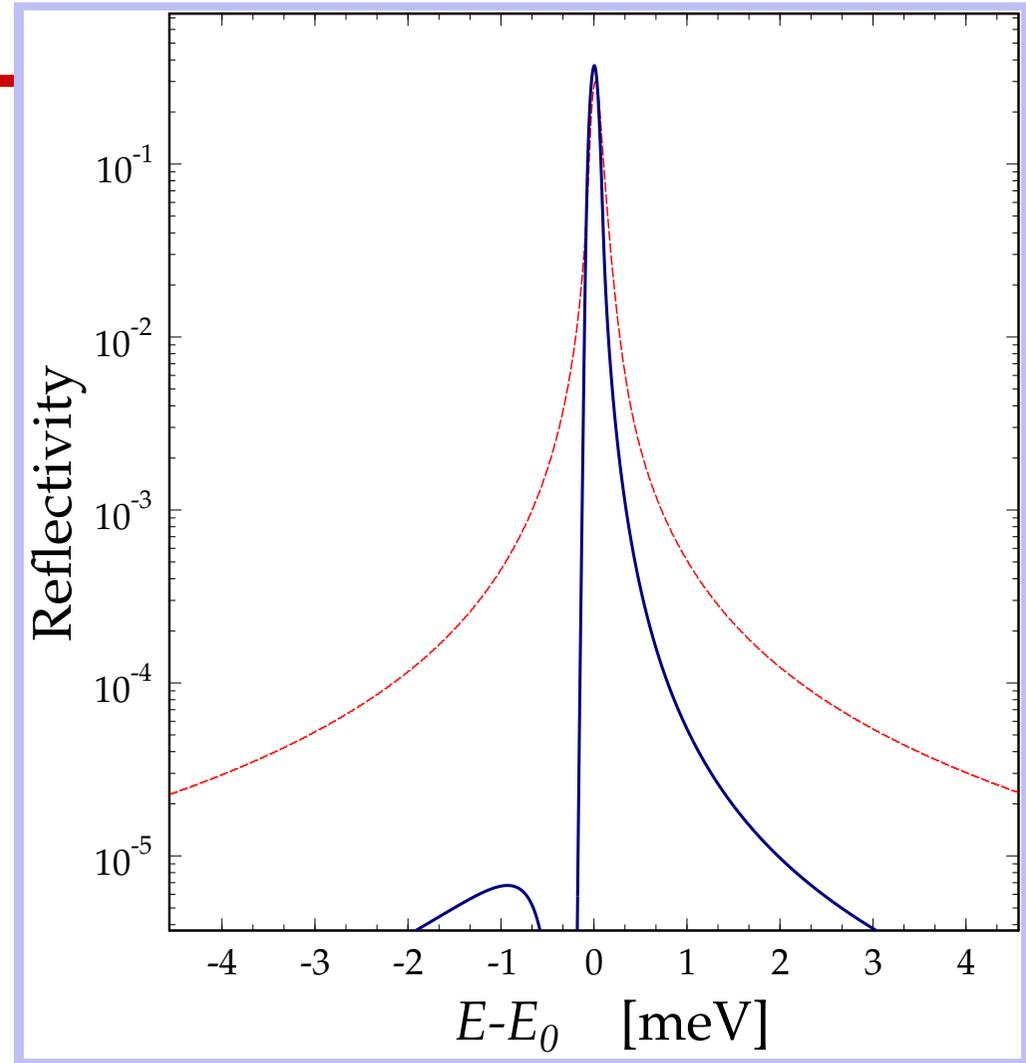
C - collimator

CDW-Segmented Analyzer

To overcome technical problems, associated with the big length (1-3 m), the dispersing element can be built of several independent segments which need not be perfectly aligned or have precisely the same temperature.



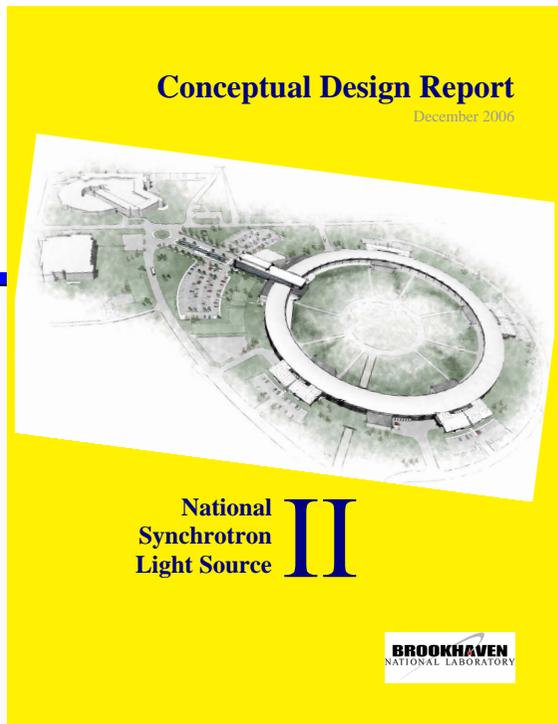
PSD - position sensitive detector
D - dispersing elements
W - wavelength selector
C - collimator



Angular-dispersive CDW analyzer:
 $E = 9.1315$ keV, $\Delta E = 0.1$ meV, D=Si(008)

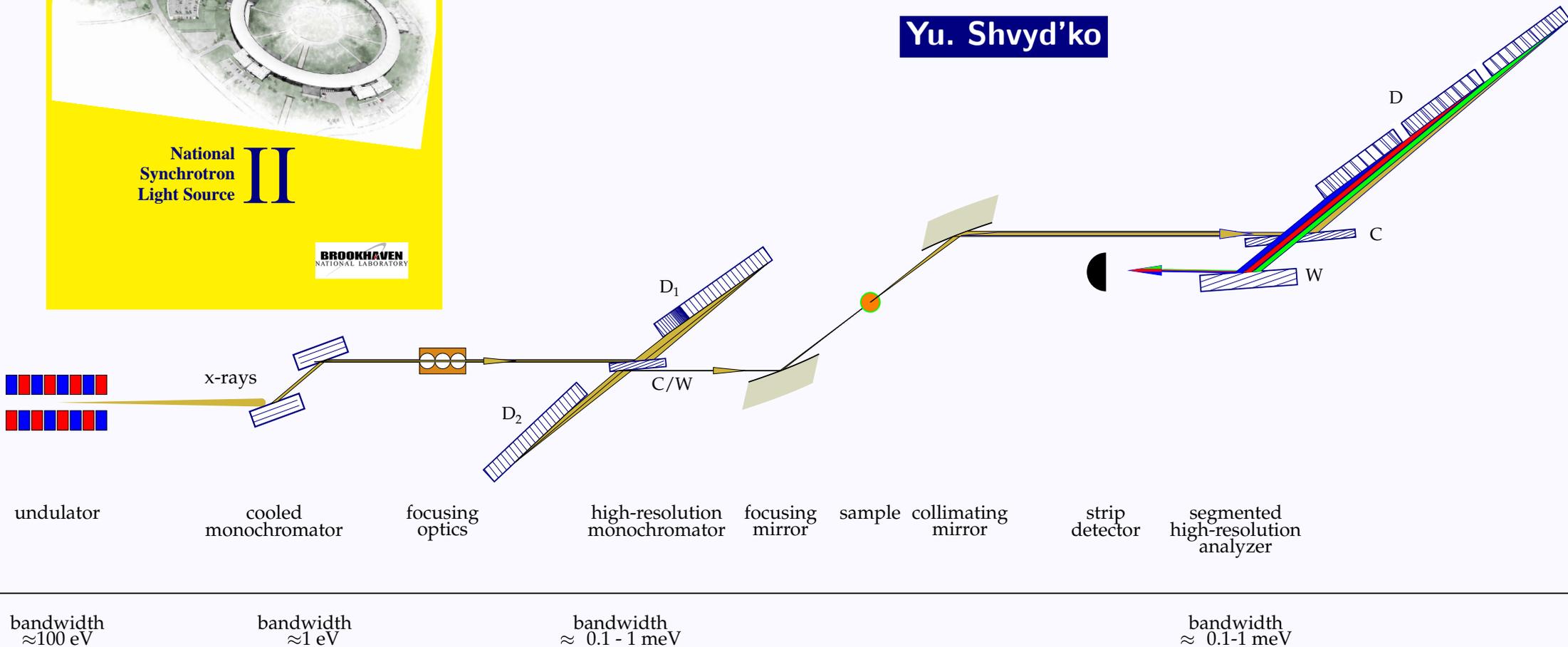
Single-bounce backscattering analyzer:
 $E = 31.02$ keV, $\Delta E = 0.1$ meV, Si(1 3 27).

0.1 meV IXS Spectrometer



An IXS spectrometer with 0.1 meV resolution, operating at 9 keV.

Yu. Shvyd'ko

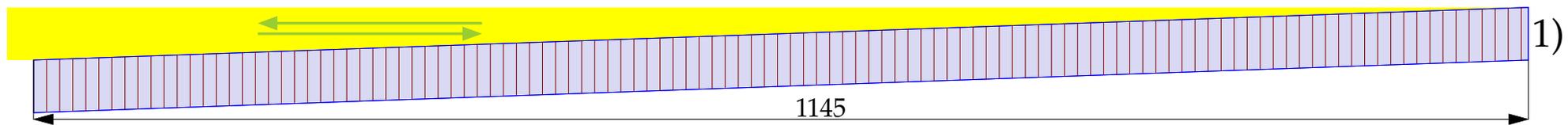


The Biggest Challenge: 1-3 m Long Crystals

are required to build a 0.1 meV IXS spectrometer

Strain free!

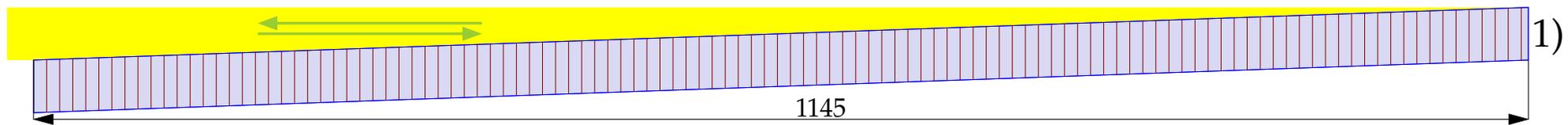
Temperature homogeneity $< 2 \text{ mK}/(1 - 3)\text{m}$!



The Biggest Challenge: 1-3 m Long Crystals

“One recognizes a really good idea by the fact that its implementation appears impossible from the very beginning”.

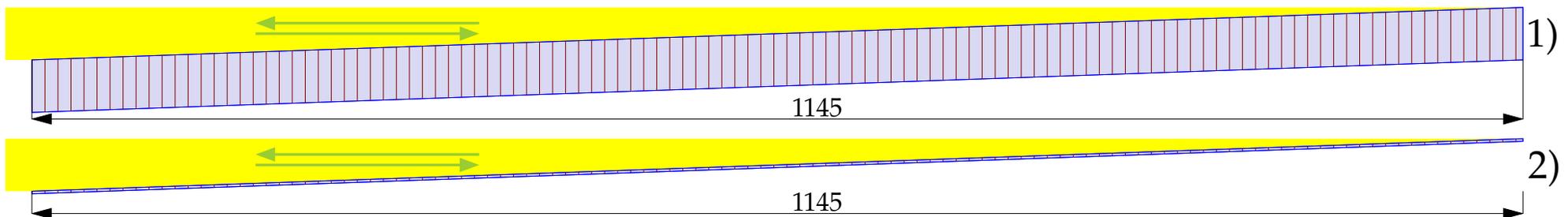
Albert Einstein



The Biggest Challenge: 1-3 m Long Crystals

“One recognizes a really good idea by the fact that its implementation appears impossible from the very beginning”.

Albert Einstein

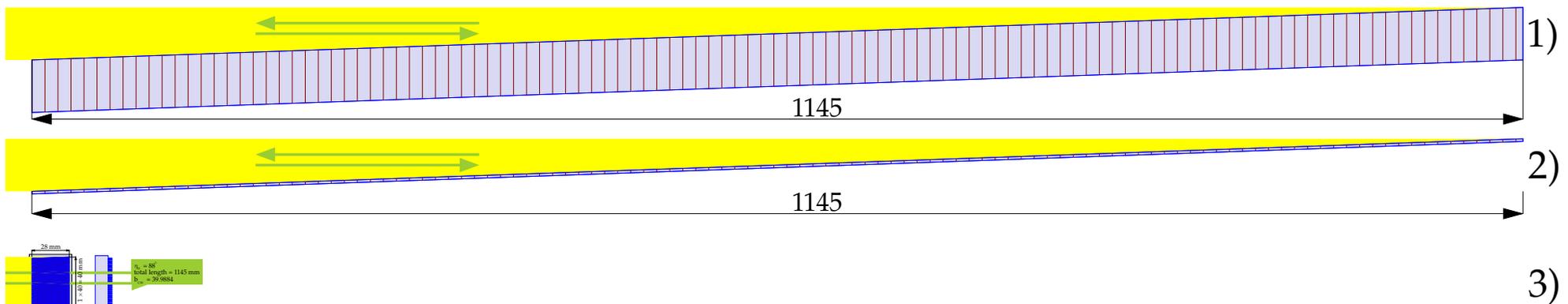


10 μm thick crystal is sufficient

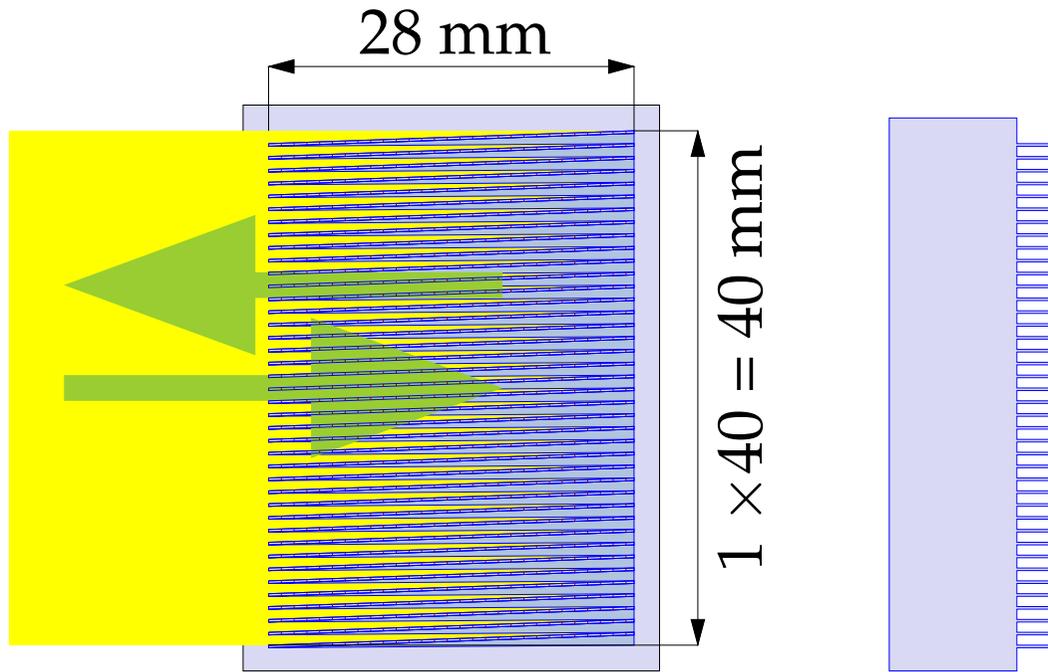
The Biggest Challenge: 1-3 m Long Crystals

“Eine wirklich gute Idee erkennt man daran, dass ihre Verwirklichung von vorne herein ausgeschlossen erscheint”.

Albert Einstein



Comb Crystal



3)

$$\begin{aligned}\eta_D &= 88^\circ \\ \text{total length} &= 1145 \text{ mm} \\ b_{CW} &= 39\end{aligned}$$

Total resolution: $\Delta Q \simeq 0.3 \text{ nm}^{-1}$.

However, combined with a position sensitive detector, this is a multianalyzer set-up with $\simeq 0.01 \text{ nm}^{-1}$ resolution.

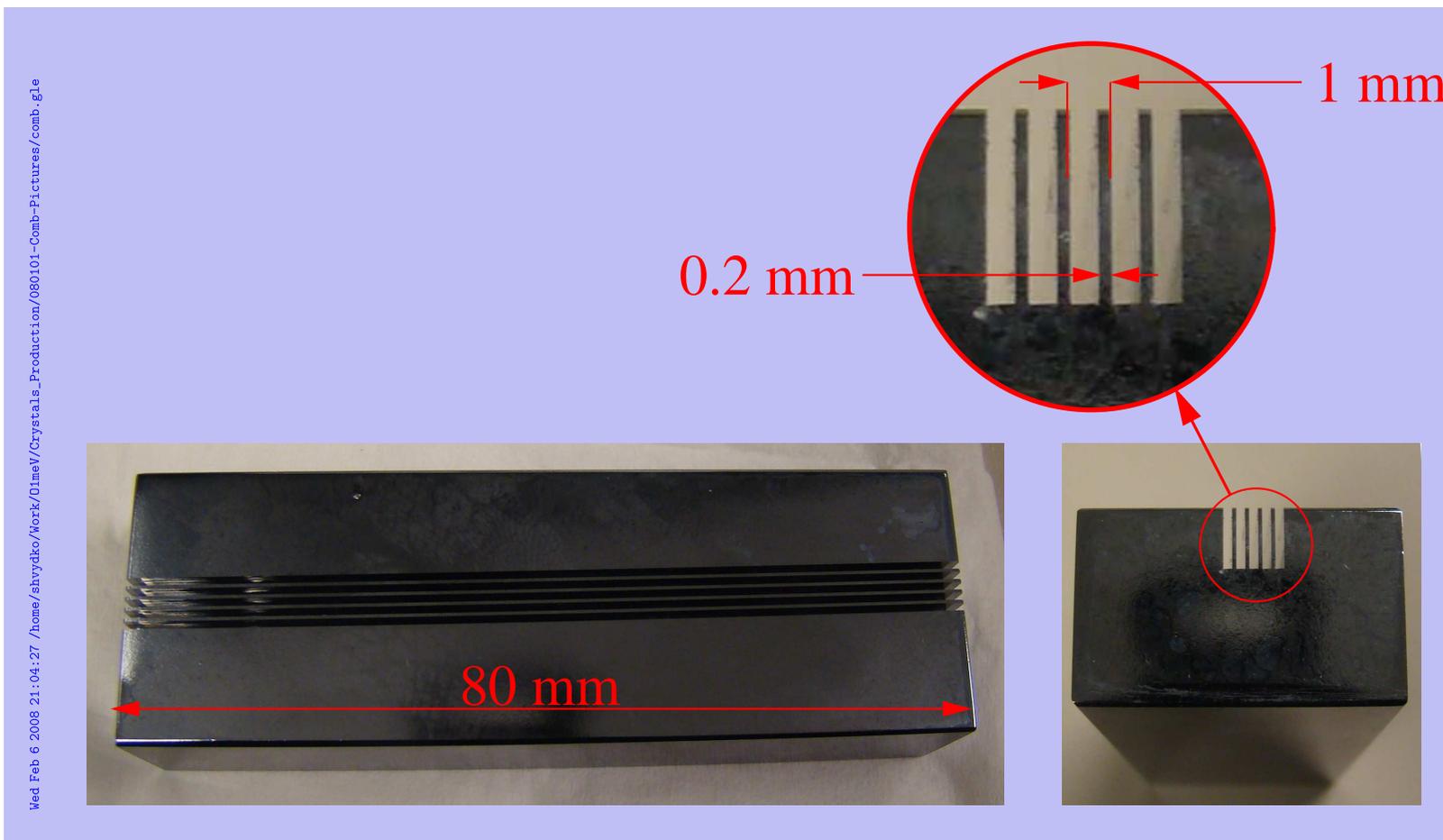
Crystal Comb



Swarovski Crystal Comb Wedding Hair Piece \$96.00

Available online: <http://www.brilliant-wedding-jewelry.com>

Comb Si Crystal



APS Comb Crystal

Available@aps.anl.gov

Current Major R&D Tasks

Development of the spectrometer components
is the major R&D task of the project at the APS:

- Comb crystals

R. Khachatryan, M. Wiczorek

- Parabaloidal graded multilayer mirror

A. Macrander, A. Khounsary R. Conley C. Liu

- Temperature stabilized enclosure, mechanical design

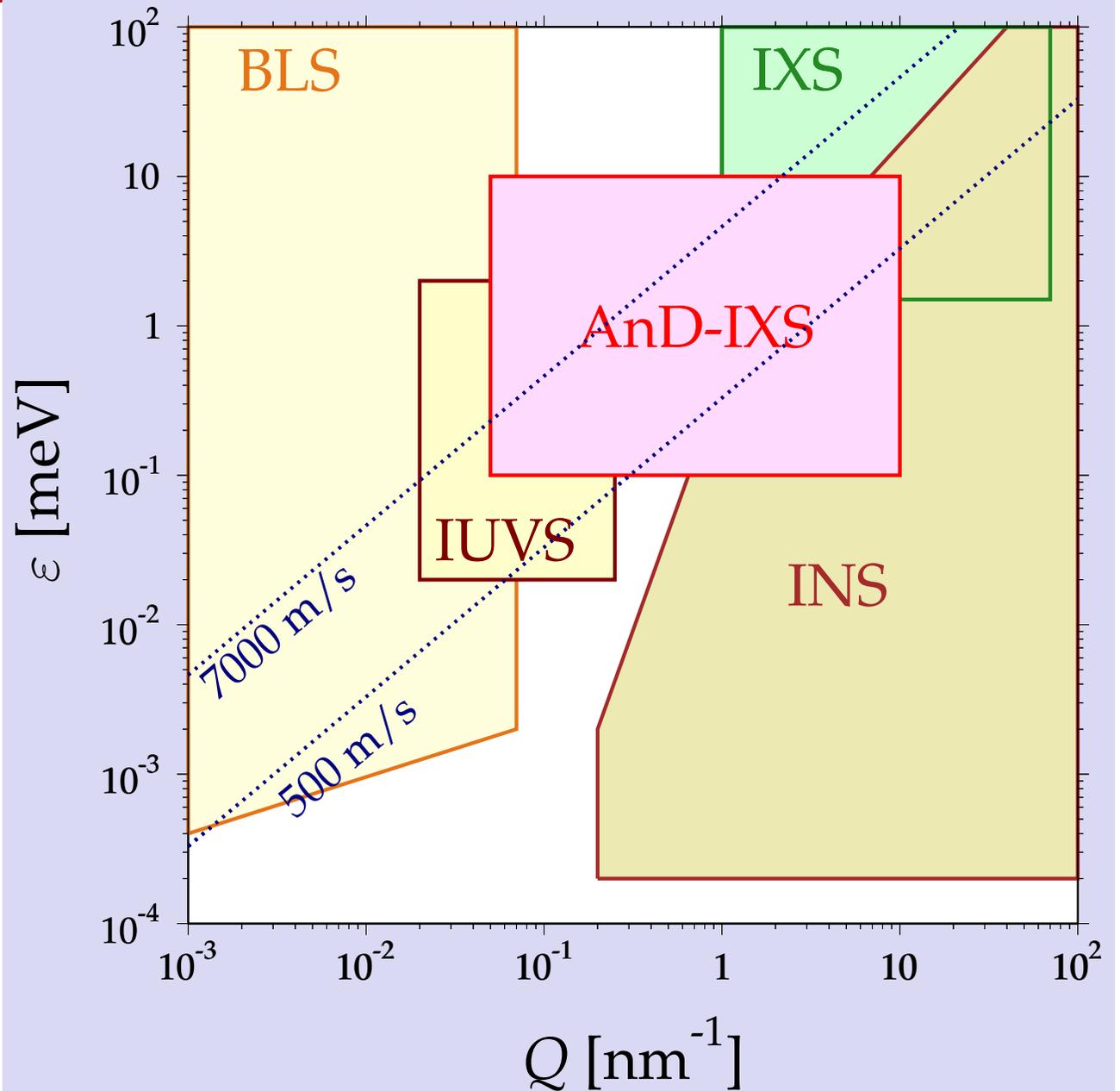
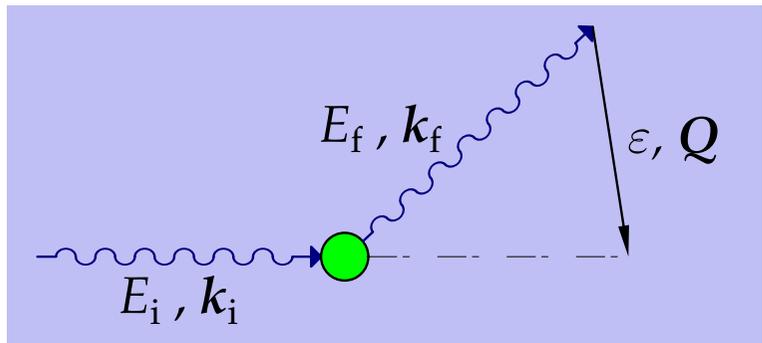
D. Shu

Expectations:

1. Energy transfer resolution $\Delta\varepsilon \approx 1 - 0.1 \text{ meV}$.
2. Momentum transfer resolution $\Delta Q \approx 0.3 - 0.01 \text{ nm}^{-1}$.
3. Spectral function with **steep wings.** (high contrast)
4. Will work at APS but also at any **intermediate energy** SR facility: NSLS-II, Diamond, etc.

Probes for Vibrational Dynamics

Angular Dispersive IXS Spectrometers



Conclusions

**To reach new challenging goals
we have to look into new ideas**

- **Position sensitive detectors:**

*A path to high-resolution, compact,
high throughput multianalyzer IXS spectrometers*

- **Effect of angular dispersion:**

A path to ultra-high resolution IXS spectrometers

- **New crystals, and many other ideas.**

The Future is Bright as the Blue Sky of Chicago

Thank you for your attention!

IXS Workshop, APS User Meeting, May 8th, 2008.

