IRIXS: an Intermediate X-Ray Energy RIXS Spectrometer

Current status and recent developments

Hlynur Gretarsson - P01 High Resolution Dynamics Beamline, DESY
11th International Conference on Inelastic X-ray Scattering
Stony Brook University, June 2019

HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

erc European Research Council

DESY.

Special thanks to…

DESY-P01: H. Gretarsson, H. Yavas (SLAC), H.-C. Wille, S. Mayer*

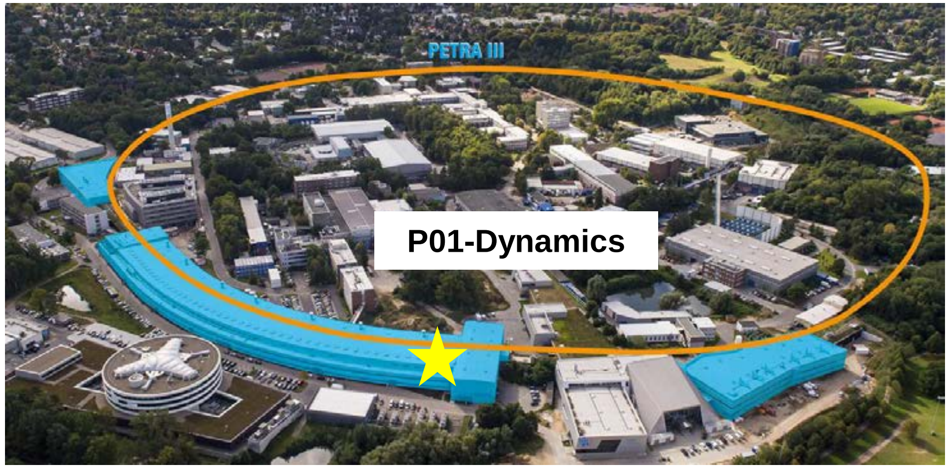
F.-U. Dill*, and C. Hagemeister**

MPI-Stuttgart: B. Keimer, G. Khaliullin, B. J. Kim (Postech), J. Bertinshaw, H. Suzuki, Lichen Wang, K. Ueda (U. Tokyo), H. Kim (Postech), J. Chaloupka (Masaryk University), Huimei Liu, and M. Minola

APS: T. Gog, Jungho Kim, A. Said, E. Kasman, and XianRong Huang (X-Ray Optics)

ESRF: R. Verbeni (X-Ray Optics)

MAXIV: K. Klementiev (ray tracing XRT)



MAX-PLANCK-GESELLSCHAFT

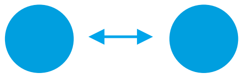
Argonne NATIONAL LABORATORY

ESRF

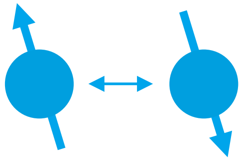
MAX IV

Beamline P01
DESY goal is 5000 hours to users/year

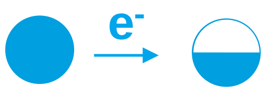
NRS (50%)



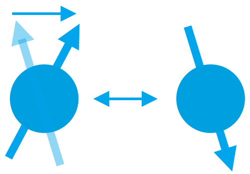
Phonon DOS
Magnetic structure



IXS (50%)

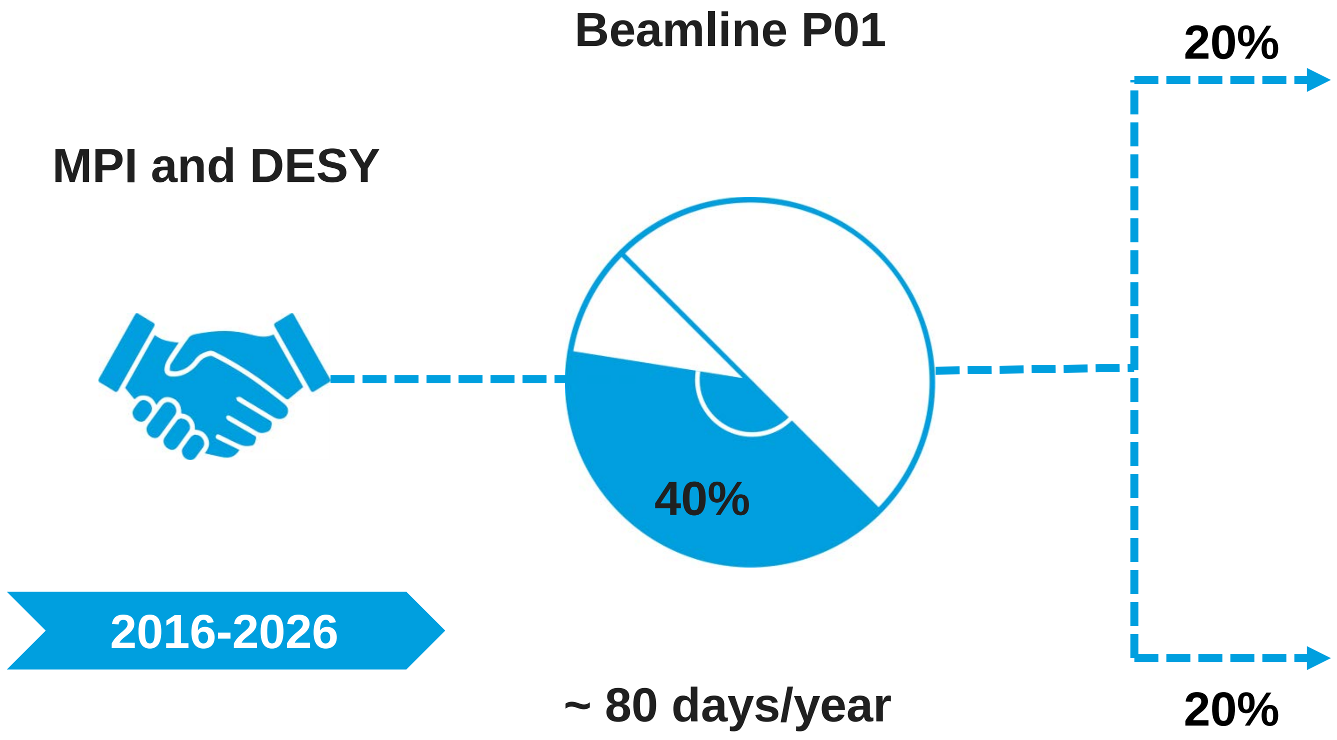


Electronic DOS
Magnetic excitations



Strong support for x-ray spectroscopy at P01

Partnership with an outside institute offers a unique scientific opportunity



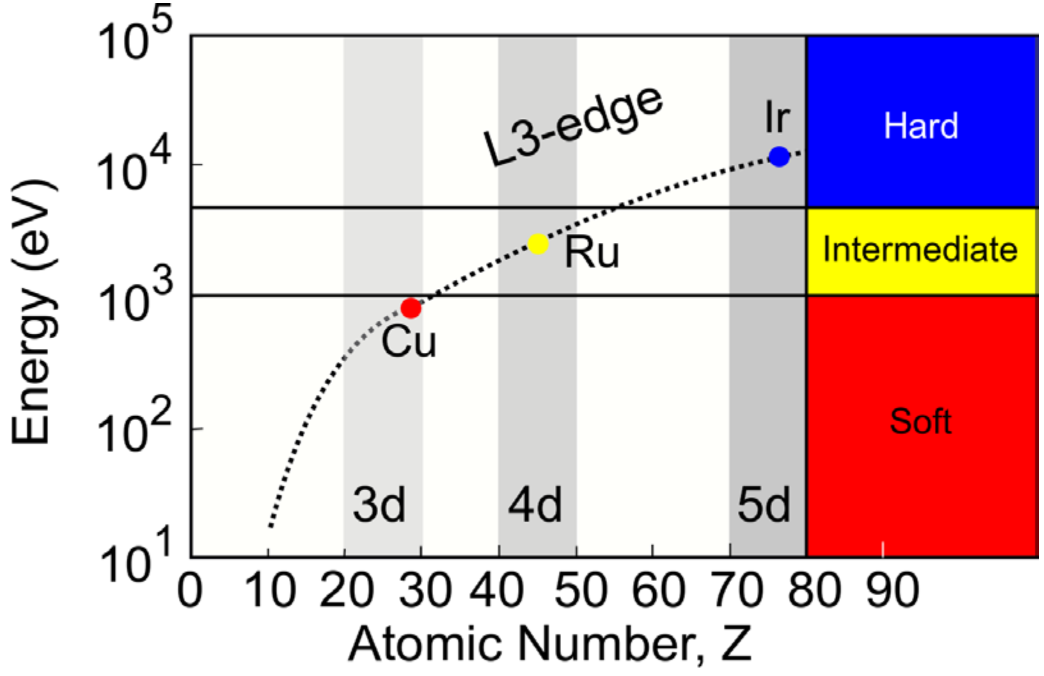
Prof. Hao Tjeng
Imaging orbitals in TMO's using XRS
MPI-Dresden
Hasan Yavas
Nature Physics (2019)
Brett Leedahl
Submitted (2019)

Prof. Bernhard Keimer
Collective modes in 4d TMO's using RIXS
MPI-Stuttgart
Hakuto Suzuki
Nature Materials (2019)
Hlynur Gretarsson
PRB (2019)

Use L_3-edge RIXS to measure collective modes (e.g. magnons)

Beamlines split into soft and hard x-rays with no overlap in energy

Figure adapted from: **Luuk J. P. Ament, Thomas P. Devereaux, et al., RMP (2011)**



	Soft	Tender	Hard
E (keV)	<1	1:5	>5
Optics	Grating	Grating /Crystal	Crystals
Vacuum	UHV	HV	V
Windows	No	No	Yes
Location	Spring-8, TPS, MAXIV, ESRF, Diamond, NSLSII		Spring-8, ESRF, Soleil, APS

There is a need for a RIXS beamline that can measure at the Ru L_3-edge

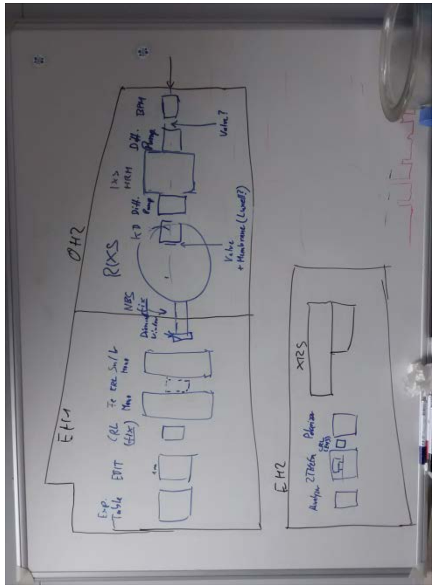
Current Status

The IRIXS Project (2016-2026)

Beamline dedicated to 4d TM's materials (e.g. E=2.840 keV, Ca_2RuO_4) with a 20 meV resolution

2016

Instrument design
Hard x-ray RIXS
Crystal optics
Si and SiO_2



2017

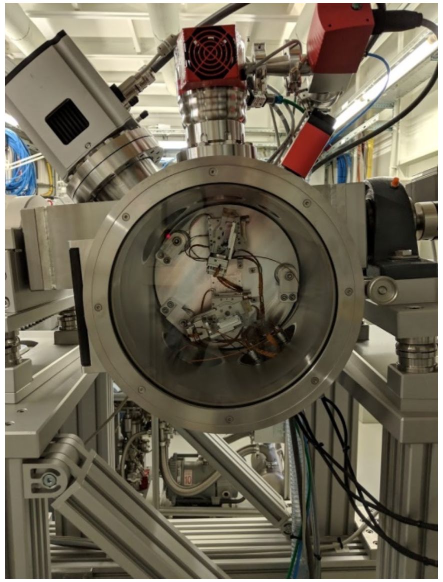
2x undulator
First beam
(2840 eV)
Spectrometer
(IRIXS v1)
HRM installed

2018

4B-HRM in use
Resolution
100 meV
Commissioning
CA-spectrometer
(IRIXS v2)

2019 - current

Commissioning
CA-spectrometer
(IRIXS v2)
More R&D
(IRIXS v3)



Overview of our IRIXS instrument (ΔE=100 meV @ 2840 eV)

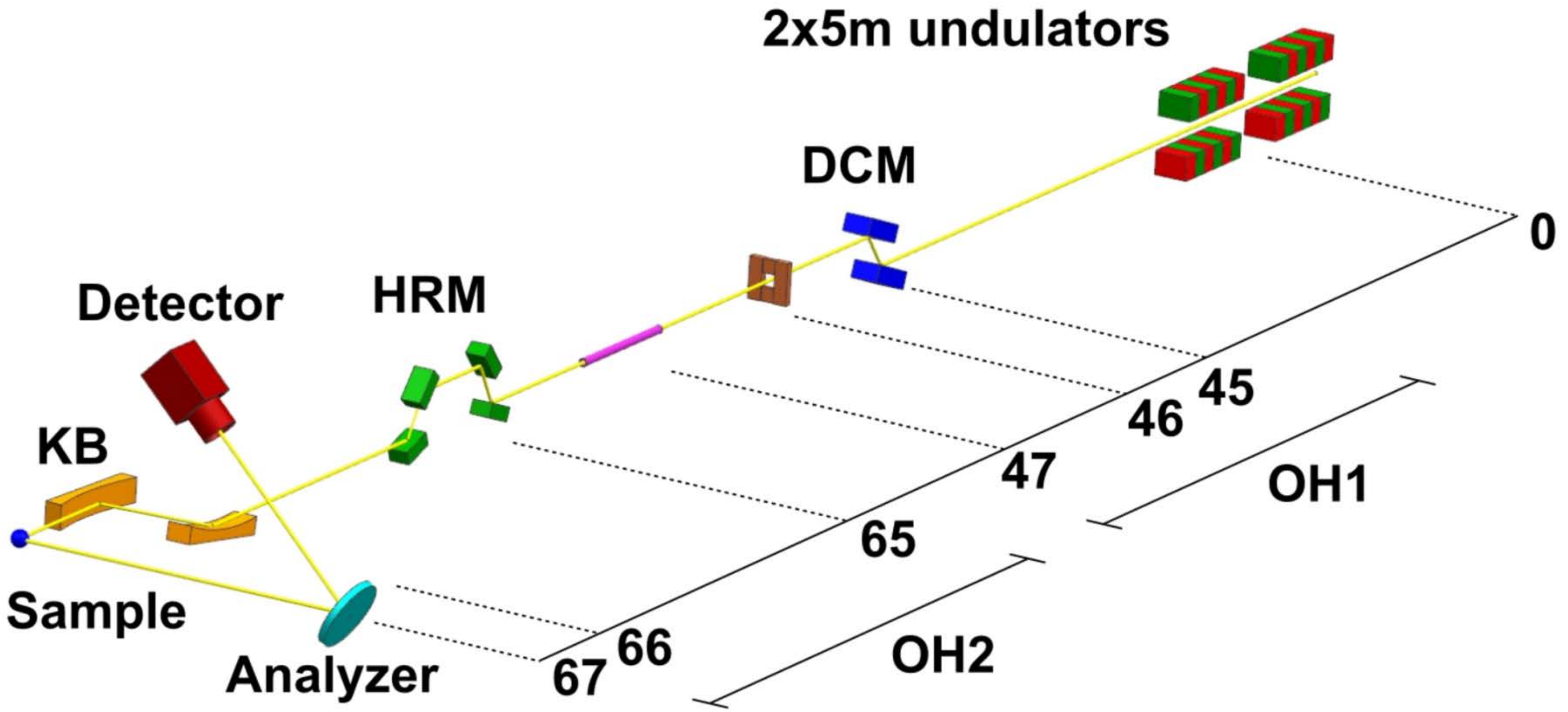
Spectrometer based on a diced analyzer – Suffers in resolving power but easy to operate

DCM
Si (111) α=32°
0.6 eV @ 2840 eV

HRM
Dispersive 4B (+ - - +)
Si (111) α=20°
60 meV @ 2840 eV

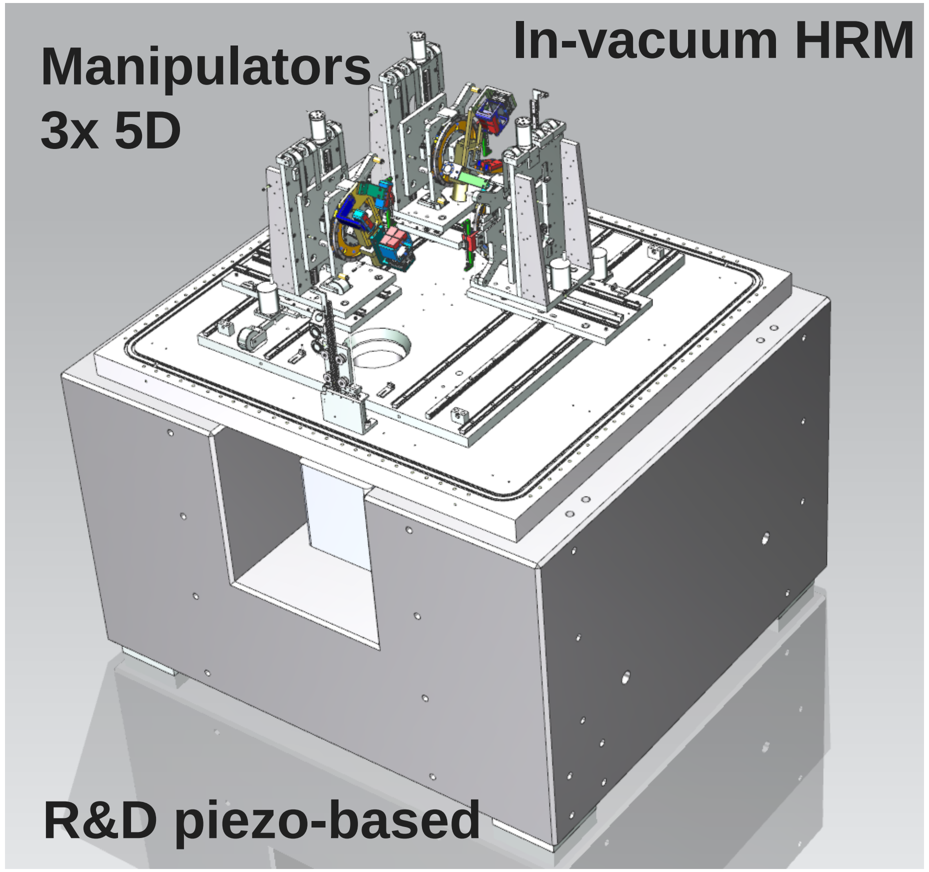
KB + Spectrometer
IRELEC mirror
SiO_2 (10-2) 60 meV
2D-pixel iKon L (13x13μm²)

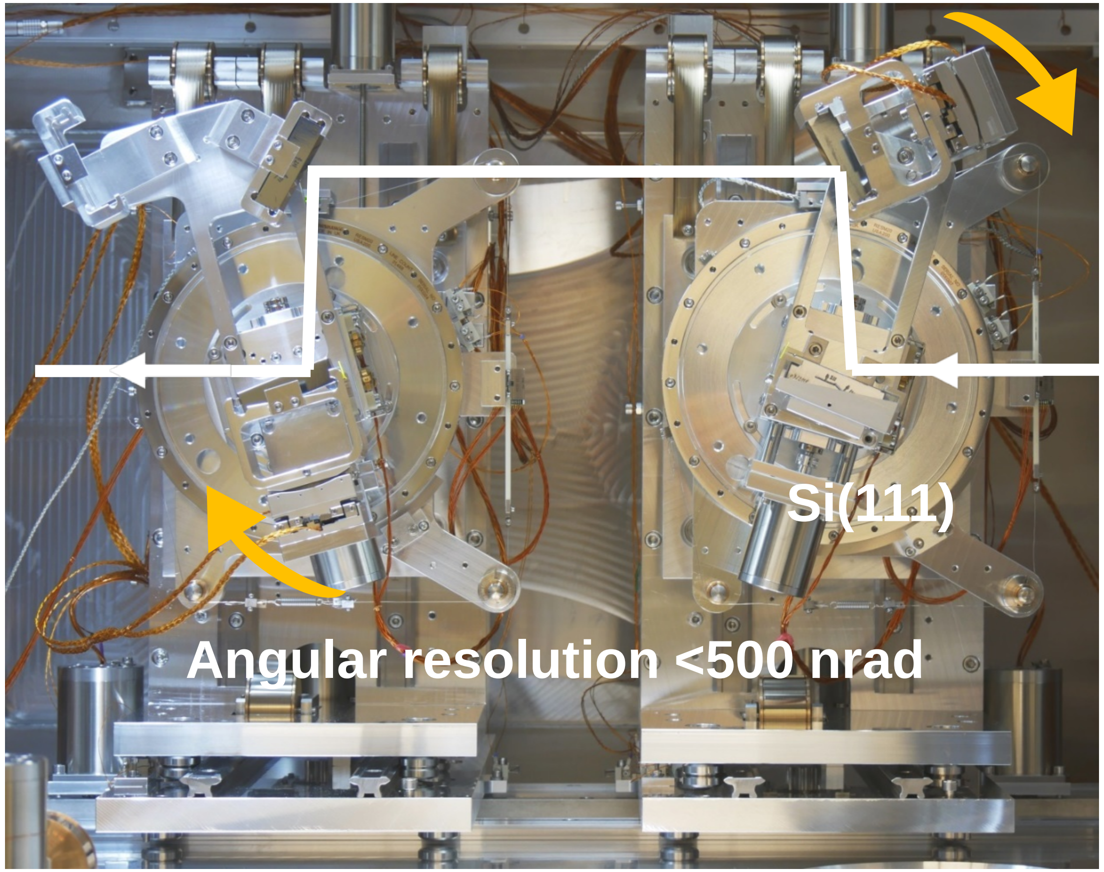
Misc.
Huber (5D)
ARS cryostat 10–300K
(Cu braids)



Dispersive (+--+) 4-bounce HRM giving 60 meV @ 2840 eV

Reflections close to backscattering are not available, a problem well known in the field of NRS





4B-HRM for NRS: M. Yabashi, et al., Rev. Sci. Instrum. (2001)

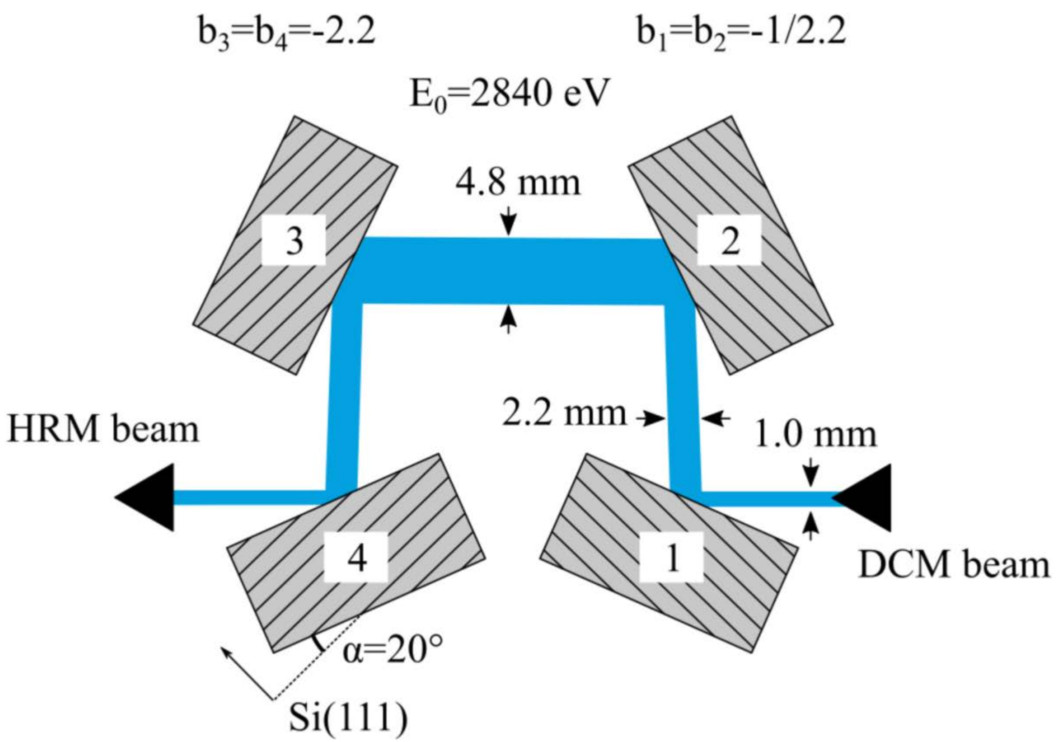
MERIXS: Yu. V. Shvyd'ko, et al., J. Electron Spectrosc. Relat. Phenom. (2013)

Dispersive (+--+) 4-bounce HRM giving 60 meV @ 2840 eV

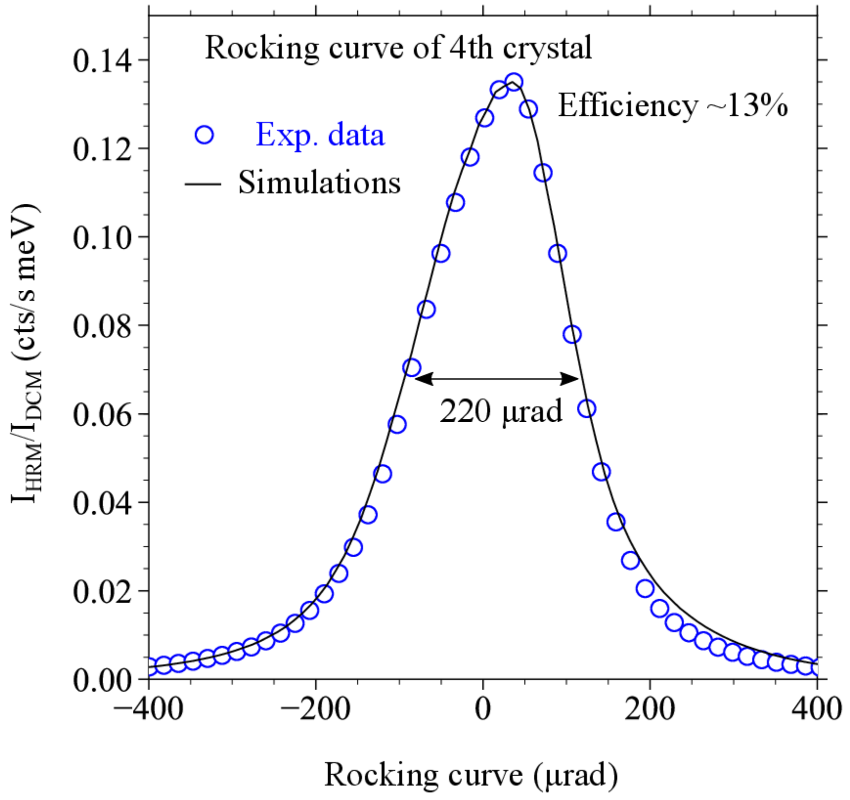
Reflections close to backscattering are not available, a problem well known in the field of NRS

Yu. Shvyd'ko, X-Ray Optics – High-Energy-Resolution Applications, vol. 98 of Optical Sciences (2004)
J.W.M. DuMond, Phys. Rev. (1937)

$$b = -\sin(\theta_B - \alpha)/\sin(\theta_B + \alpha)$$



No offset of the HRM beam
Smaller bandwidth compared to 2B
Reflectivity is low

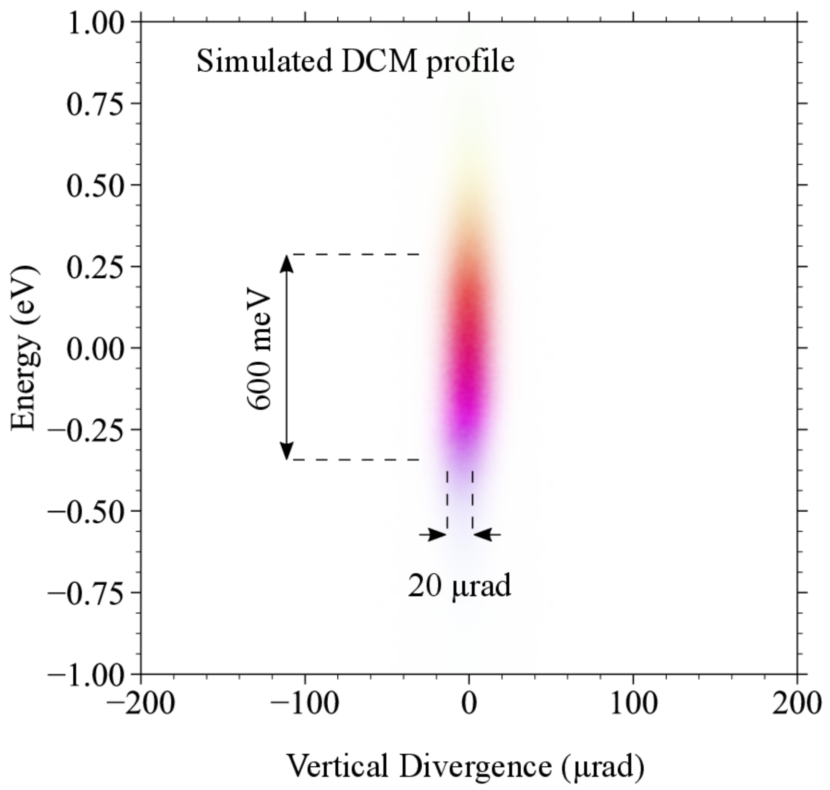


Good agreement with XRT results

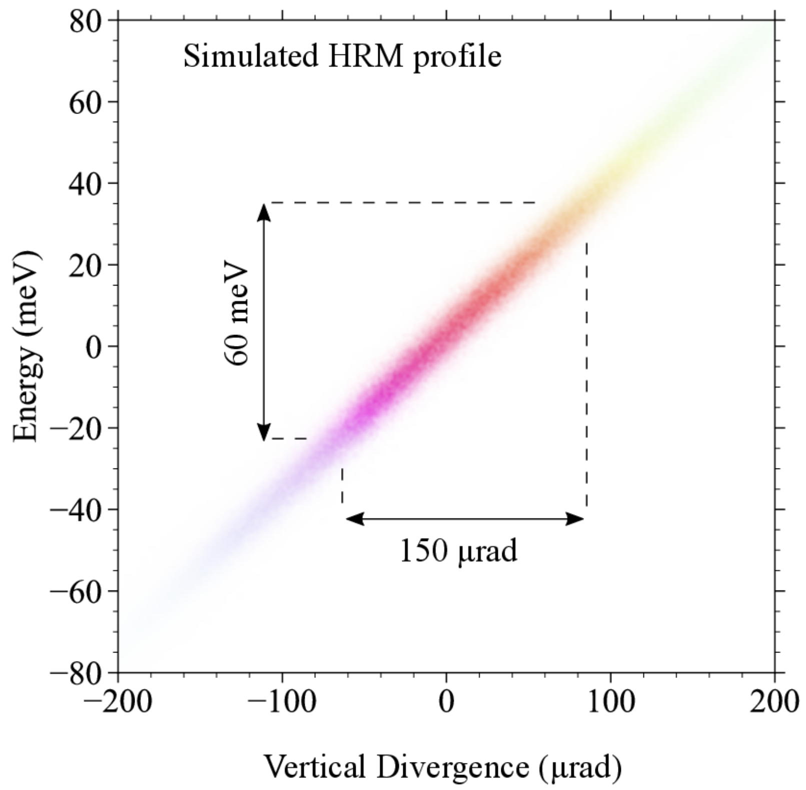
Ray tracing simulations of our 4-bounce HRM

Angular beam profile is not intact, the monochromator acts as a prism!

Incoming beam is highly collimated
…but broad energy bandwidth



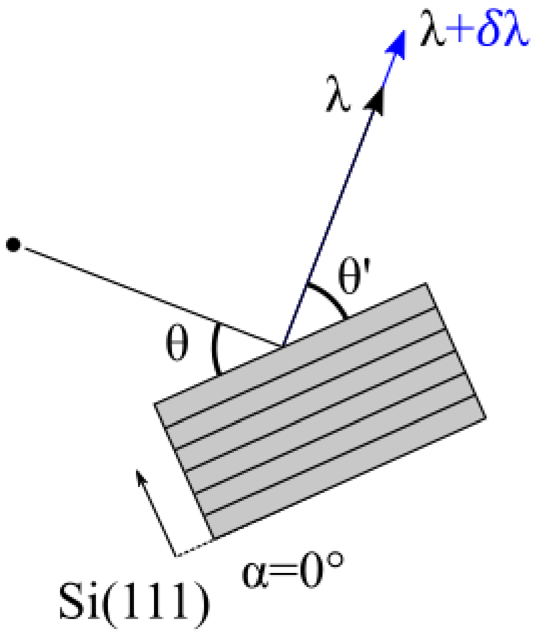
Outgoing beam has low energy bandwidth
…but badly collimated

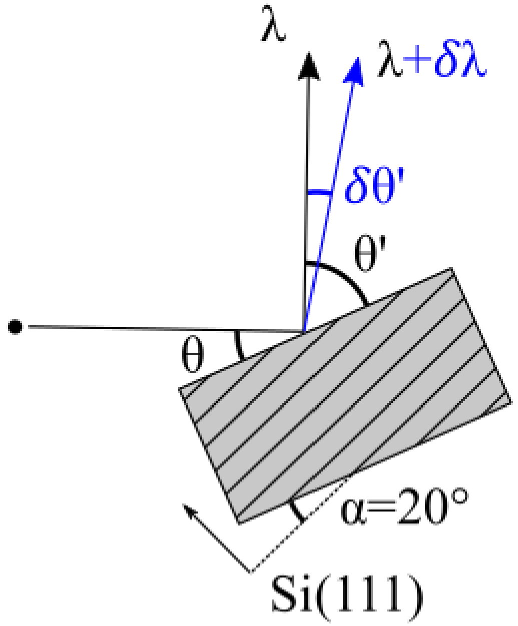


Reflection from asymmetric crystals can alter the beam profile

A complicated energy/divergence distribution emerges

Figures are adapted from: X. R. Huang, et al., J. Appl. Cryst. (2012)

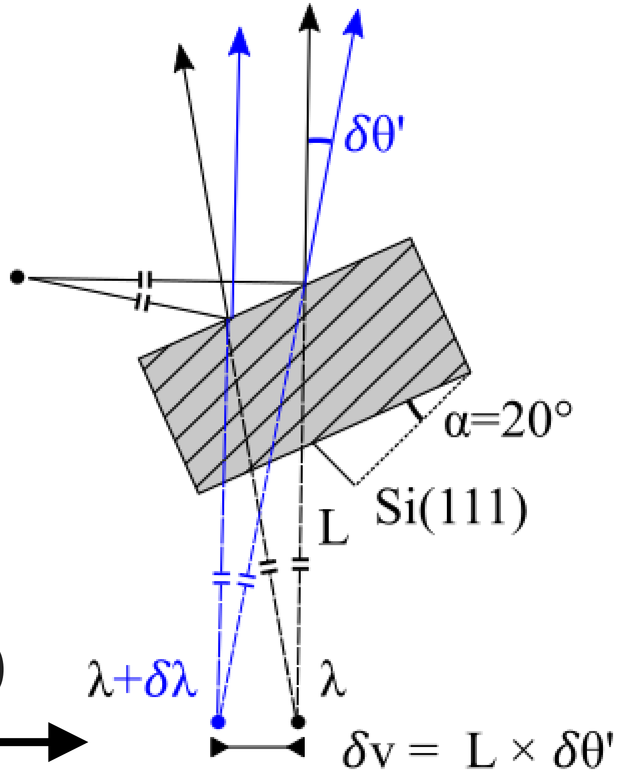




$$\delta\theta' = \delta\lambda \times \sin(\alpha) / d\sin(\theta')$$

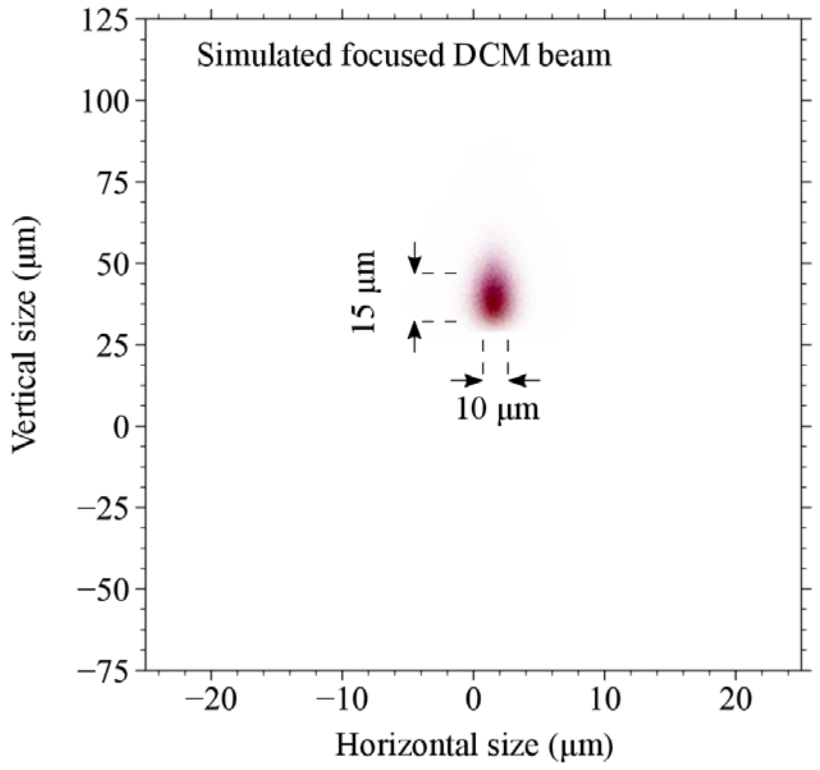
Energy is sorted
(in angle space)

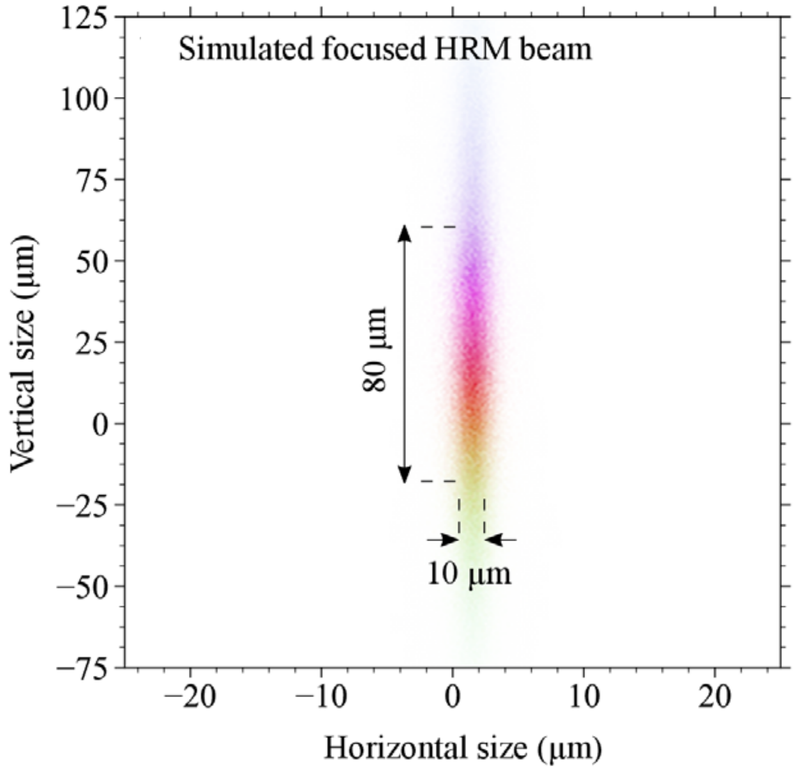
“Rainbow” virtual source
(not a point source anymore)



Implications for the focusing optics

KB mirror will convert the large angular dispersion into real space, creating a “rainbow”





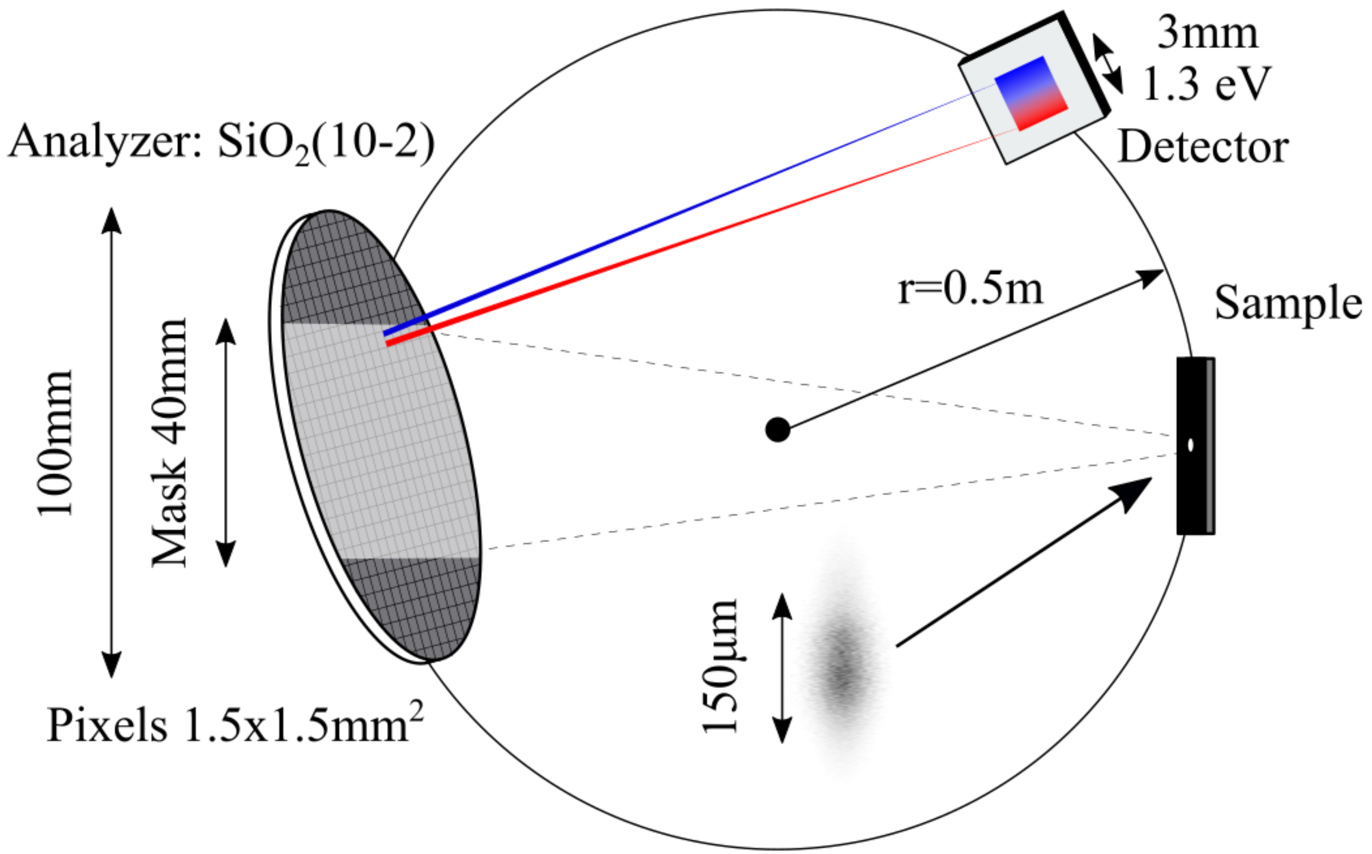
Ray-tracing results confirm the virtual source problem

Experimentally we get 150 µm in vertical height

Our beam is therefore still scrambled

Performance of the IRIXS spectrometer

Diced analyzers away from backscattering suffer from large Johann error



ID20 ESRF: M. M. Sala, et al., J. Synchrotron Rad. (2018)

Finite pixel size give use >1 eV window

At these angles mask is crucial
$\theta_B = 73°$ → Johann error
~ 15 meV (100 meV)

Dispersion rate of our spectrometer:
6 meV/pixel (0.4 meV/μm)
Source size error is 60 meV for 150 μm

$$\Delta E^2 = \Delta E_i^2 + \Delta E_a^2 + \Delta E_g^2$$

$$\Delta E^2 = 60^2 + 60^2 + 60^2$$

Estimated ΔE is 100 meV

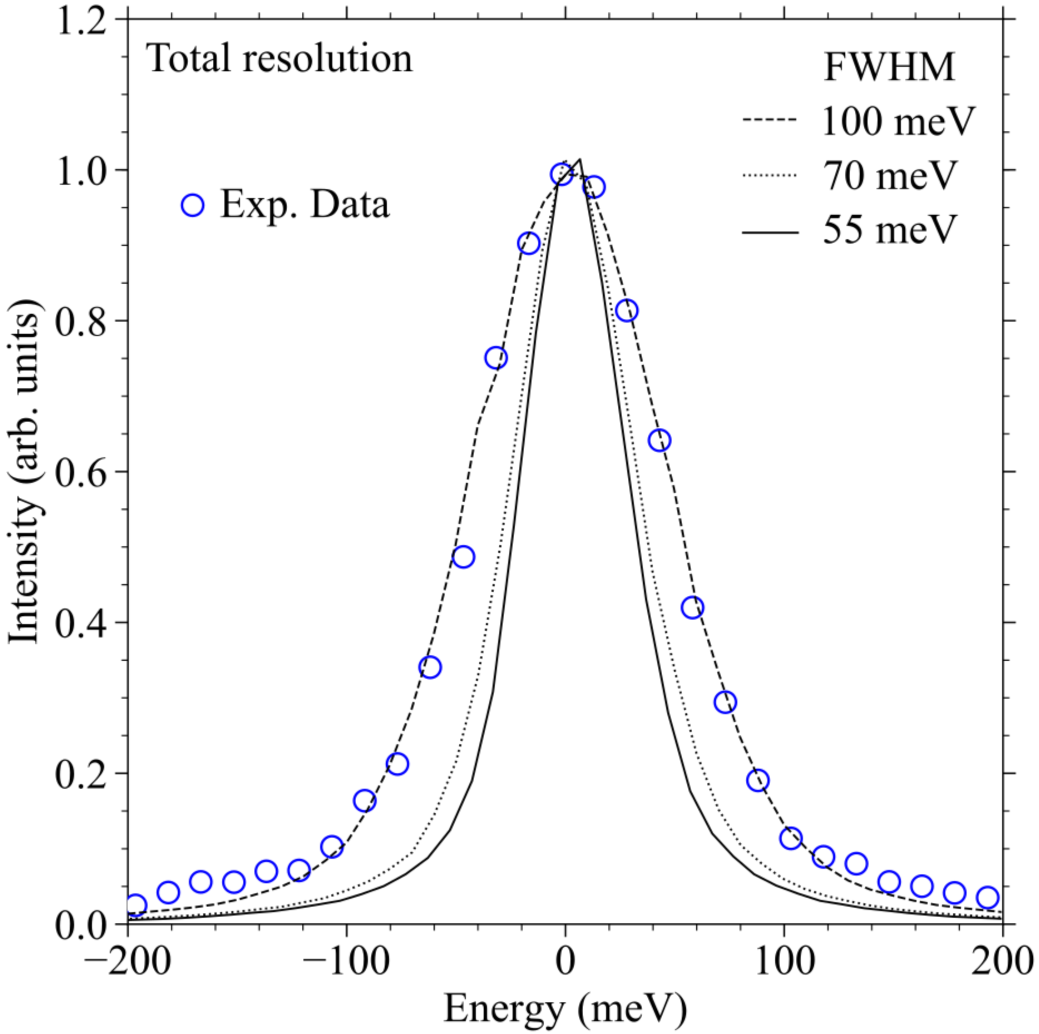
Performance of the IRIXS spectrometer

There is still a room for improvements

Simulations based on the XRT code from:
D. Ketenoglu, H. Yavas, et al.,
J. Synchrotron Rad. (2015)

Intrinsic resolution is 55 meV

Eliminate the source size error
improve the incoming bandwidth
→ 70 meV

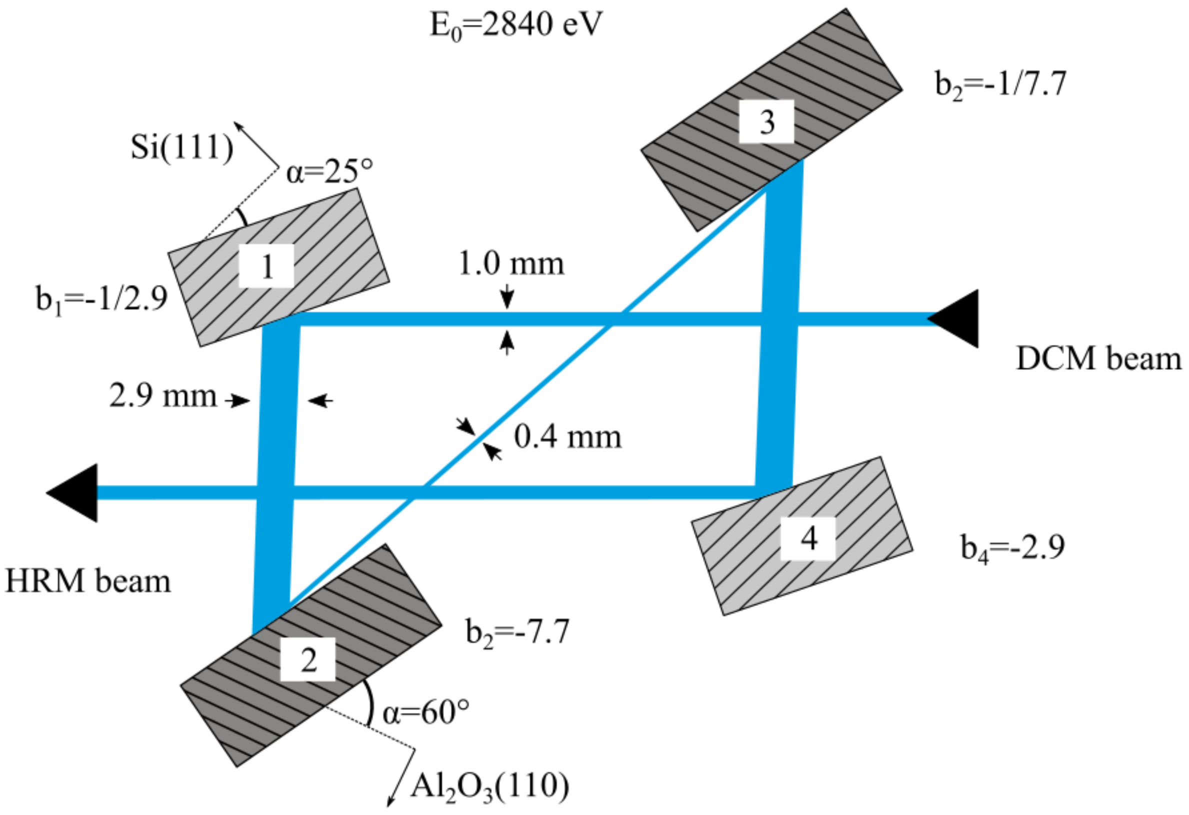


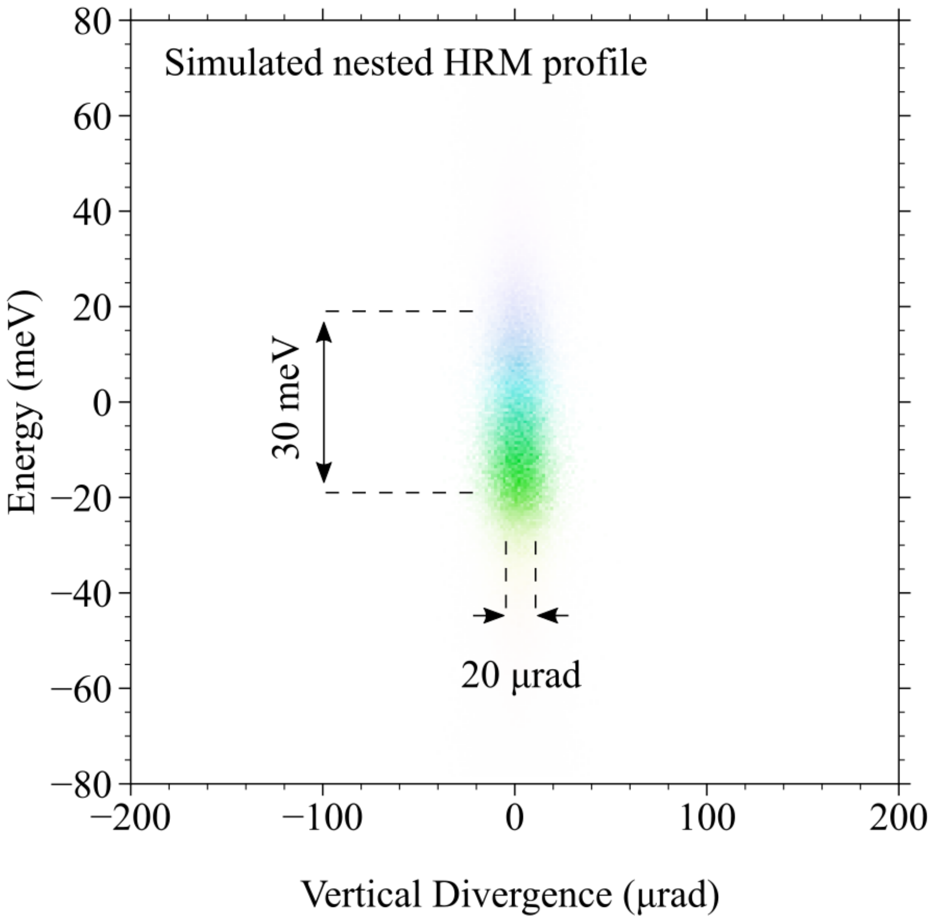
Recent Developments

Revisiting the HRM with a nested concept

We need a "non-dispersive" monochromator that can give small bandwidth

"…negligible VS spread" : X. R. Huang, et al., J. Appl. Cryst. (2012)

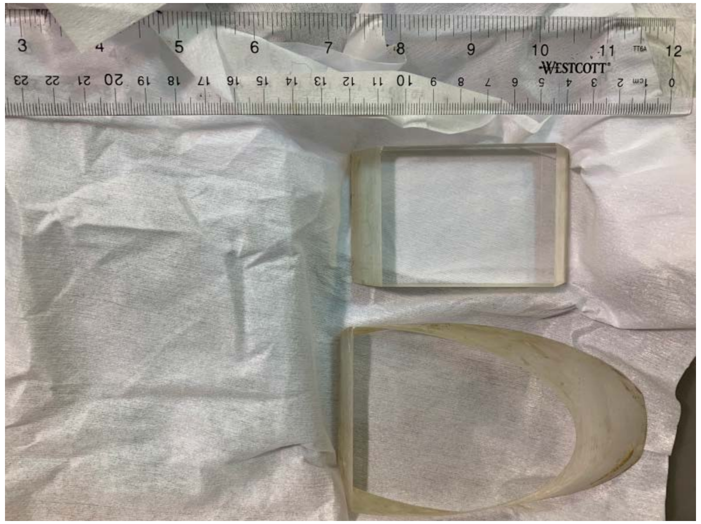




Revisiting the HRM with a nested concept

We need a "non-dispersive" monochromator that can give small bandwidth

Sapphire boules from Rubicon
Oriented, cut, and polished at APS
[A. Said, E. Kasman, and XianRong Huang]



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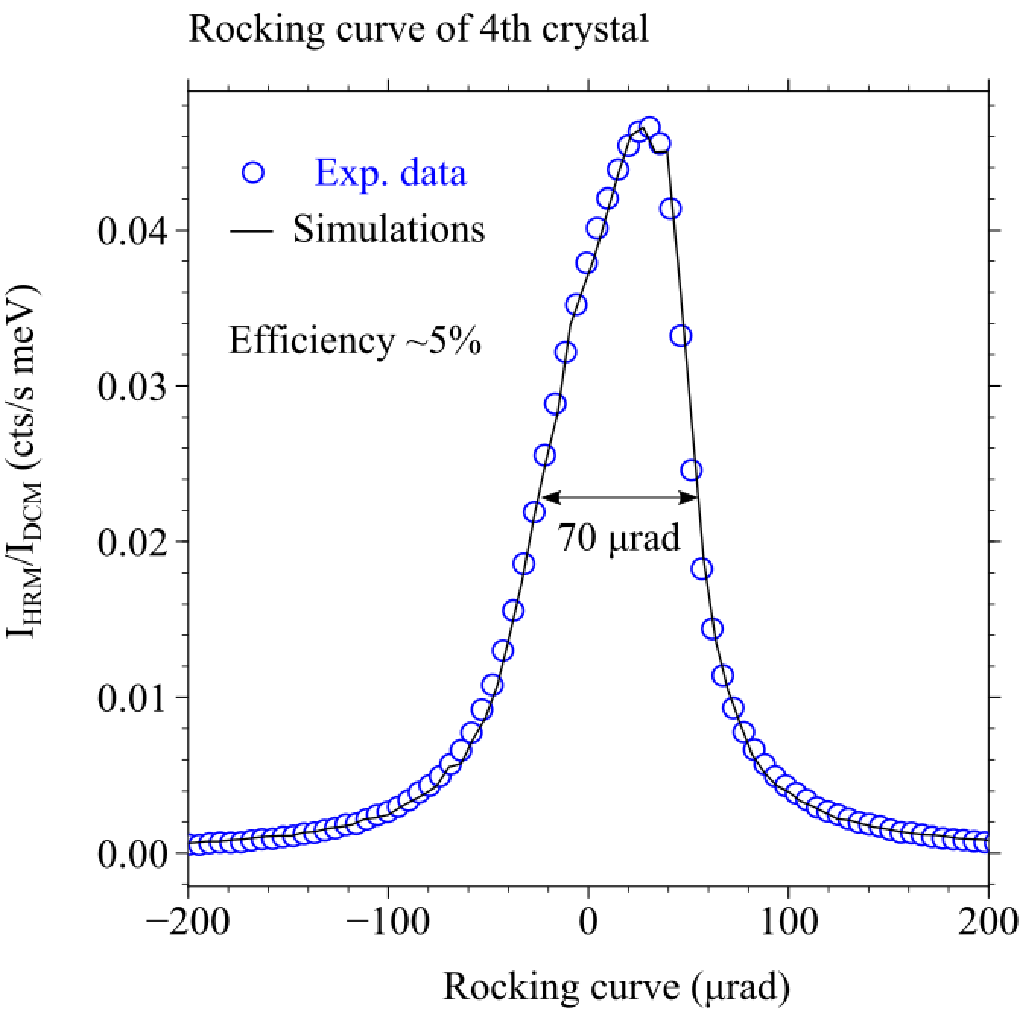


A new (C)A-Spectrometer based on Montel optics

Spherical analyzer has limitations – poor efficiency when looking at magnons

HRM

Nested 4B (+ + - -)

Si(111) α=25°

Al_2O_3(111) α=-60°

30 meV @ 2840 eV

Spectrometer

Montel

Incoatec (100μrad)

A-spect. SiO_2(10-2)

Darwin 60μrad

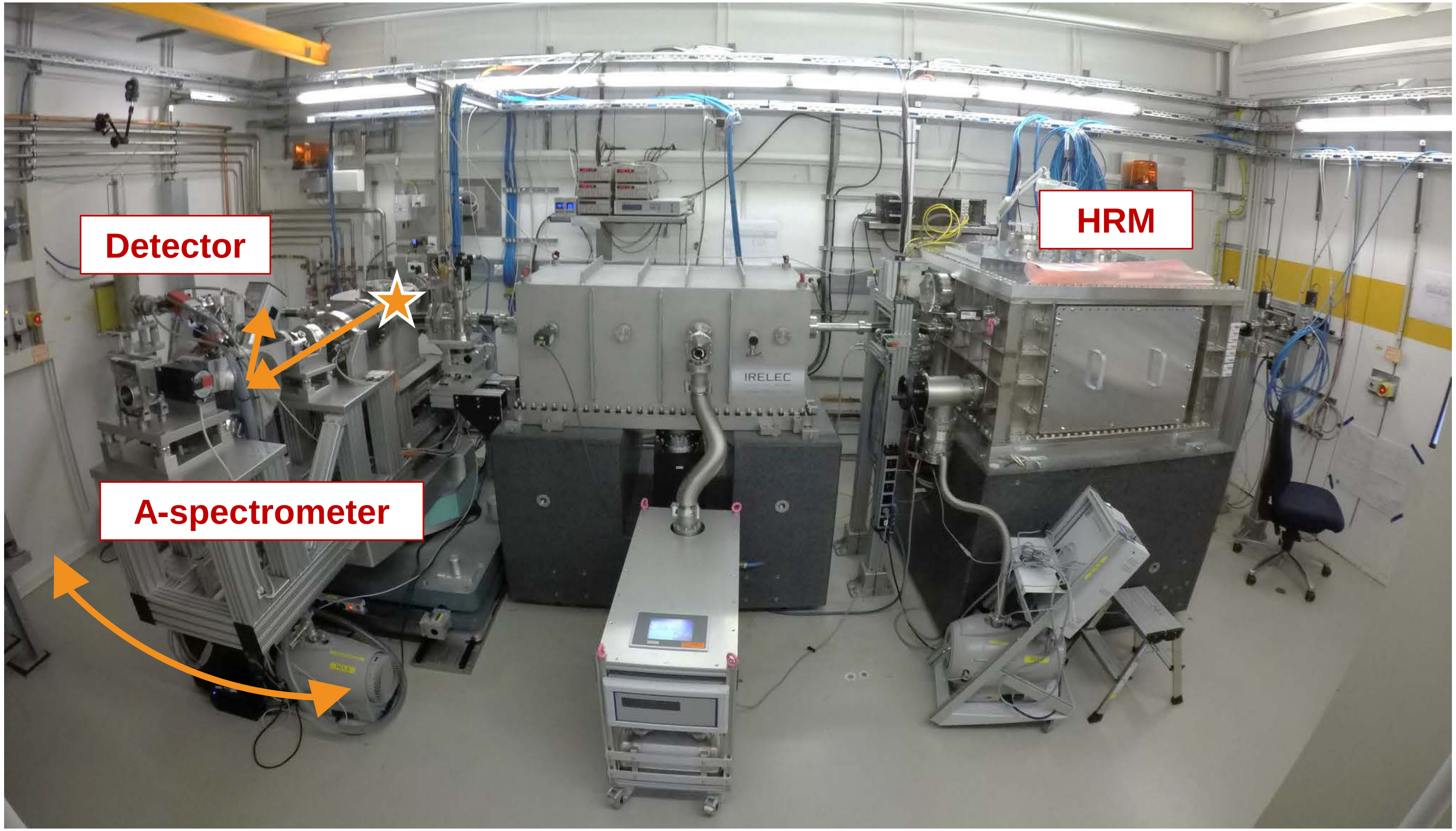
100 meV @ 2840 eV

CA-spect. SiO_2(111)

α=-67°

Darwin 50μrad

35 meV @ 2840 eV



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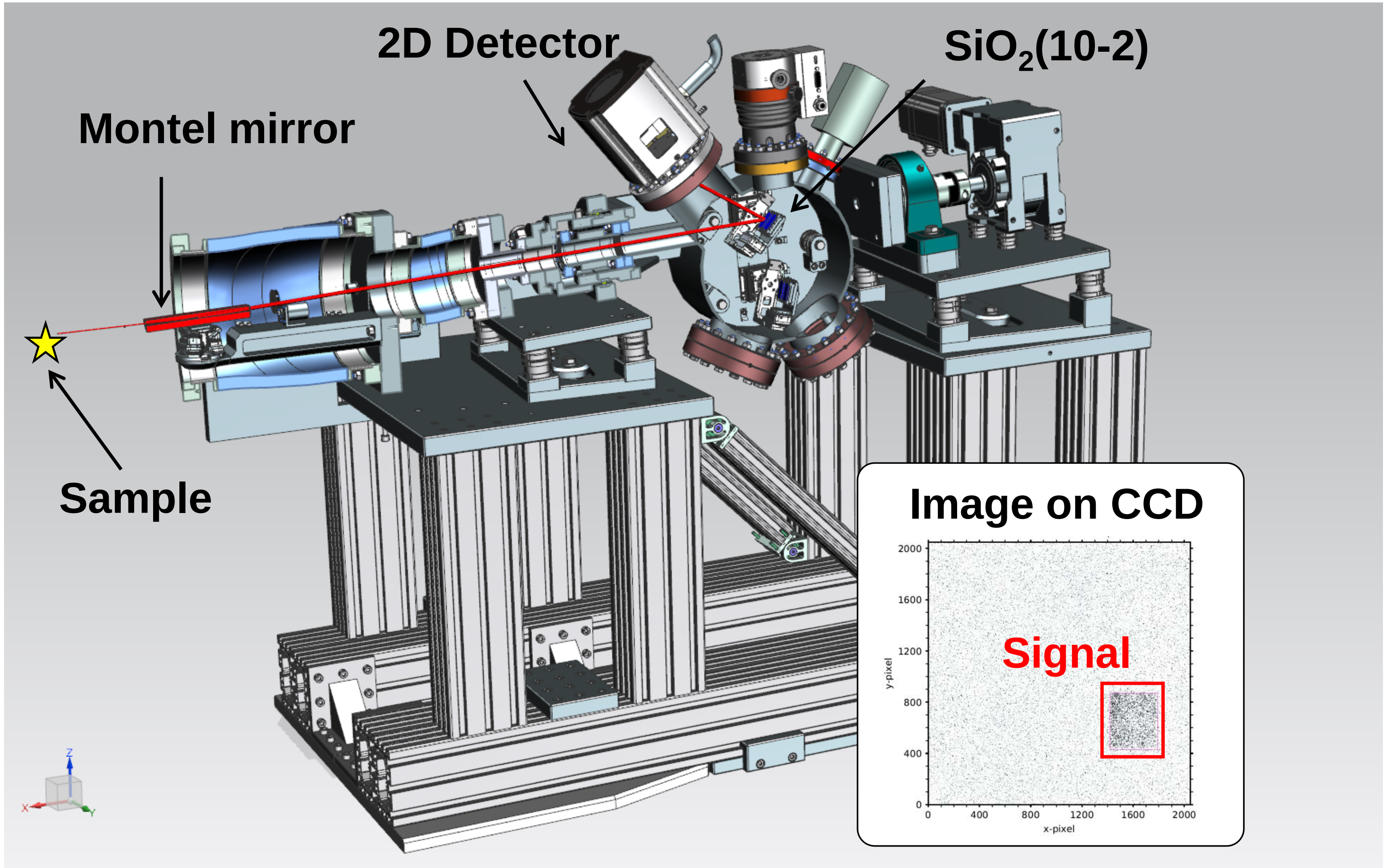
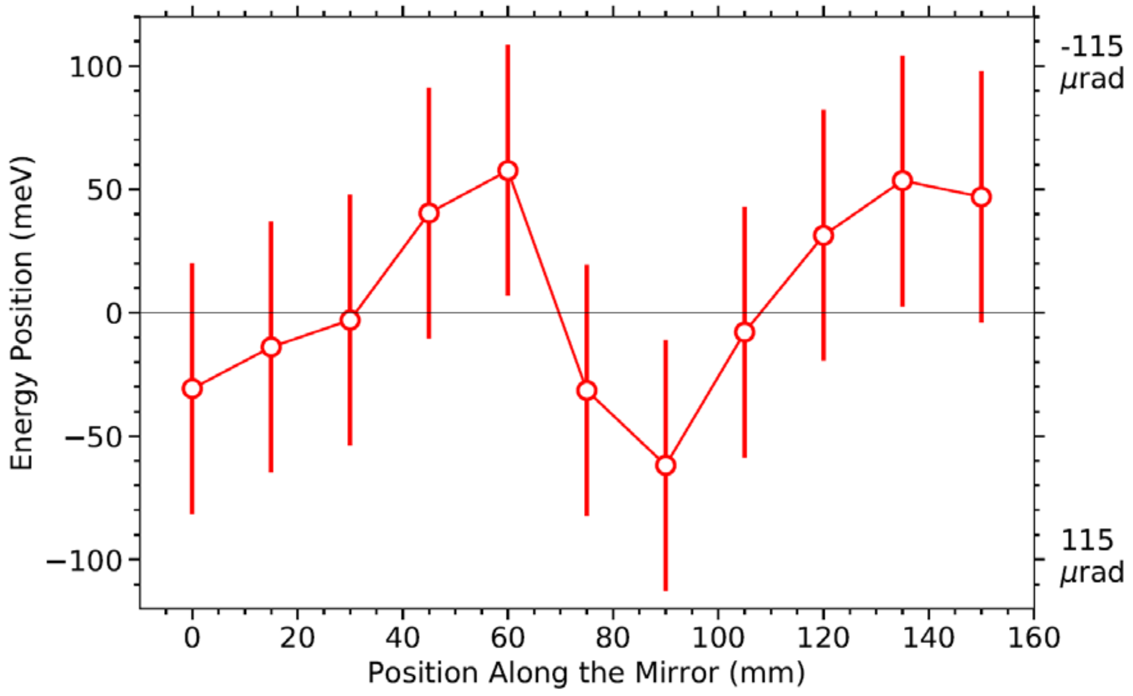
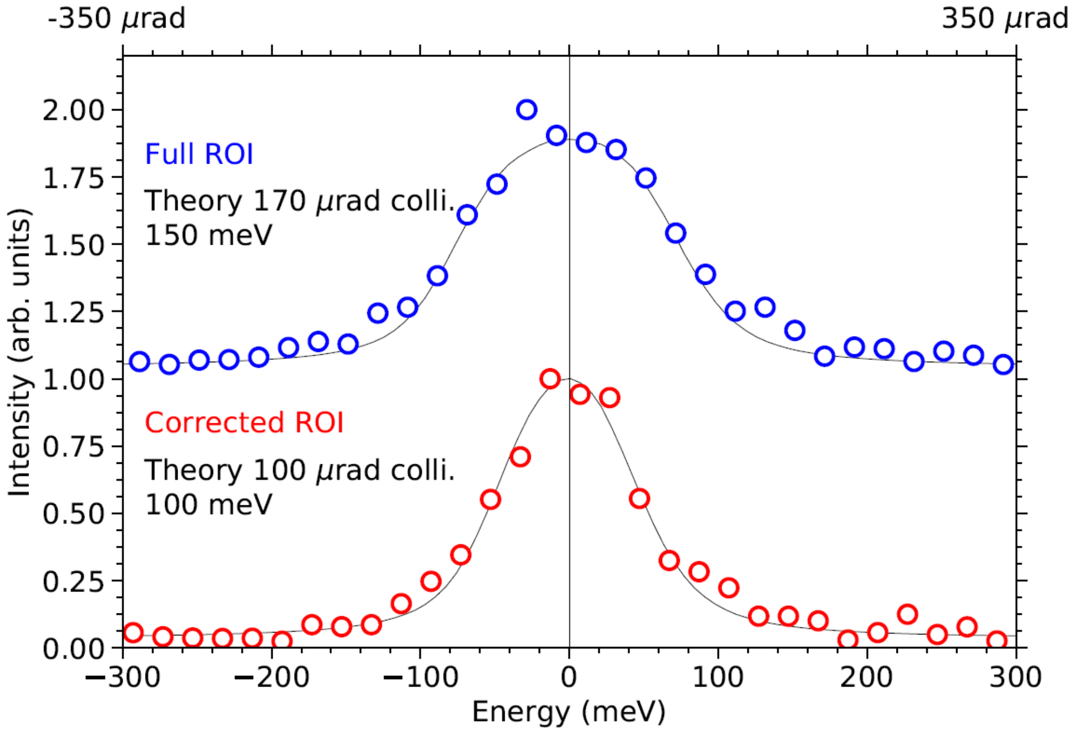


Performance of the A-Spectrometer

Alignment has to be done close to 90° – Elastic scattering is very weak





Large variations in the energy

Measured slope error: <15 µrad rms

Translates to worse performance

Correction → Theoretical value

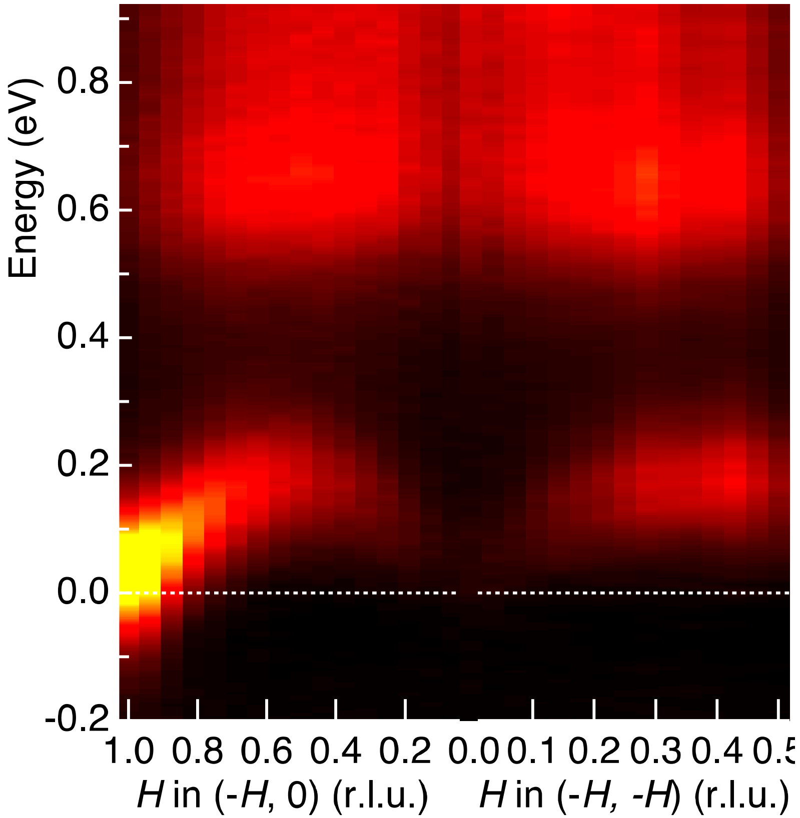
Conclusion

Magnon in a microcrystal ($SrRu_2O_6$)
ΔE = 150 meV

IRIXS = *i*ntermediate x-ray energy *RIXS*
located at P01 DESY and run by MPI-Stuttgart

Current: Resolution of ΔE = 100 meV at Ru L_3-edge (2840 eV)

Future: Spherical Analyzer and/or CA-Spectrometer ΔE = 70 meV



H. Suzuki, H. Gretarsson, H. Ishikawa, K. Ueda, Z. Yang, H. Liu, H. Kim, D. Kukusta, A. Yaresko, M. Minola, J. A. Sears, S. Francoual, H.-C. Wille, J. Nuss, H. Takagi, B. J. Kim, G. Khaliullin, H. Yavas & B. Keimer,
Nature Materials 18, 563–567 (2019)

Thank you

Contact

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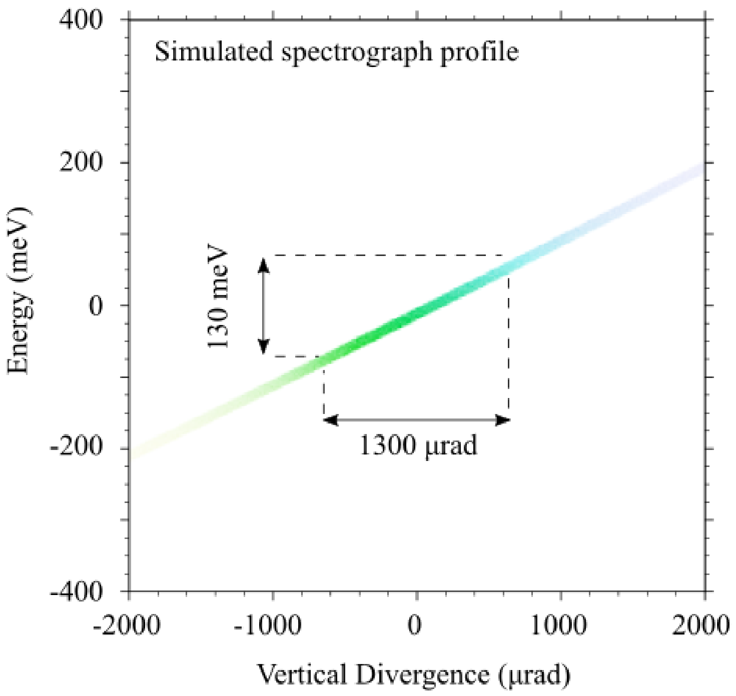
Future Perspectives

Are there other options out there?

A spectrometer with a large angular dispersion rate is needed

“…imaging a spectrum of photons…” : Y. Shvyd’ko, et al., PRA (2013)

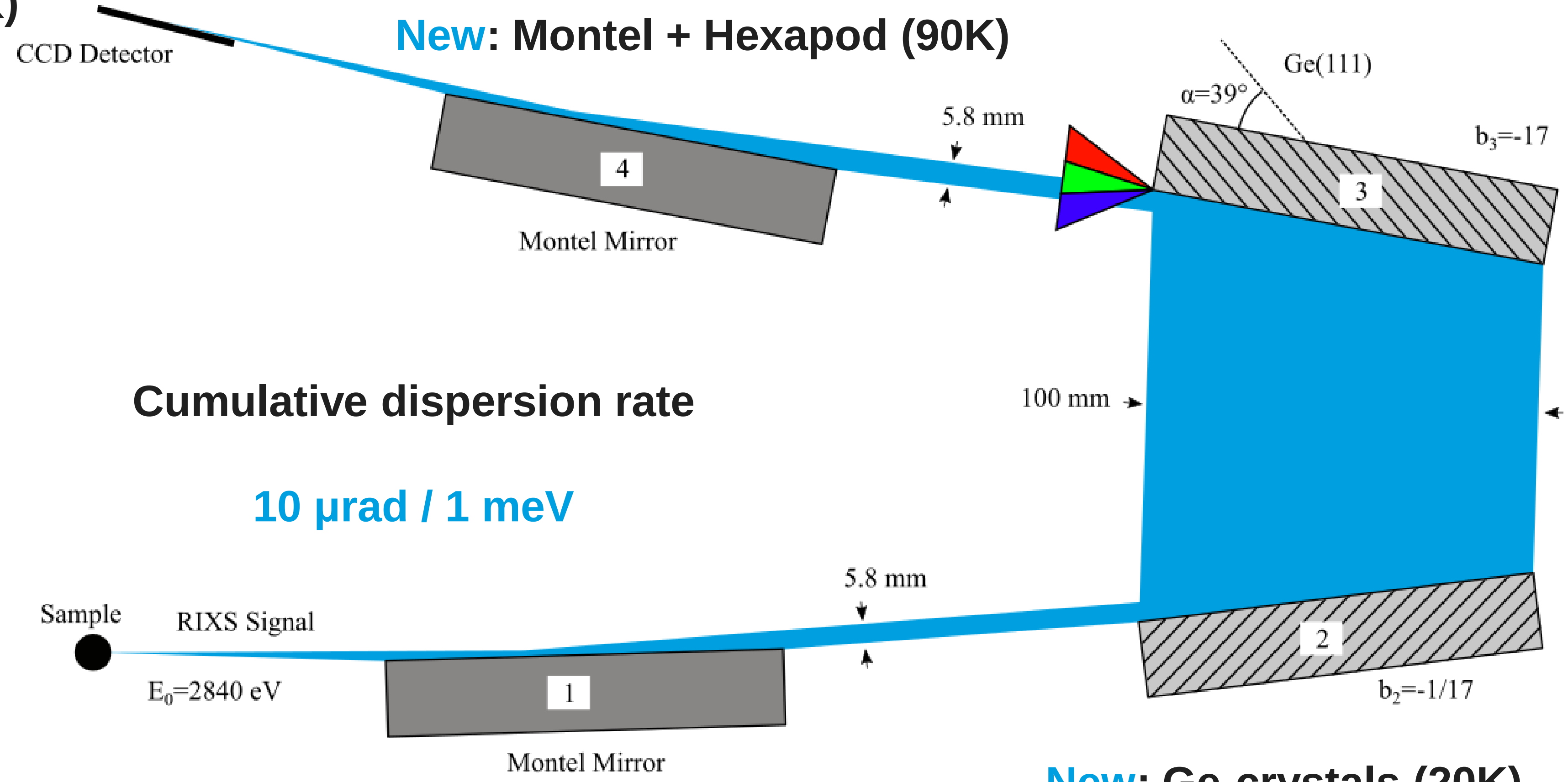
New: Grazing incident CCD (60K)



New: Montel + Hexapod (90K)

Cumulative dispersion rate

10 µrad / 1 meV



New: Ge-crystals (20K)

Is it too good to be true?

Extensive ray tracing work by Joel supports 20 meV resolution

Caveat: Stepping into the unknown. Will require considerable R&D