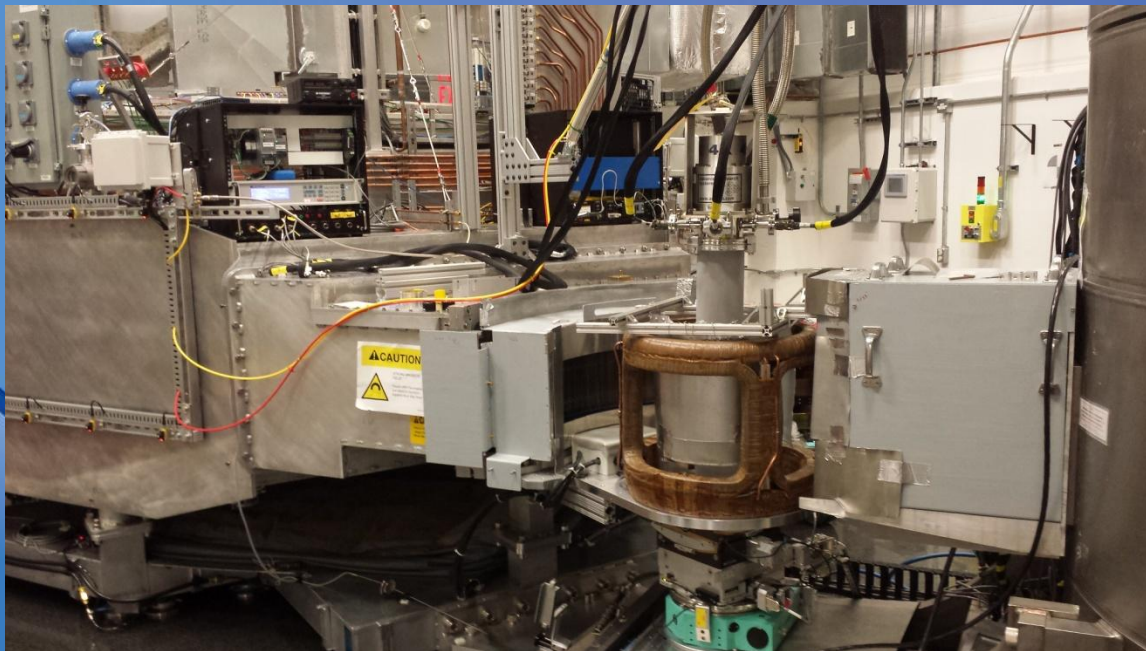


Polarized inelastic neutron scattering on HYSPEC HYbrid SPECtrometer at SNS

Igor Zaliznyak

*Condensed Matter Physics and Materials Science Division
PNCMI, July 6, 2016*



BROOKHAVEN
NATIONAL LABORATORY

a passion for discovery

 **Office of
Science**
U.S. DEPARTMENT OF ENERGY



Related presentations

- At PNCMI 2016
 - B. Winn: “*3D Polarization Analysis with a Polarizing Supermirror Array Analyzer at HYSPEC*” – Session 9
 - A. Savici: “*Data processing workflow for time of flight polarized neutrons inelastic measurement*” – Session 3
- At ACNS 2016
 - O. Garlea: “*The first results from the HYSPEC polarization analysis capability*”



History: HYSPEC timeline

2000

- The Concept of the Hybrid Spectrometer proposed at BNL

2001

- Direct Geometry Hybrid Spectrometer presented to SNS EFAC
- HYSPEC Instrument Development Team (IDT) formed

2002

- HYSPEC IDT filed Letter of Intent with SNS
- HYSPEC proposal submitted to DOE

2003

- DOE CD0, HYSPEC is approved as part of the SING project

2004

- HYSPEC's placement approved on BL14B; Design & Engineering begins

2005

- DOE CD2, HYSPEC's performance baseline approved

2006

- DOE CD3, construction begins

2011

- DOE CD4, HYSPEC commissioning & operation begins

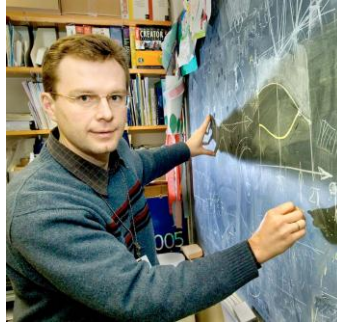
2013

- HYSPEC enters SNS User Program

2015

- Polarized beam operation on HYSPEC is commissioned

HYbrid SPECtrometer, HYSPEC: BNL Instrument Design Group



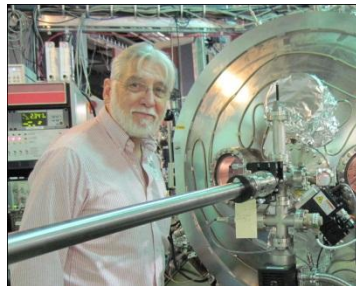
Igor Zaliznyak, PI



Steve Shapiro, co-PI



Larry Passell, advisor



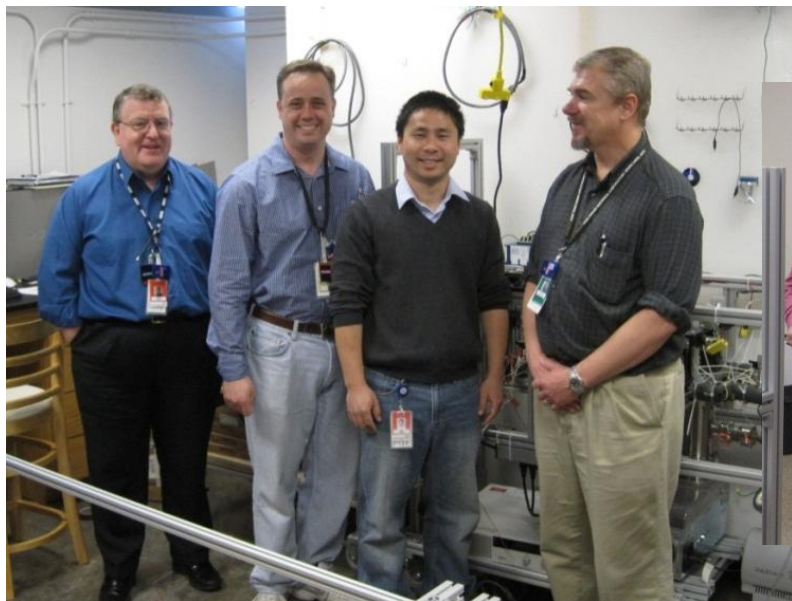
Bill Leonhardt, engineer



Vinita Ghosh, scientist – MC simulations

HYbrid SPECtrometer, HYSPEC – ORNL Instrument Team

HYSPEC: SNS Instrument
Construction Team (... - 2013)



HYSPEC SNS Instrument Team now



Mark Hagen Lead Scientist (now @ ESS)
Barry Winn Scientist
Tony Tong Scientist
David Anderson Engineer

Melissa Graves-Brook
Science Associate

Ovidiu Garlea,
Scientist
Joined in May, 2013

Barry Winn,
Scientist

HYSPEC Team - 2002

Instrument Development Team

<u>I. Zaliznyak</u> , co-PI	BNL
<u>S. M. Shapiro</u> , co-PI	BNL
G. Shirane	BNL
J. Tranquada	BNL
L. Passell	BNL
D. Abernathy	SNS
L. Daemen	Los Alamos
M. Greven	Stanford
B. Gaulin	McMaster
V. Kiryukhin	Rutgers
Y. Lee	MIT
S. Nagler	ORNL
R. Osborn	ANL
J. Rhyne	U. Missouri
C. Stassis	Ames/Iowa St.
A. Zheludev	ORNL

Instrument design team

- I. Zaliznyak (BNL)
- S. M. Shapiro (BNL)
- L. Passell (BNL)
- V. J. Ghosh (BNL) Monte-Carlo simulations
- S. Doran (SNS/ANL) Engineering design concept

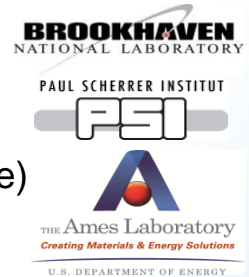
HYSPEC Team - 2015

Instrument Development Team

I. Zaliznyak (co-PI, EC member)	BNL
S. Shapiro (co- PI, EC member)	BNL
M. Kenzelmann (EC member)	PSI
L. Daemen	LANL
J. Fernandez-Baca	ORNL
J. Gardner	NIST/Indiana U.
B. Gaulin	McMaster U.
M. Greven	Stanford
V. Ghosh	BNL
M. Hagen	SNS =>ESS
M. Huecker	BNL
V. Kiryukhin	Rutgers
G. Lander	EITU
Y. Lee	MIT
S.-H. Lee	U. Virginia
C. Majkrzak	NIST
A. Goldman (EC member)	Ames/Iowa U.
S. Nagler	ORNL
R. Osborn	ANL
L. Passell	BNL
L. P. Regnault	CEA-Grenoble
T. Sato (EC member)	Tohoku University
J. Tranquada (EC member)	BNL
G. Xu	BNL
A. Zheludev	ETH-Zurich

IDT Executive Committee

- I. A. Zaliznyak, PI (BNL)
- S. M. Shapiro, PI (BNL)
- M. Kenzelmann (PSI)
- A. Goldman (Ames/Iowa State)
- T. Sato (Tohoku)
- J. Tranquada (BNL)



HYSPEC science case: polarization first

- **Characterization of spin-dependent cross-sections by means of polarization analysis**
- **Coherent collective excitations in single crystals:**
 - lattice dynamics (phonons)
 - spin dynamics (magnons, critical scattering)
- **Structure and dynamics of partially ordered and glassy phases**
 - spin glasses
 - charge glasses
 - correlated amorphous phases
 - small angle
- **Study of the microscopic physical properties of samples in extreme environments:**
 - temperature
 - pressure
 - magnetic field

HYSPEC place among the SNS inelastic instruments.

epithermal

High energy transfer

10-1000 meV Fermi Chopper Spectrometer

- $E = 10 - 1000 \text{ meV}$
- $Q = 0.1 - 22 \text{ \AA}^{-1}$

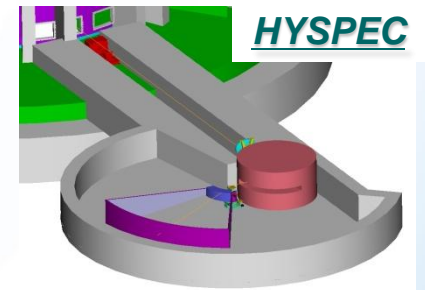


thermal

High intensity at moderate resolution and medium energy transfer + polarized beam

Crystal-Focussing Hybrid Spectrometer

- $E = 3.8 - 90 \text{ meV}$
- $Q = 0.1 - 8 \text{ \AA}^{-1}$

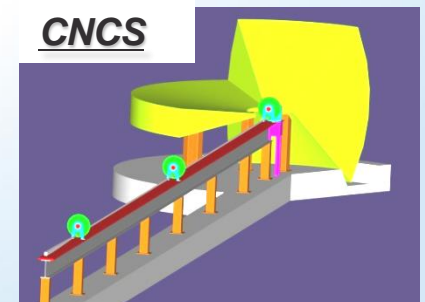


subthermal

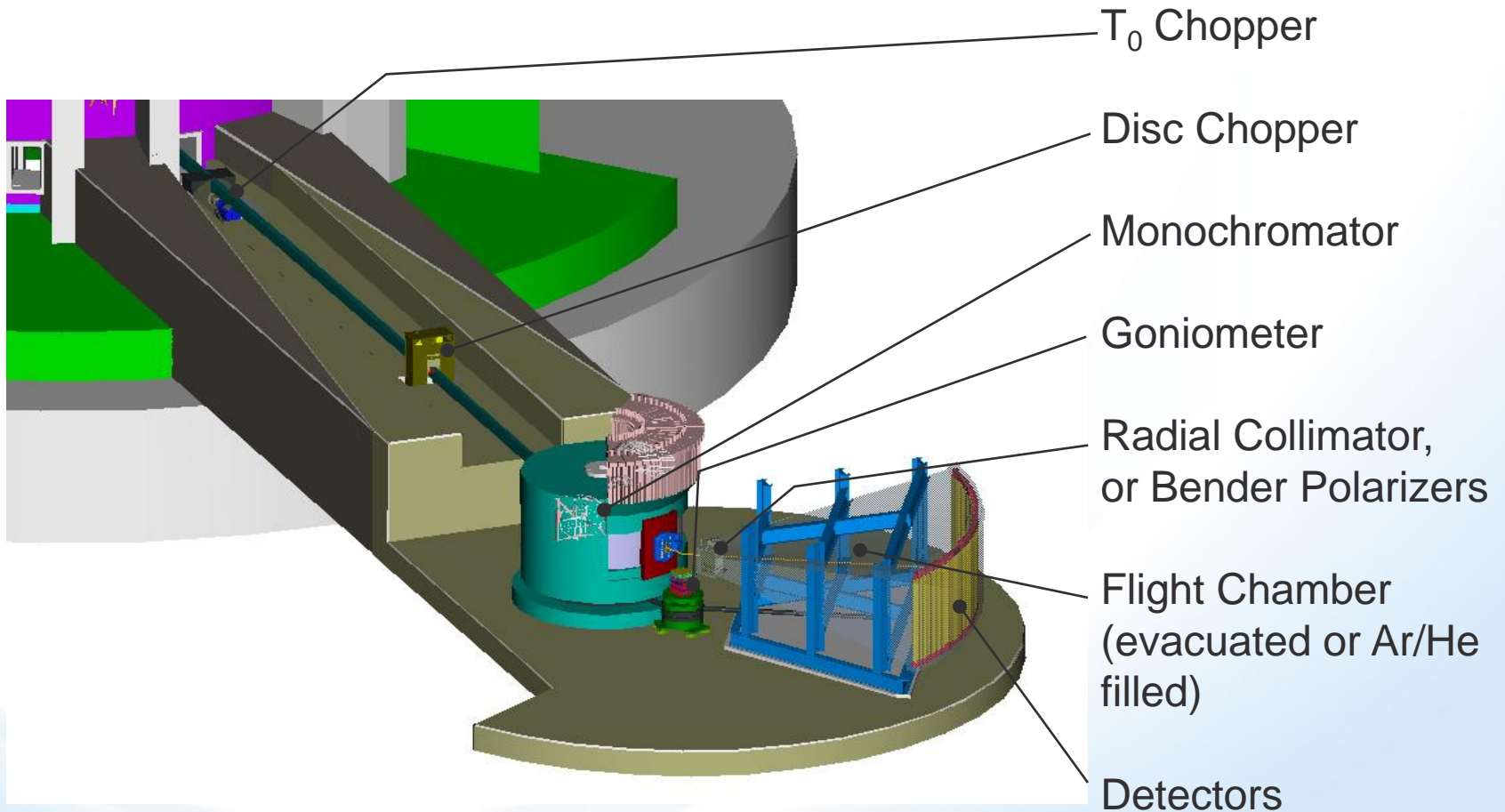
High resolution and low energy transfer

10-100 μeV Multichopper Spectrometer

- $E = 2 - 20 \text{ meV}$
- $Q = 0.1 - 4 \text{ \AA}^{-1}$



HYSPEC conceptual design - 2003

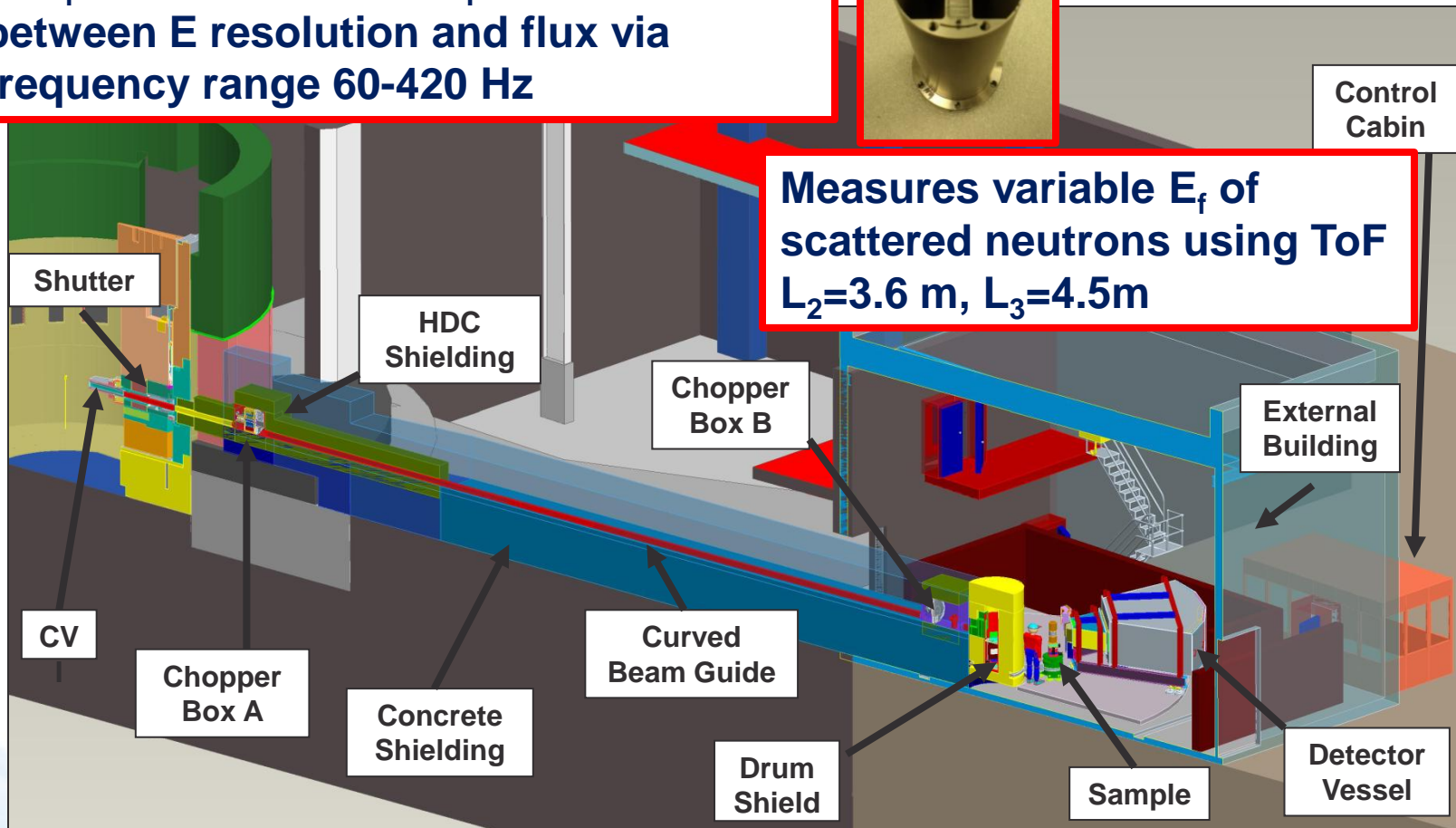


HYSPEC layout (design – 2008)

Short strait blade Fermi chopper at $L_1=37.2$ m to select E_i ; trade off between E resolution and flux via frequency range 60-420 Hz



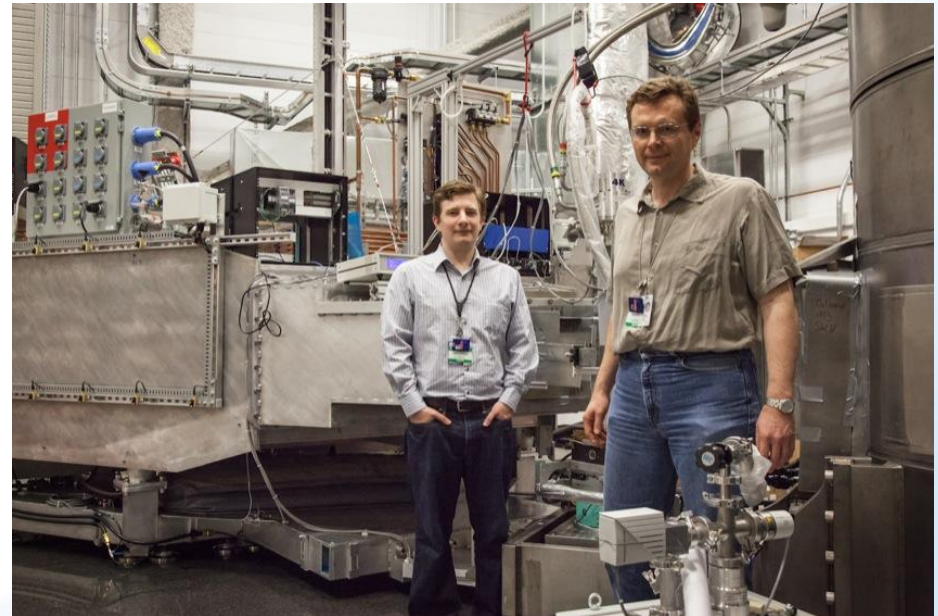
Measures variable E_f of scattered neutrons using ToF
 $L_2=3.6$ m, $L_3=4.5$ m



HYSPEC in operation - 2012



Commissioning Experiments,
D. Fobes and I. Zaliznyak (2012)



HYSPEC in operation - 2013

Tune-up complete: apertures, beam stop, shielding, shielding

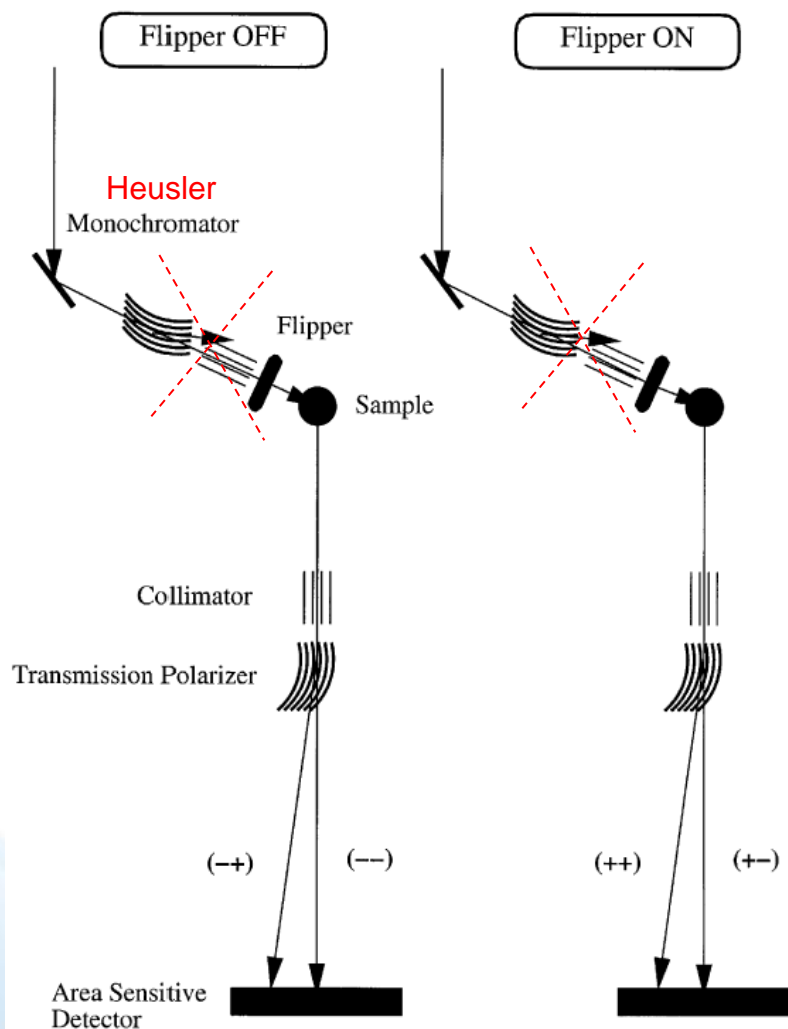


HYSPEC in operation - 2013

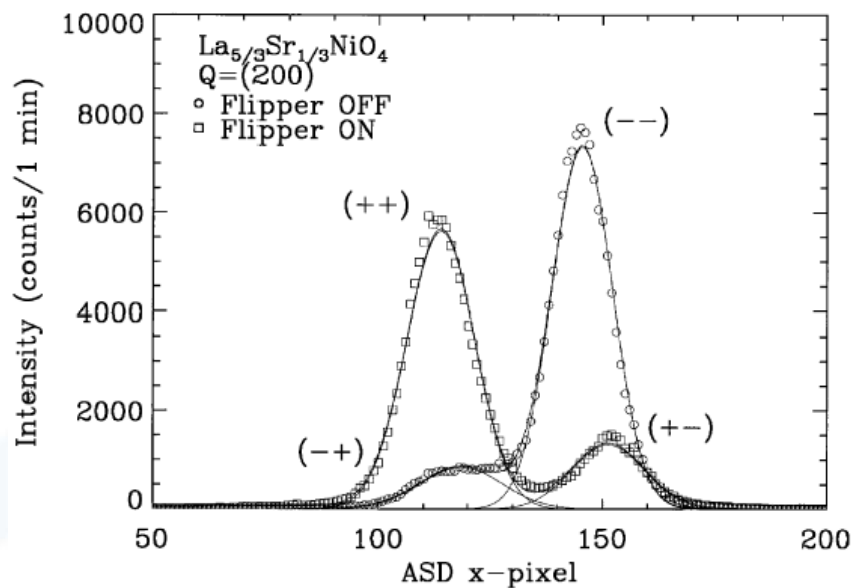
Tune-up complete: apertures, beam stop, shielding, shielding



Initial HYSPEC concept for polarized beam measurement with a Position Sensitive Detector (PSD)

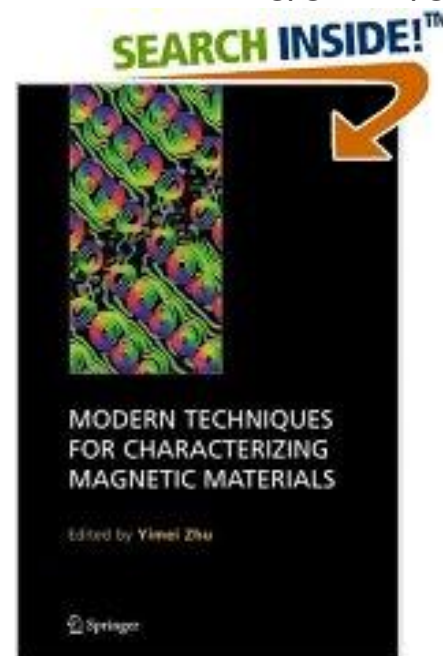
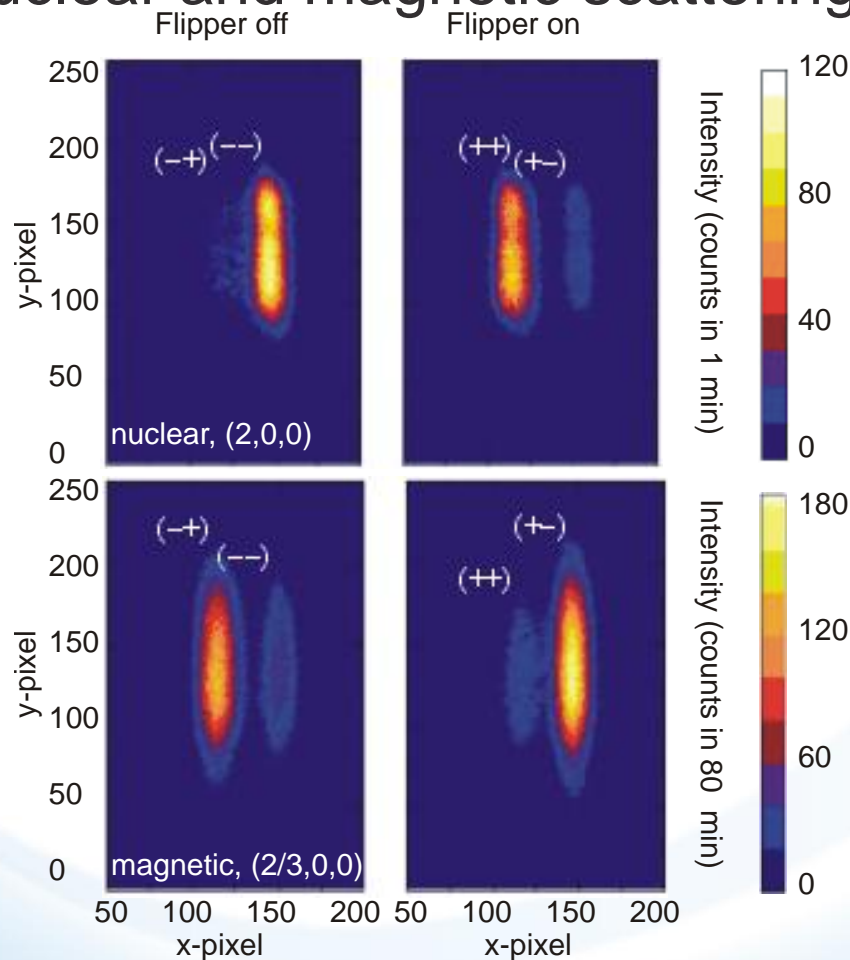


S.-H. Lee, C. F. Majkrzak,
Physica B 267-268, 341 (1999)



Initial concept for HYSPEC polarization analysis: experimental demonstration with PSD on SPINS

Nuclear and magnetic scattering intensities in $\text{La}_{5/3}\text{Sr}_{1/3}\text{NiO}_4$



I. A. Zaliznyak and S.-H. Lee, in Modern Techniques for Characterizing Magnetic Materials, ed. Y. Zhu (Springer, 2005)

HYSPEC setup for polarization analysis (2002 design)

❑ Polarized incident beam is supplied by reflection from the vertically focusing Cu_2MnAl (Heusler alloy) crystal monochromator

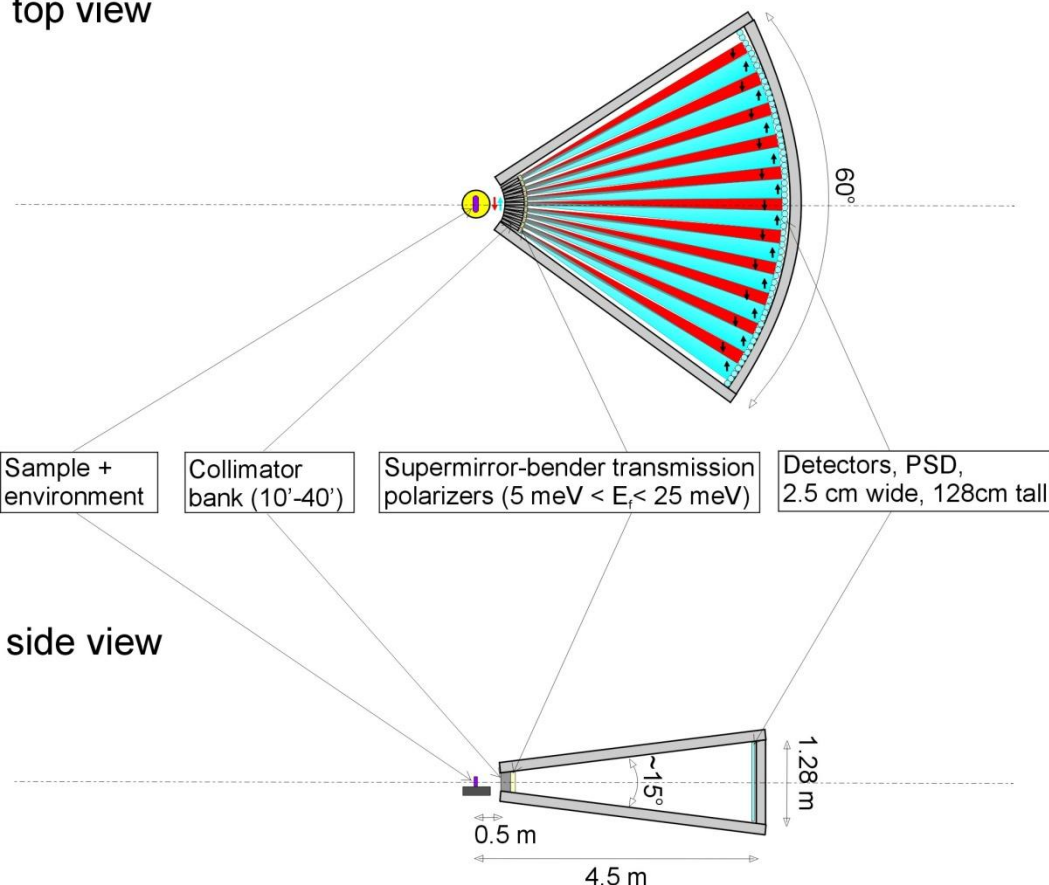
$$10 \text{ meV} < E_i^{\text{pol}} < 90 \text{ meV}$$

❑ Polarization analysis of the scattered neutrons is performed by a set of 18-22 supermirror-bender transmission polarizers, each 2 cm wide, 5 cm thick and 15 cm high,

$$3.7 \text{ meV} < E_f^{\text{pol}} < 15\text{-}25 \text{ meV}$$

Polarized-beam analyzer setup

top view

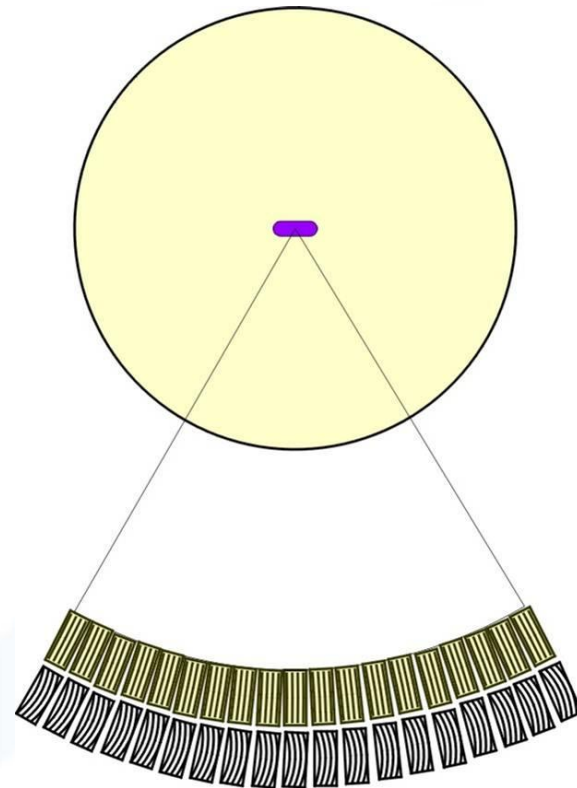
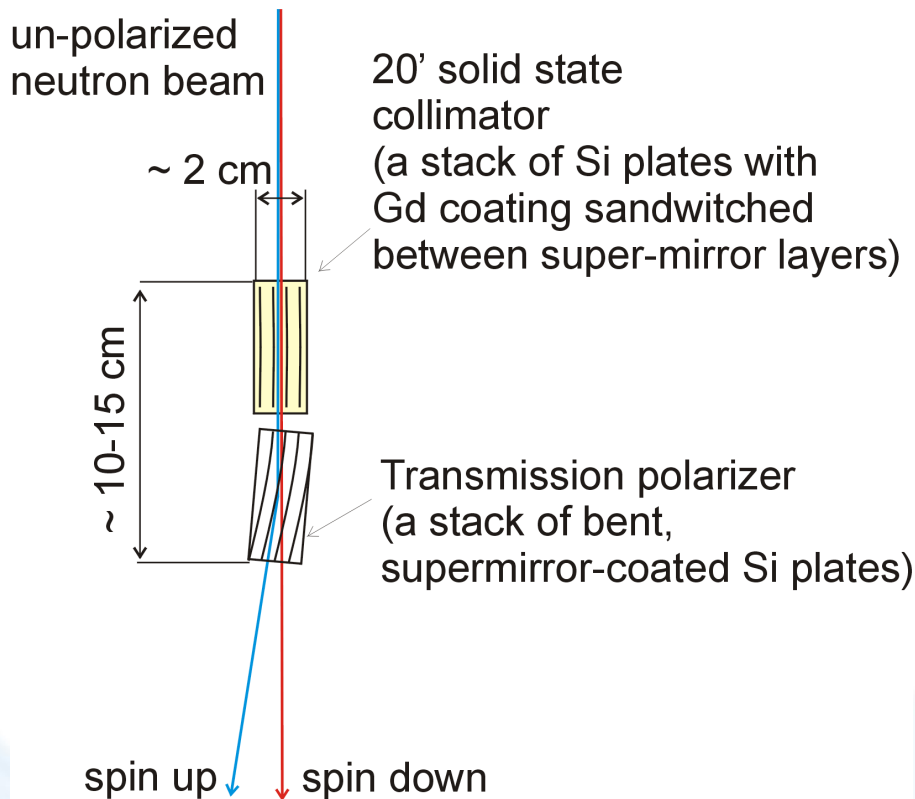


I. Zaliznyak, et. al., Physica B **356**, 150-155 (2005); [cond-mat/0410040](http://arxiv.org/abs/cond-mat/0410040).

A supermirror-bender transmission polarizer setup for HYSPEC (2002)

A very compact device
(but needs a saturating magnetic field)

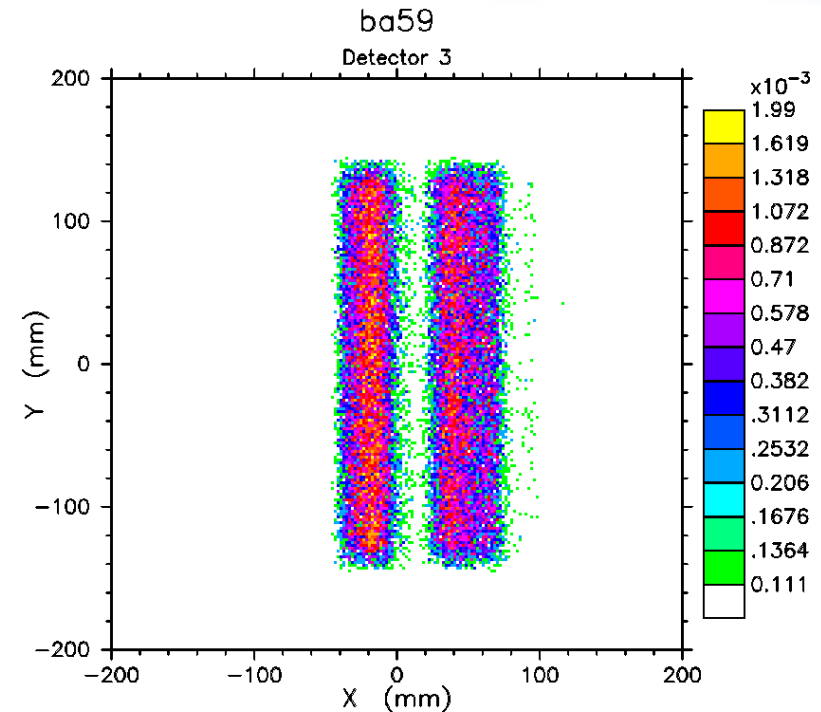
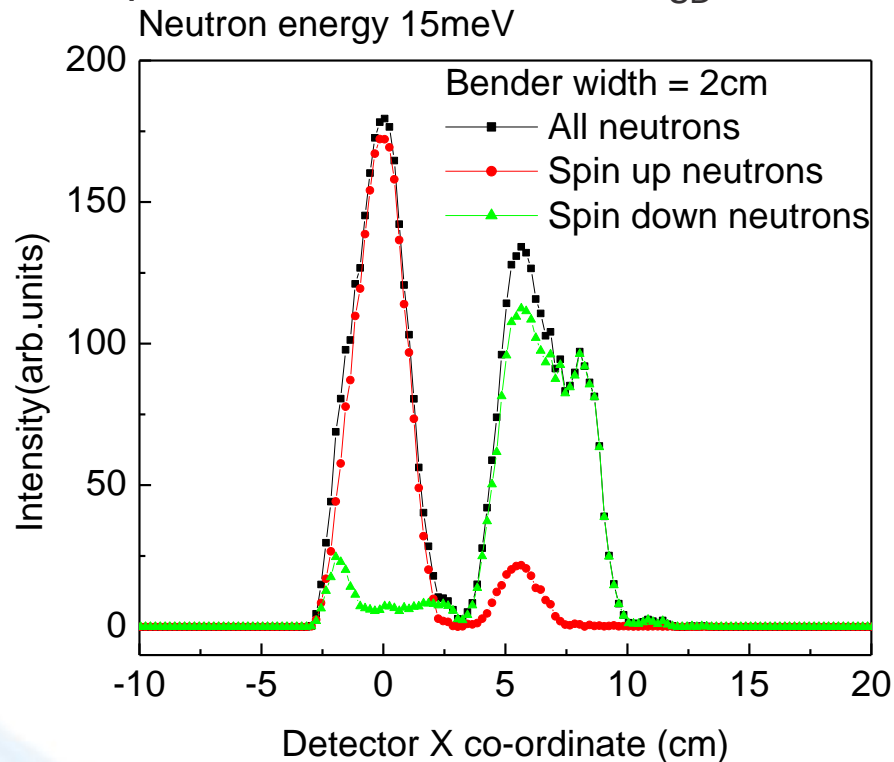
An array of 20 benders covers 60 deg.
acceptance of the detector bank.



I. Zaliznyak, et. al., Physica B **356**, 150-155 (2005); [cond-mat/0410040](https://arxiv.org/abs/cond-mat/0410040).

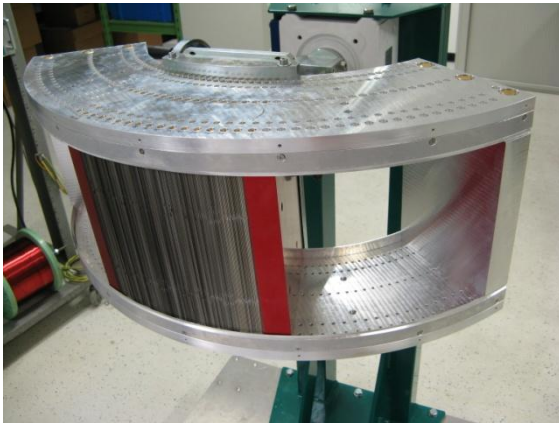
MC simulation (NISIP) of HYSPEC operation in the polarized beam mode: beam separation

Simulation for the bender geometry optimized for $E=14.7$ meV (C. Majkrzak, 1995)
Sample-to-detector distance L_{SD} is 4.5 m



I. Zaliznyak, et. al., Physica B **356**, 150-155 (2005); [cond-mat/0410040](https://arxiv.org/abs/cond-mat/0410040).

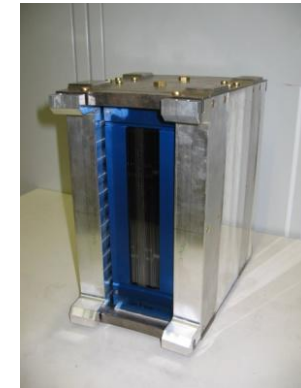
Opportunistic change of plan: PSI Supermirror Polarization Analyzer



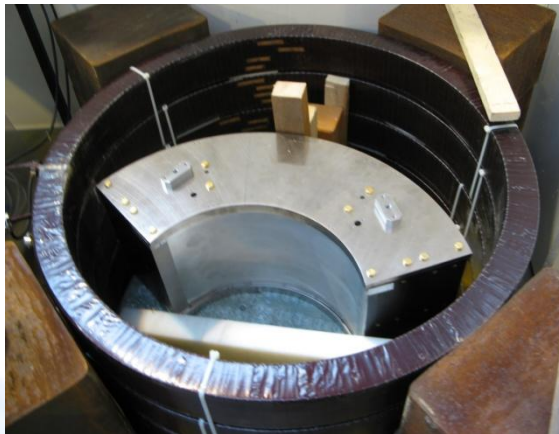
Supermirror analyzer assembled with around 200 supermirrors



Prototype I (1.8 deg)



Prototype II (4.0 deg)

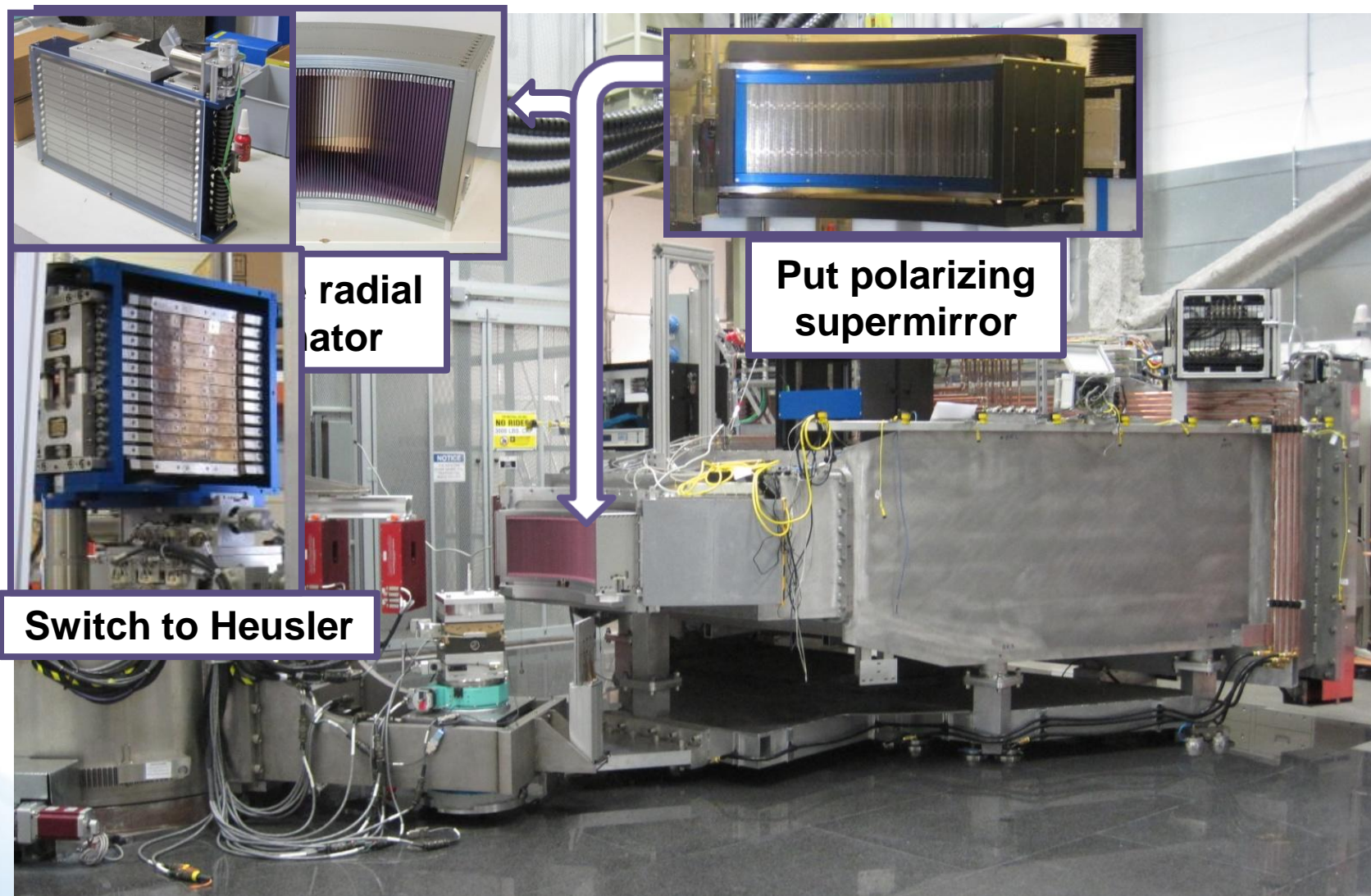


supermirror analyzer inside the magnetization unit (500 G)

2011 status:

- 780 out of 960 polarizers produced
- ~100 polarizers per month
- 200 polarizers installed in housing & tested on BOA (optics beamline at SINQ, PSI)
- Anticipated completion in March 2011, followed by tests at SINQ

Polarized beam setup with the PSI Polarizing Supermirror Array (B. Winn)



Intensity at sample, V scatterer

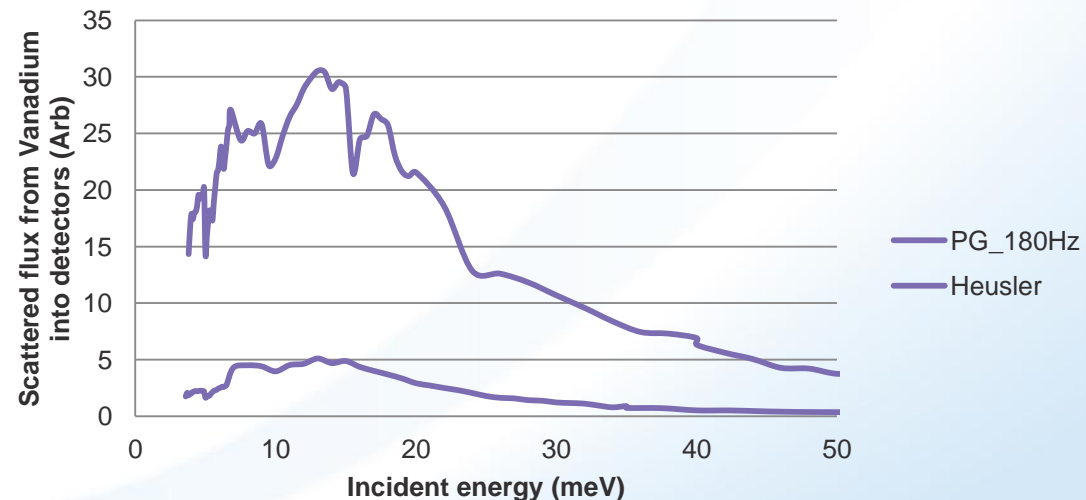
- 15 cm high beam from guide vertically focused to sample
~2.5 cm x 2.5 cm FWHM
- $4.2E5$ n/s/MW/cm²: Gold foil measurement at sample position, PG focus array to sample 1.8 m, $E_i=15$ meV, Fermi 180 Hz
- Plot: Vanadium incoherent isotropic scatter integrated over detector array at $40^\circ < 2\Theta < 100^\circ$, PG & Heusler

3.8 meV < E_i < 50 meV

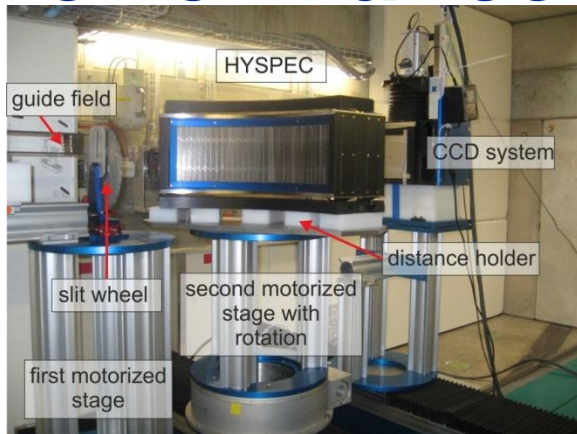
Common E_i 's:

3.8, 7, 15, 20, 27, 35 meV

Rare E_i : 50 meV



Performance of the Polarizer

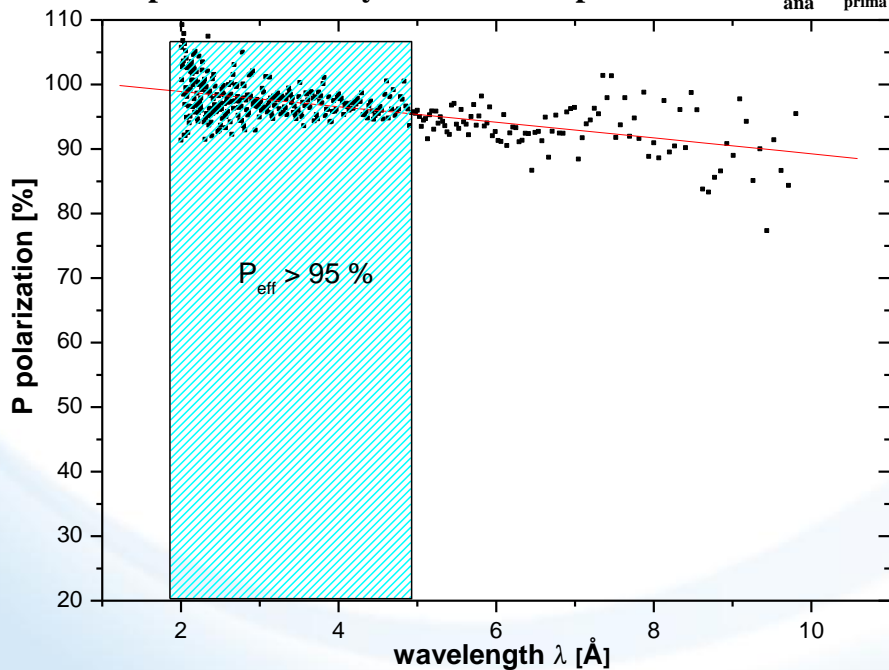


960 supermirrors, 60°
 U. Filges
 BOA beamline at SINQ
 Ready to ship

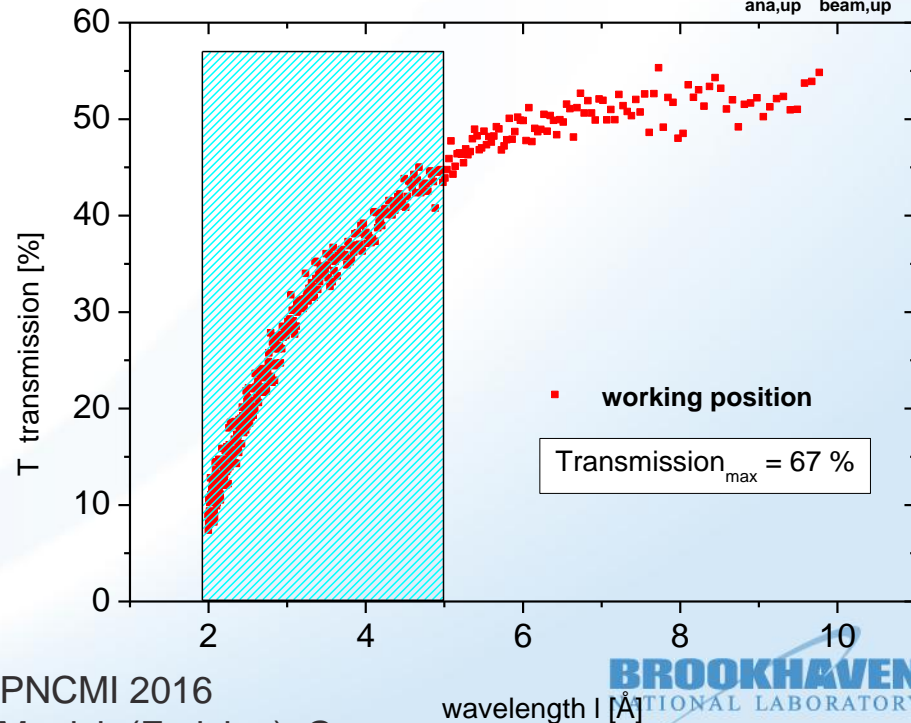


Magnetization unit at HYSPEC

supermirror analyzer - effective polarization P_{ana}/P_{prima}



supermirror analyzer - transmission $I_{ana,up}/I_{beam,up}$



Polarized beam commissioned (2015)

Neutron Sciences FUTURE FOR USERS ABOUT SCIENCE INSTRUMENTS & SUPPORT PUBLICATIONS NEWS CAP

<https://neutrons.ornl.gov/news/supermirroruser>



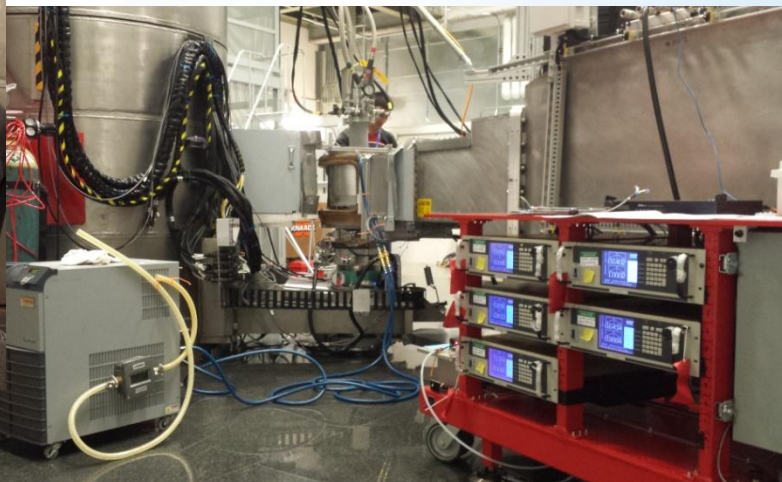
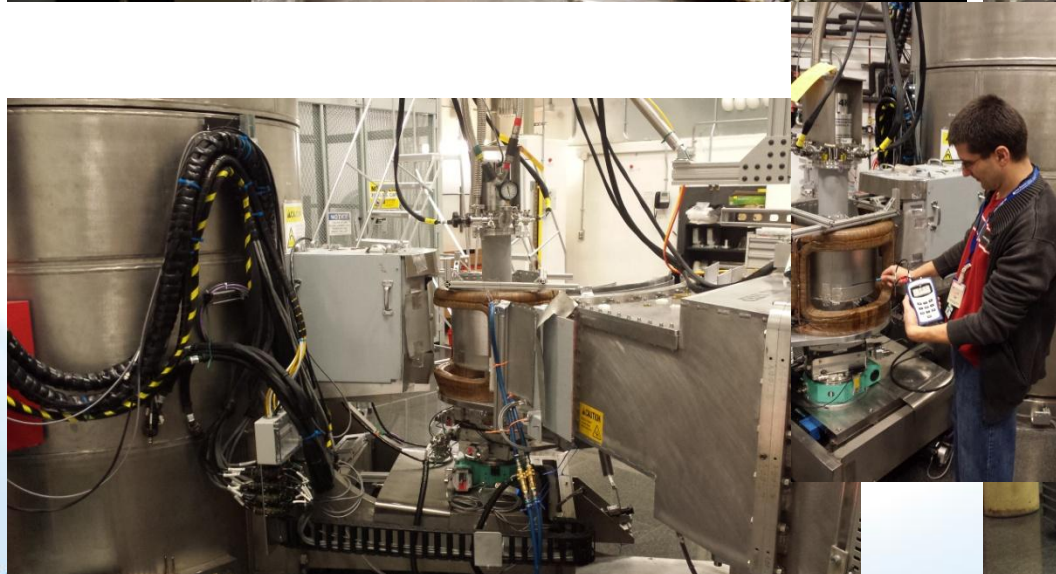
More Power to HYSPEC

November 11, 2015

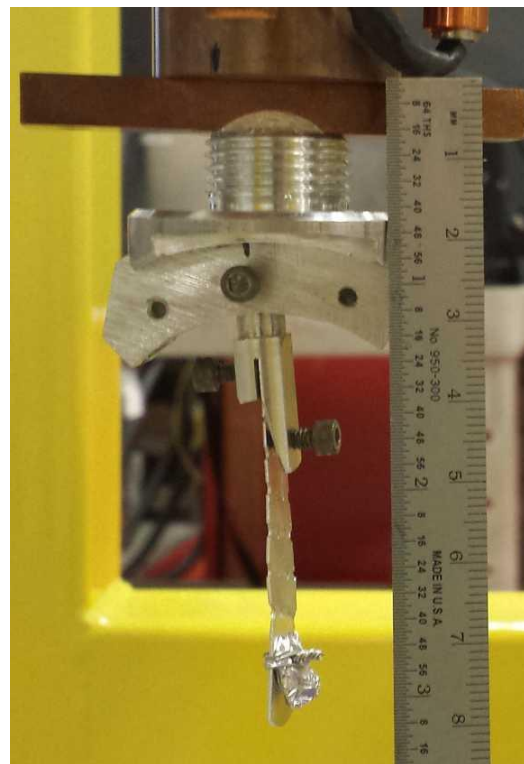
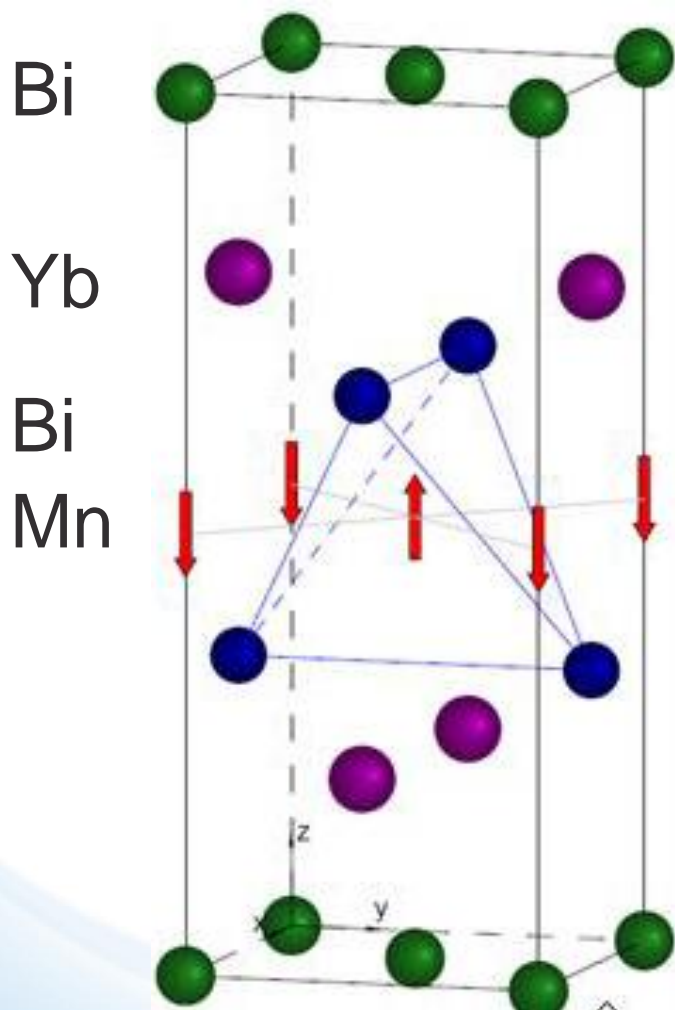
After installing the new wide-angle super mirror array at SNS's hybrid spectrometer, beam line 14B, HYSPEC is ready to tackle new problems using fully polarized neutron scattering.



HYSPEC polarized beam setup in operation



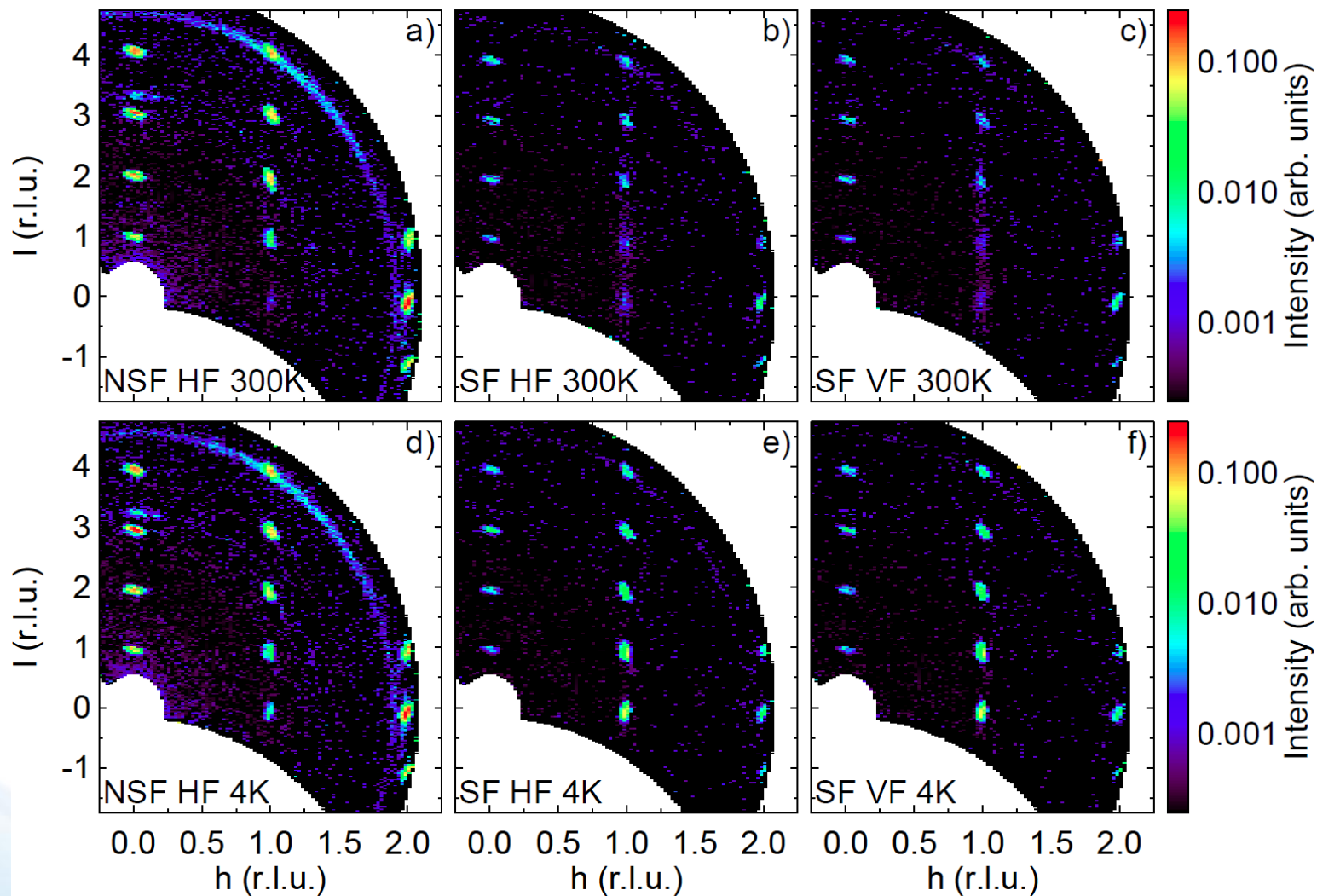
First test: antiferromagnetic structure of the layered semimetal YbMnBi_2



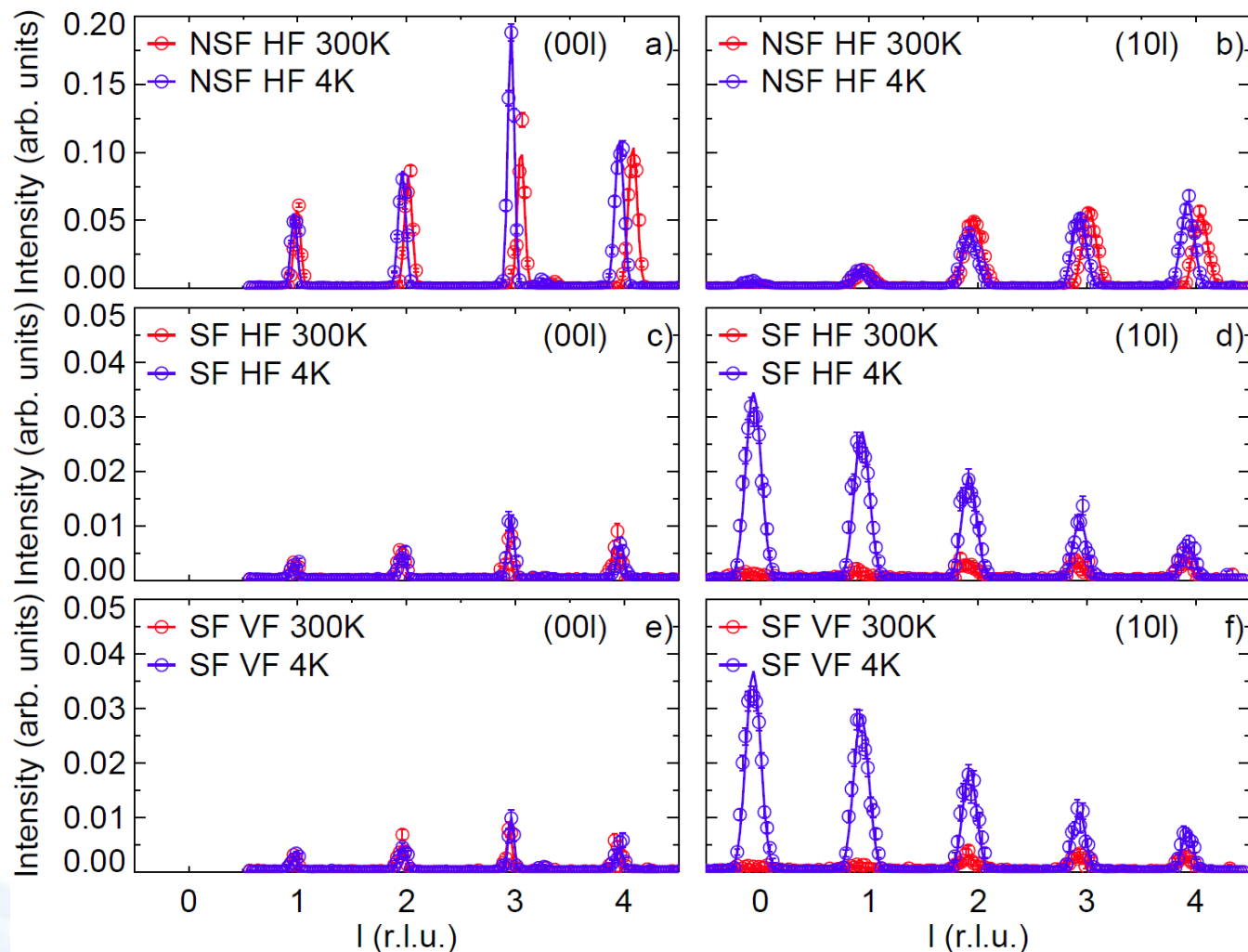
YbMnBi_2 (~0.5g)
single crystal



Polarized diffraction measurement of YbMnBi_2 : one night on HYSPEC



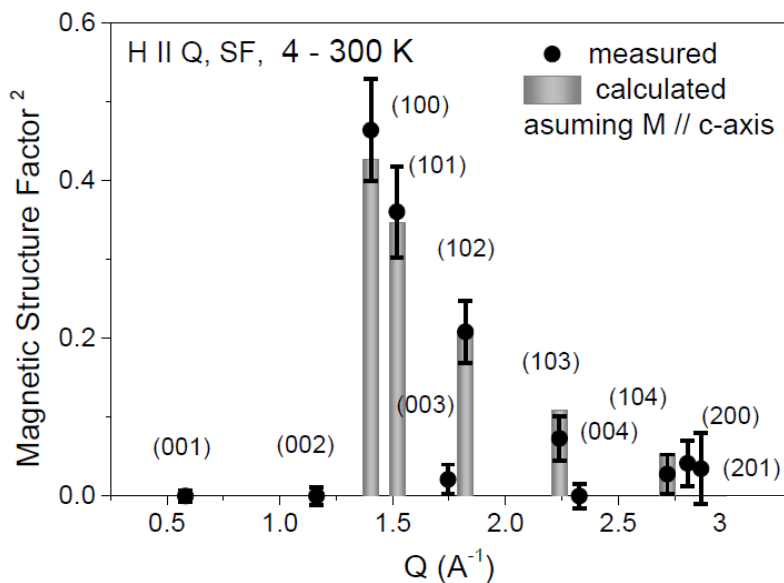
Polarized diffraction scans on YbMnBi_2 Bragg peaks



HYSPEC is not a diffractometer, but... can do diffraction, if needed

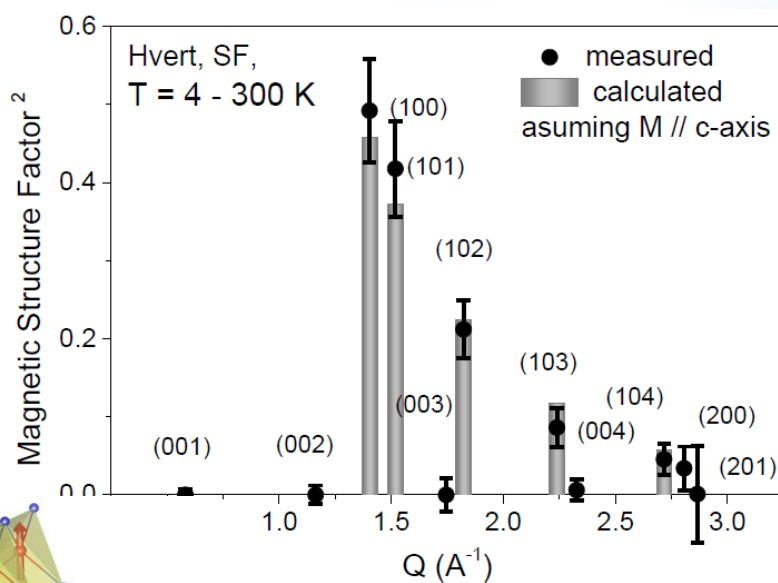
The refinement compares favorably to HB3 diffractometer

Fit of the 4K – 300 K data with $P \parallel Q$.
AFM model with spins along c axis gives ordered moment amplitude of $4.37(18) \mu_B$

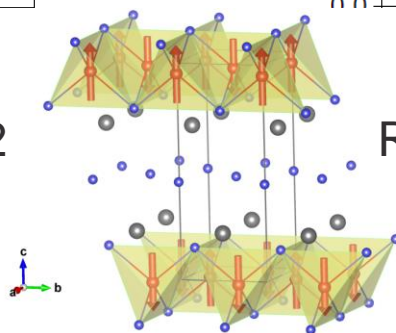


RF-factor: 25.9, $\chi^2(\text{Intensity})$: 0.72

Fit of the 4K – 300 K data with P vertical ($\perp Q$).
AFM model with spins along c axis gives ordered moment amplitude of $4.52(17) \mu_B$



RF-factor: 17, $\chi^2(\text{Intensity})$: 0.46

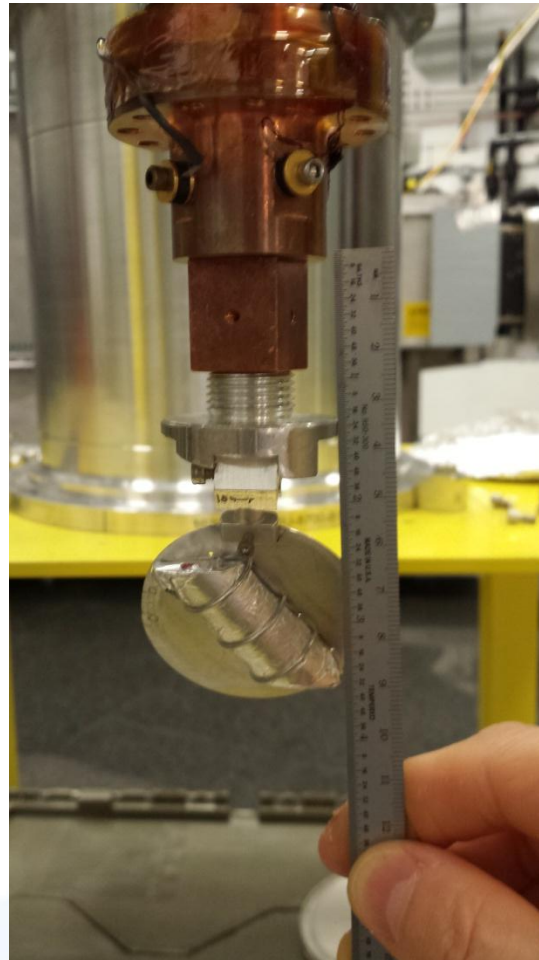
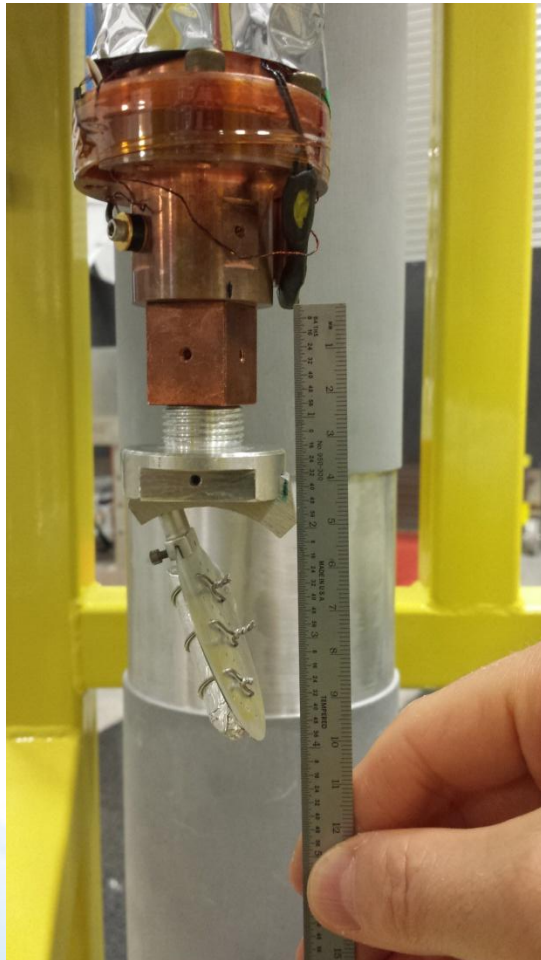


PNCMI 2016

4-7 July 2016, Munich (Freising), Germany

Magnetic dynamics in $\text{FeTe}_{0.45}\text{Se}_{0.55}$ superconductor: sample geometry

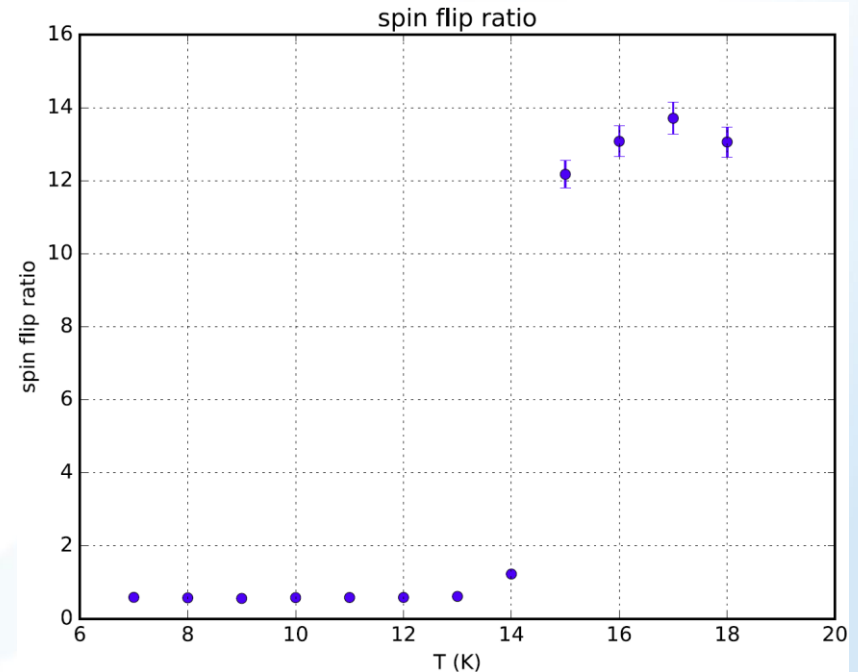
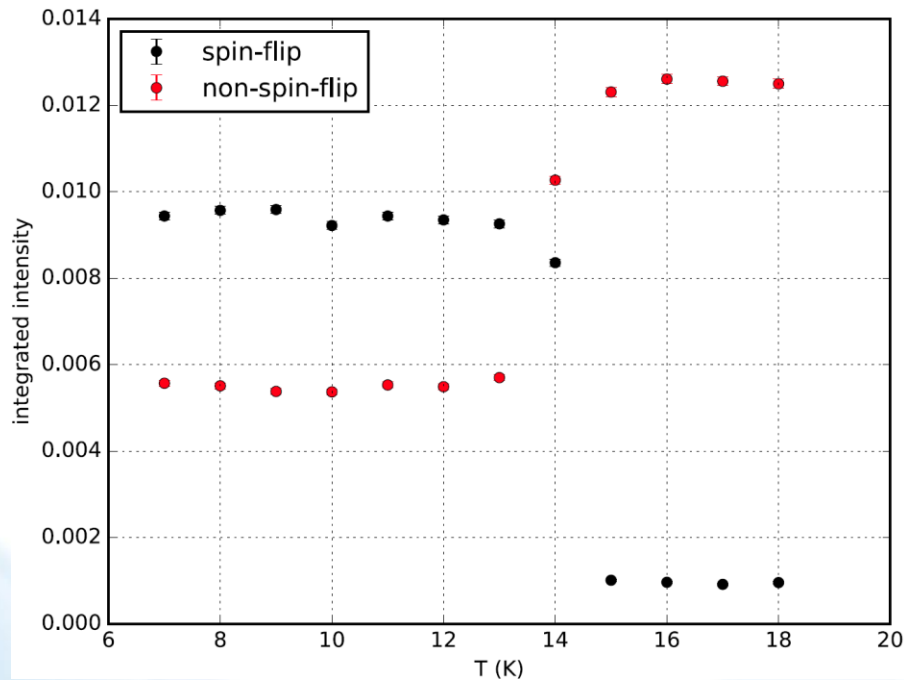
Large (~ 23g) bulk single crystal, irregularly mounted on Al plate



Beam depolarization in superconducting $\text{FeTe}_{0.45}\text{Se}_{0.55}$

Sample is cooled in guide field $\sim 10\text{--}20\text{G} \Rightarrow$ the beam is fully depolarized at $T < T_c$!

Flipping Ratio ($T > T_c$) = 13(1)



Zero field cooling: $FR = 5 \sim 8$

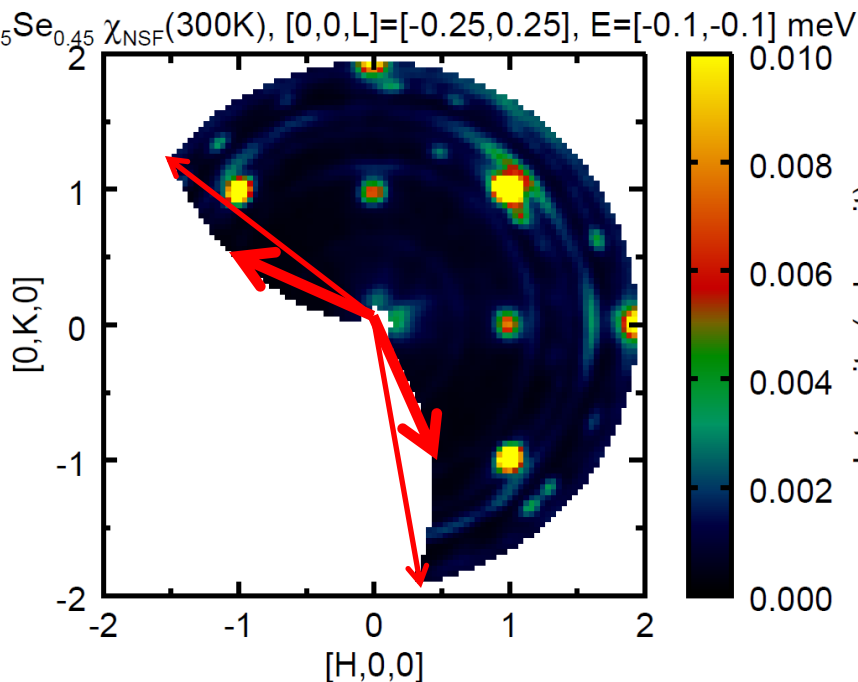
- Cooled in a mu-metal shield from 16 K to 5 K
- Cooled on the instrument sample table, in a compensating guide field providing zero field environment
- Effect is similar: flipping ratio improved.
- FR varies from 5 to 8, depending on the sample rotation angle



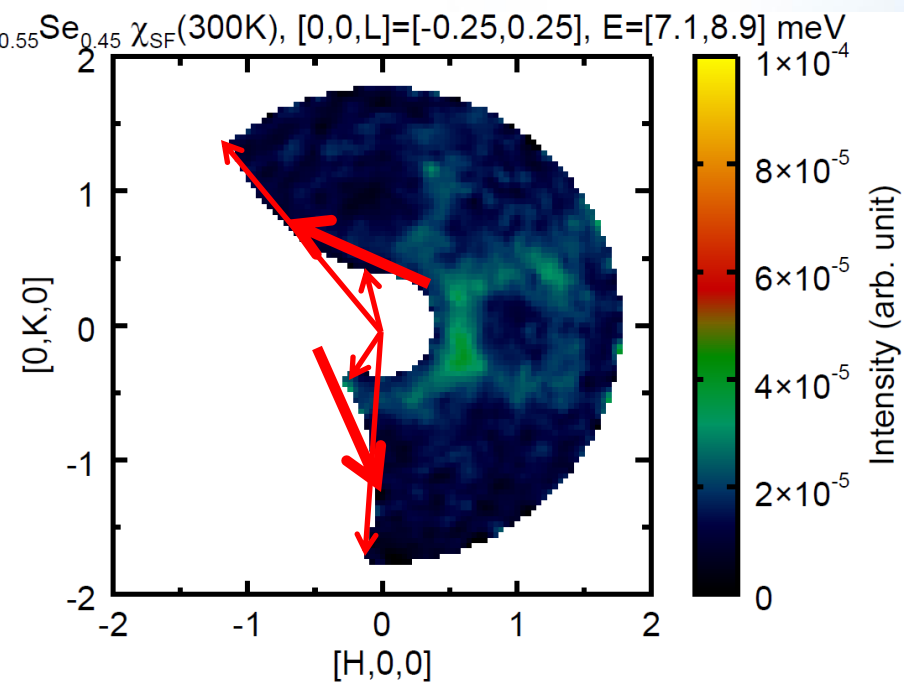
“P||Q” setup: align polarization with the middle of detector at E=0

Change of the mutual alignment of **P** and **Q** with energy transfer

E=0 meV

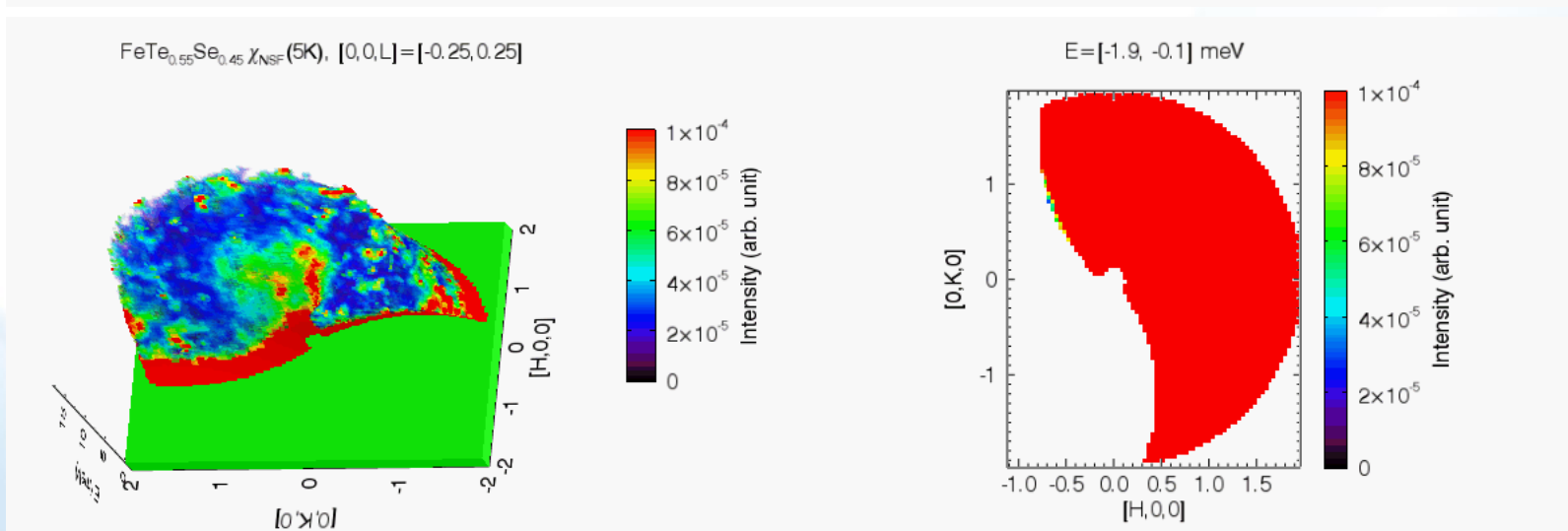
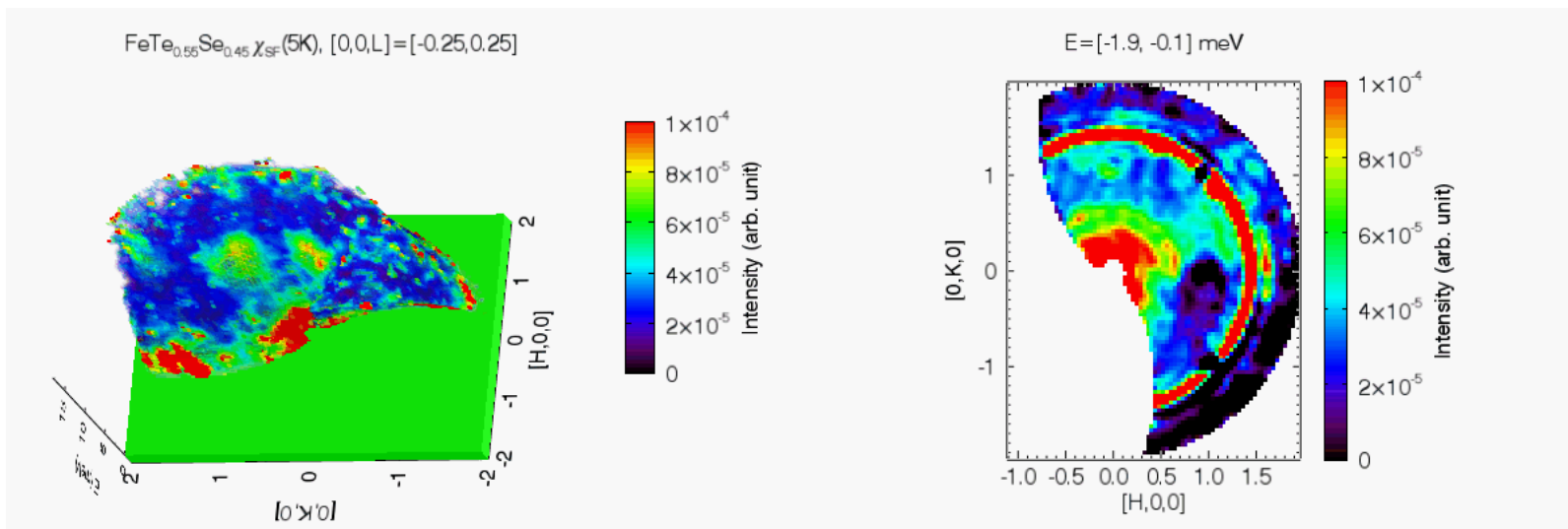


E=8.0(9) meV

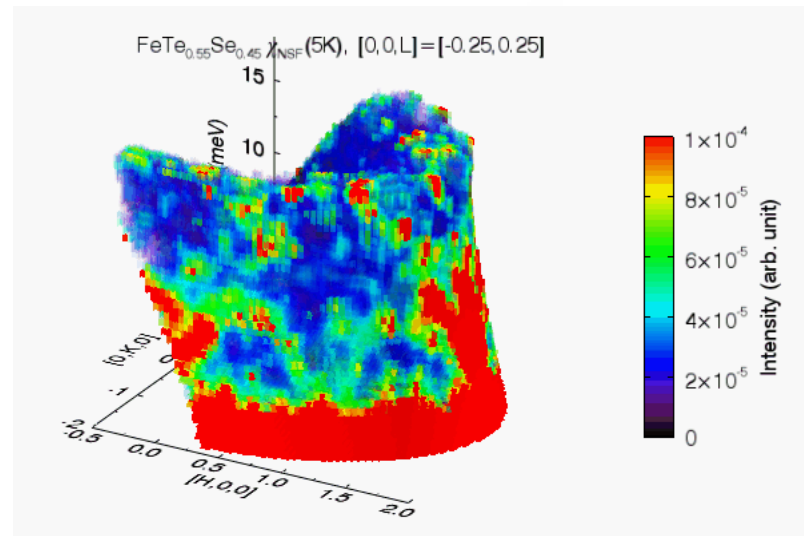
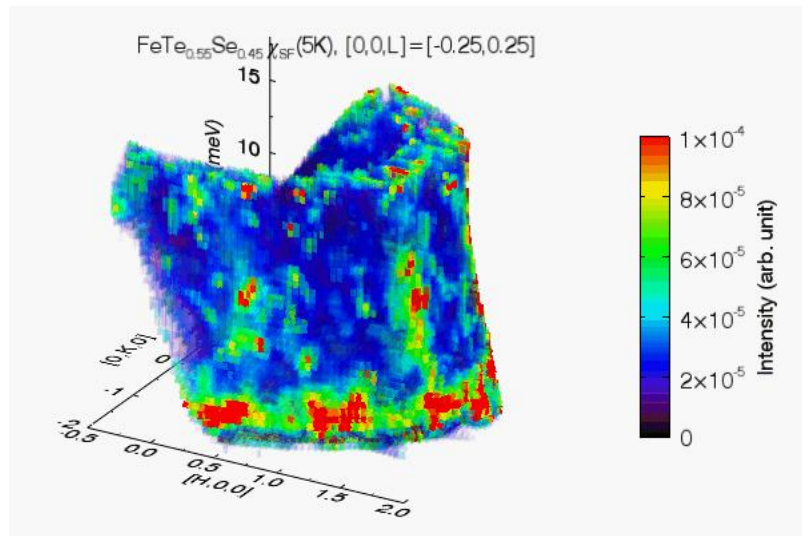


SNS @ 1 MW. $E_i = 20$ meV. Each dataset is approximately 24 hours on HYSPEC: 6-8 min for each of the 191 angular positions of the sample.

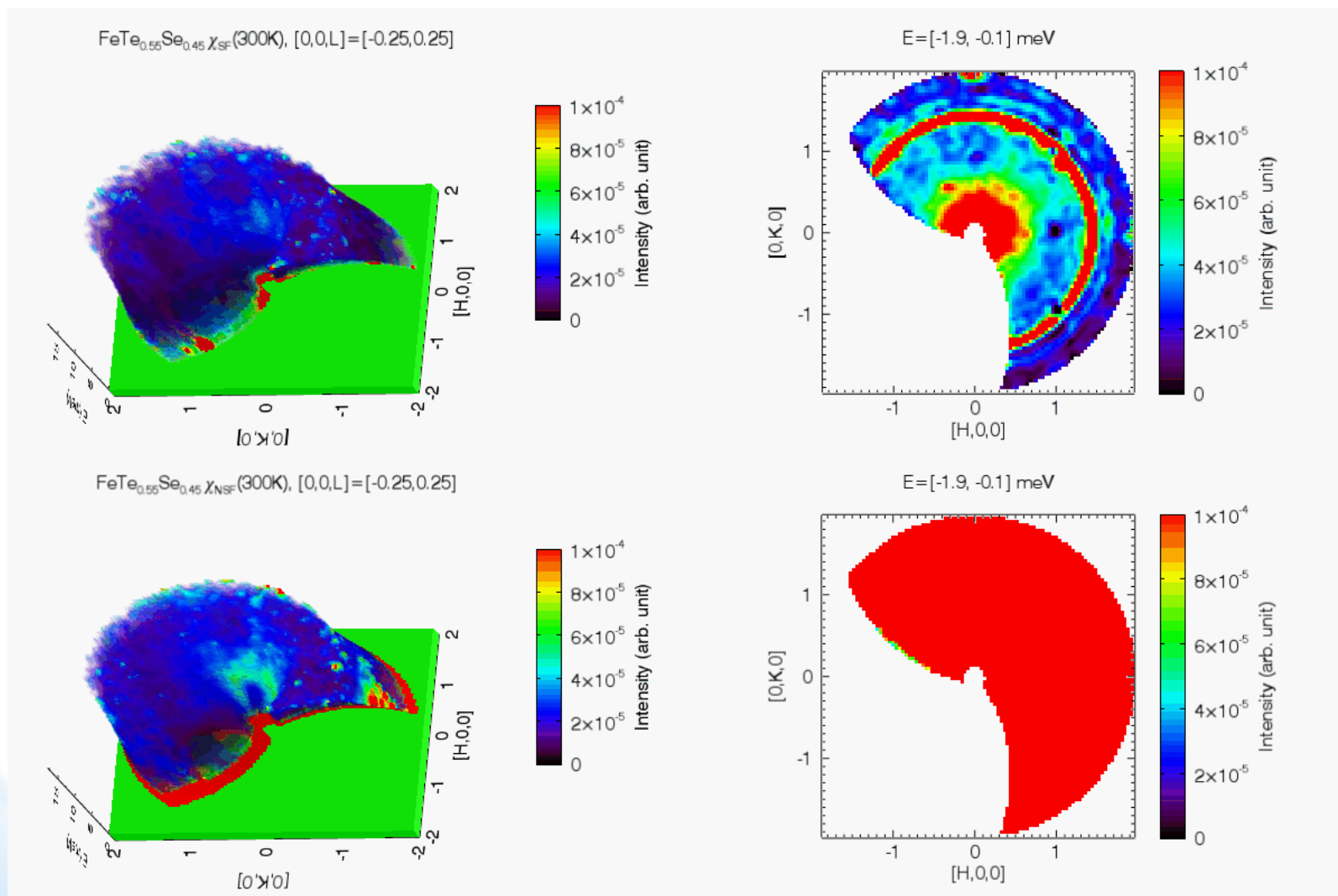
SF and NSF at 5 K



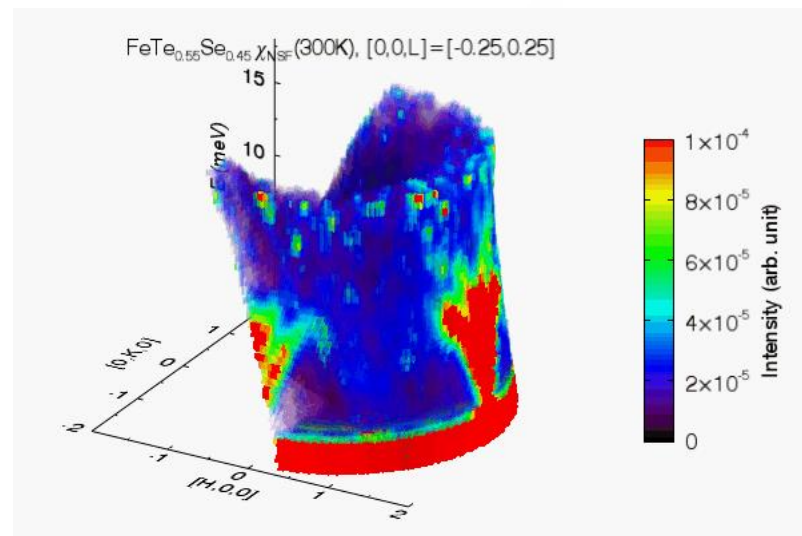
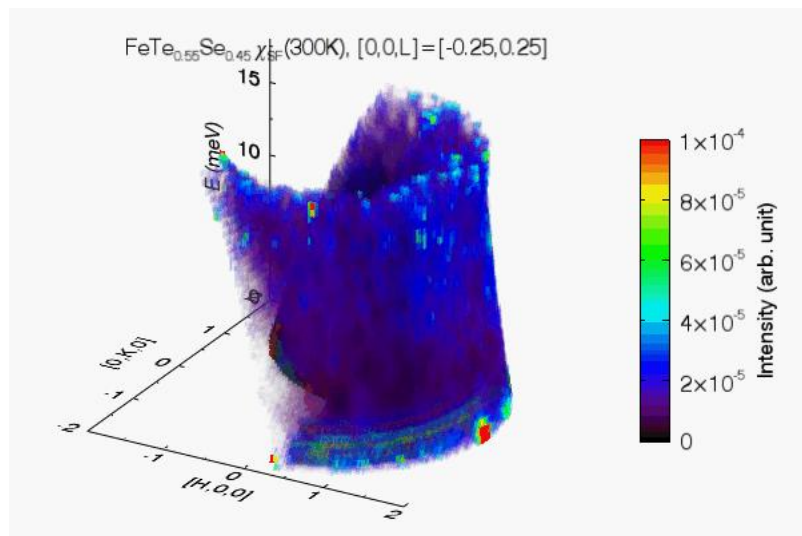
SF and NSF at 5 K



SF and NSF at 300 K



SF and NSF at 300 K



Magnetic and non-magnetic excitations in $\text{FeTe}_{0.55}\text{Se}_{0.45}$ by polarized neutron scattering on HYSPEC

I. Zaliznyak , O. Garlea, A. Savici, J. Schneeloch, J. Tranquada, Z. Xu , G. Xu , G. Gu

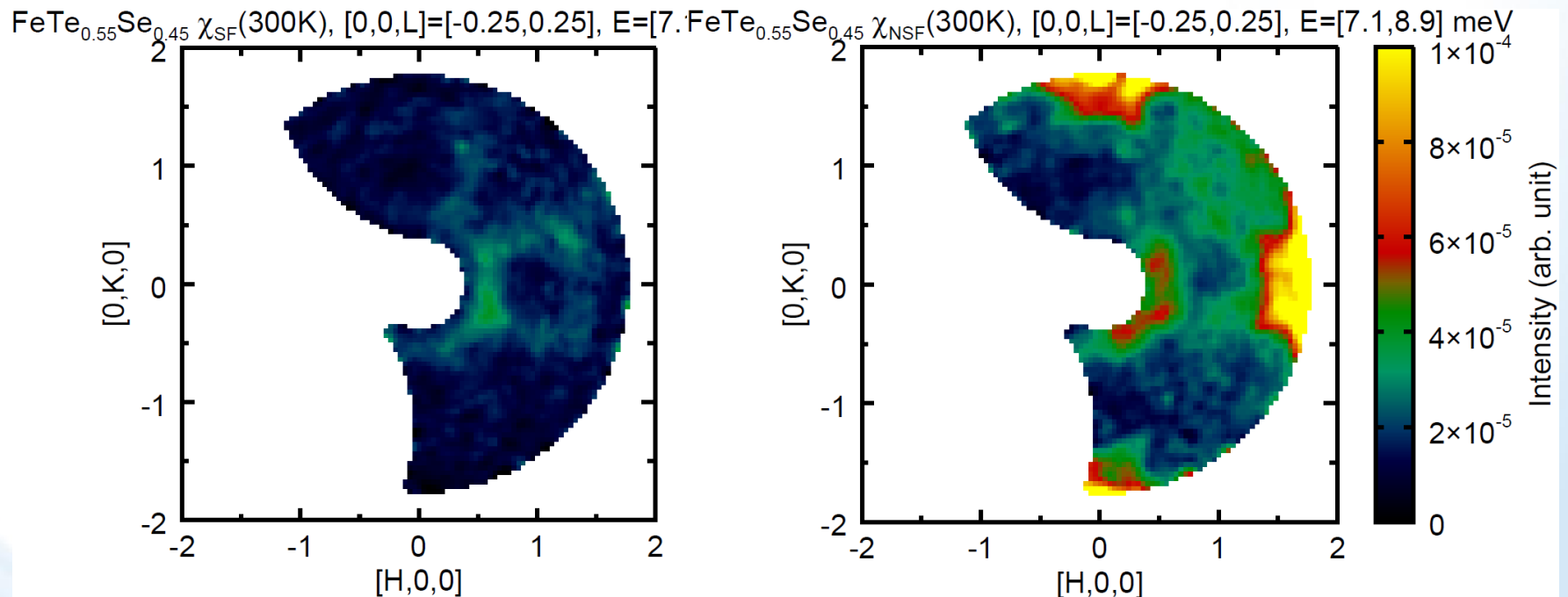
Comparison of the equivalent slices from the Spin-Flip (left) and the Non-Spin-Flip (right) data sets

Spin-Flip Scattering (magnetic)

$I_{\text{SF}}(\mathbf{Q}, E)$ at $T = 300$ K

Non-Spin-Flip Scattering (phonon)

$I_{\text{NSF}}(\mathbf{Q}, E)$ at $T = 300$ K



SNS @ 1 MW. $E_i = 20$ meV. Each dataset is approximately 24 hours on HYSPEC: 6-8 min for each of the 191 angular positions of the sample.

Magnetic and non-magnetic excitations in $\text{FeTe}_{0.55}\text{Se}_{0.45}$ by polarized neutron scattering on HYSPEC

I. Zaliznyak , O. Garlea, A. Savici, J. Schneeloch, J. Tranquada, Z. Xu , G. Xu , G. Gu

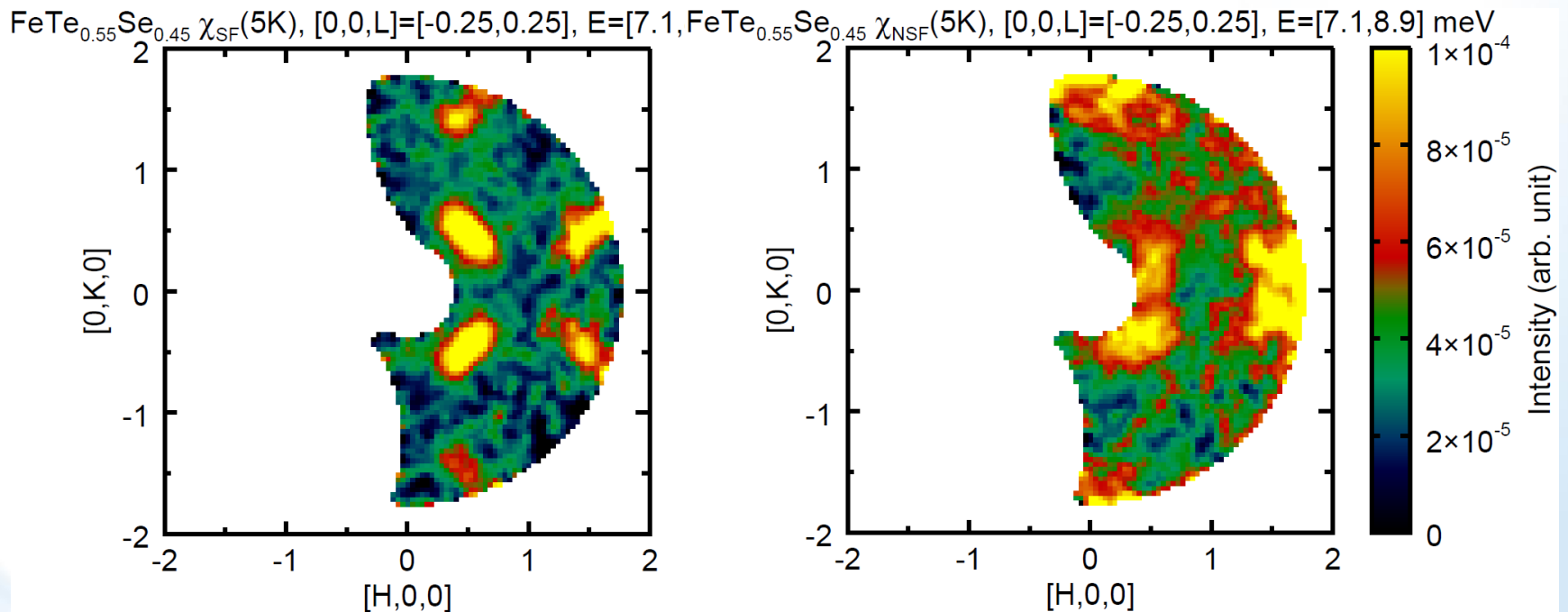
Comparison of the equivalent slices from the Spin-Flip (left) and the Non-Spin-Flip (right) data sets

Spin-Flip Scattering (magnetic)

$I_{\text{SF}}(\mathbf{Q}, E)$ at $T = 5 \text{ K}$

Non-Spin-Flip Scattering (phonon)

$I_{\text{NSF}}(\mathbf{Q}, E)$ at $T = 5 \text{ K}$



SNS @ 1 MW. $E_i = 20 \text{ meV}$. Each dataset is approximately 24 hours on HYSPEC: 6-8 min for each of the 191 angular positions of the sample.

Magnetic and non-magnetic excitations in $\text{FeTe}_{0.55}\text{Se}_{0.45}$ by polarized neutron scattering on HYSPEC

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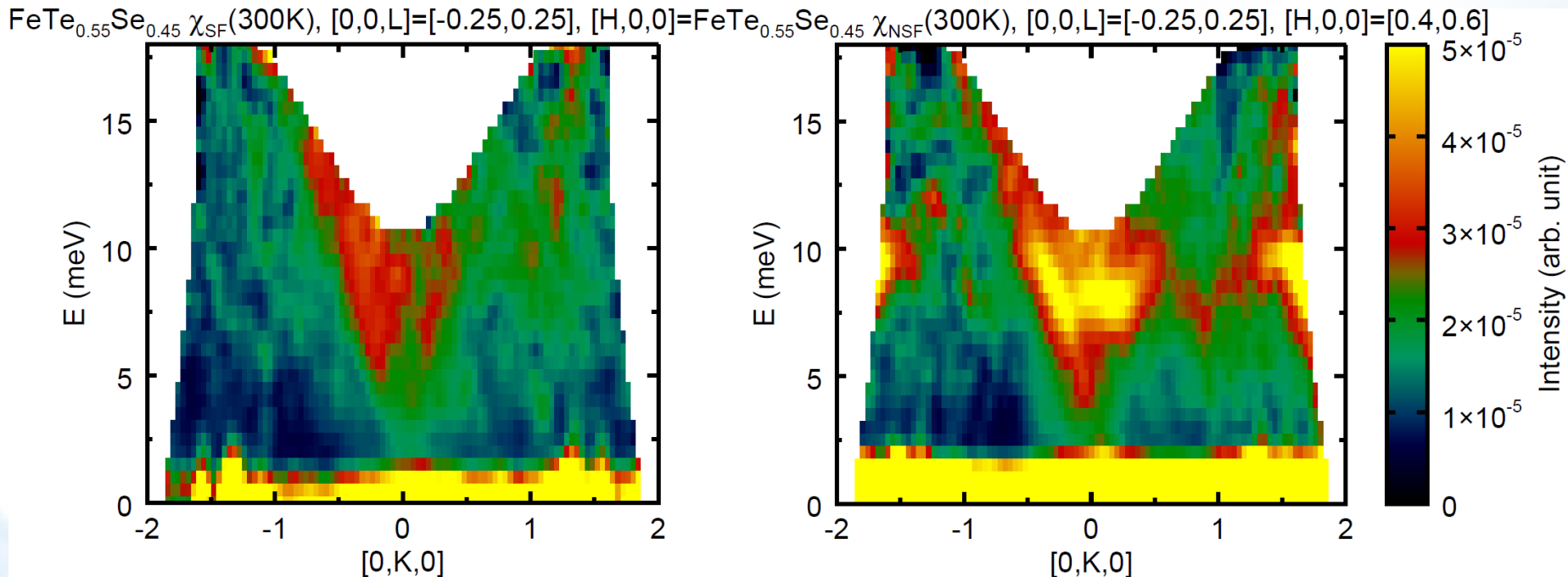
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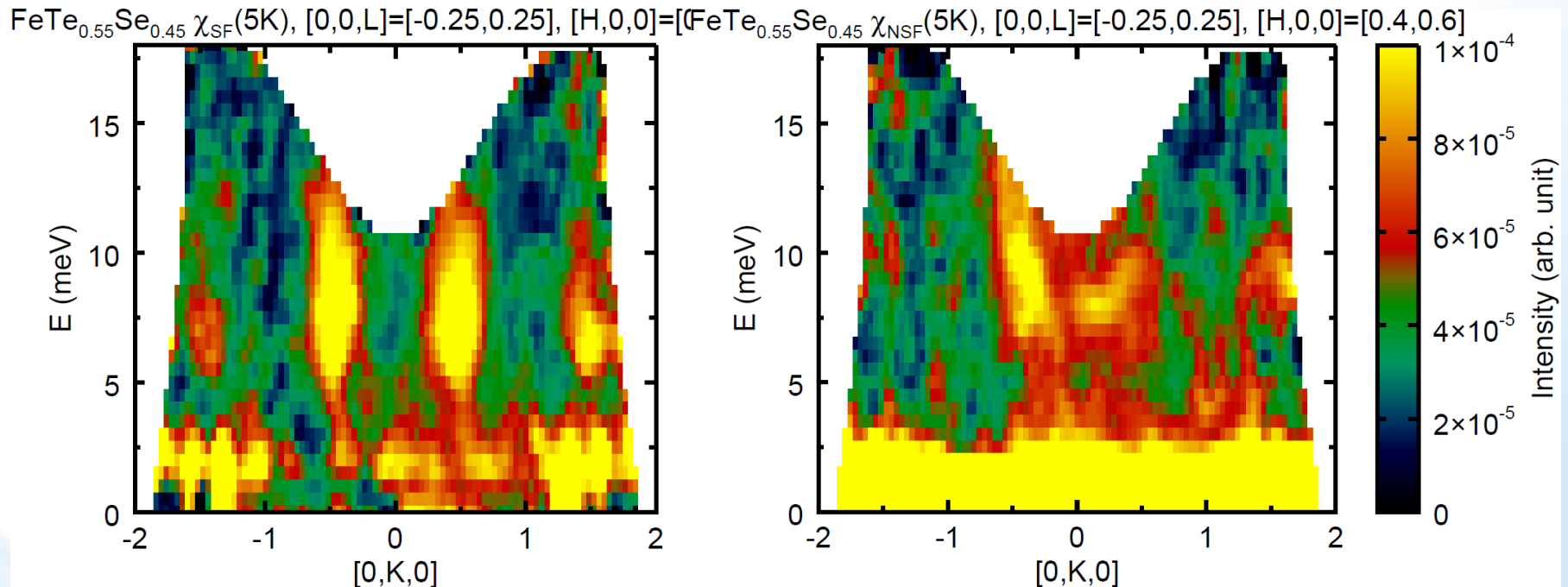
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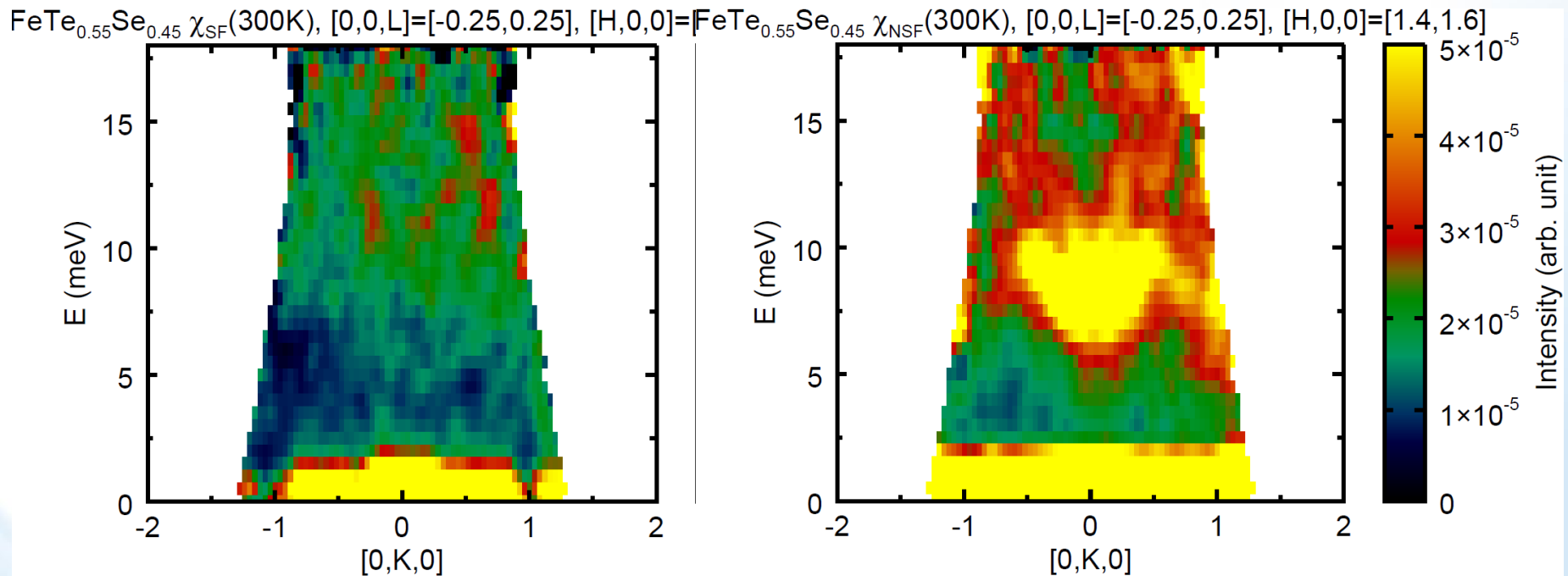
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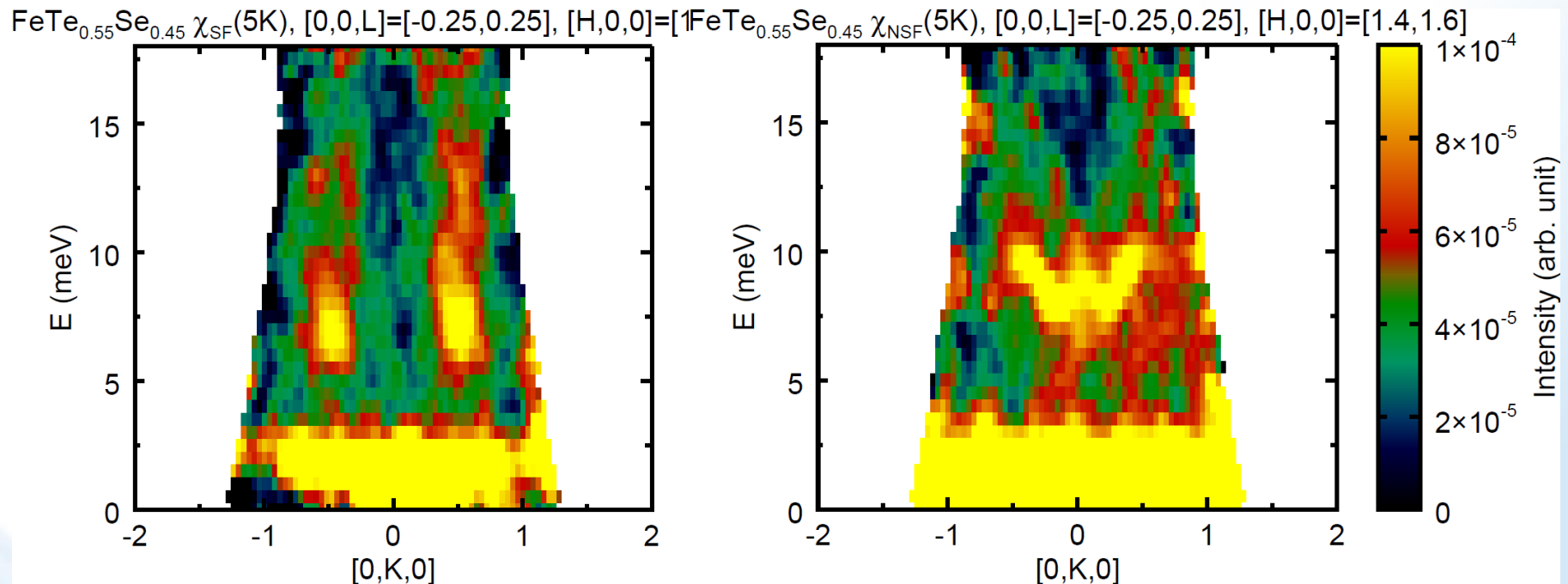
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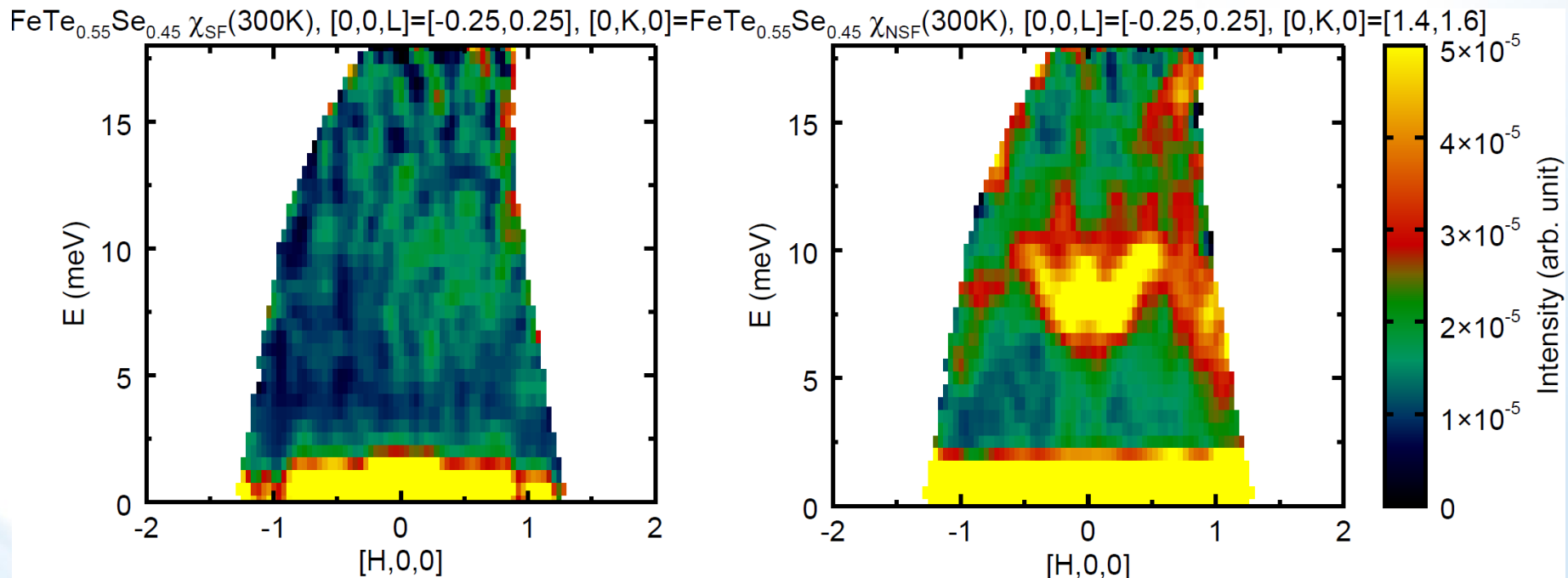
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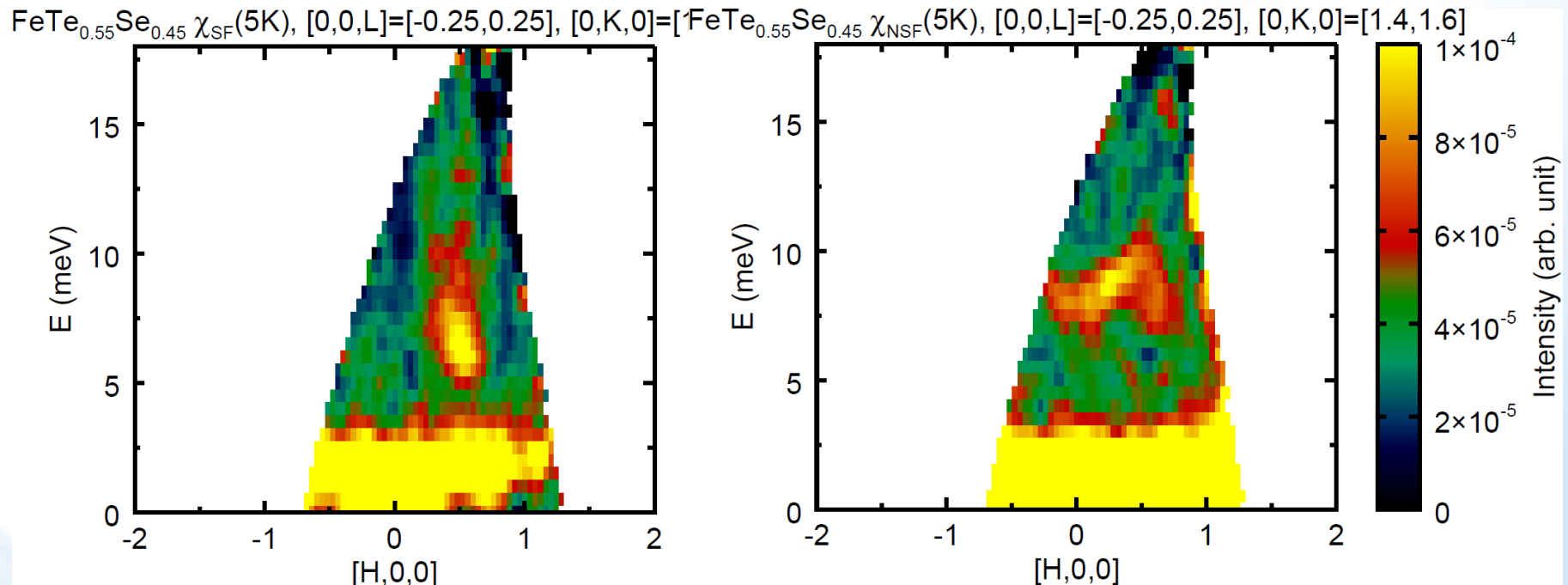
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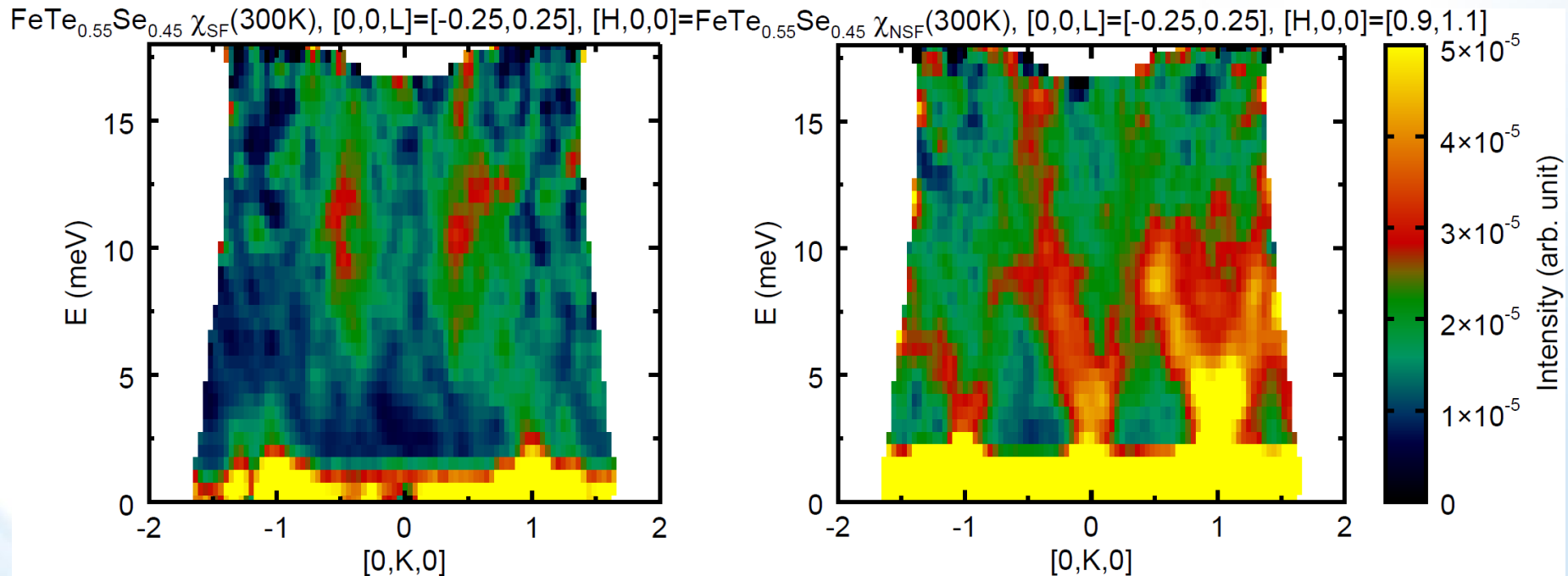
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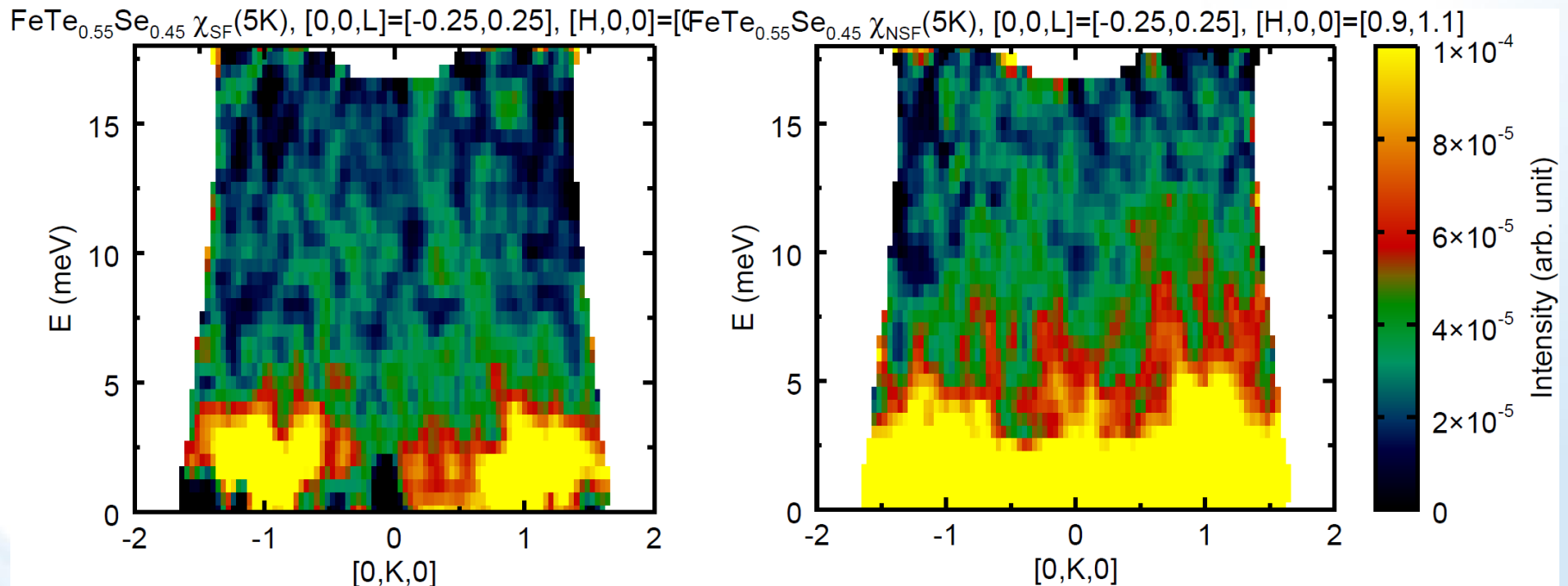
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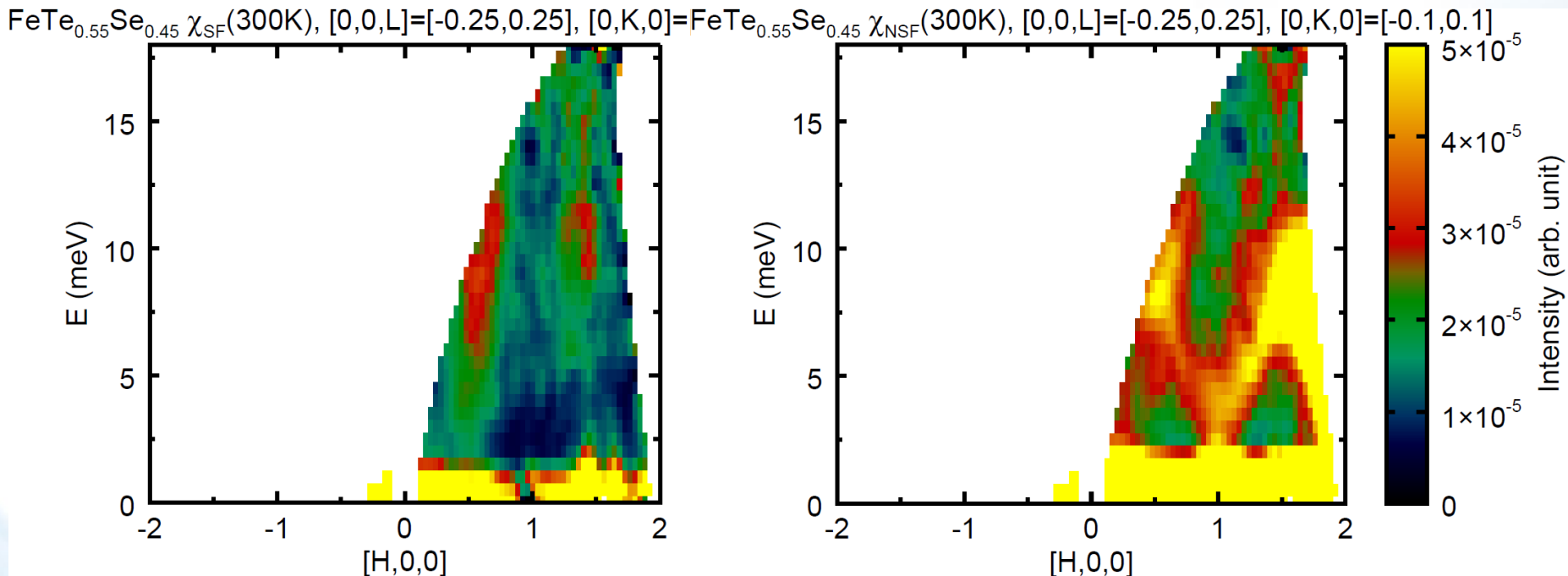
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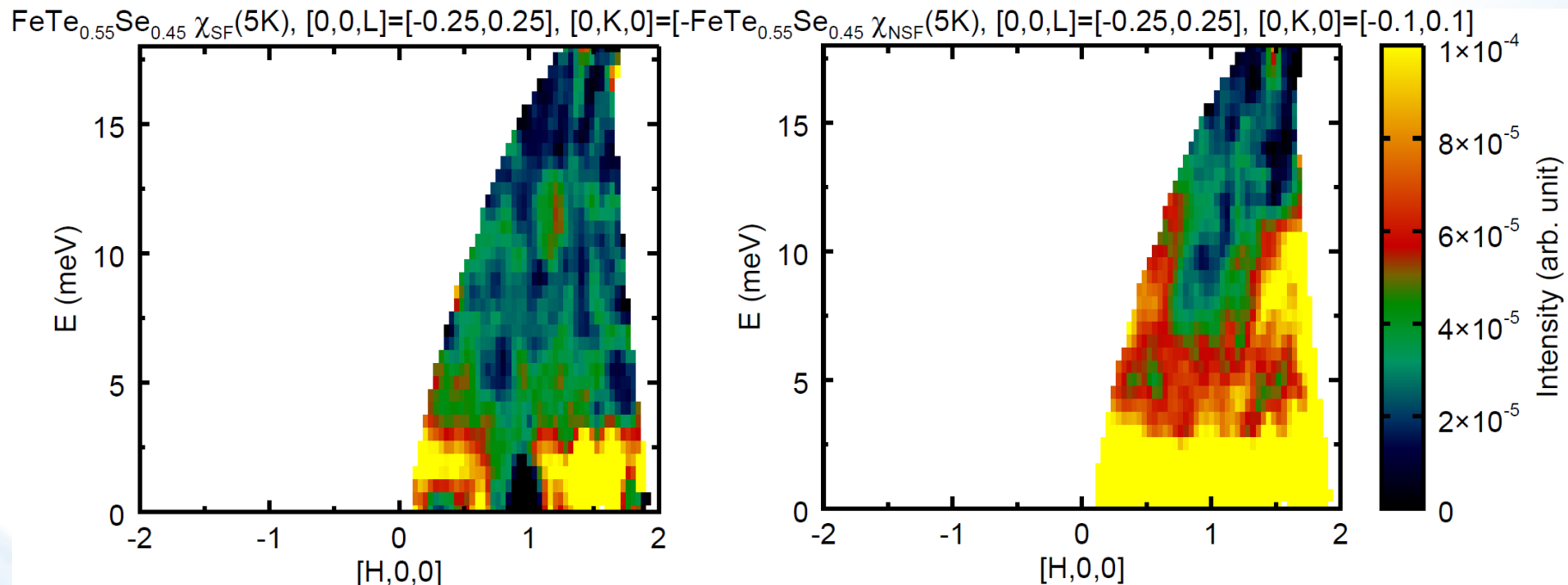
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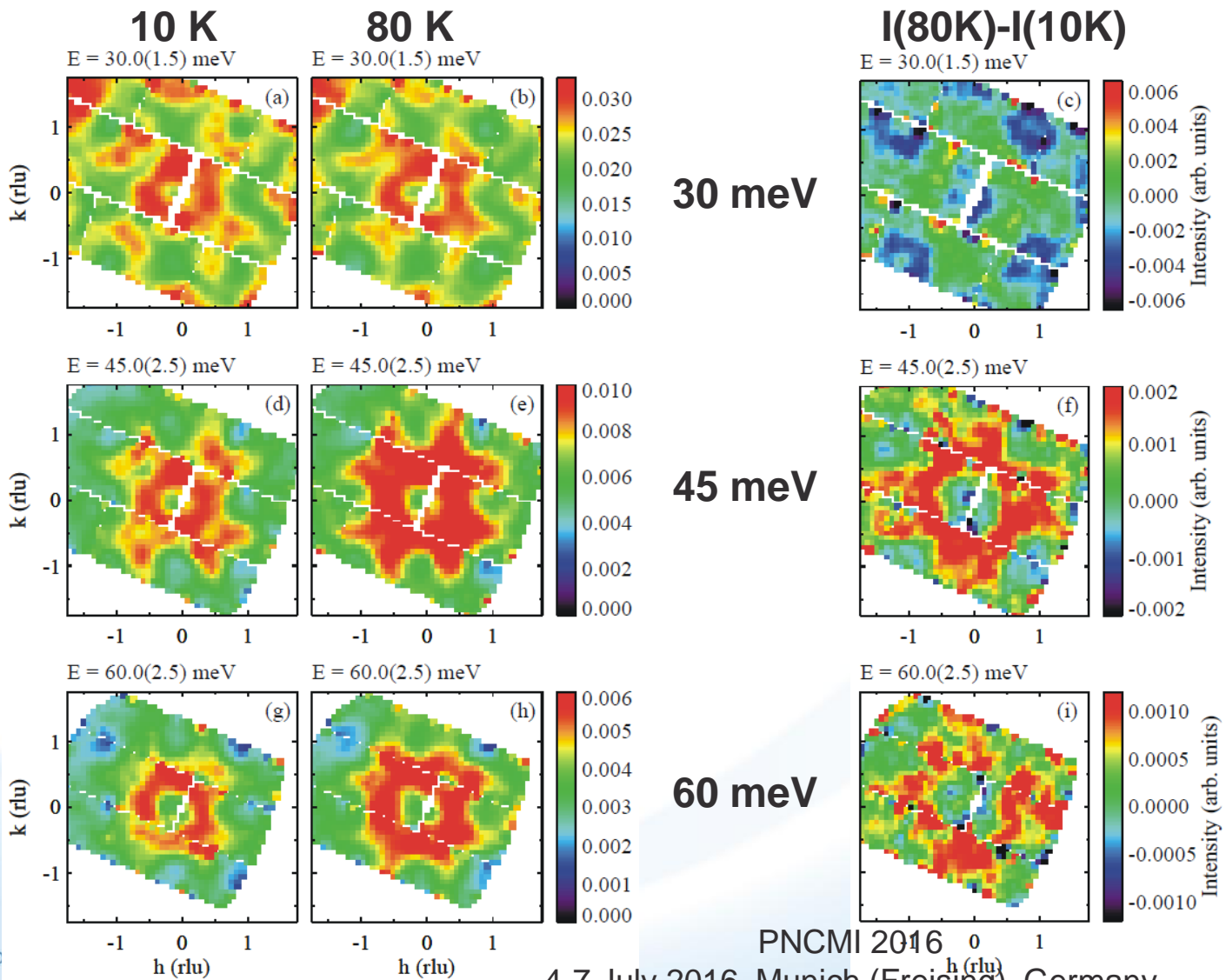
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Temperature-induced dynamical magnetism in $\text{Fe}_{1.1}\text{Te}$

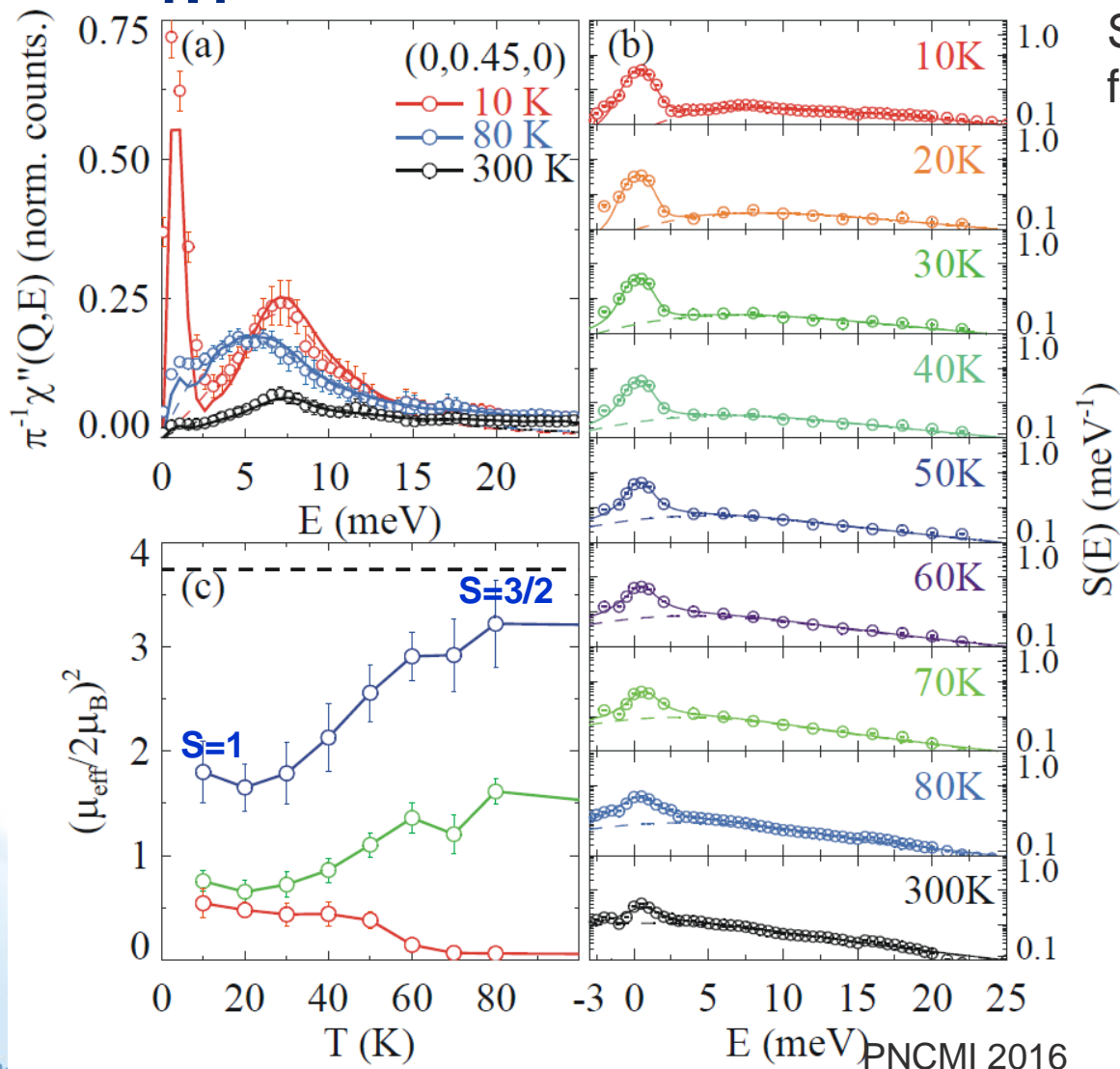
FeTe on ARCS,
 $E_i = 100$ meV
 Zaliznyak, et. al.,
 arXiv:1103.5073
 Phys. Rev. Lett. **107**,
 216403 (2011).



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Temperature induced magnetism in $\text{Fe}_{1.1}\text{Te}$



Sum rule defines the effective fluctuating magnetic moment

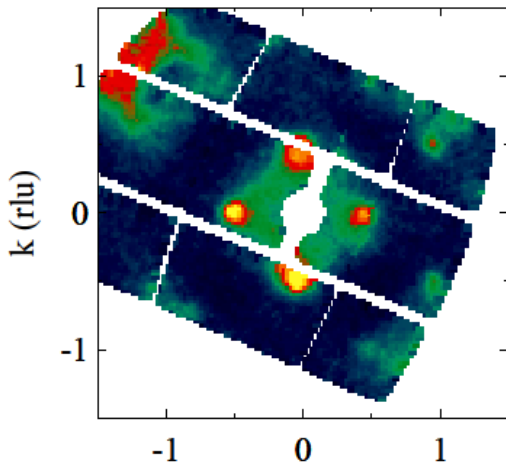
$$\left[\mu_{\text{eff}} / (g\mu_B) \right]^2 = \int S(Q, E) d^3\mathbf{Q} dE = S(S+1)$$

Zaliznyak, et. al.,
PRL **107** 216403 (2011);
PRB **85**, 085105 (2012).

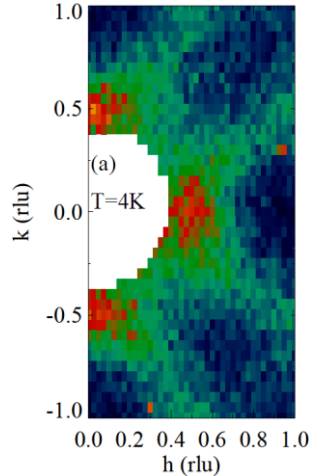
Dynamical spin response in $\text{FeTe}_{1-x}\text{S}_x$

$x \text{S}_x$

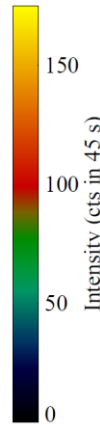
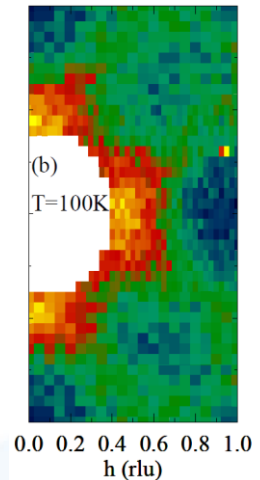
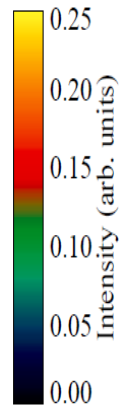
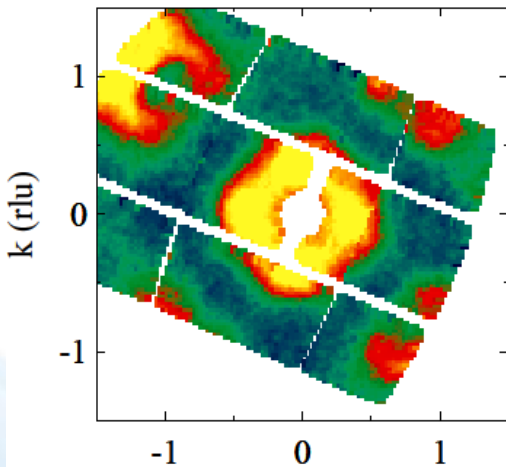
$T = 10 \text{ K}$ (hk0) zone



(hk0) zone

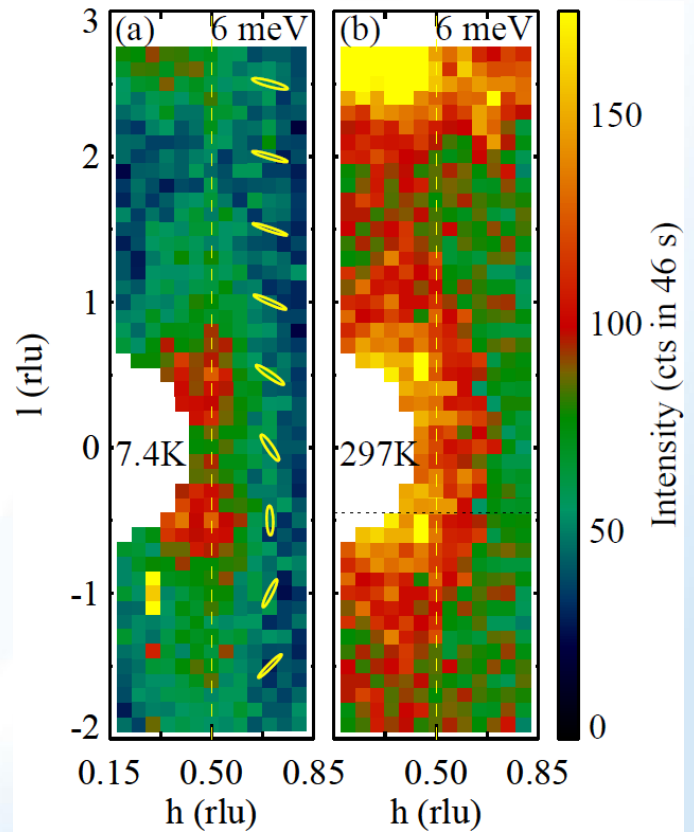


$T = 80 \text{ K}$



$\text{FeTe}_{1-x}\text{S}_x$ ($x \approx 0.13$) on HB3.
I. Zaliznyak, et. al, PNAS 112,
10316–10320 (2015)

(h0l) zone



$\text{Fe}_{1.1}\text{Te}$, ARCS ($E = 6 \text{ meV}$).

Brookhaven Science Associates

$\text{FeTe}_{1-x}\text{S}_x$ ($x \approx 0.13$) on HB3.

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BROOKHAVEN
NATIONAL LABORATORY

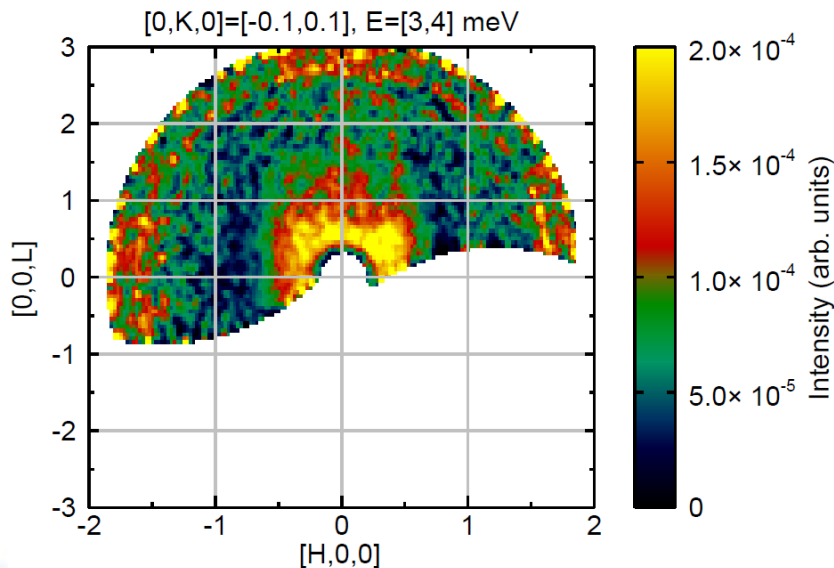
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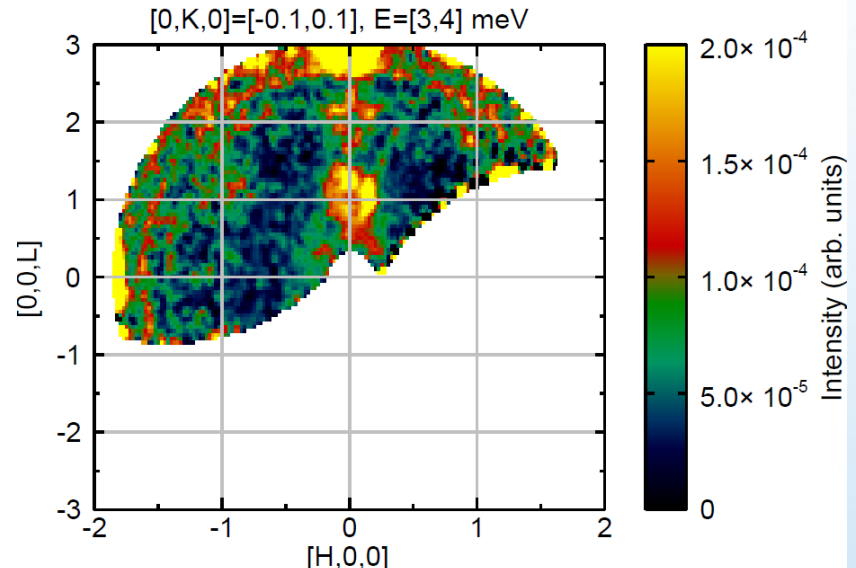
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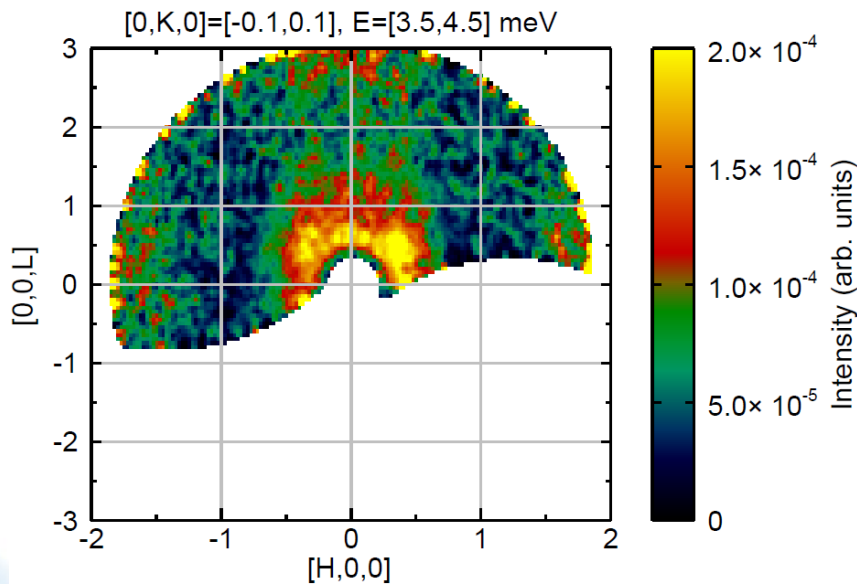
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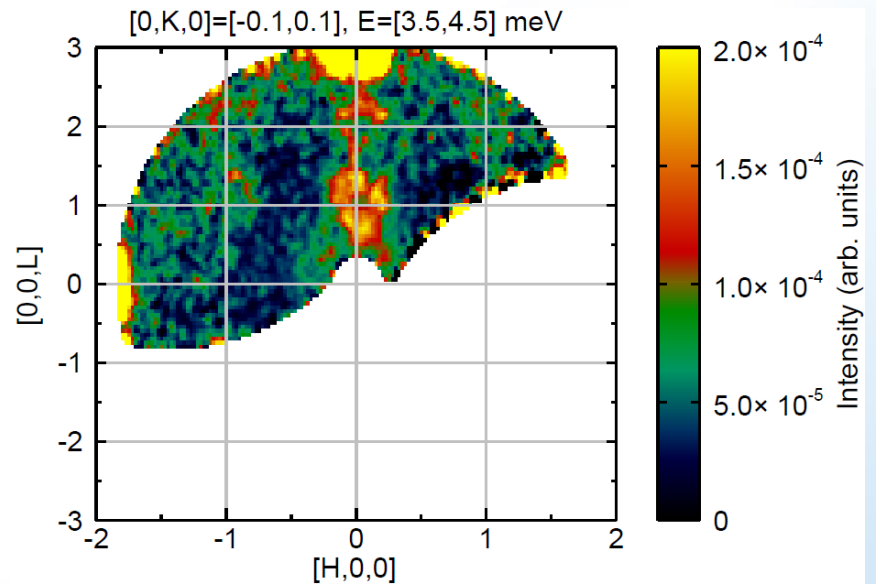
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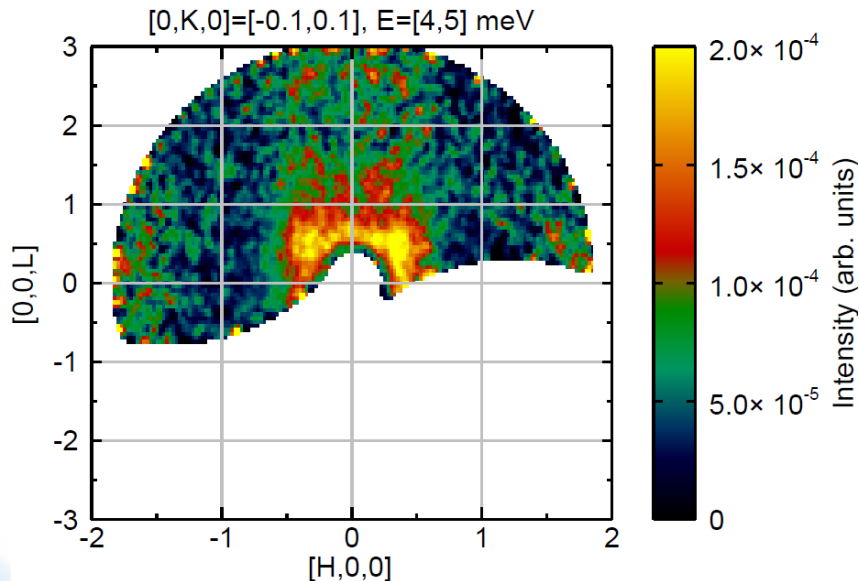
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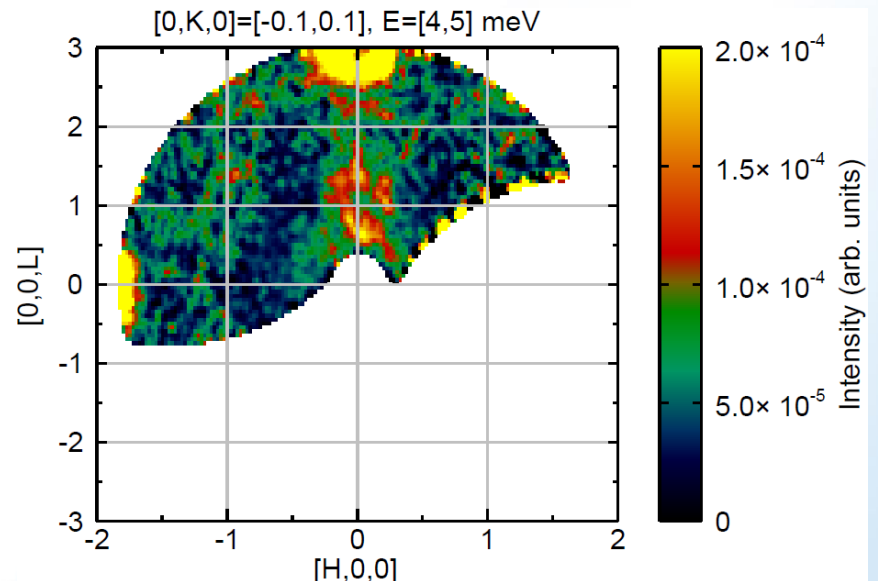
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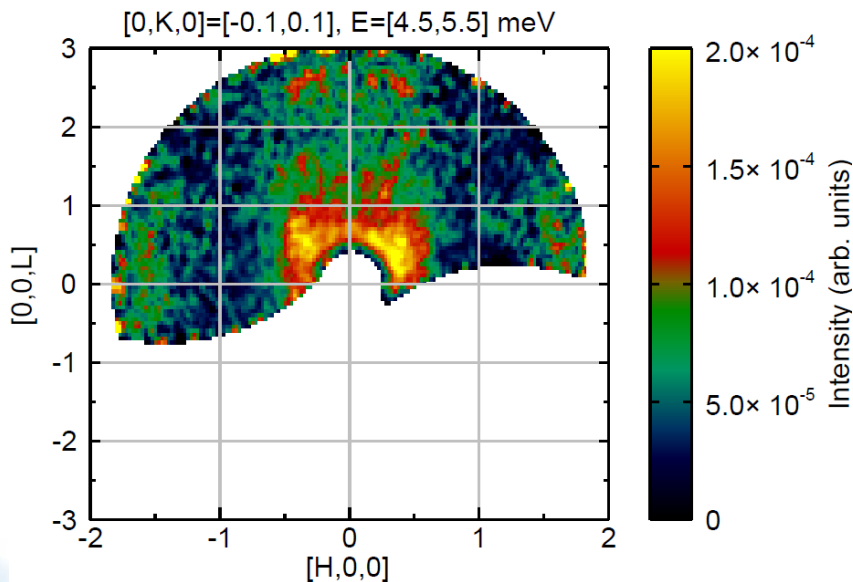
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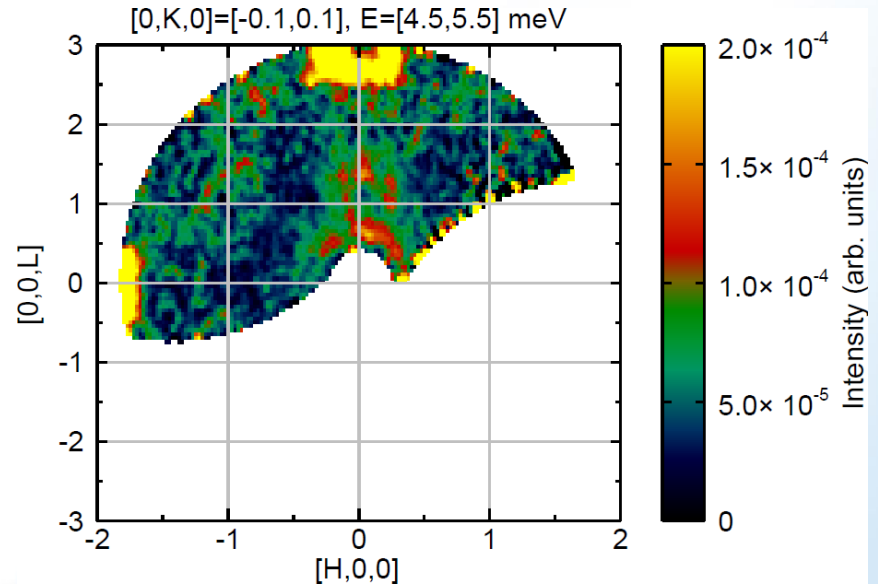
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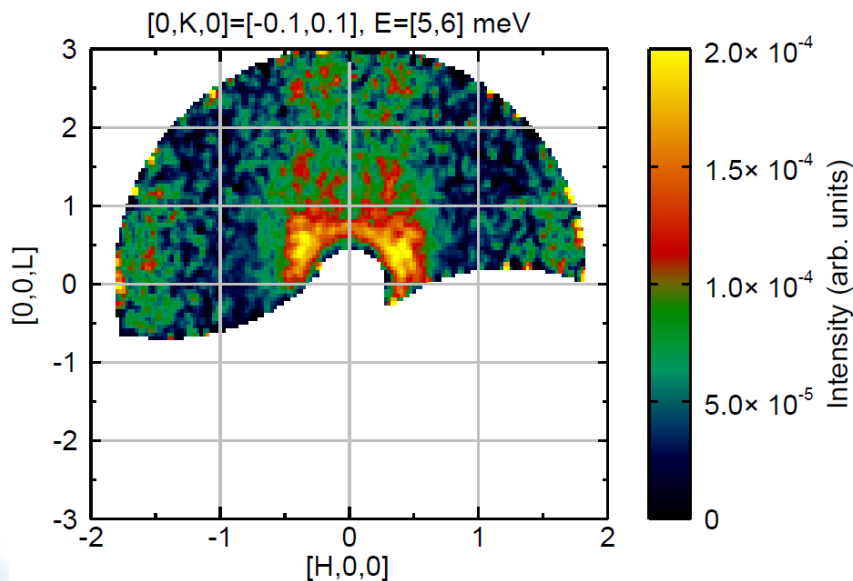
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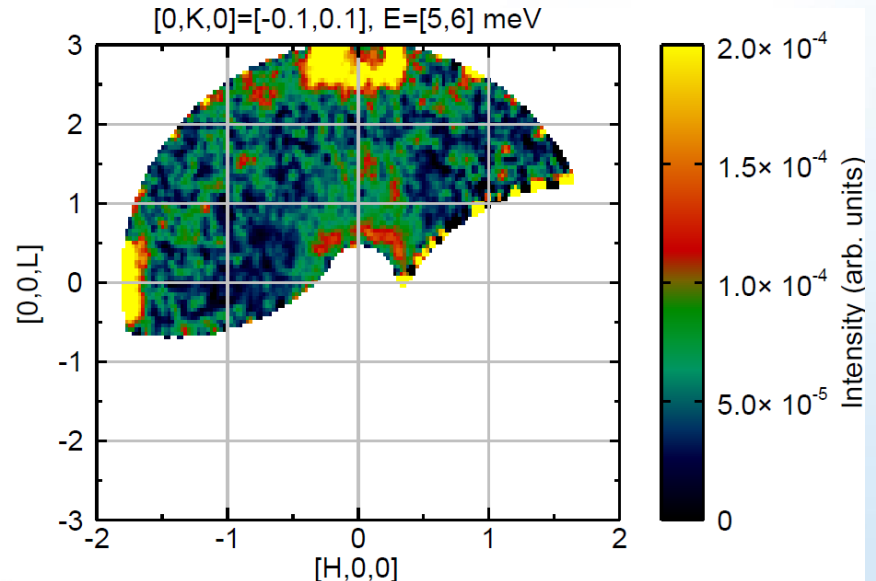
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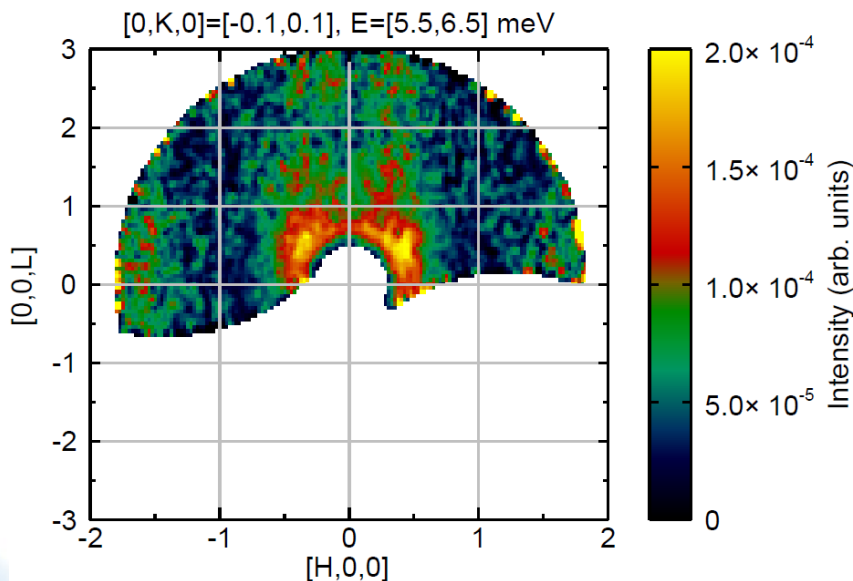
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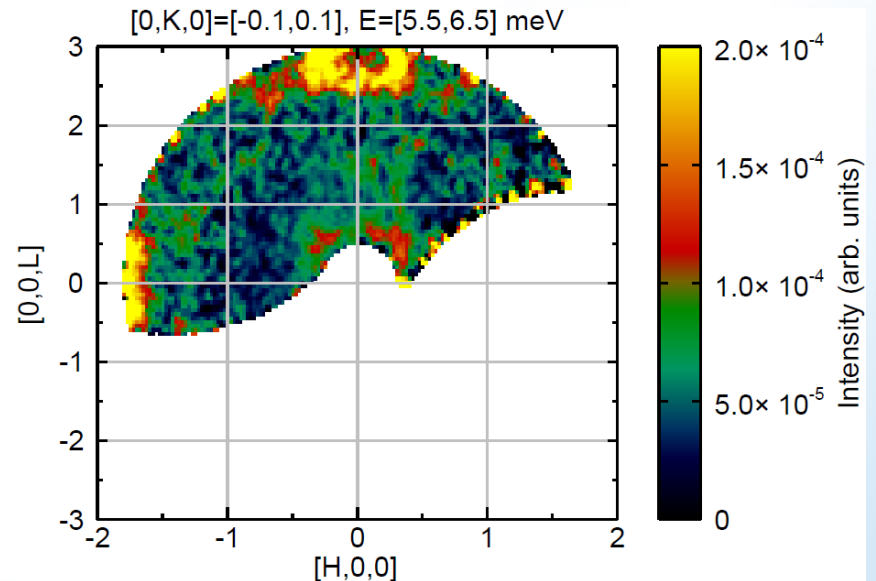
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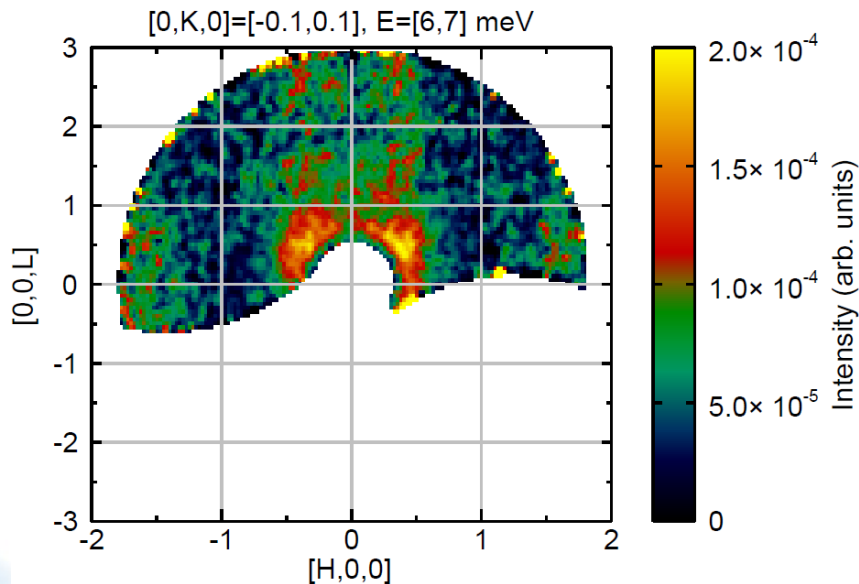
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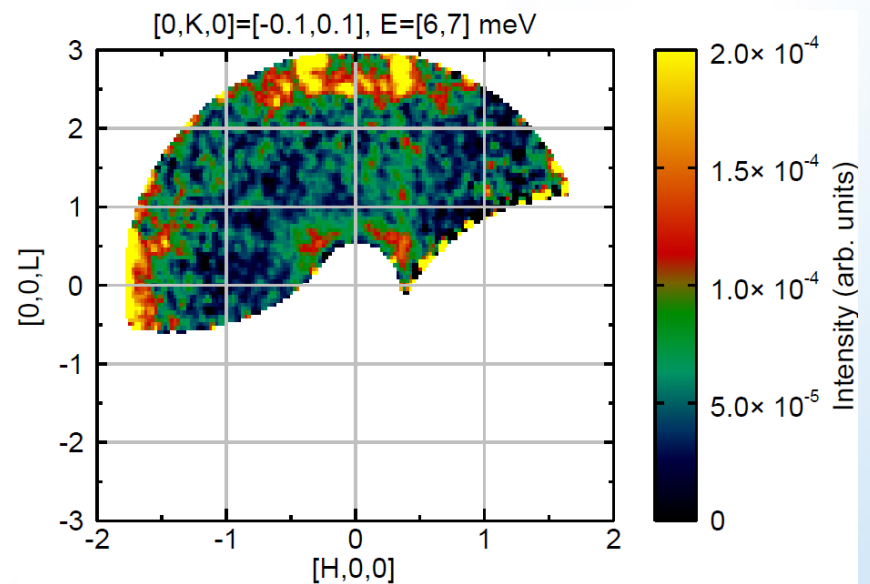
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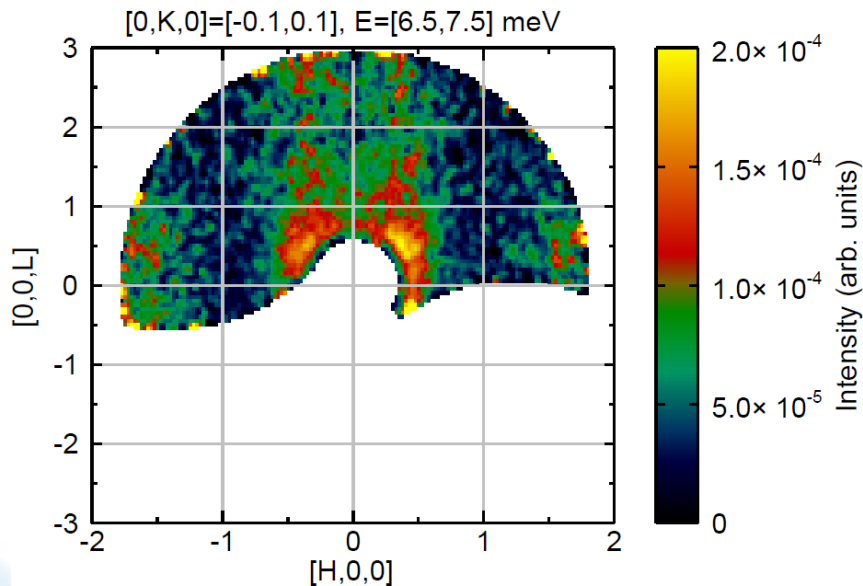
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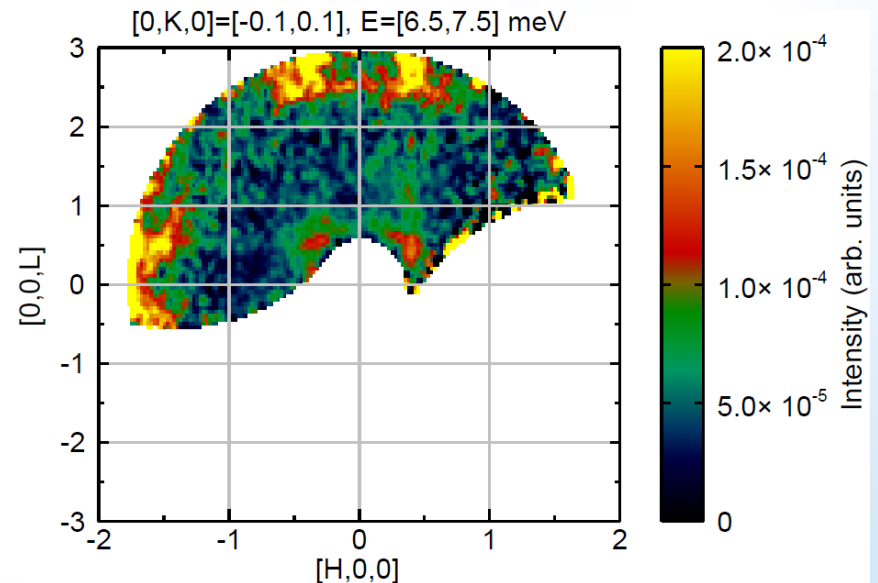
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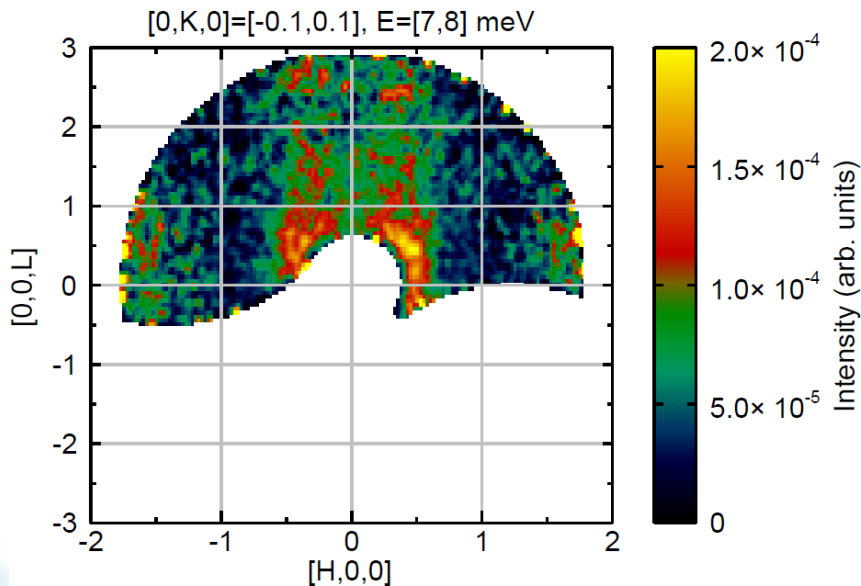
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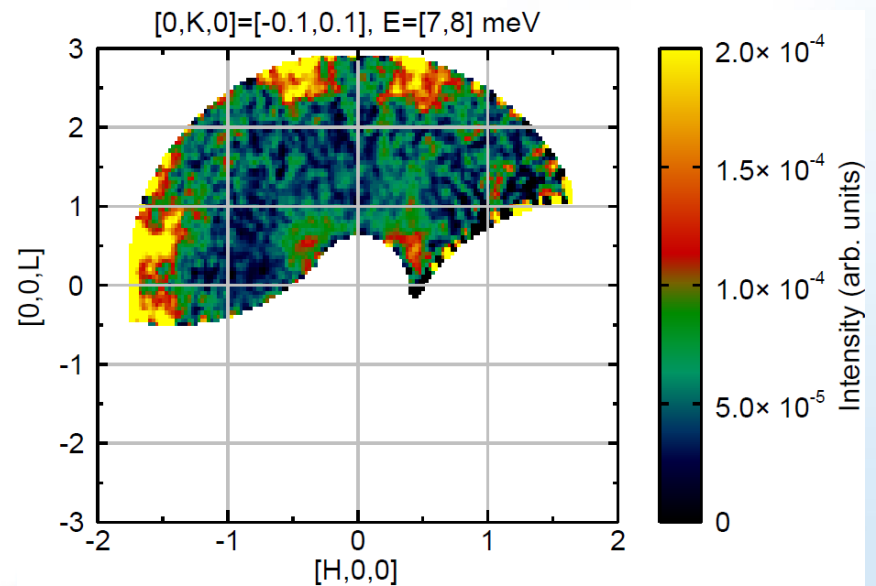
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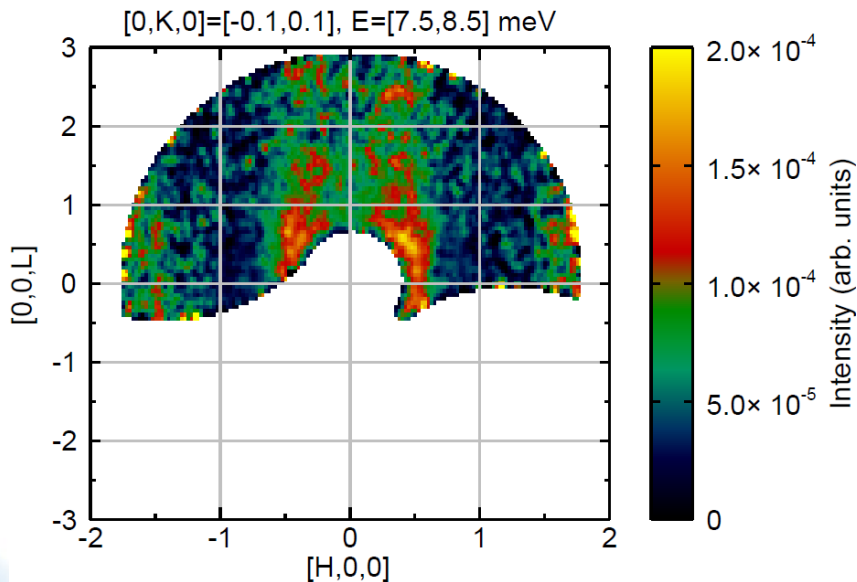
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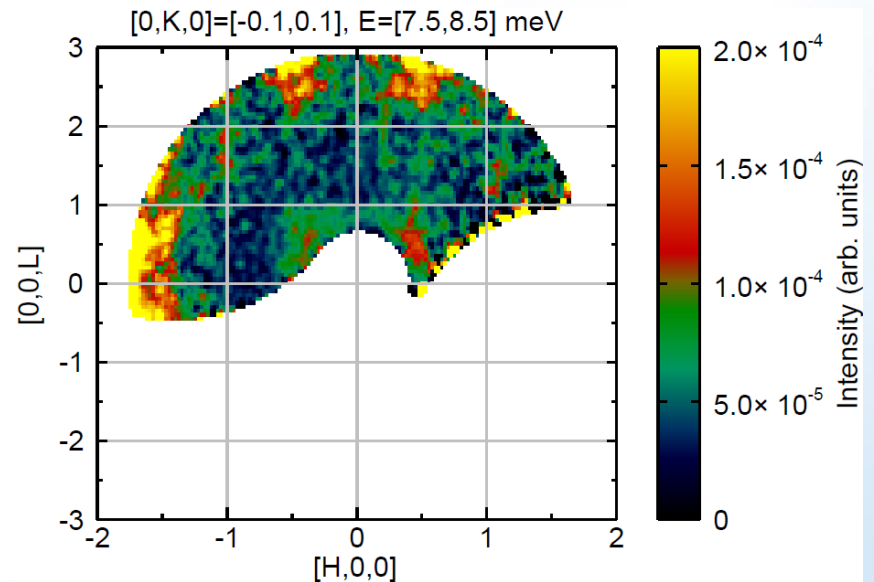
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SNS @ 1.3MW. $E_i = 20$ meV. Each dataset is approximately 20 hours on HYSPEC: 6 min for each of the 191 angular positions of the sample.

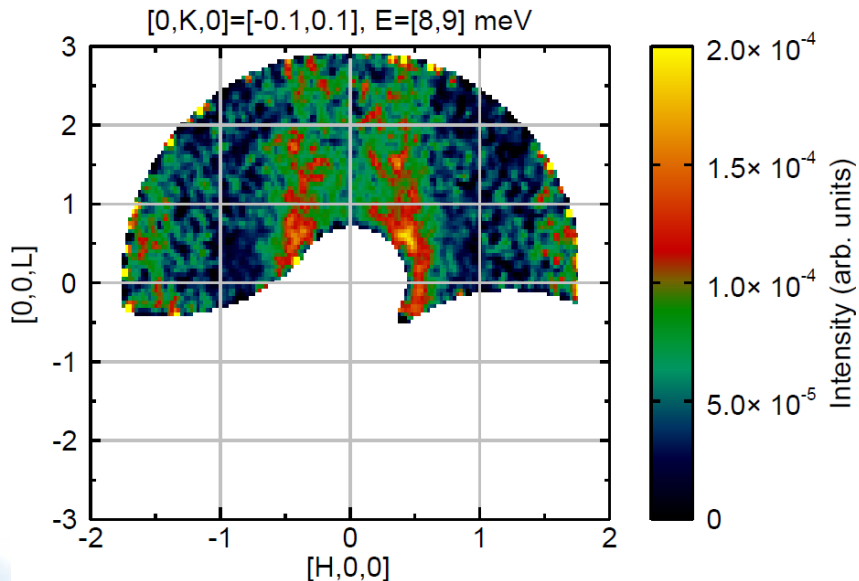
Magnetic and non-magnetic excitations in $\text{Fe}_{1.1}\text{Te}$ by polarized neutron scattering on HYSPEC

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Comparison of the equivalent slices from the Spin-Flip (left) and the Non-Spin-Flip (right) raw data sets

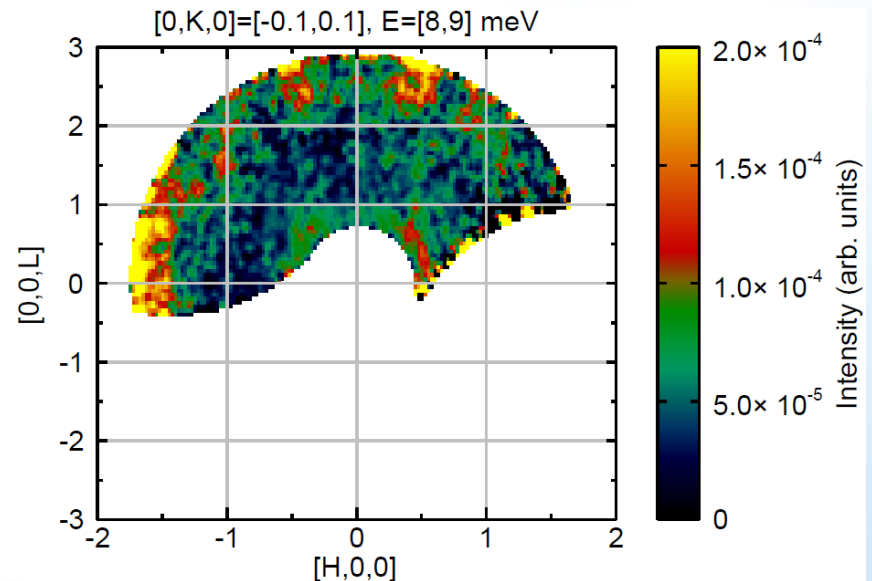
Spin-Flip Scattering (magnetic)

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Non-Spin-Flip Scattering (phonon)

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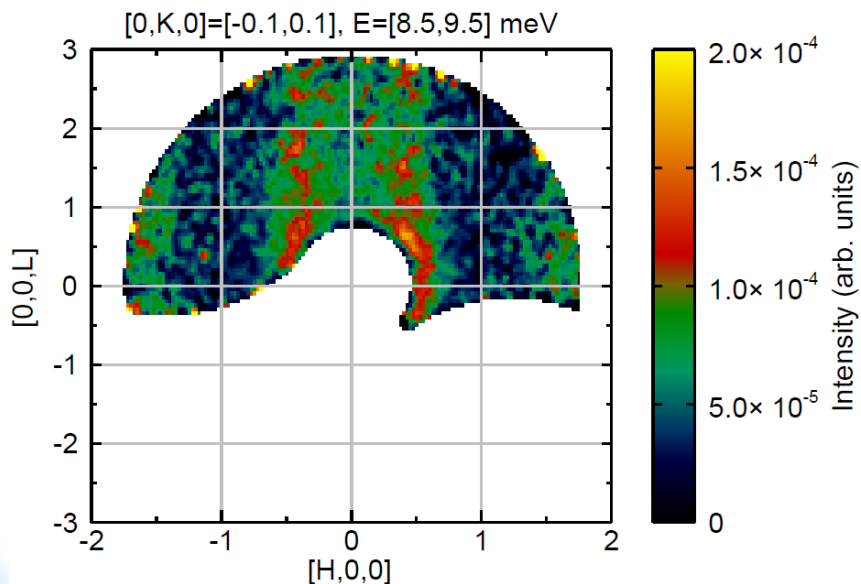
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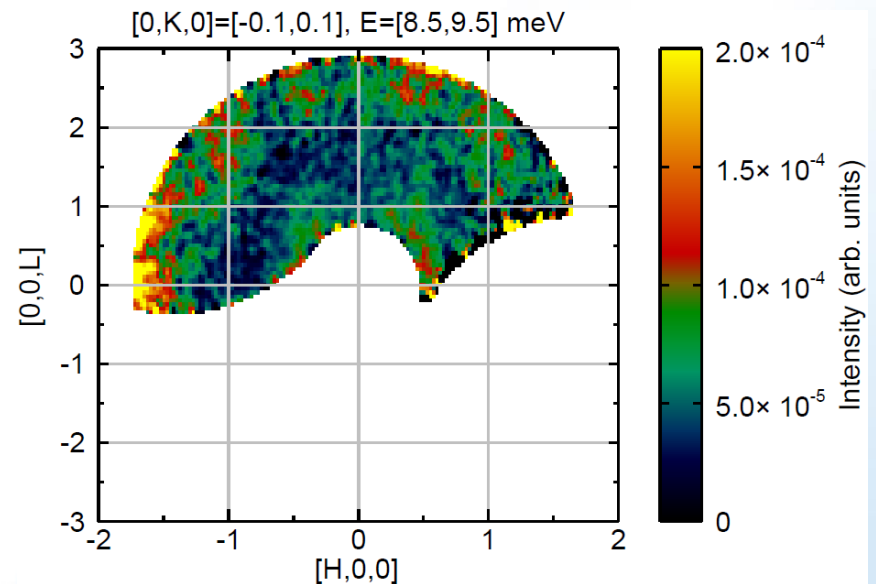
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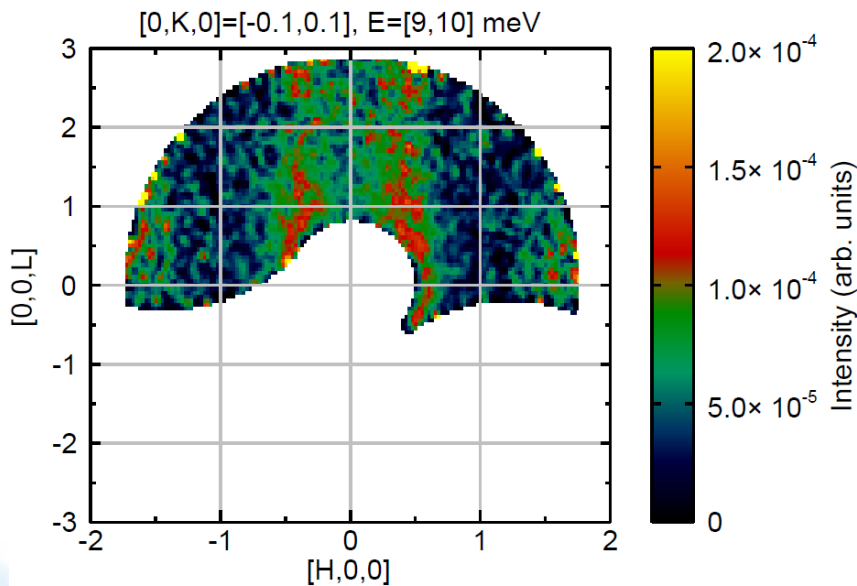
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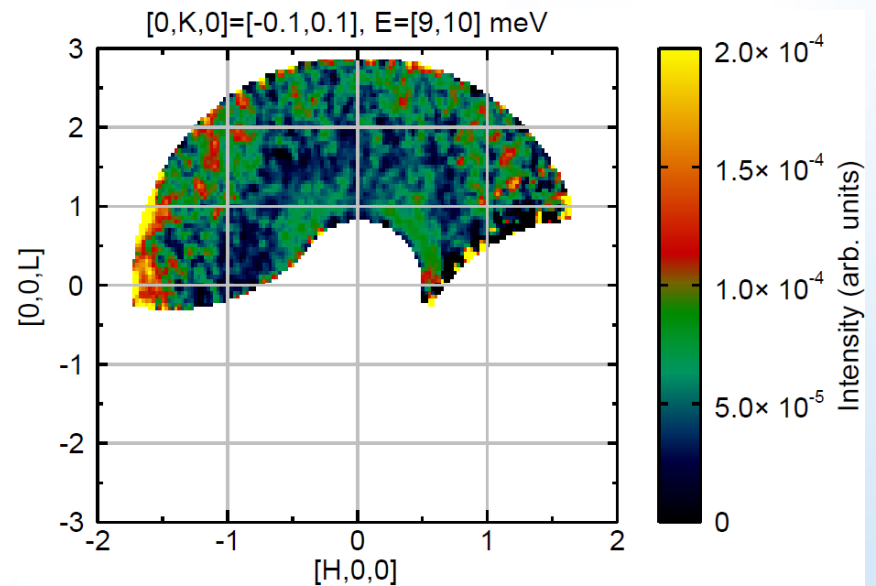
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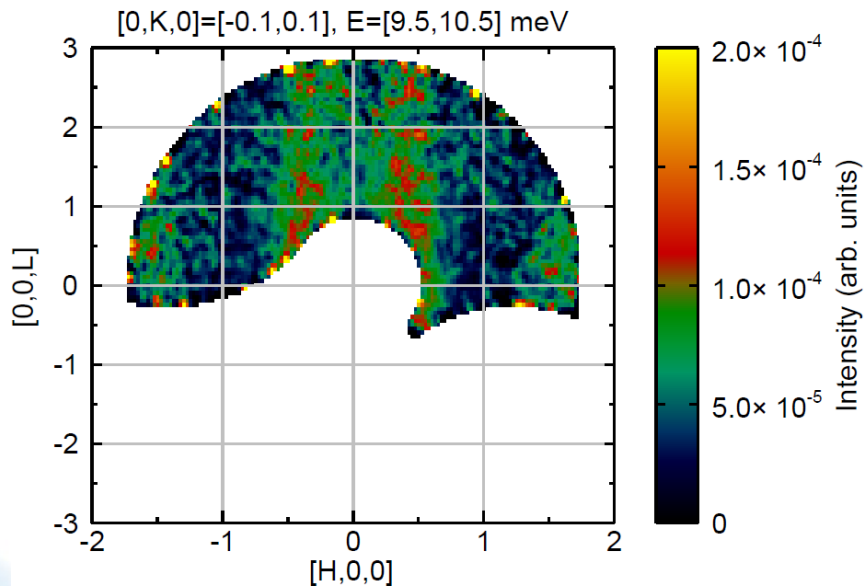
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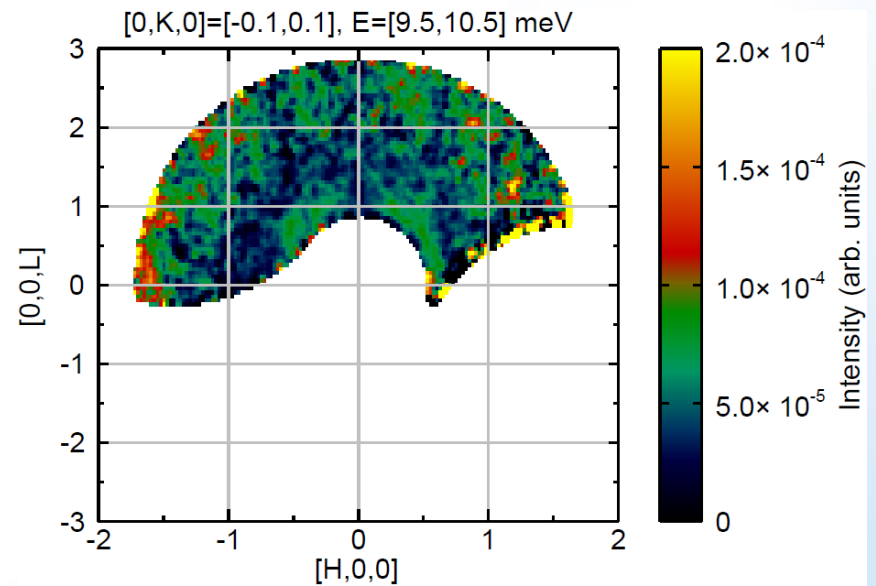
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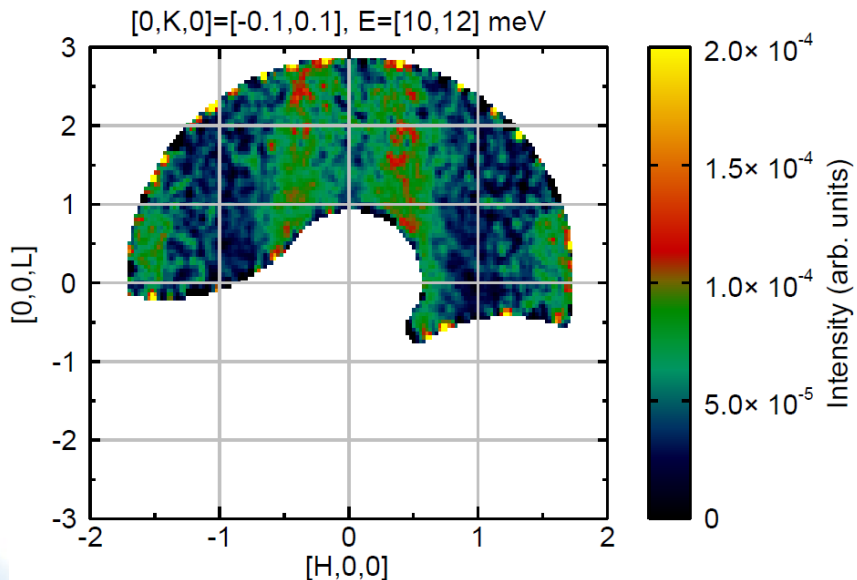
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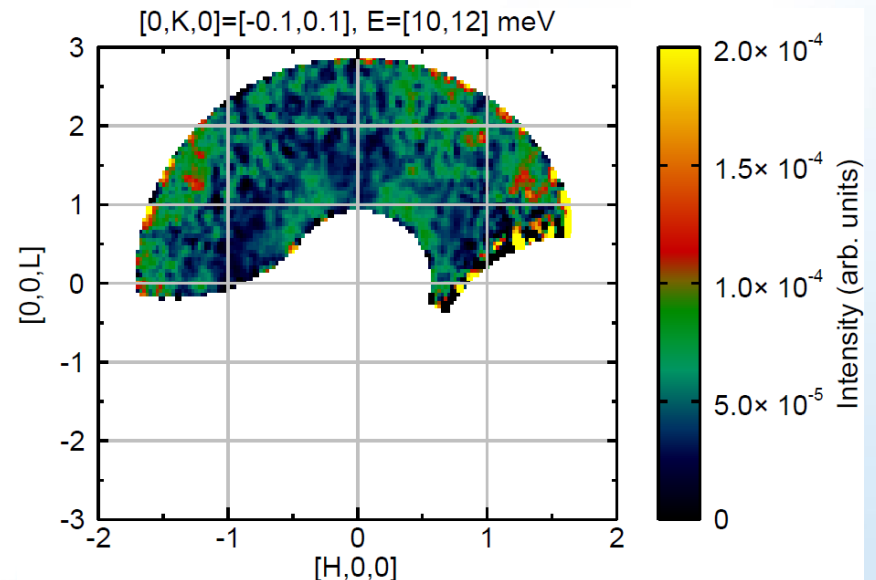
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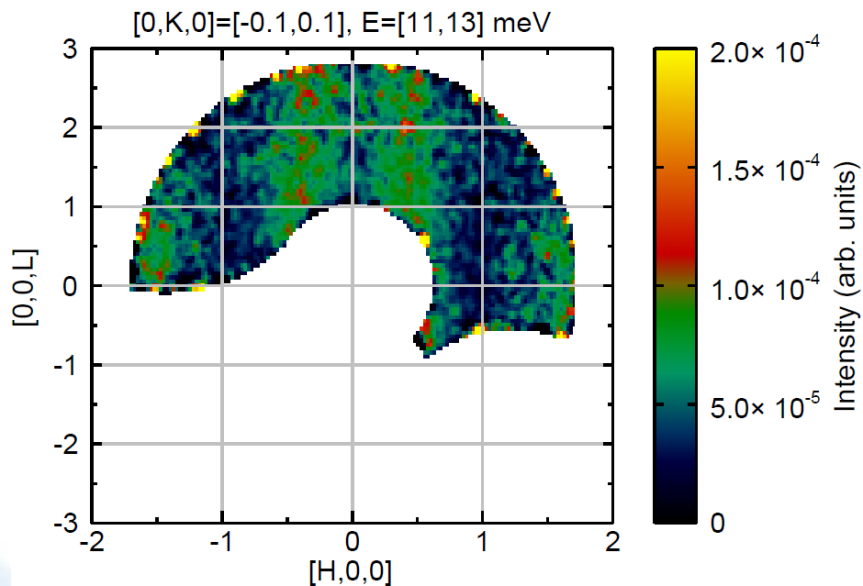
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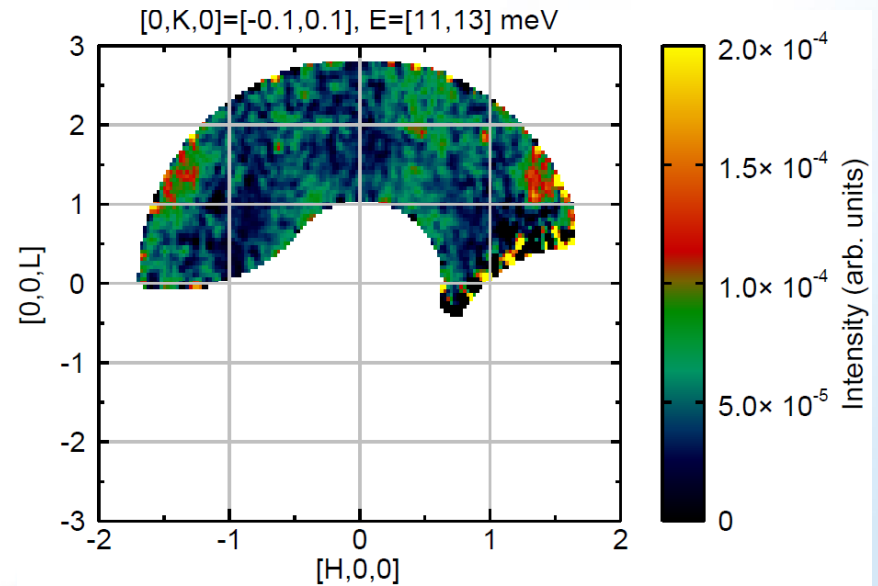
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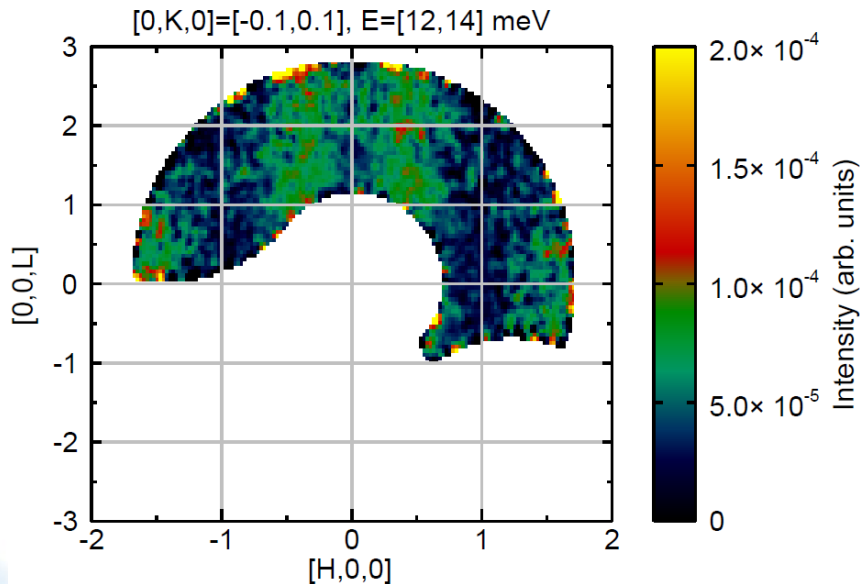
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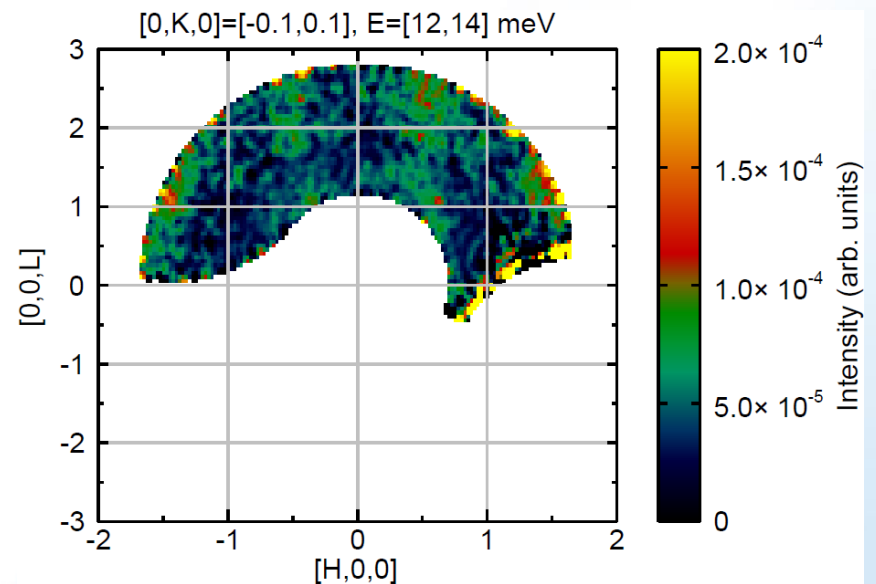
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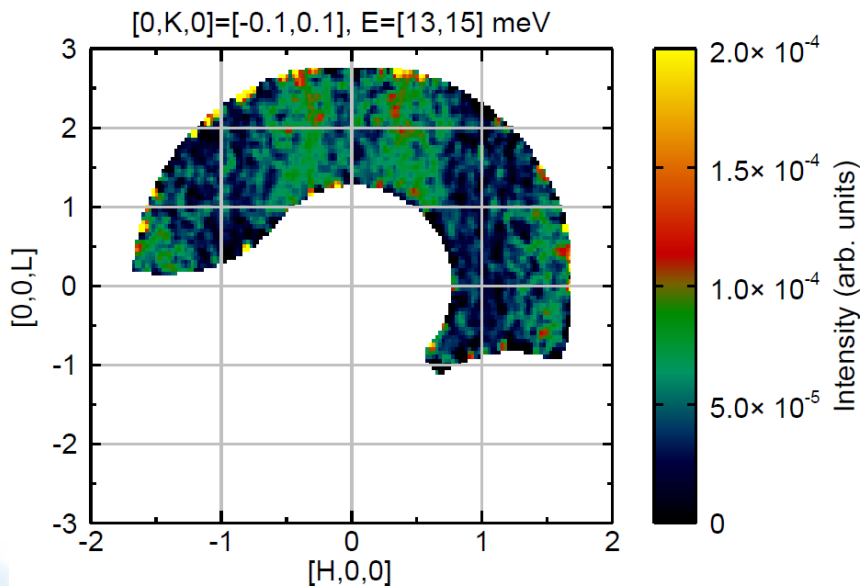
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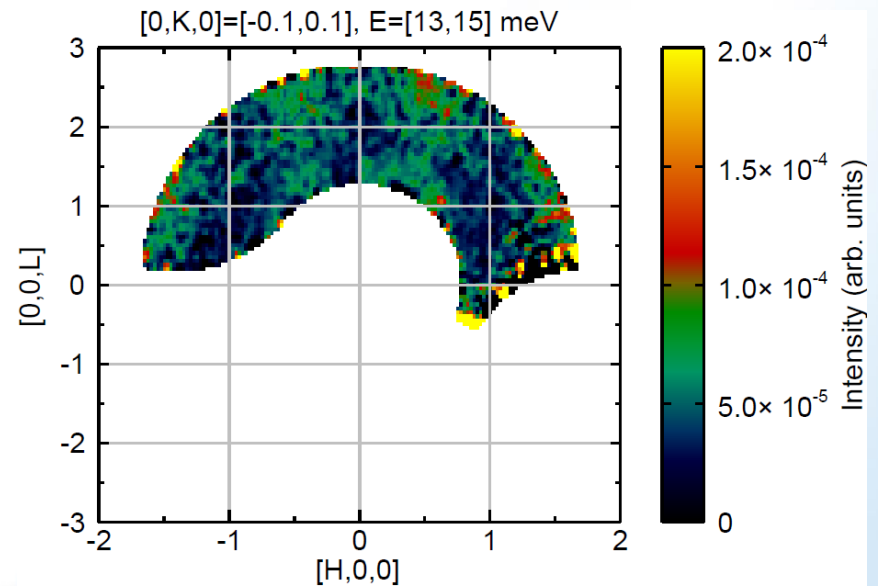
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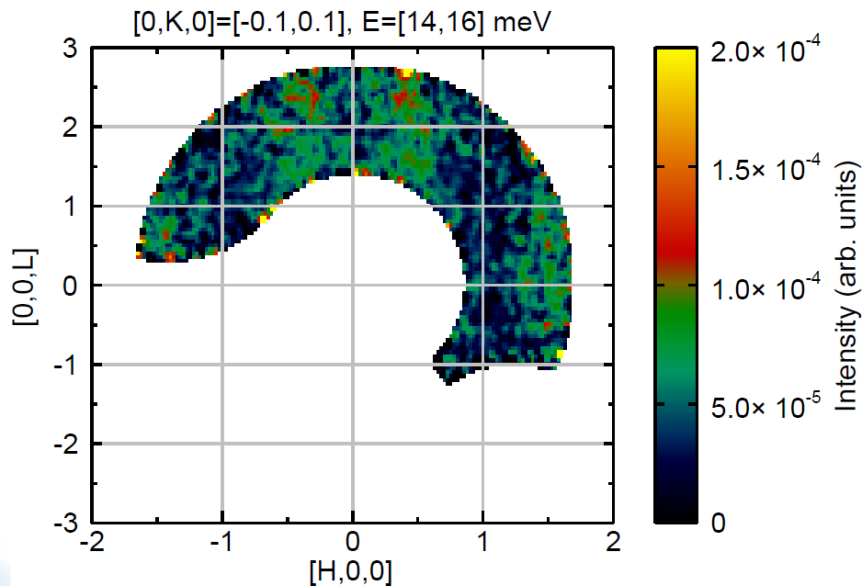
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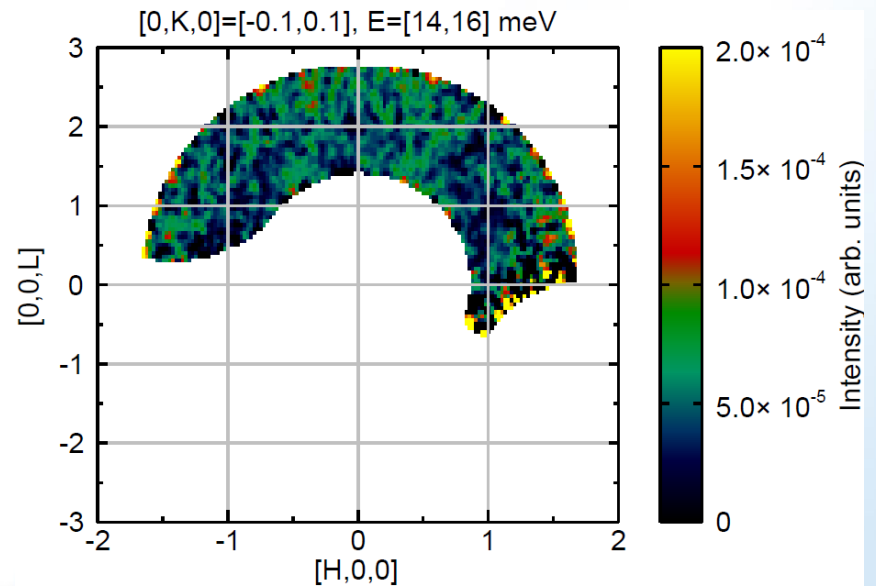
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Summary

- Polarized neutron surveys of a large volume of the sample's phase space are possible despite
 - Factor 20 to 80 transmission losses in the polarized setup
 - Restricted field of view at the focus of the radial supermirror array
 - Large number of corrections for transmission and deflection in the polarized setup (talks by A. Savici and B. Winn)
- It's a miracle?
 - Careful experiment planning and execution
 - Precise instrument and sample alignment
 - Steady and maintenance-free setup
- It's a miracle!

