The Neutron Resonance Spin Echo Option @ V2/FLEXX at BER II

Klaus Habicht

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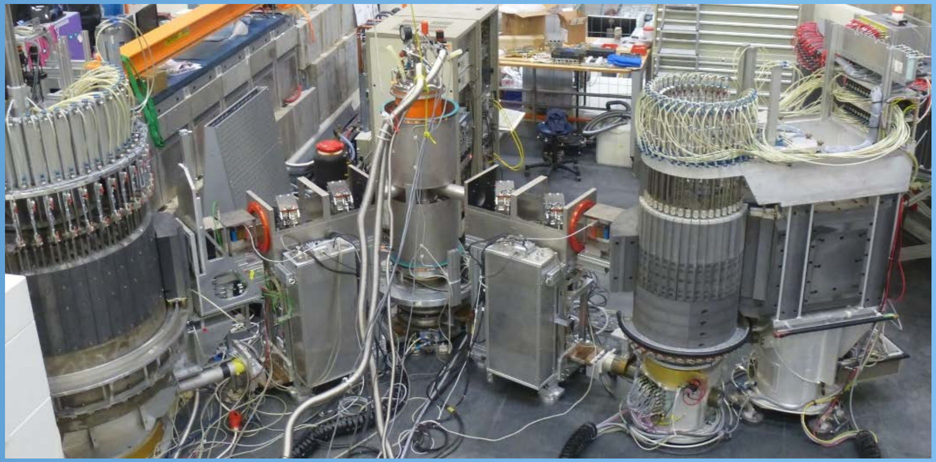
für Materialien und Energie



Key Question

Is an NRSE option better than a dedicated instrument?

V2/FLEXX, the cold-neutron host spectrometer

Features of the NRSE option at V2/FLEXX

Acknowledgements

FLEX-upgrade project

Duc Manh Le – now STFC, ISIS, UK
Markos Skoulatos – now MLZ, Germany
Kirrily Rule – now ANSTO, Australia

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now Univ. Stavanger, Norway
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Zhilun Lu, HZB, Germany
Zita Hüsges, HZB, Germany
Siqin Meng, HZB, Germany

Thomas Krist, HZB, Germany

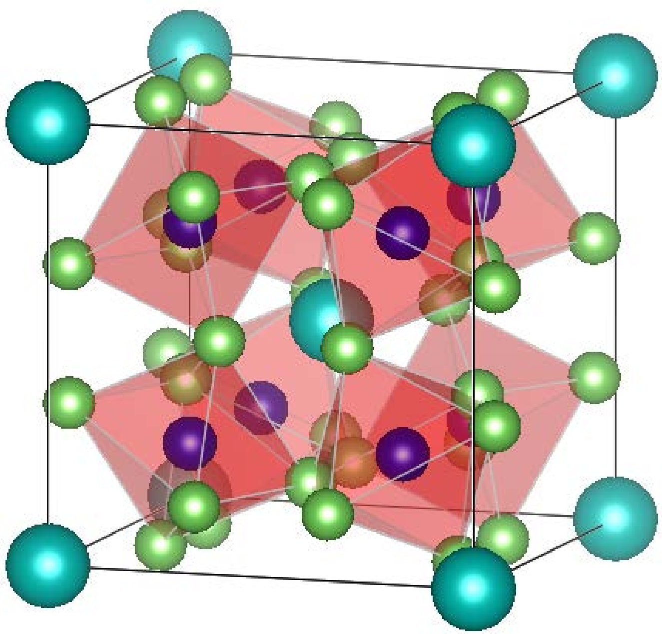
NRSE

Felix Groitl – now at EPFL and PSI,
Thomas Keller, MPI Stuttgart, Germany

Probing Material Structures: Scattering Techniques

structure

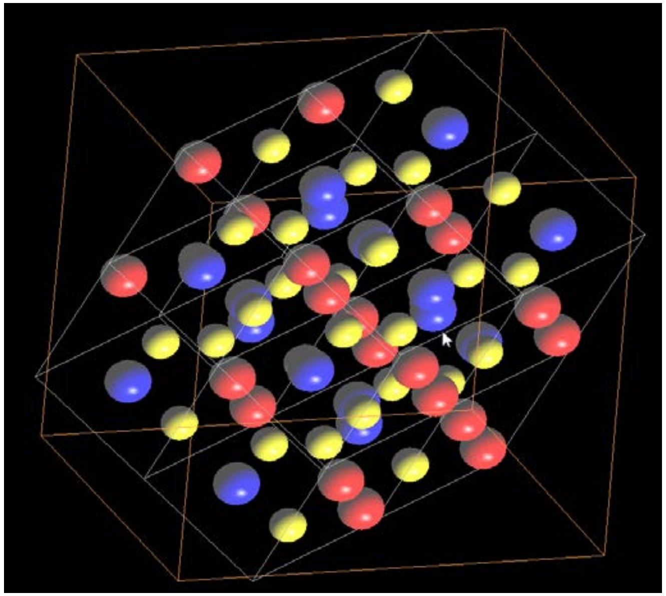
Intensity (arbitrary units)



Distance of lattice planes d (Å)

dynamics

Energy transfer (meV)

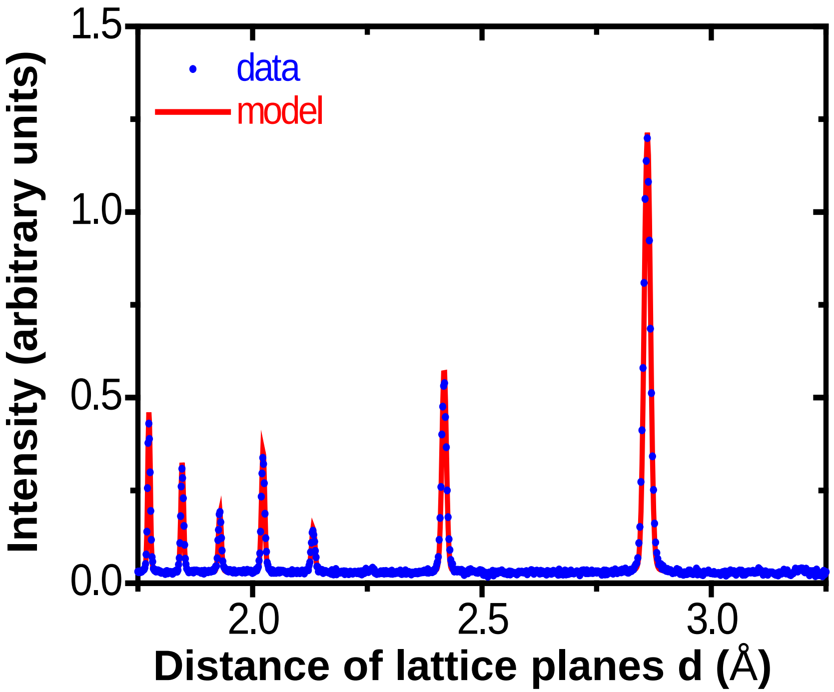


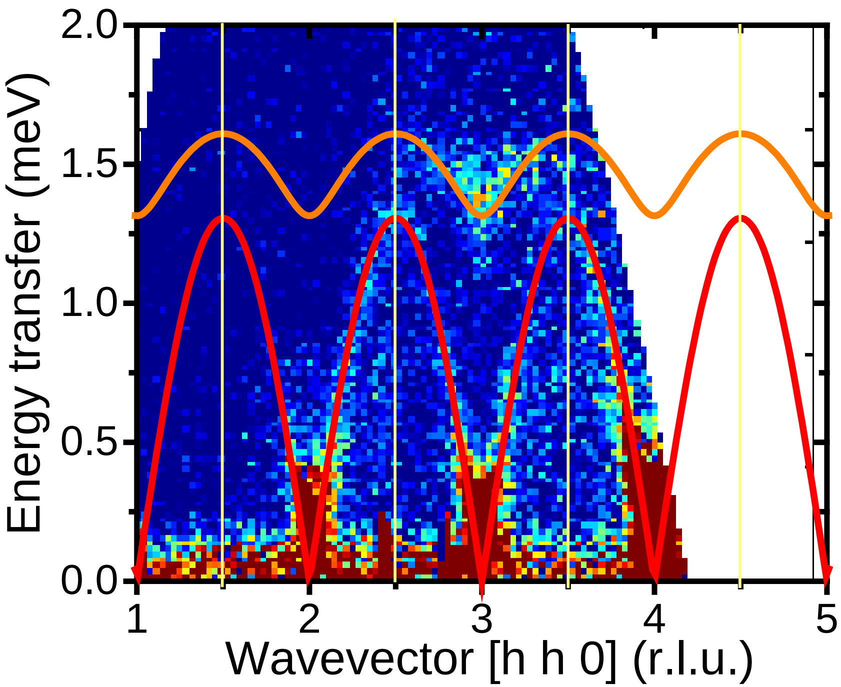
Wavevector q [h h 0] (r.l.u.)

Neutron scattering techniques probe static or dynamic correlations

Probing Material Structures: Scattering Techniques

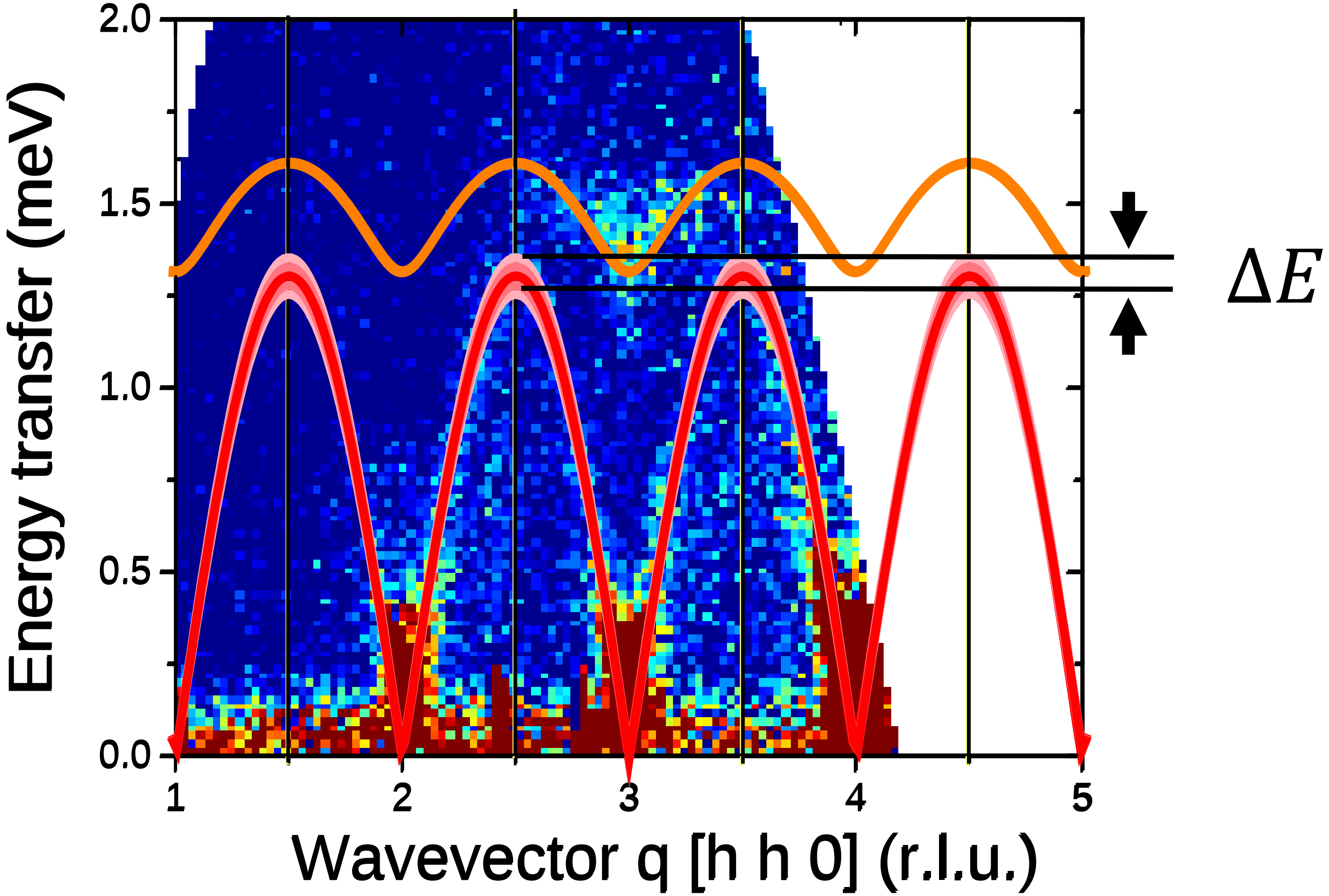
structure | **dynamics**





Neutron scattering techniques probe static or dynamic correlations

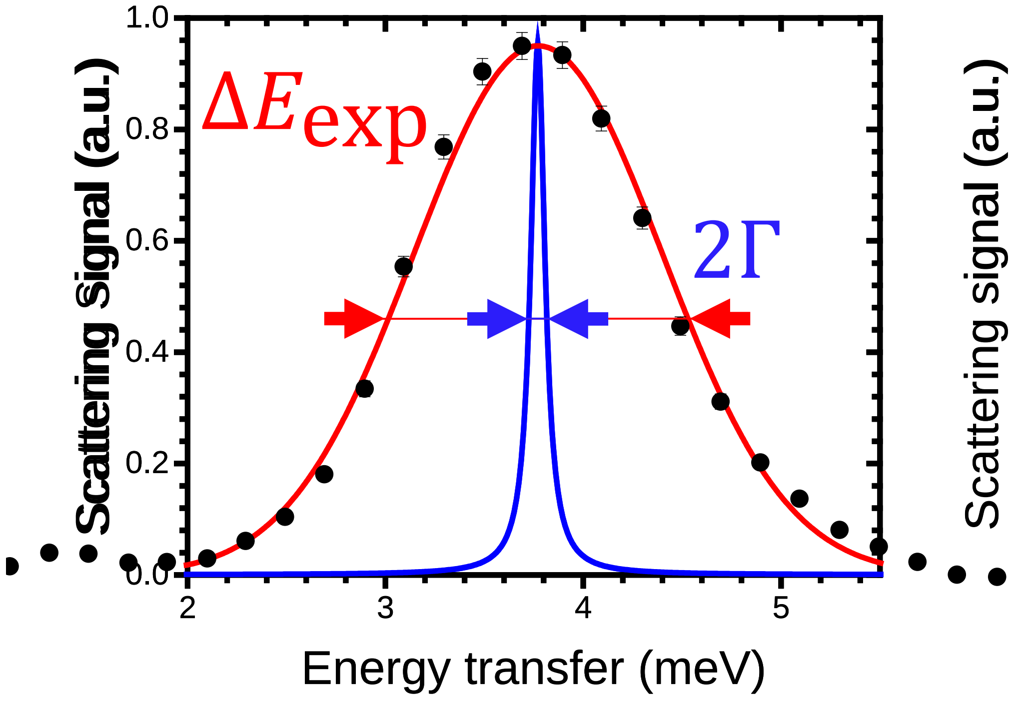
NRSE Motivation: Quasiparticle Linewidth

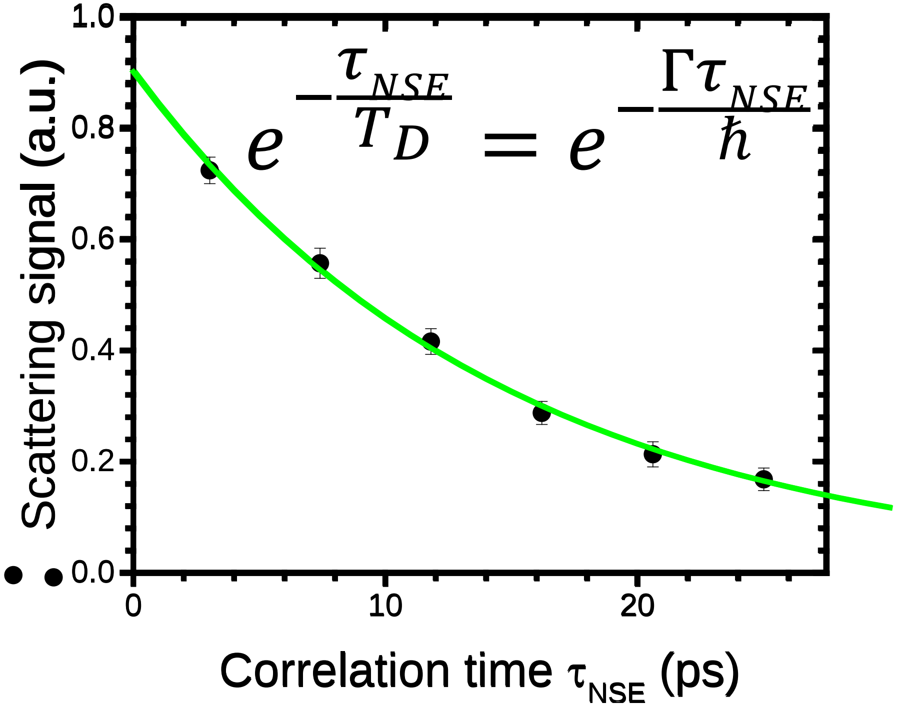


Dispersion relates quasiparticle energy to quasiparticle momentum
Energy *width* in the dispersion encodes quasiparticle lifetime

Quasiparticle Linewidth and Lifetime

energy domain **time domain**



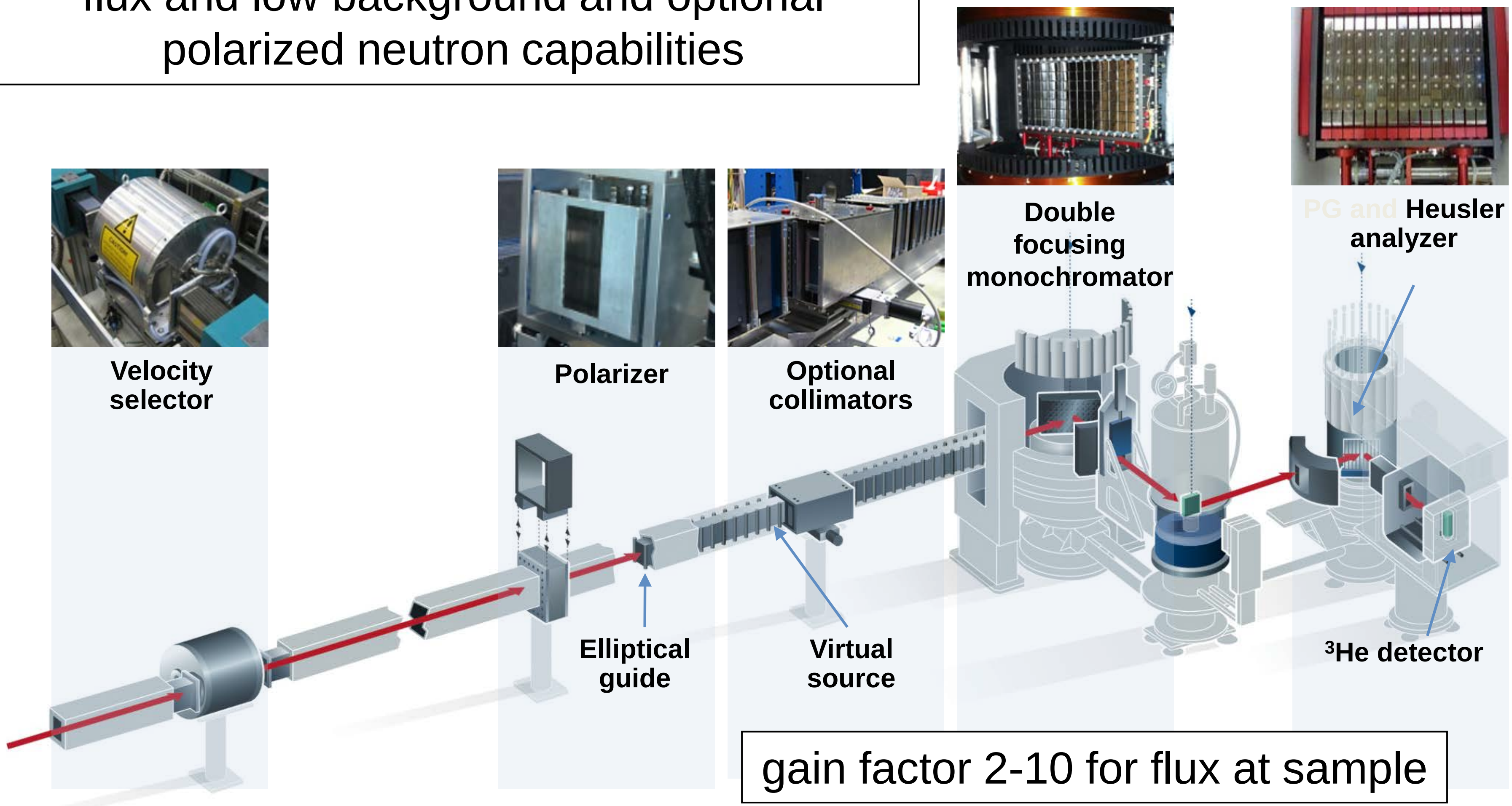


Energy *linewidth* Γ inversely proportional to *lifetime* T_D :

$$\Gamma = \hbar / T_D$$

The Upgraded Cold Neutron TAS FLEXX

new primary spectrometer optimized for high flux and low background and optional polarized neutron capabilities



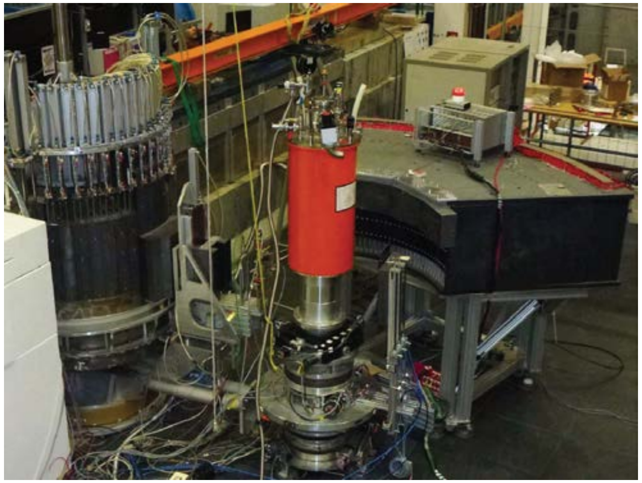
gain factor 2-10 for flux at sample

M. D. Le, et al., Nucl. Inst. Meth. A 729, 220-226 (2013)

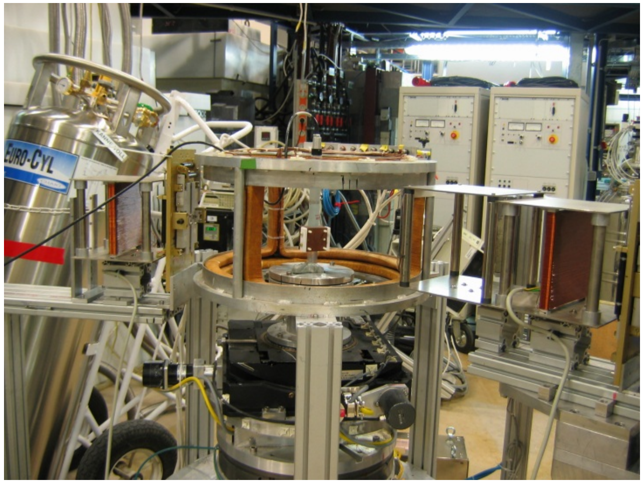
FLEXX Options

FLEXX standard TAS mode

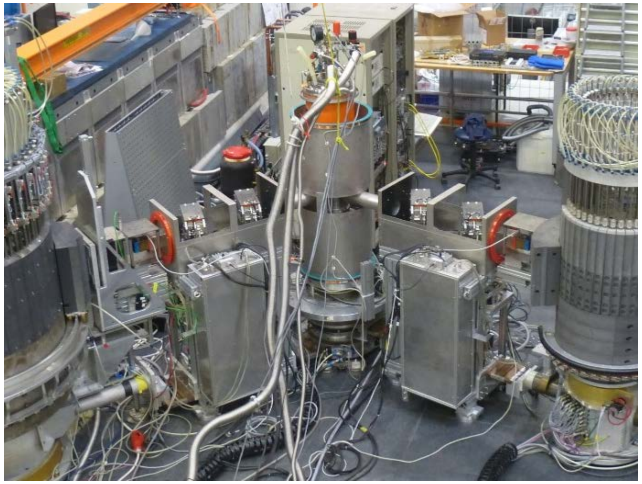
MultiFLEXX backend



XYZ polarization analysis



Neutron Resonance Spin Echo Option



FLEXX Polarizer: S-Bender

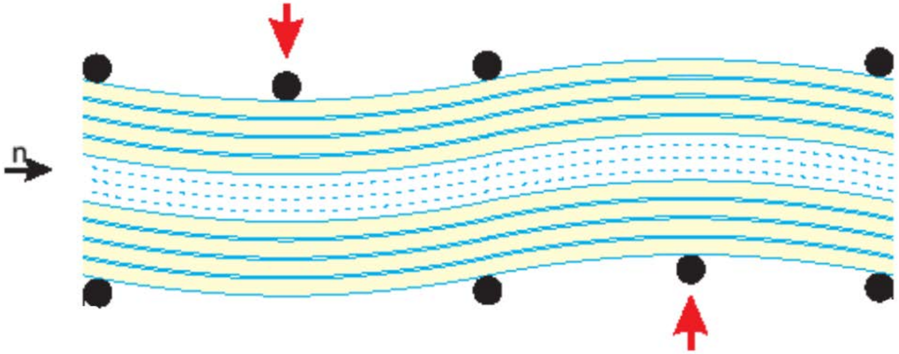
beam cross section: 60 mm x 125 mm

400 wafers 0.15 x 125 x 120 mm^3

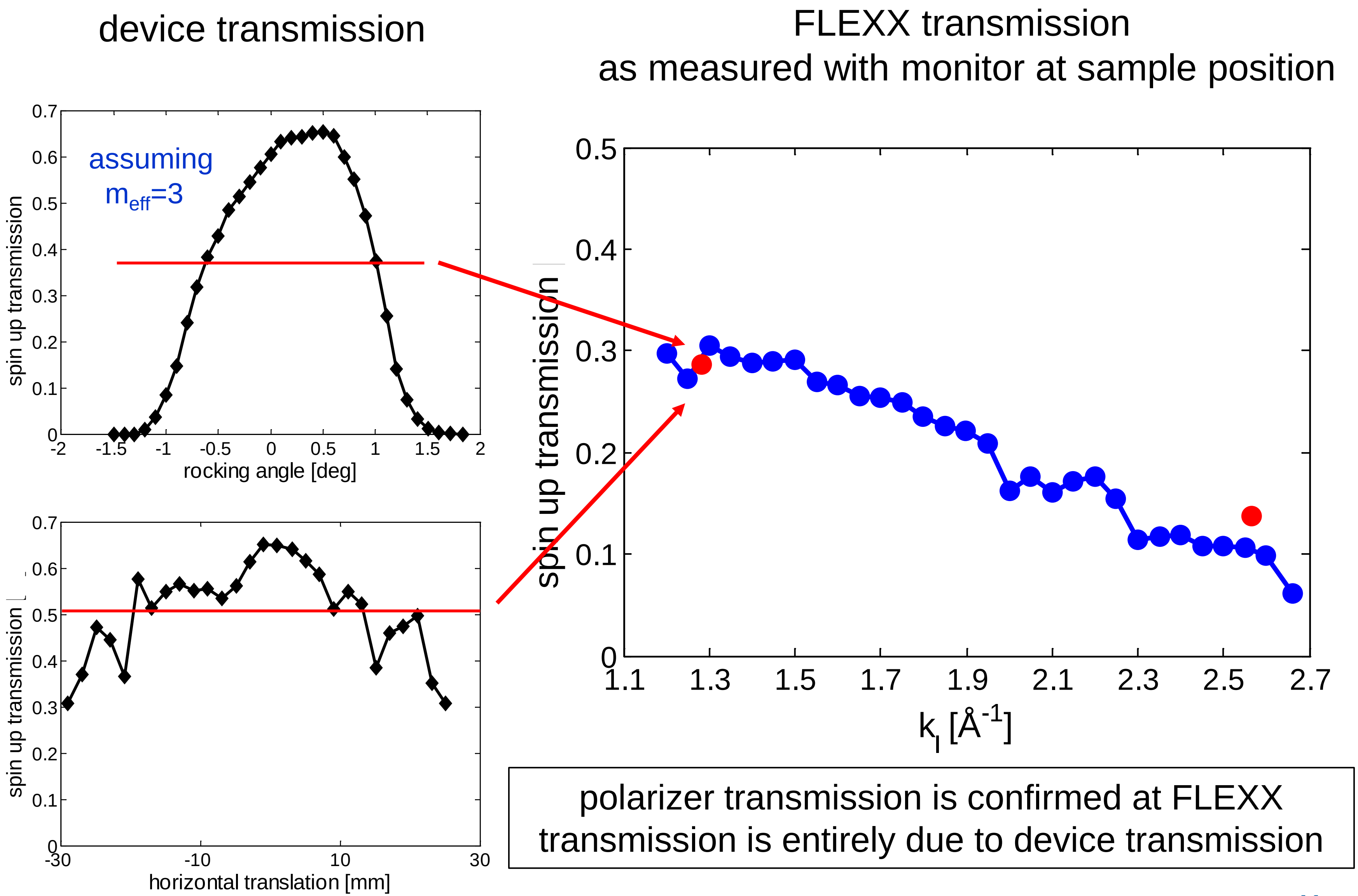
Fe-Si multilayer with m = 3

anti-reflecting Gd-layer/Si/Gd-layer

magnetization field > 300 G



FLEXX S-Bender Transmission

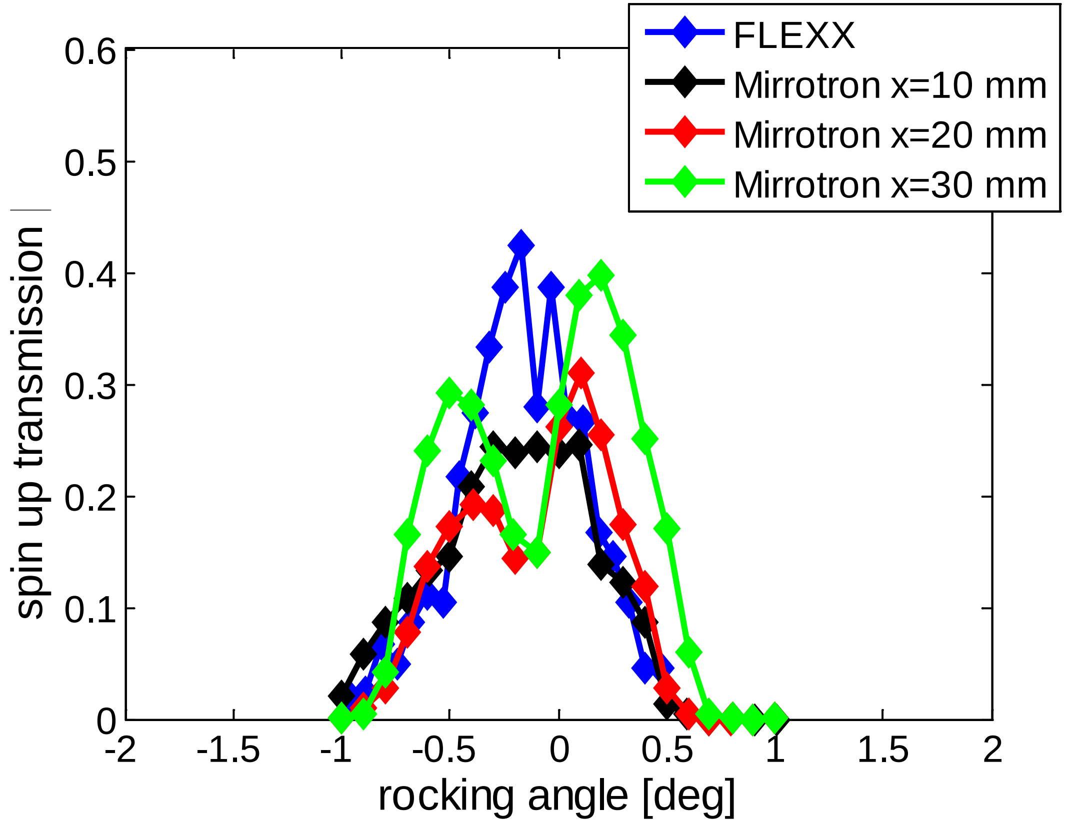


polarizer transmission is confirmed at FLEXX
transmission is entirely due to device transmission

FLEXX S-Bender Transmission

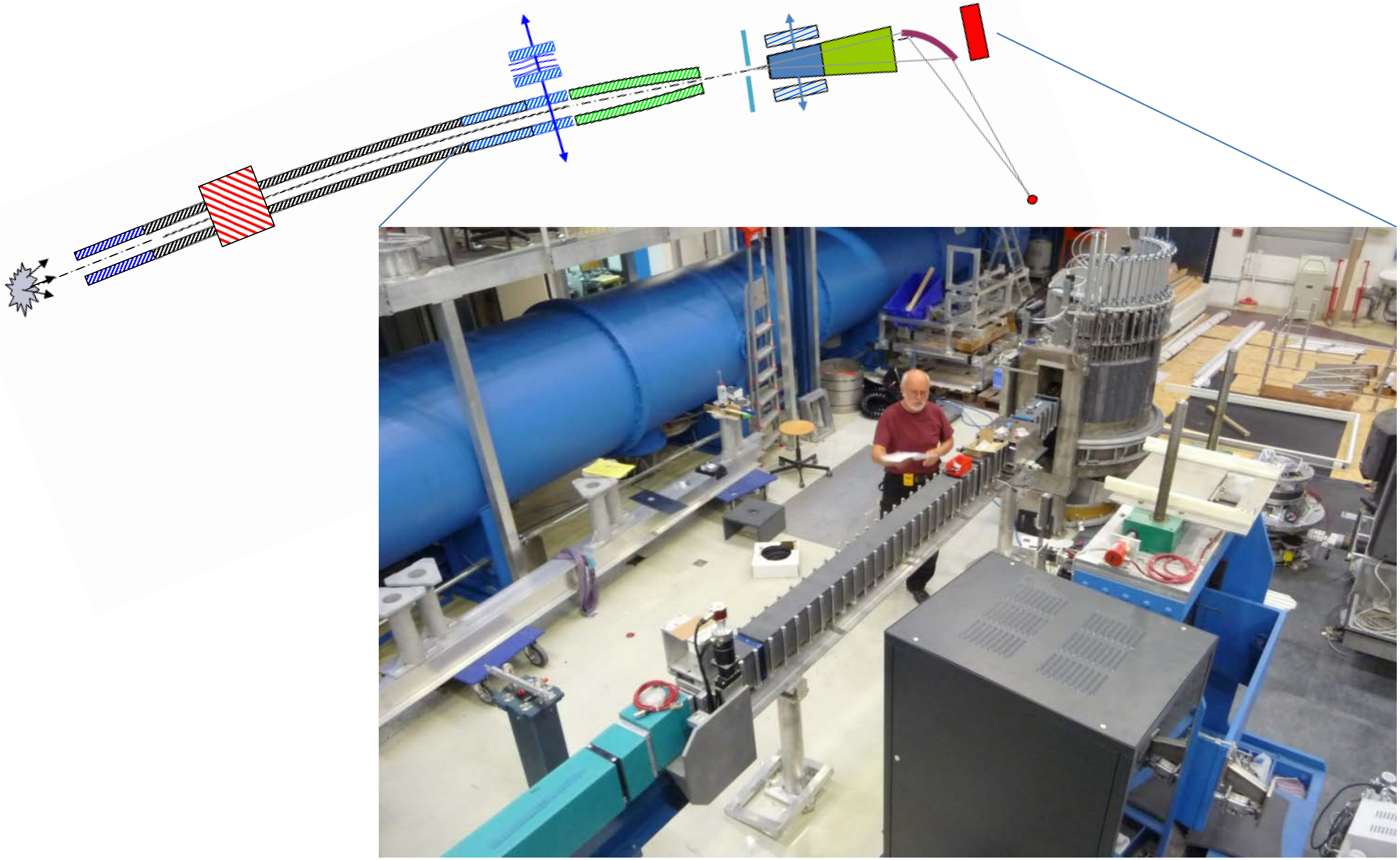
polarizer rocking scans k_I=2.56 $Å^{-1}$
(measurements by Mirrotron)

polarizer rocking scan at FLEXX k_I=2.66 $Å^{-1}$
as measured with monitor at sample position



angular acceptance of polarizer is confirmed at FLEXX

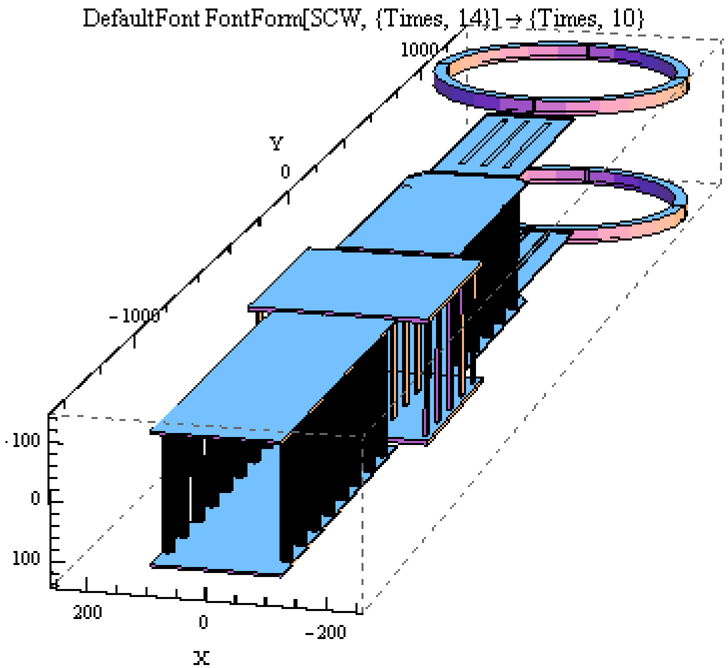
FLEXX Primary Spectrometer Guide Field

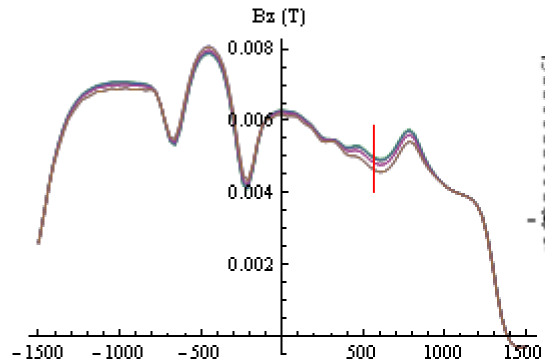


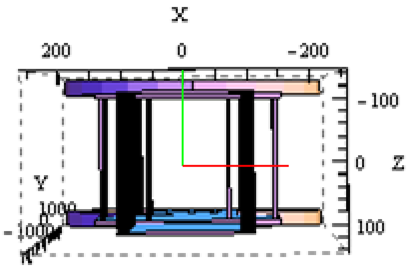
M. Skoulatos, K. Habicht, *NIM A* **647** 100 (2011)

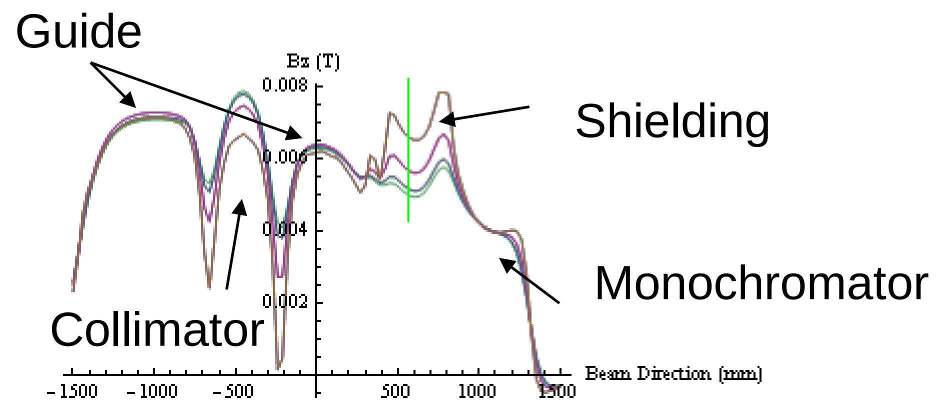
Guide Field Design Checks

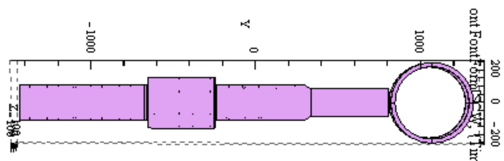
- **Calculations using Radia code from ESRF in Mathematica**
- **Magnetic field from Radia used to calculate beam depolarization using a depolarization formalism by Rosman and Rekveldt [1]**
- **McStas simulations**











[1] Rosman and Rekveldt,
Z. Phys. B – Cond.Mat. **79**, 61-68 (1990)

Guide Field Design Checks

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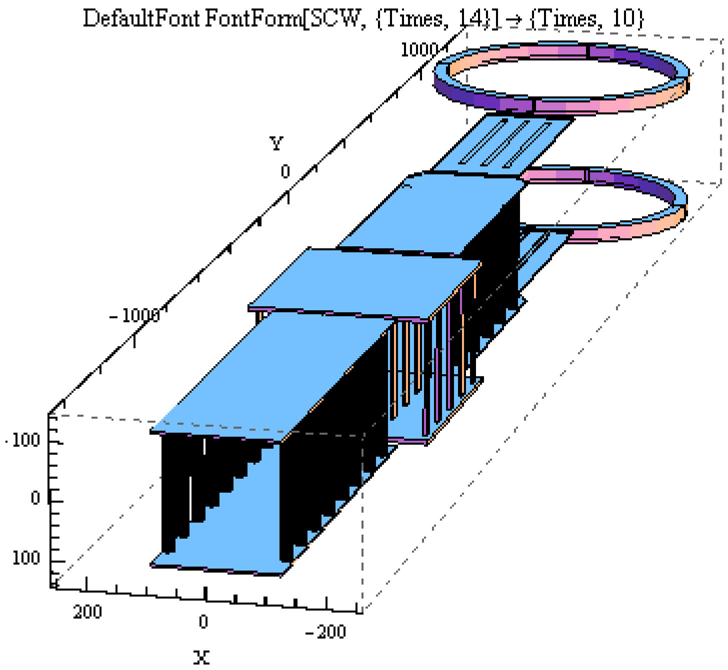
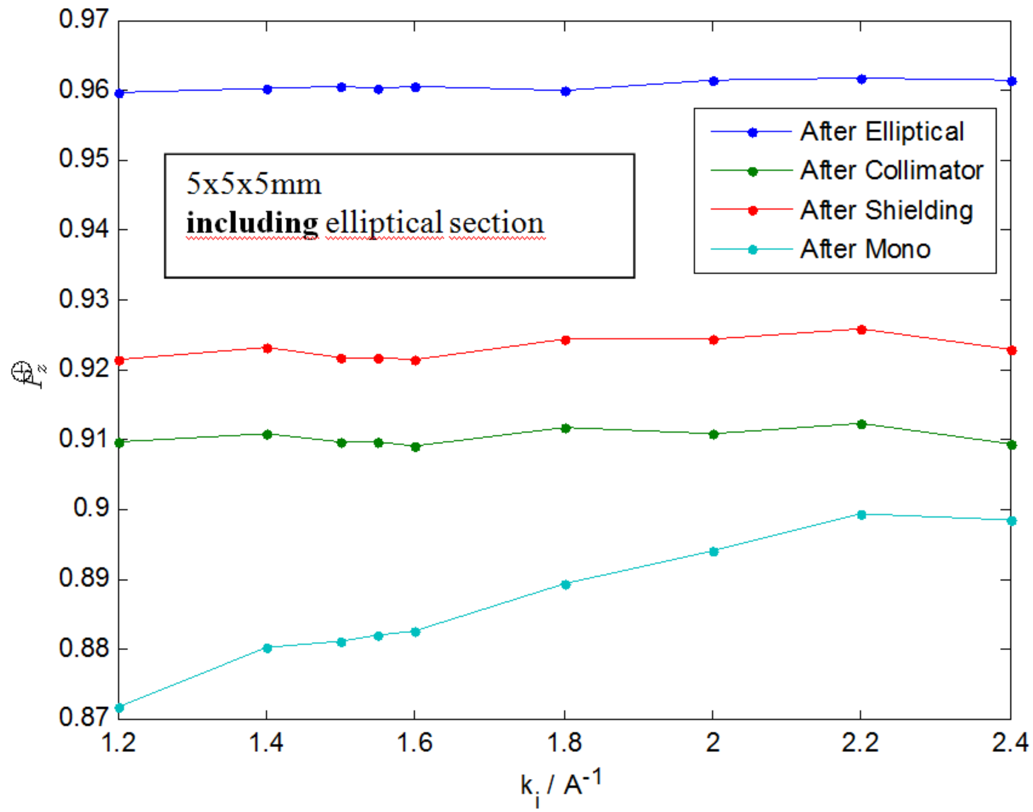
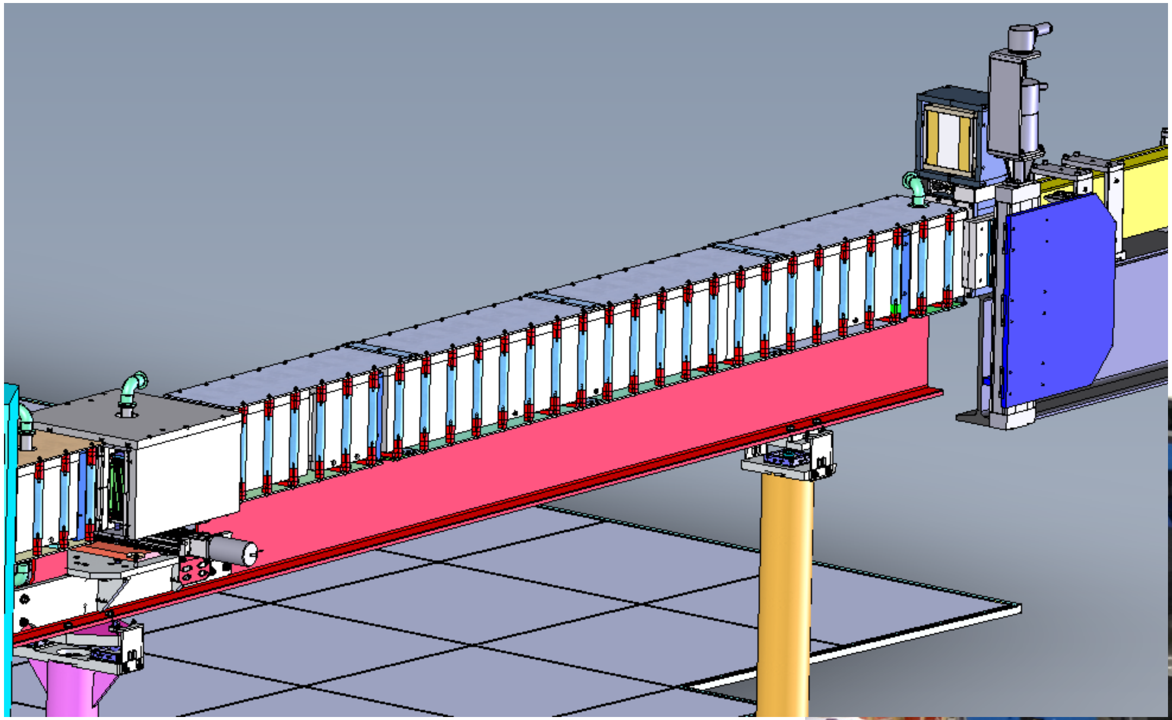


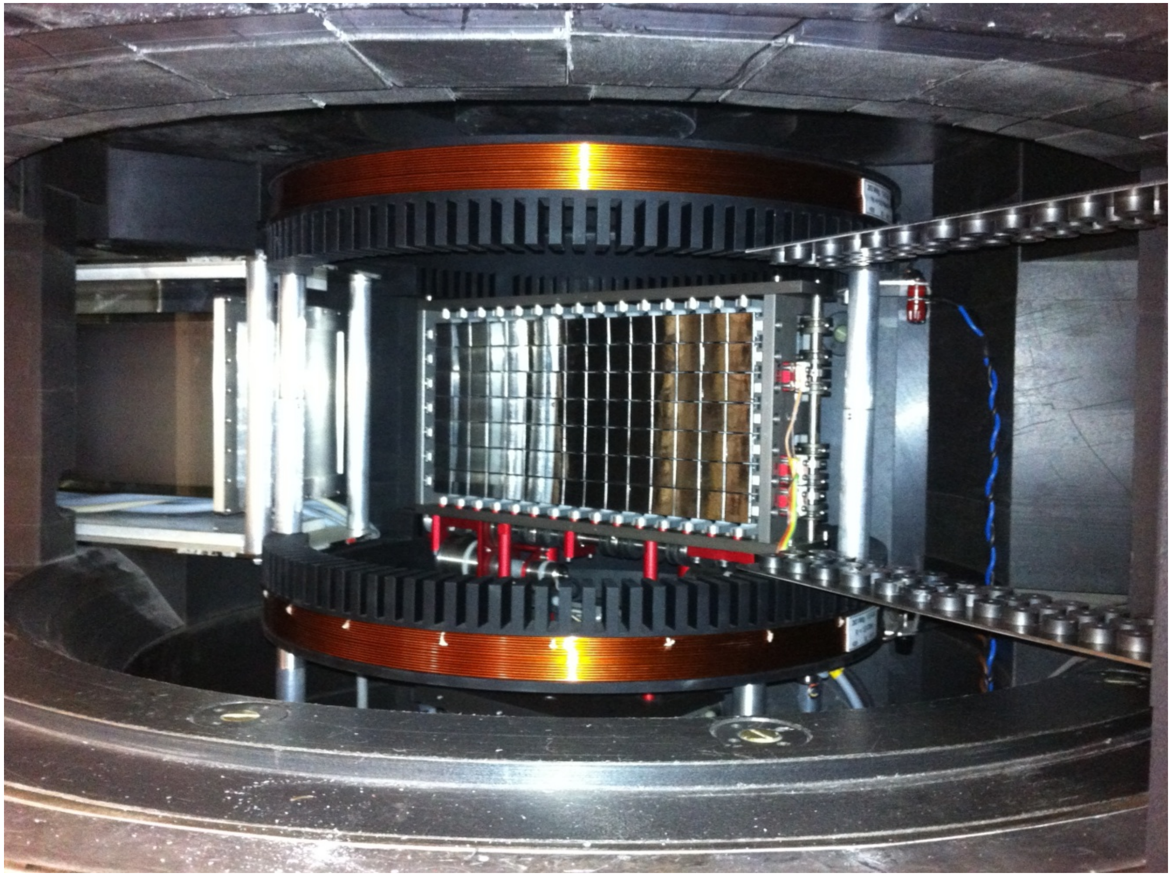


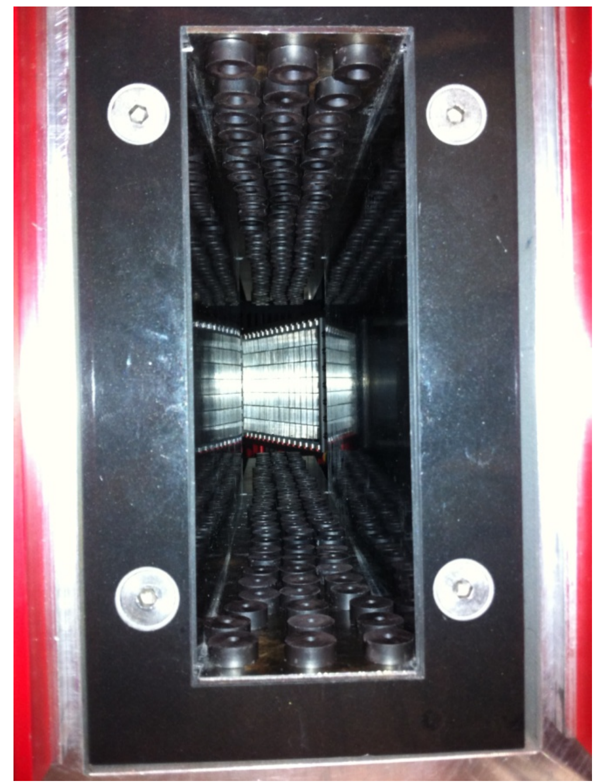
[1] Rosman and Rekveldt,
Z. Phys. B – Cond.Mat. **79**, 61-68 (1990)

FLEXX Guide Field Realization

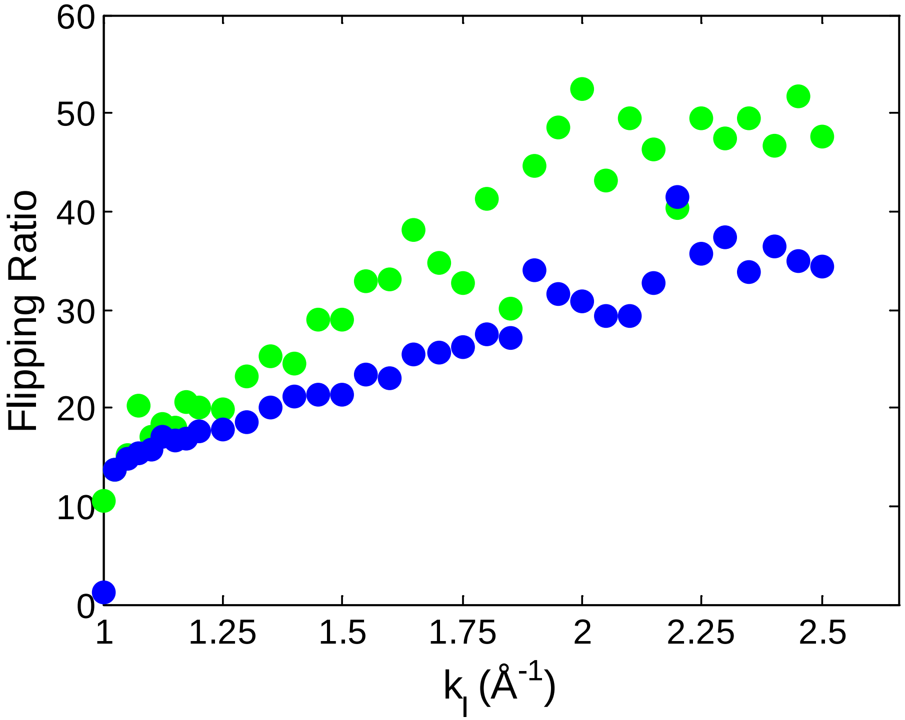


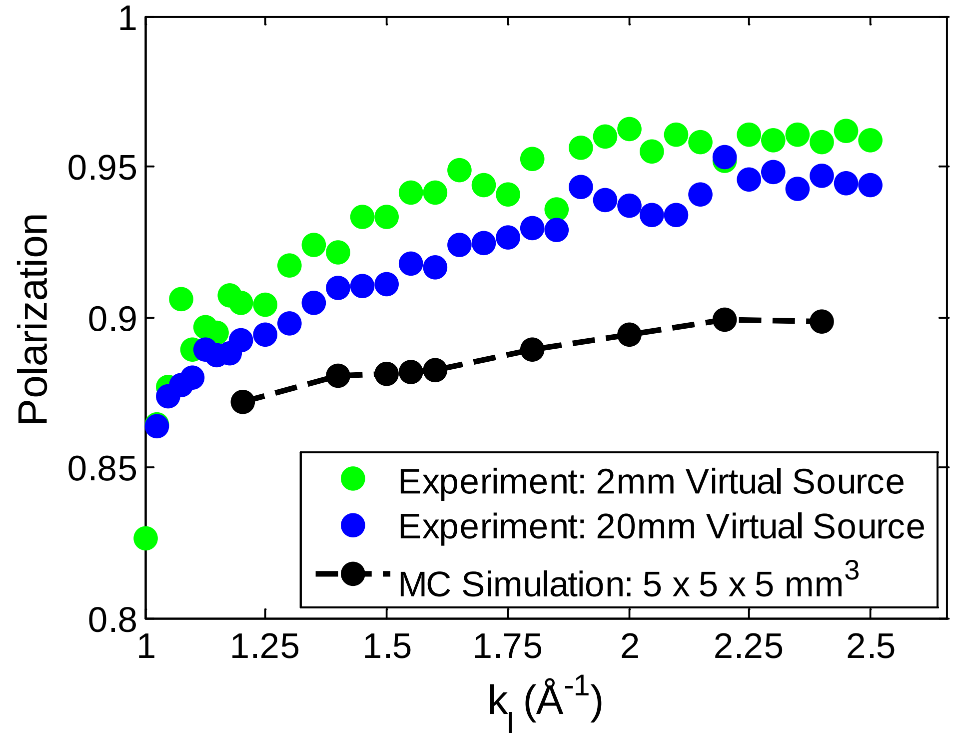
FLEXX Monochromator Helmholtz Coils





FLEXX Polarisation



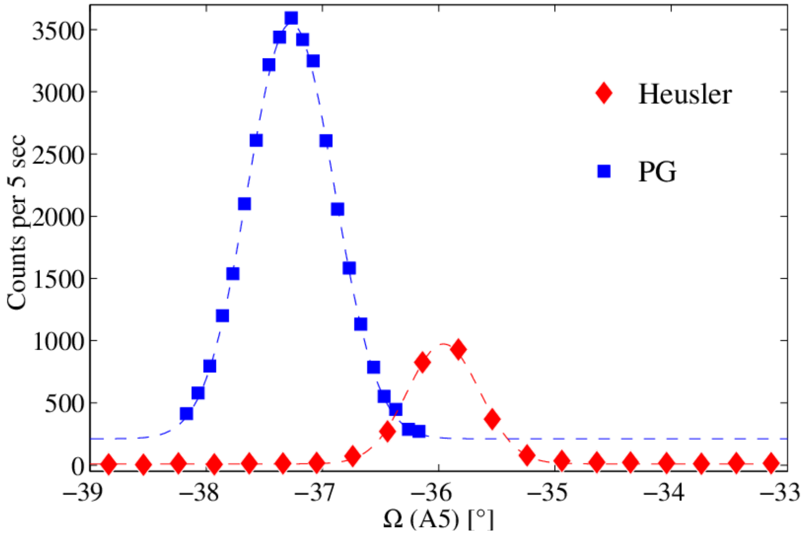


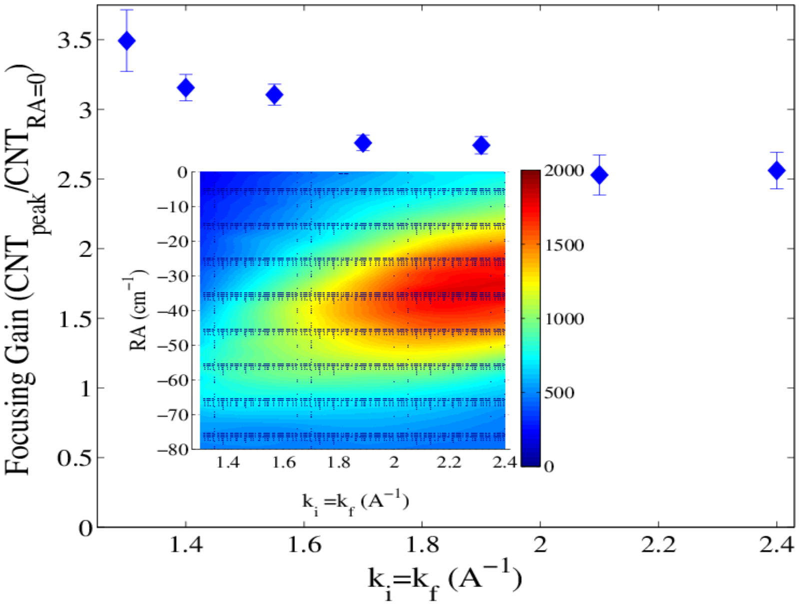
experimental polarization

- decreases towards larger wavelengths as expected from MC simulation
- does depend on virtual source width and monochromator curvature

FLEXX Heusler Analyzer Performance

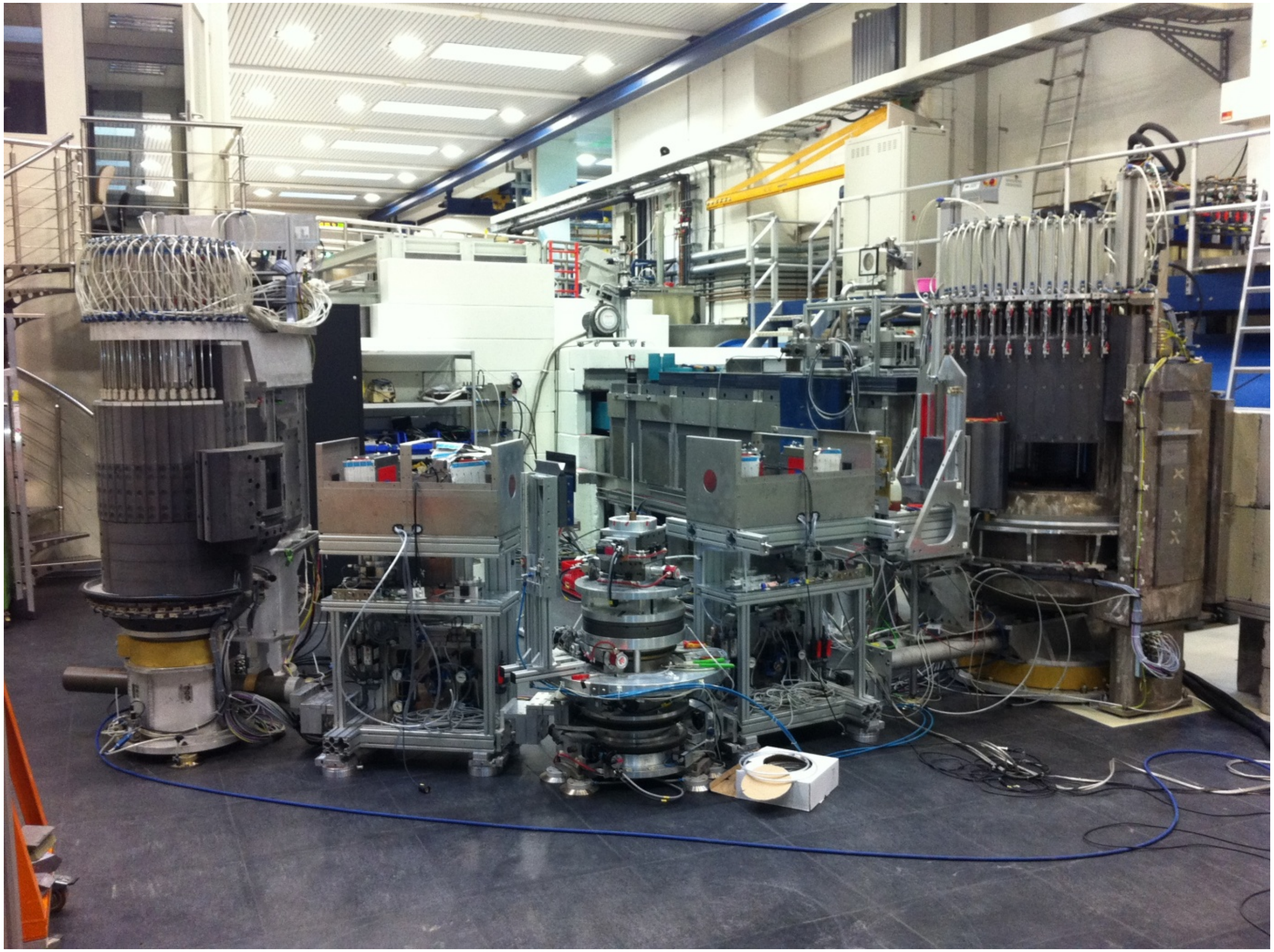
3 rows, 15 crystals each
Cu_2MnAl (111) Bragg peak
0.42° mosaic (individual crystals)
fixed vertical, variable horizontal curvature
vertical 0.17 T magnetization field beam cross section: 60 mm x 125 mm





horizontal focussing gain ~2.5-3

NRSE Option at V2/FLEXX

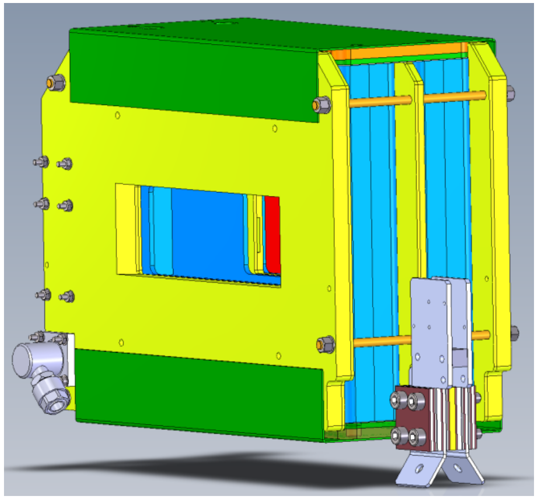


Upgrade of NRSE Option at V2/FLEXX

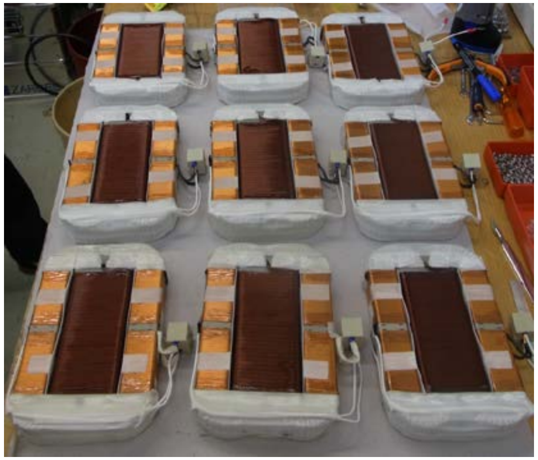
New bootstrap coils for the NRSE option at FLEX

(in collaboration with MPI Stuttgart / FRM II)

- **increase in accepted beam width**
- **access to steeper dispersion by larger coil tilt angles**
- **access to larger scattering angles for Larmor diffraction**
- **improved magnetic shielding in the NRSE arms**



courtesy: Max Planck-Institut für Festkörperphysik Stuttgart



F. Groitl *et al.*, Rev. Sci. Instrum. 86, 025110 (2015)

Upgrade of NRSE Option at V2/FLEXX

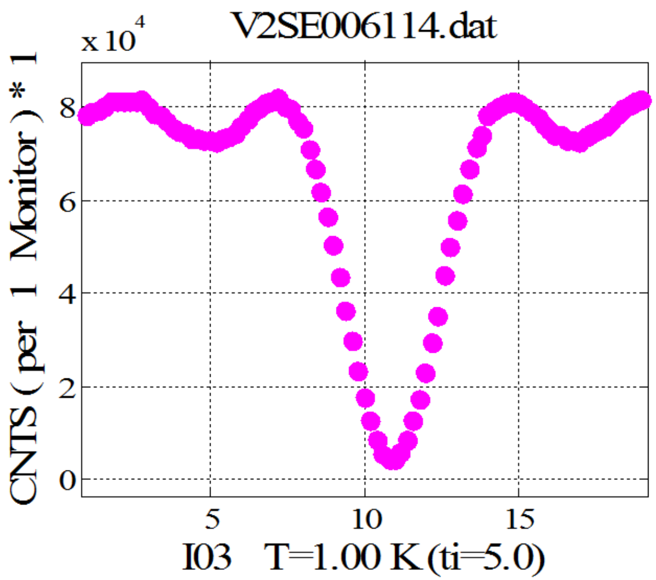
Ne … option at FLEX

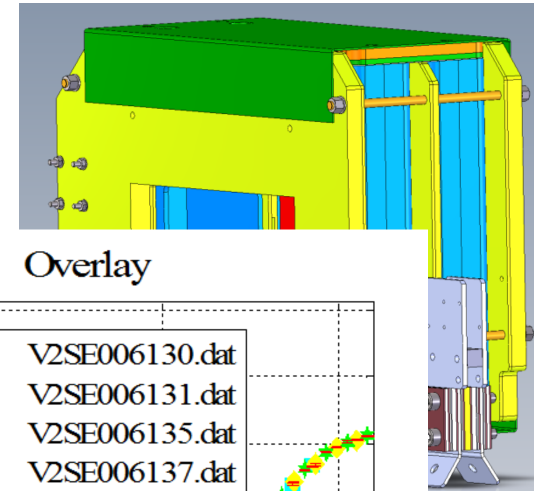
(ir … rt / FRM II)

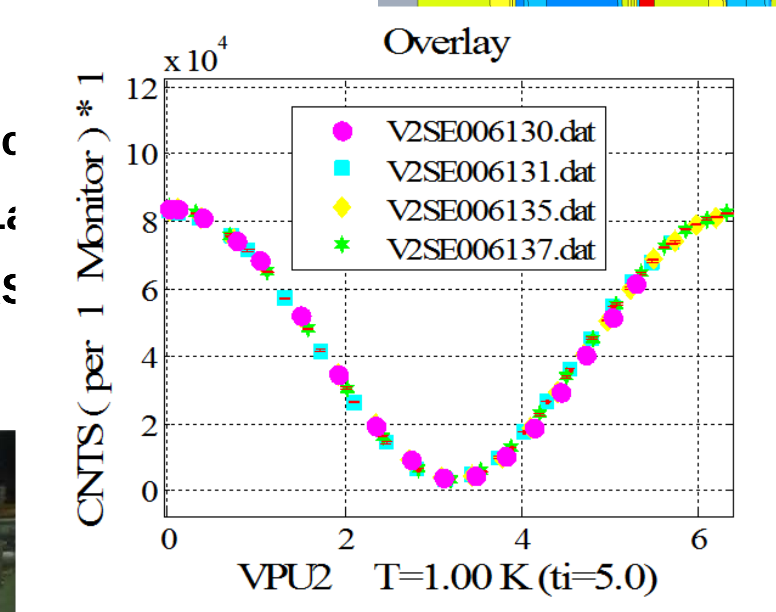
- **in … er c**
- **a… r La**
- **a… NRS**
- **in**

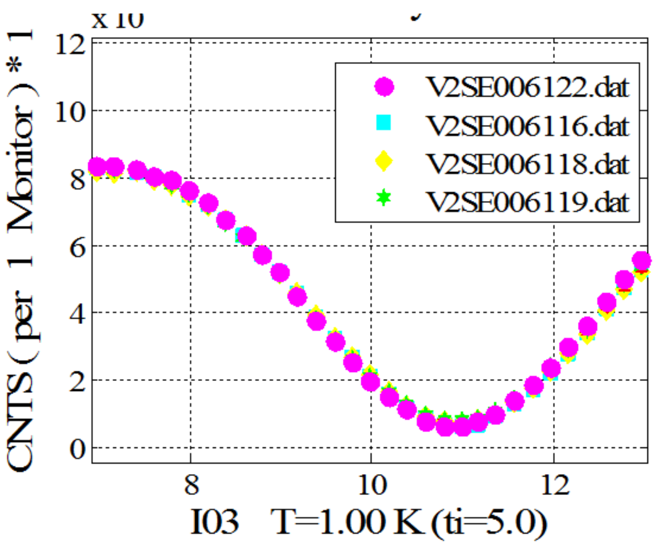
… nstitut

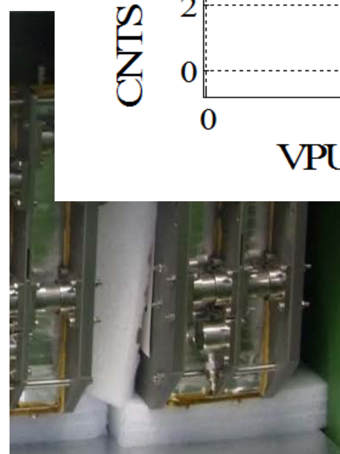
… tuttgart

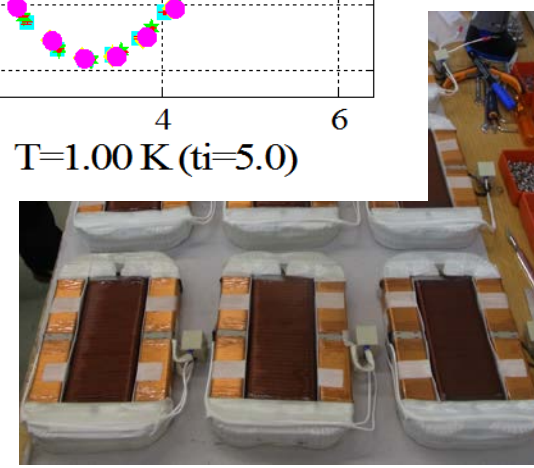






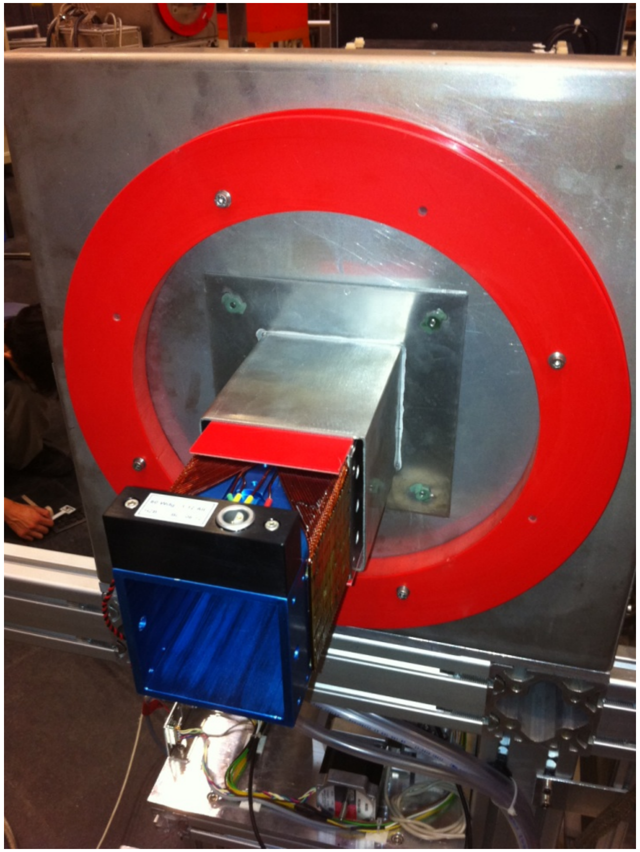


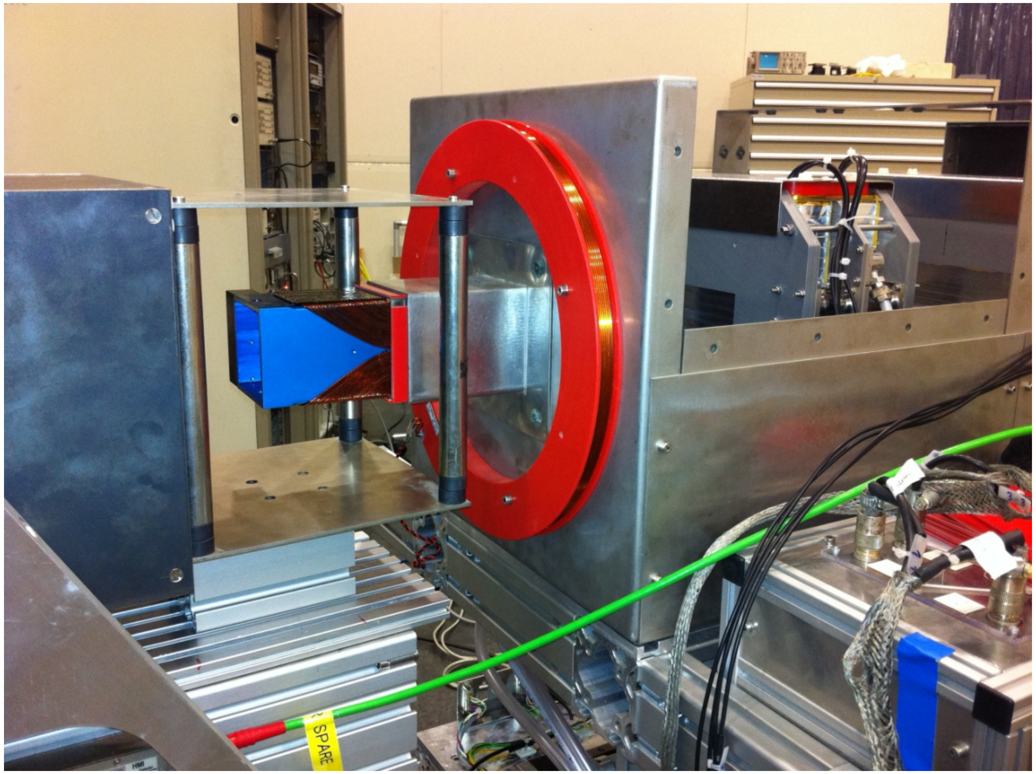




F. Groitl *et al.*, Rev. Sci. Instrum. 86, 025110 (2015)

NRSE Coupling Coils





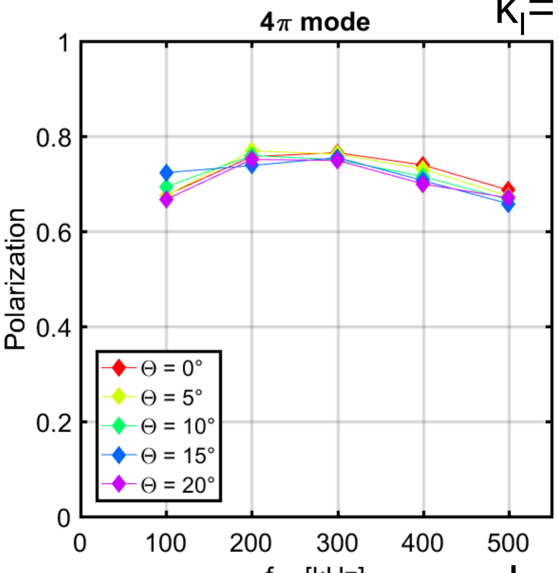
F. Groitl *et al.*, Rev. Sci. Instrum. 86, 025110 (2015)

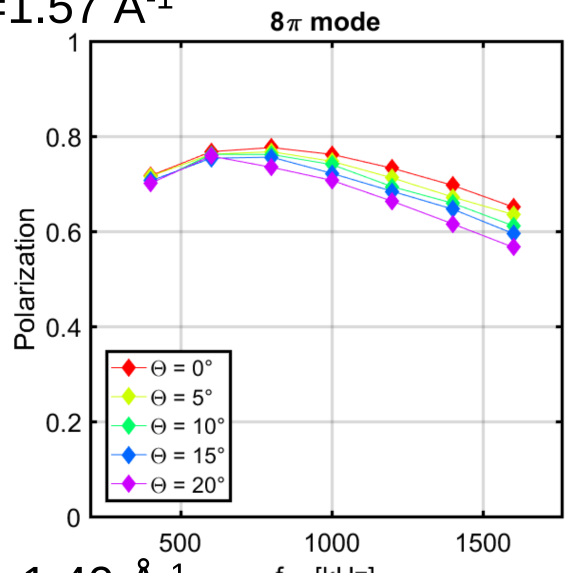
NRSE Option at V2/FLEXX

F. Groitl *et al.*, Rev. Sci. Instrum. 86, 025110 (2015)

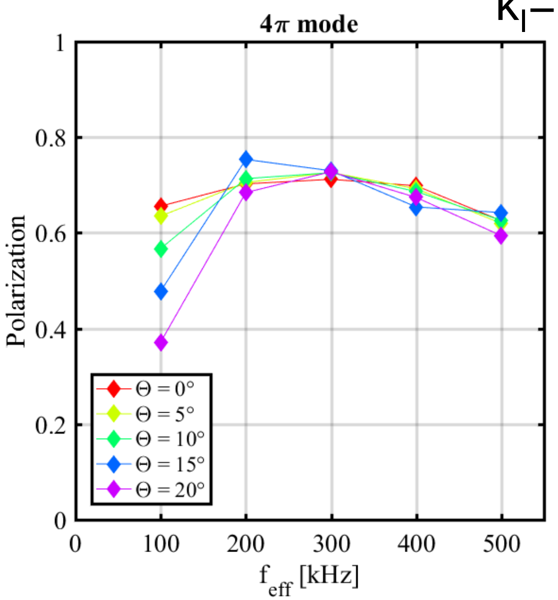
Direct Beam Calibration Measurements

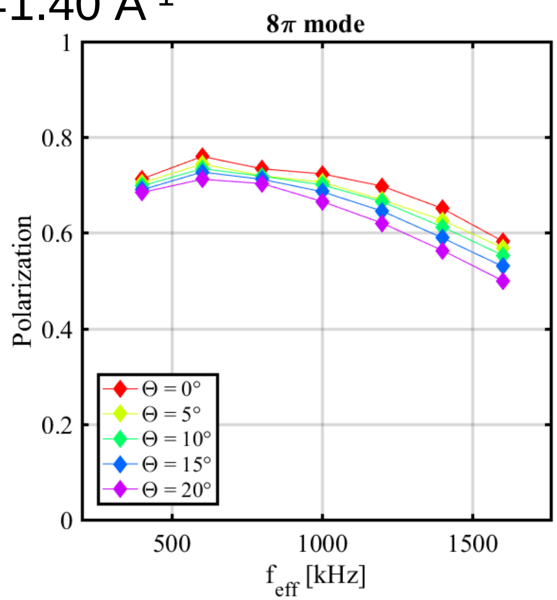
$k_I = k_f = 1.57$ Å^{-1}

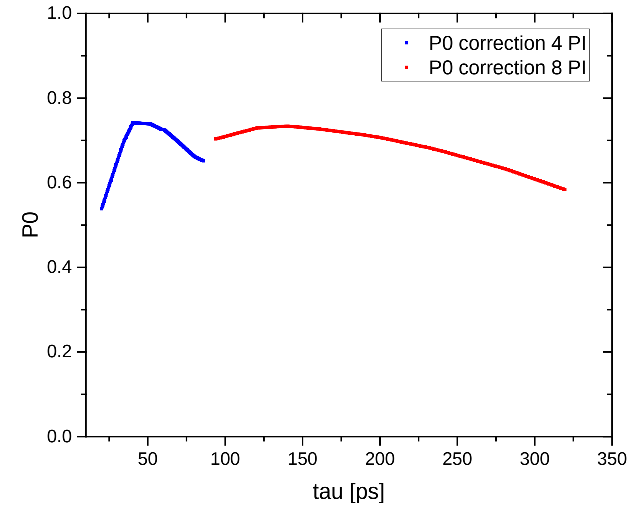




$k_I = k_f = 1.40$ Å^{-1}

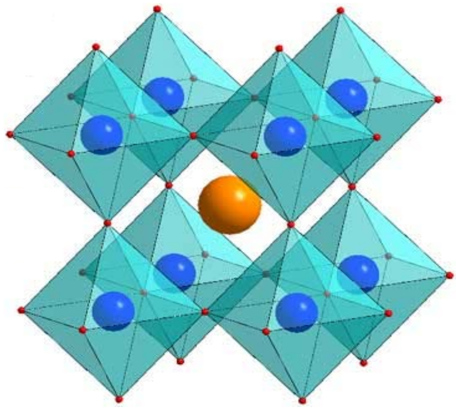






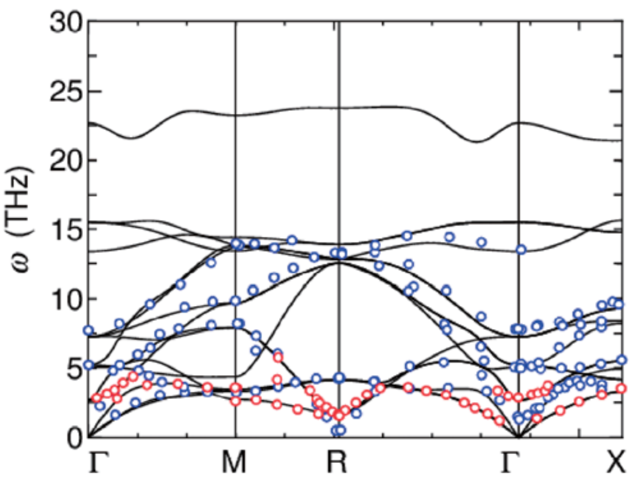
NRSE Science at V2/FLEXX and TRISP !

thermal transport in **thermoelectric $SrTiO_3$**

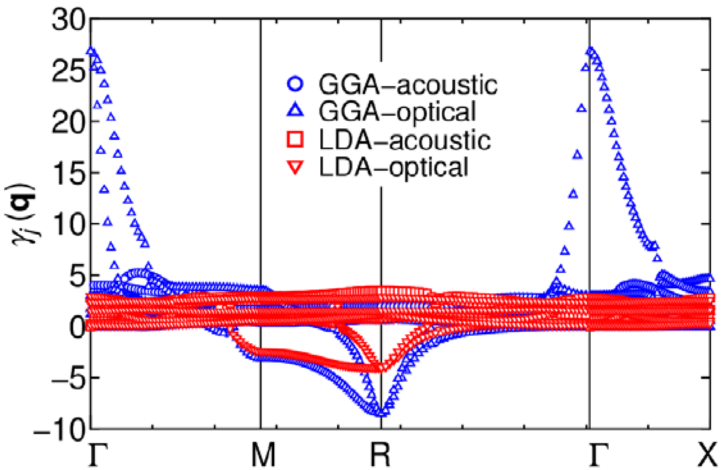


Goal: benchmark first-principles DFT / MD simulations with interatomic force constants including anharmonic lattice dynamics

$SrTiO_3$ phonon dispersion



calculated mode Grüneisen parameters

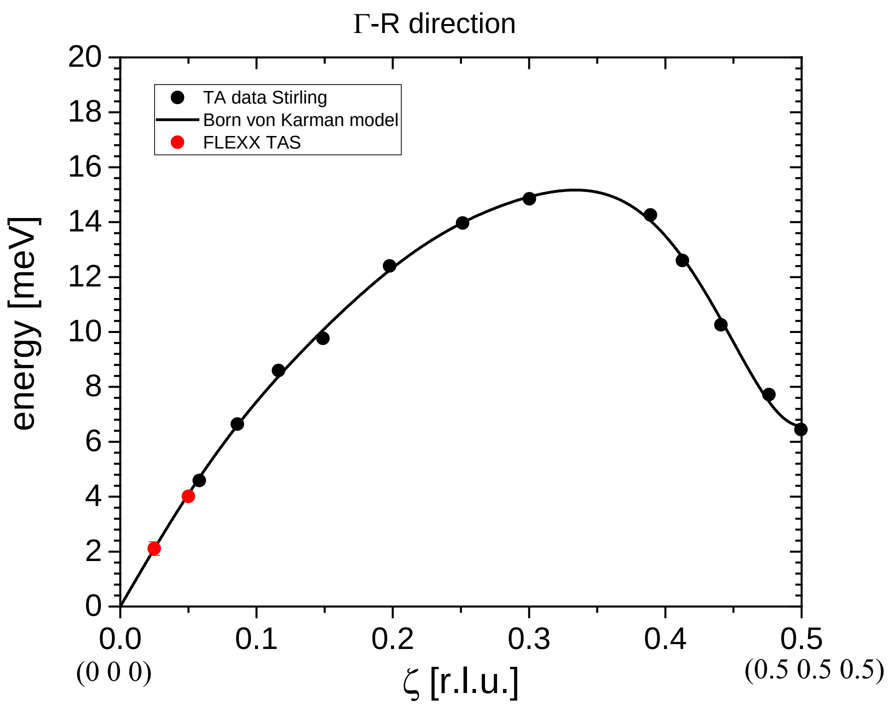


L. Feng, T. Shiga, J. Shiomi, Appl. Phys. Express **8**, 071501 (2015)

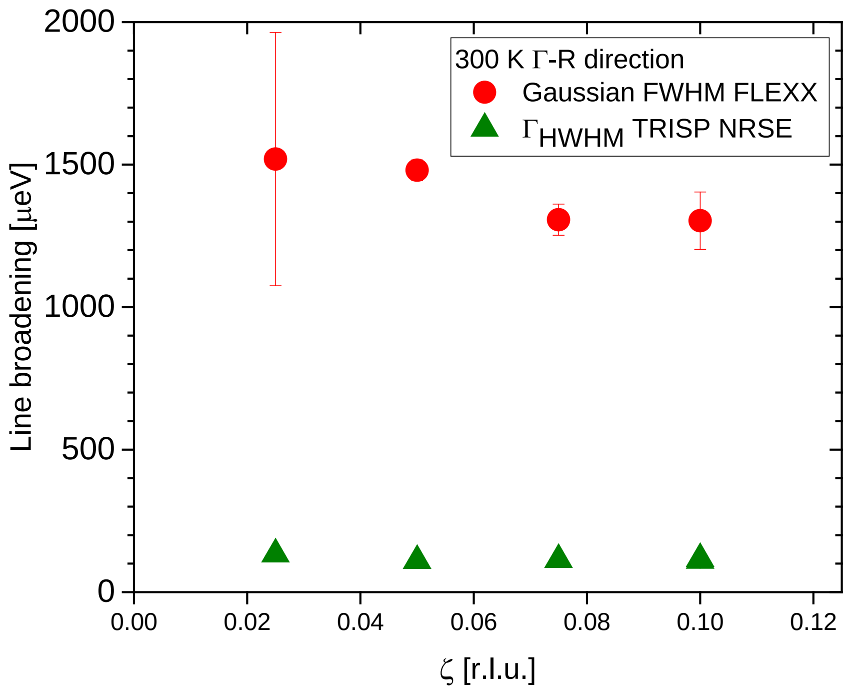
needs experimental access to phonon lifetimes at low spin echo times

Thermoelectric $SrTiO_3$

$SrTiO_3$ phonon dispersion



experimental line broadening

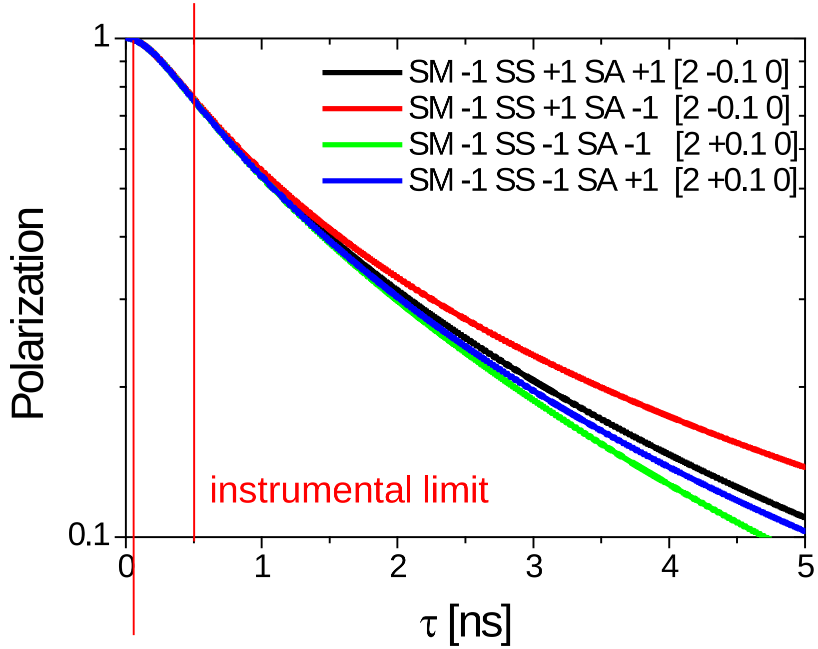


"Instrumental" Resolution for NRSE

beam divergence

$$P = \frac{1}{N}\int S(\mathbf{Q},\Delta\omega) T_{TAS}(\mathbf{k}_i,\mathbf{k}_f) e^{i\phi(\mathbf{k}_i,\mathbf{k}_f)} d^3k_i d^3k_f + c.c.$$

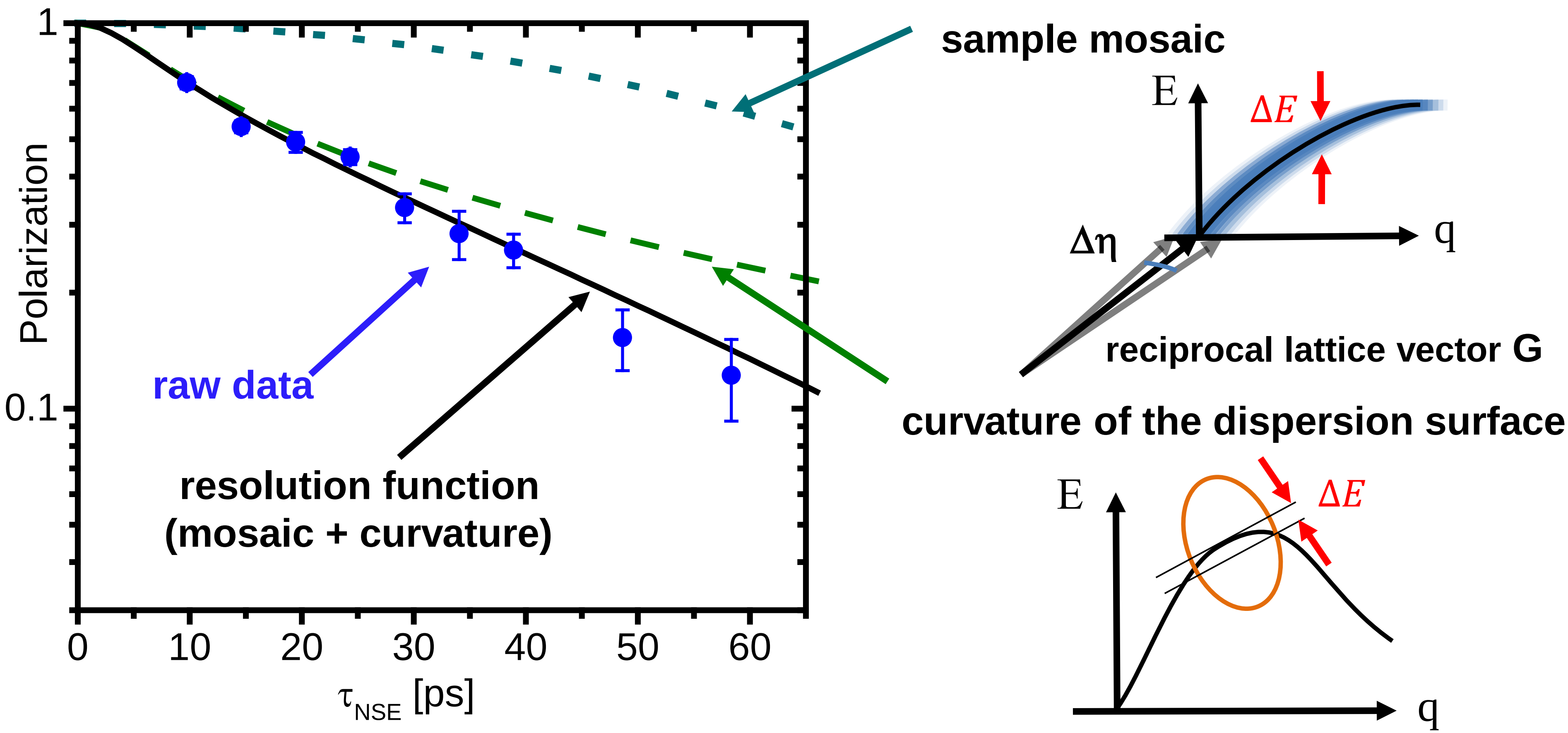
- **use Gaussian approximation of TAS transmission probability $T_{TAS}(k_i,k_f)$**
- **expand total Larmor phase $\phi(k_i,k_f)$ to second order**
- **expand energy conservation to second order**
- **integrate by matrix technique**



upper limit typical phonon measurements

at very large spin echo times instrumental resolution has to be considered

Development of Resolution Theory



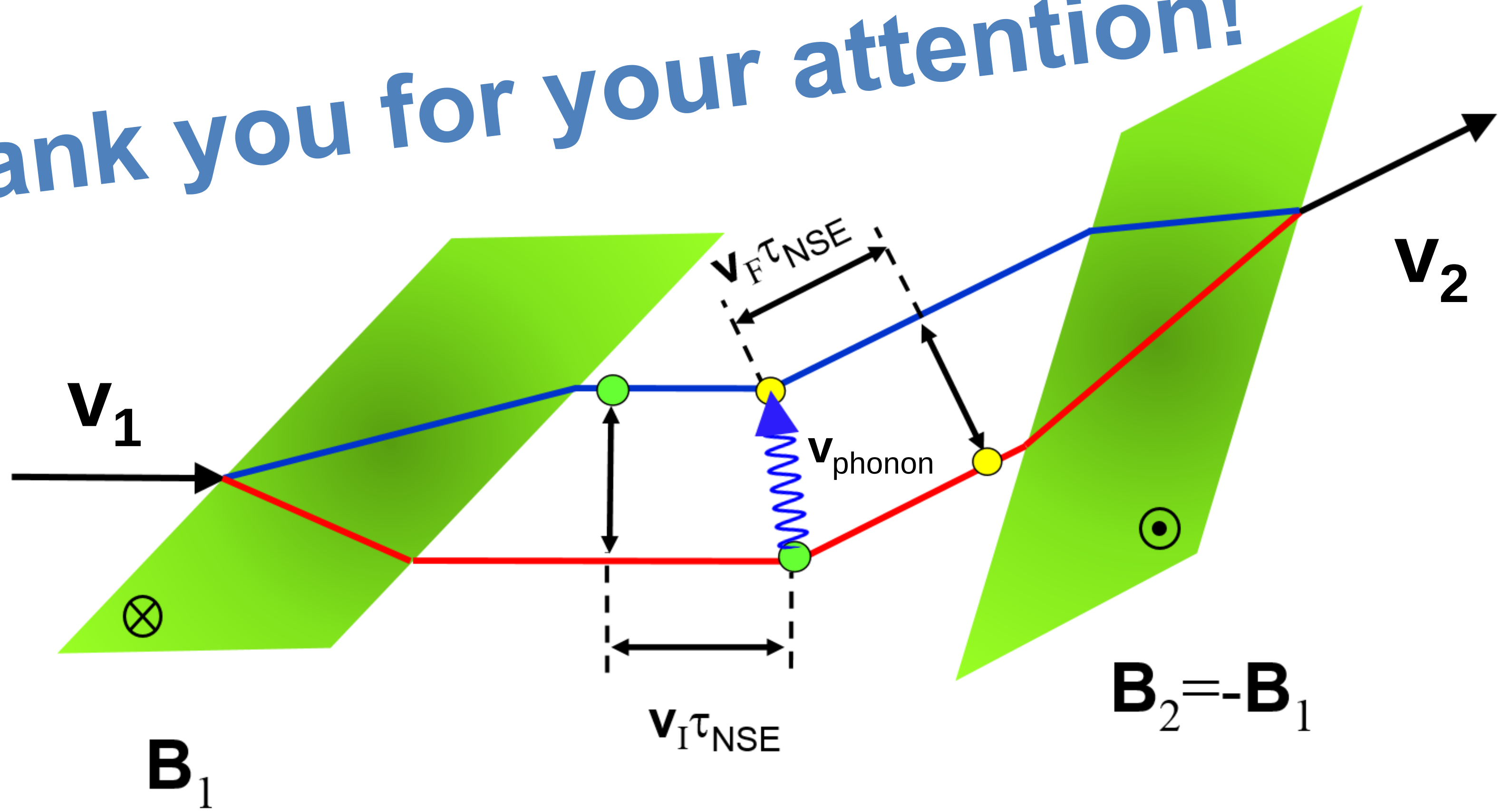
Development of *analytical resolution function for NRSE spectroscopy*

Data correction: no convolution ➡ divide data by calculated resolution function

K. Habicht *et al.*, *J. Appl. Cryst.* **36**, 1307 (2003) K. Habicht *et al., Physica B* **350** E803-E806 (2004)

Neutron Spin-Echo: Semi-Classical Model

Thank you for your attention!



Dispersive excitations require tilted magnetic field regions