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

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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

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### NRSE
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- Thomas Keller, MPI Stuttgart, Germany
Neutron scattering techniques probe static or dynamic correlations.
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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

\[ \Delta E_{\text{exp}} = 2\Gamma \]

Energy linewidth \( \Gamma \) inversely proportional to lifetime \( T_D \):

\[ \Gamma = \frac{\hbar}{T_D} \]

Time domain

\[ e^{-\frac{\tau_{\text{NSE}}}{T_D}} = e^{-\frac{\Gamma \tau_{\text{NSE}}}{\hbar}} \]
The Upgraded Cold Neutron TAS FLEXX

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

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

device transmission

as measured with monitor at sample position

assuming $m_{\text{eff}}=3$

polarizer transmission is confirmed at FLEXX transmission is entirely due to device transmission
polarizer rocking scans $k_i = 2.56 \text{ Å}^{-1}$ (measurements by Mirrotron)

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

angular acceptance of polarizer is confirmed at FLEXX
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

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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$_2$MnAl (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
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

Upgrade of NRSE Option at V2/FLEXX

Ne

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NRSE Option at V2/FLEXX

Direct Beam Calibration Measurements

$k_i = k_f = 1.40 \, \text{Å}^{-1}$

$k_i = k_f = 1.57 \, \text{Å}^{-1}$
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

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needs experimental access to phonon lifetimes at low spin echo times

Thermoelectric SrTiO$_3$

SrTiO$_3$ phonon dispersion

![SrTiO$_3$ phonon dispersion graph]

Experimental line broadening

![Experimental line broadening graph]

- TA data Stirling
- Born von Karman model
- FLEXX TAS

- 300 K $\Gamma$-R direction
- Gaussian FWHM FLEXX
- $\Gamma$ HWHM TRISP NRSE
“Instrumental” Resolution for NRSE

beam divergence

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

- 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

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

Polarization vs. \( \tau \) [ns]

- instrumental limit
- upper limit typical phonon measurements
Development of Resolution Theory

Development of **analytical resolution function for NRSE spectroscopy**

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

Neutron Spin-Echo: Semi-Classical Model

Dispersive excitations require tilted magnetic field regions

Thank you for your attention!