Inelastic neutron scattering at DNS-IV

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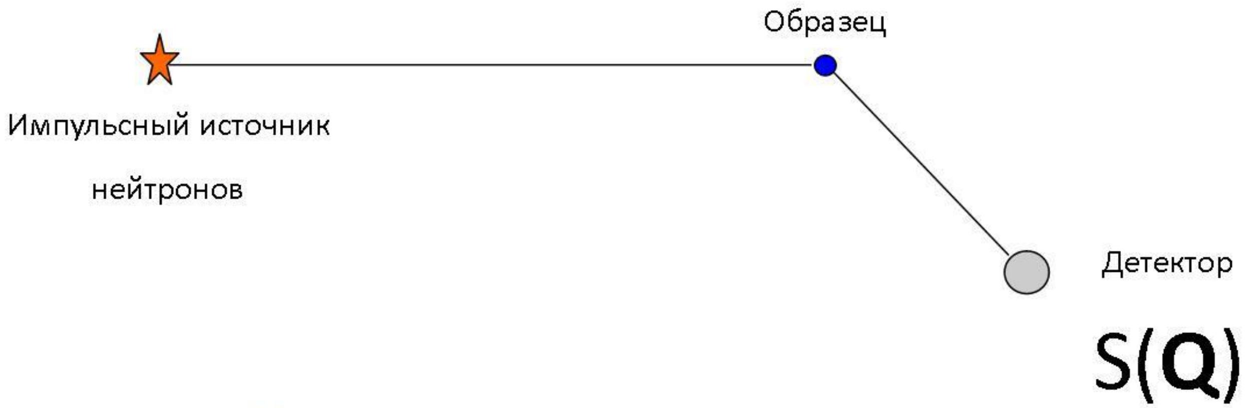
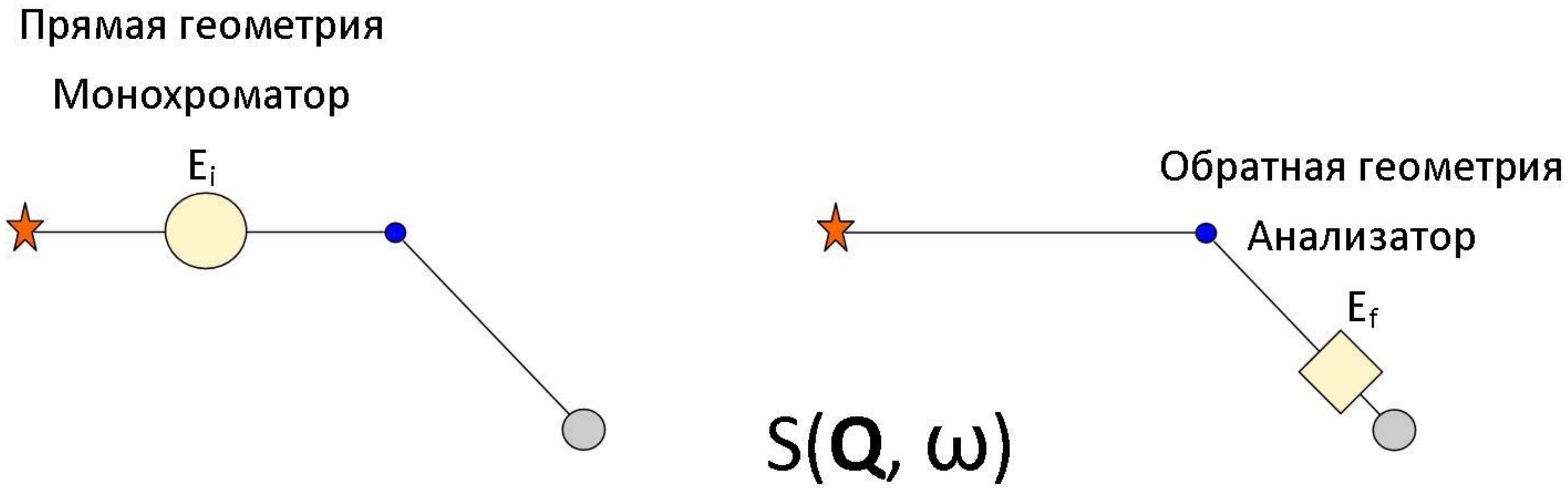
Дифракция



Неупругое рассеяние



Science with INS

$$S(\mathbf{Q},\omega,T) = \chi''(\mathbf{Q}, \omega, T)\,(1 - \exp(-\,\omega/k_B T))^{-1}$$

- ***Magnetic dynamics of strongly correlated electron systems***
  - High temperature superconductors
  - Quantum magnets
  - Non Fermi liquid systems
  - Systems with proximity to quantum critical point
  - Mixed valence, Kondo effect, Heavy Fermions
- ***Phonons, Molecular dynamics, Biomolecular Dynamics***

4D S(Q,ω,T)

ISIS 8 spectrometers

Merlin direct geometry, general purpose single crystal and powder

LET direct geometry, high resolution, general purpose single crystal and powder **(TS2)**

Tosca inverse geometry, molecular spectroscopy

Iris inverse geometry, high resolution QES and INS

Osiris inverse geometry , high resolution QES and INS and diffraction

Maps direct geometry, general purpose single crystal and powder

Vesuvio inverse geometry, deep inelastic scattering

Mari direct geometry, general purpose powder samples

SNS 6 spectrometers

ARCS direct geometry Atomic-level dynamics in materials science, chemistry, condensed matter sciences

CNCS direct geometry, cold neutron Condensed matter physics, materials science, chemistry, biology

HYSPEC direct geometry Measures excitations in small single-crystals with optional polarization analysis

SEQUOIA direct geometry Dynamics of complex fluids, quantum fluids, magnetism, condensed matter, materials science

BASIS back scattering, inverse geometry Dynamics of macromolecules, constrained molecular systems, polymers, biology, chemistry, materials science

VISION inverse geometry Vibrational dynamics in molecular systems, chemistry

J-PARC 5 spectrometers

4SEASONS direct geometry, general purpose single crystal and powder

DNA inverse geometry , high resolution Biomolecular Dynamics Spectrometer

HRC direct geometry, general purpose single crystal and powder

AMATERAS direct geometry, high resolution

POLAND (project) direct geometry + polarisation analysis

IBR-2 2 spectrometers

NERA inverse geometry Vibrational dynamics in molecular systems, chemistry

DIN 2PI direct geometry, general purpose powder samples

ESS 5 spectrometers

BIFROST Indirect Geometry Spectrometer. Swiss-Danish team to build a pioneering crystal analyzer spectrometer optimized to study dynamics in quantum materials and matter under extreme conditions.

MIRACLES Indirect Geometry Spectrometer high resolution backscattering. It will be one of the ESS long instruments (L_1=162.5 m).

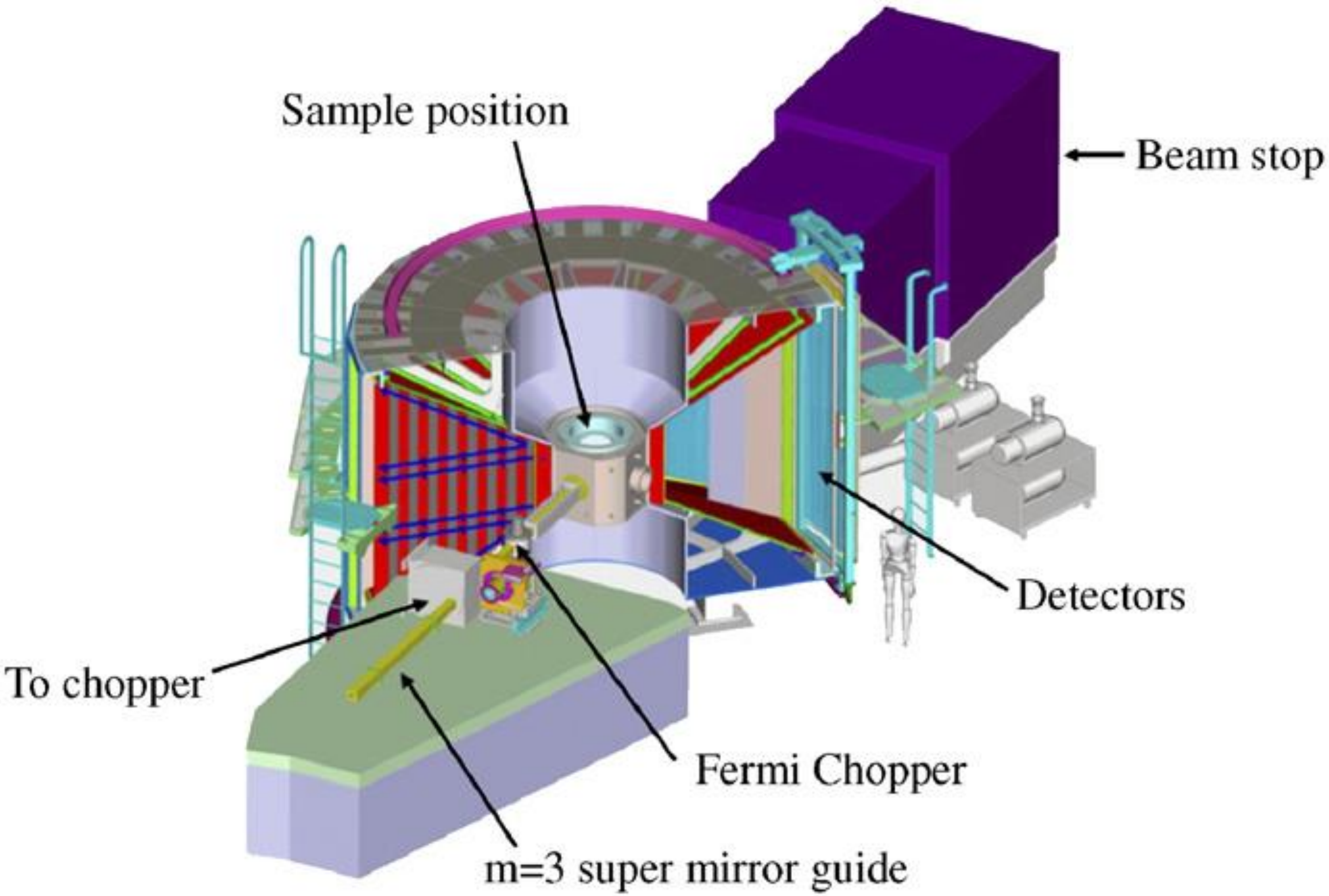
VESPA Indirect Geometry Vibrational Spectrometer TOSCA/NERA like at L_1 = 60m

CSPEC is a direct geometry time of flight spectrometer L_1 = 160m L_2 = 3.5m

T-REX is a direct geometry time of flight spectrometer L_1 = 170m L_2 = 3.0m Polarization analysis. Wide energy range from μeV to hundreds meV

MERLIN - a high count rate, medium energy resolution, direct geometry chopper spectrometer

Merlin has been in user operation since 2008.



- Supermirror converging m3 guides
- Incident energy 7-2000 meV
- Energy Resolution: Depends on the choice and speed of Fermi chopper $\Delta h\omega/E_i$=3-5 % FWHM at the elastic line
- Fermi chopper: 10 m from the moderator 50-600 Hz phased to ISIS pulse ±0.1ms
- Background chopper: 8.5m at 50Hz
- Beam size at the sample: 50x50 mm, motorized jaws can define a smaller beam size
- Intensity at the sample(E_i= 45 mev, $\Delta h\omega/E_i$=5%) 6×10^4 ($n \cdot cm^{-2} \cdot s^{-1}$)

MERLIN detector : 2.5 m from the sample position

Position sensitive ^{3}He tubes (10 bar partial pressure) 2.5 cm diameter, 3 m long, resolution 21 mm along the tube

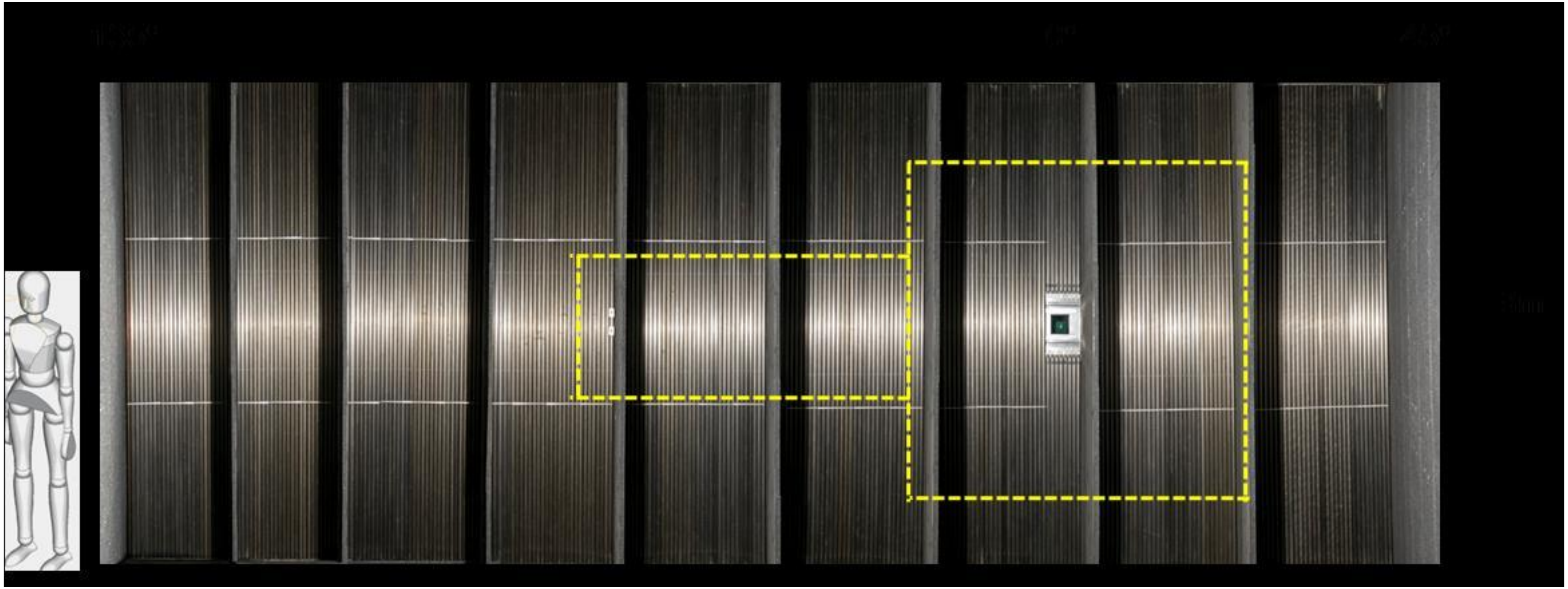
Angular range: -45° to 135° horizontal

±30° vertical direction

Smallest scattering angle 3°

Detector Pixels: 69632

Solid Angle: 3.1Sr



R.A. Ewings, A. Buts, M.D. Le, J. van Duijn, I. Bustinduy, T.G. Perring
"Horace: Software for the analysis of data from single crystal spectroscopy experiments at time-of-flight neutron instruments" Nuclear Instruments & Methods A 834, 132-142 (2016).

Mslice, Horace, Mantid

Fixed angle between k_i and one of the high symmetry direction in the crystal (k_i is parallel to c):

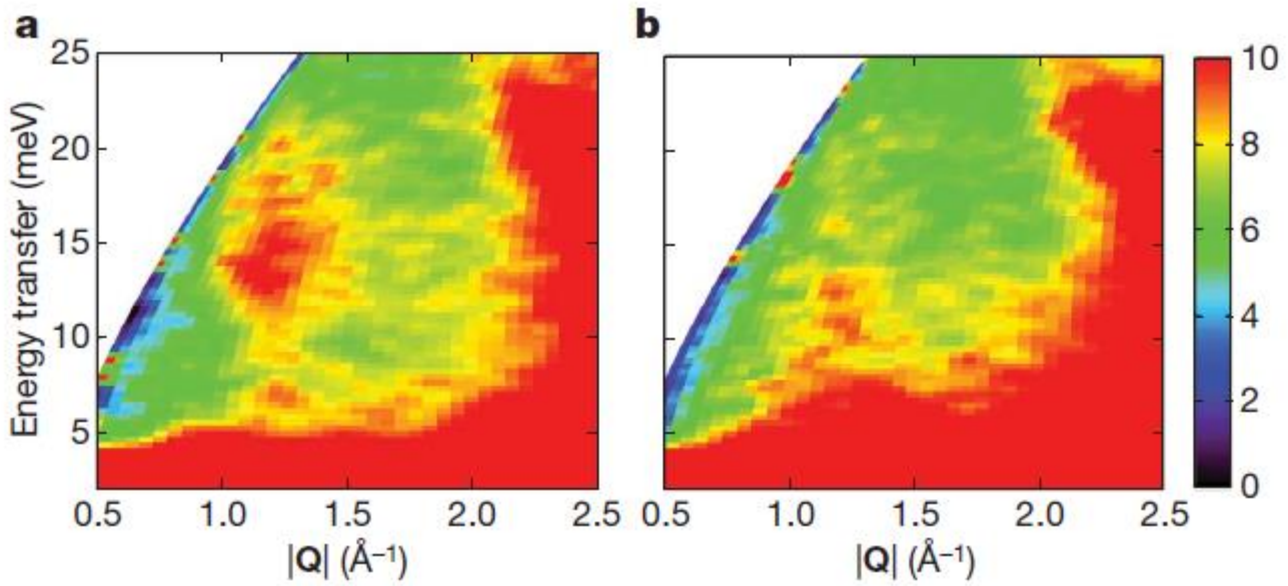
$(\phi,\theta,t) \rightarrow (Q_x, Q_y, \omega)$ Q_z is not defined

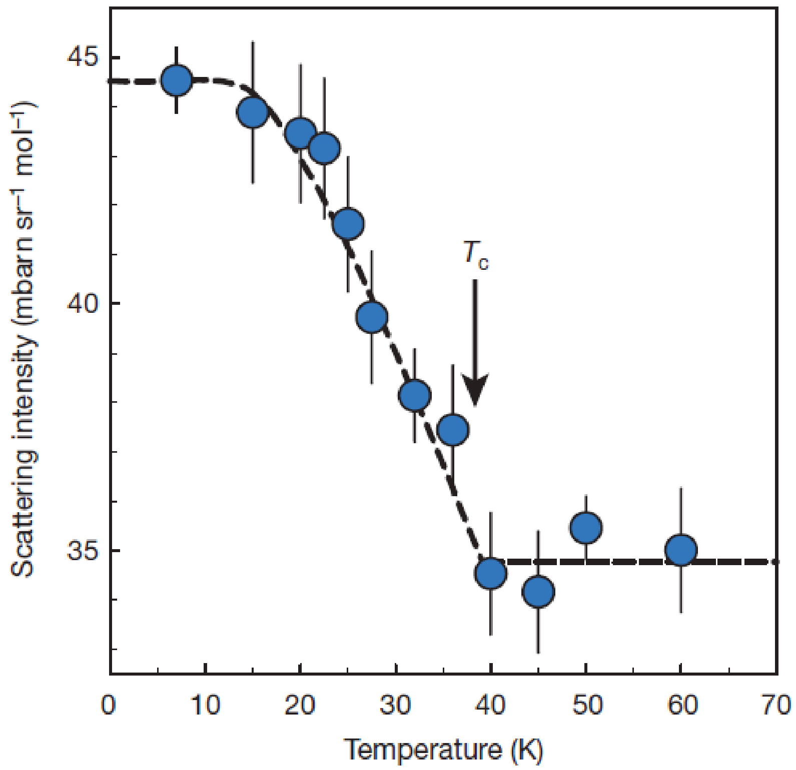
Multiple crystal angle (crystal rotated about vertical axis (1,-1,0) with (HHL) scattering plane) :

Full four dimensional scattering function $S(Q_x, Q_y, Q_z, \omega)$

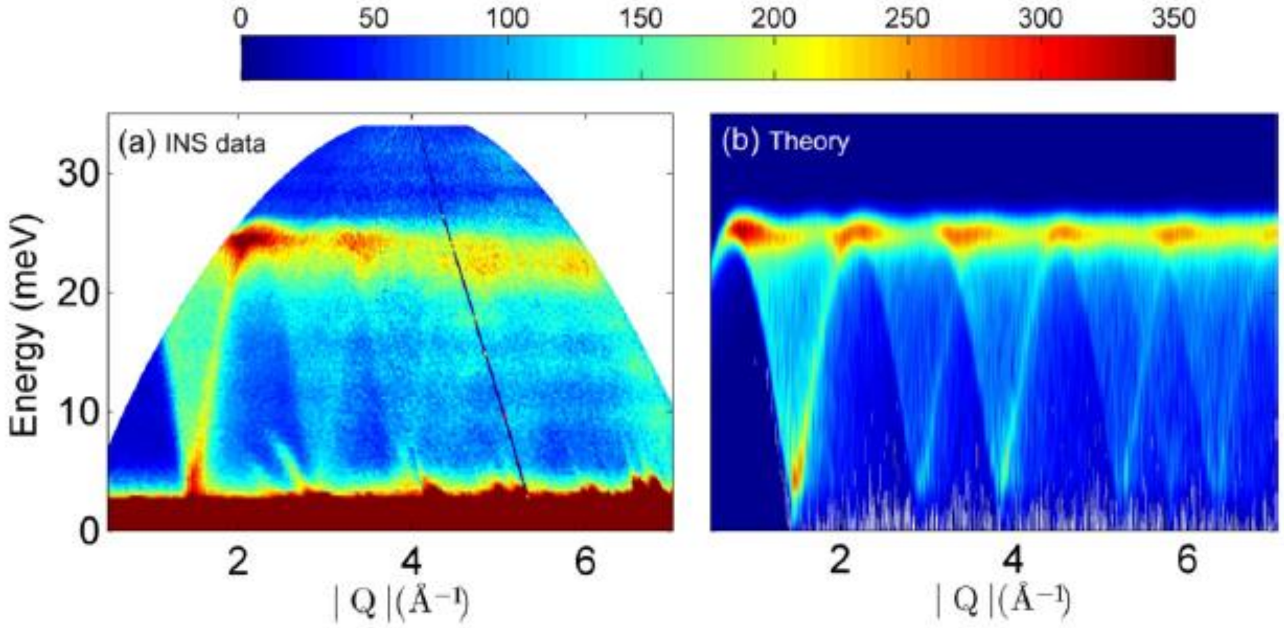
$(\phi,\theta,t, \psi) \rightarrow (Q_x, Q_y, Q_z, \omega)$

A.D. Christianson, E. A. Goremychkin, R. Osborn *et al.*,
“Unconventional superconductivity in $Ba_{0.6}K_{0.4}Fe_2As_2$ from inelastic neutron scattering”
Nature **456**, p. 930 (2008)



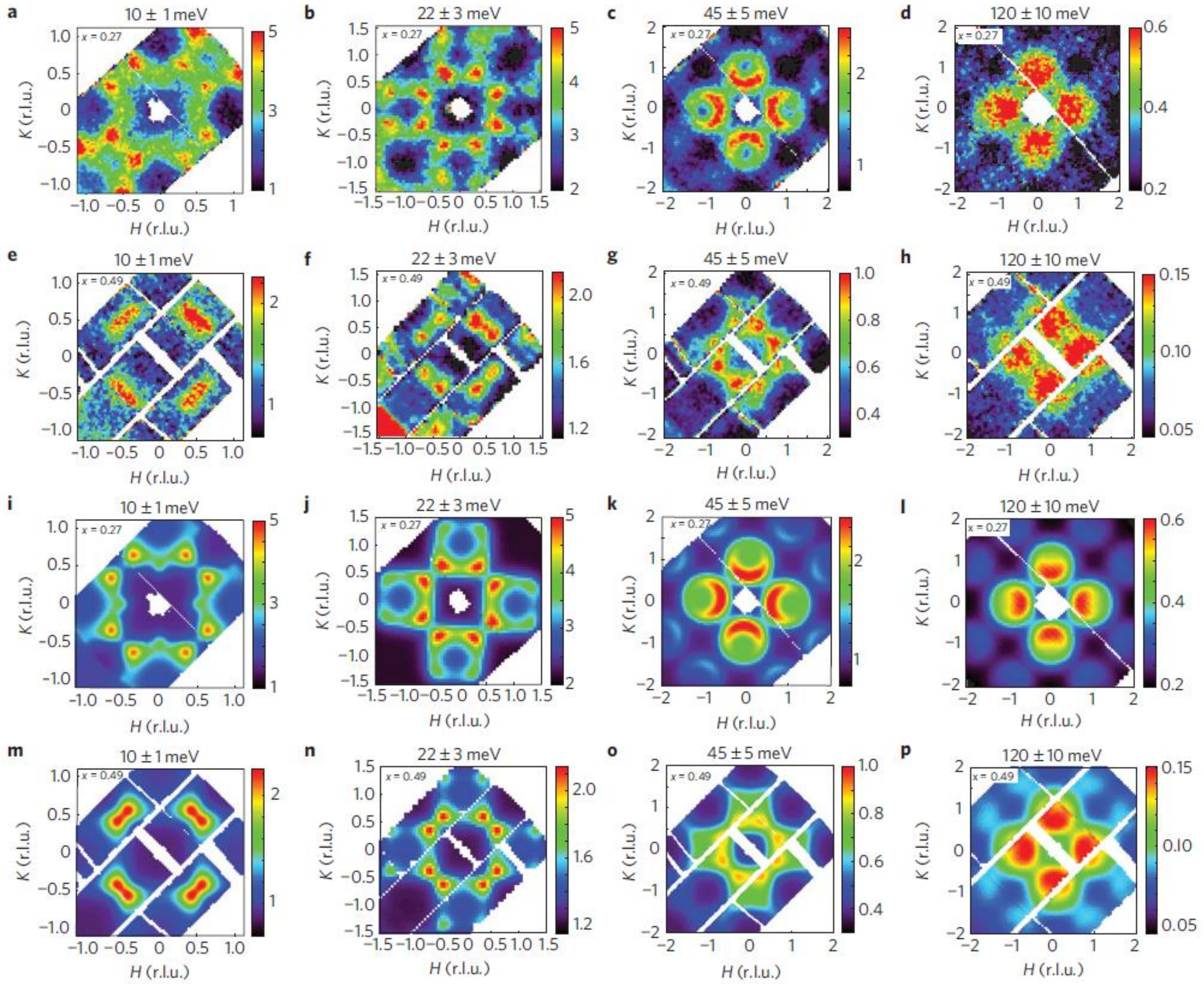


E. S. Klyushina *et al.*, PHYSICAL REVIEW B **96**, 214428 (2017)



(a) INS data measured on a powder sample at T = 5 K using the Merlin spectrometer with an incident energy of 35 meV.
(b) Spin-wave simulations of the powder excitation spectrum of $BaNi_2V_2O_8$ performed for the Hamiltonian (3) with the parameters J_n = 12.3 meV, J_{nn} = 1.25 meV, J_{nnn} = 0.2 meV, J_{out} = −0.00045 meV, D_{EP} = 0.0695 meV, D_{EA} = −0.0009 meV

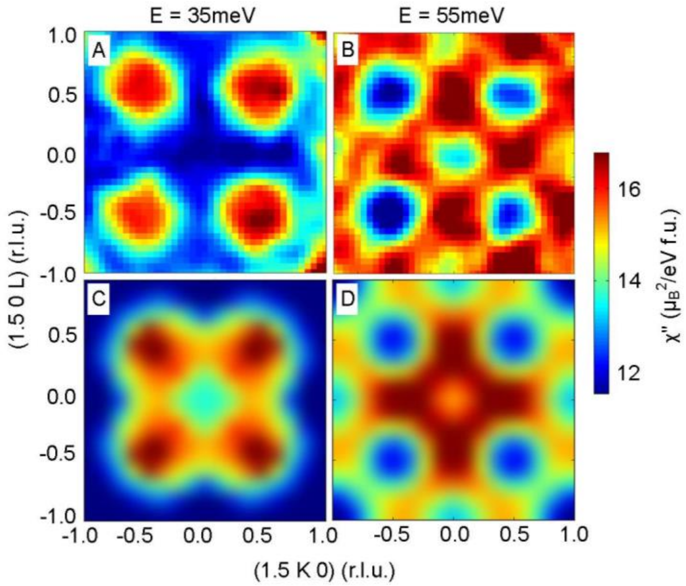
M. D. Lumsden, A. D. Christianson, E. A. Goremychkin *et al.*,
"Evolution of spin excitations into the superconducting state in $FeTe_{1-x}Se_x$"
NATURE PHYSICS **6**, 182 (2010)

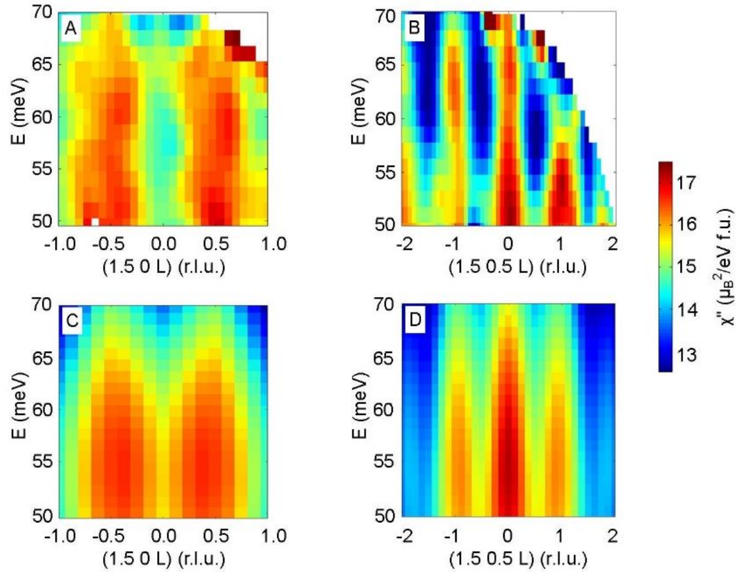


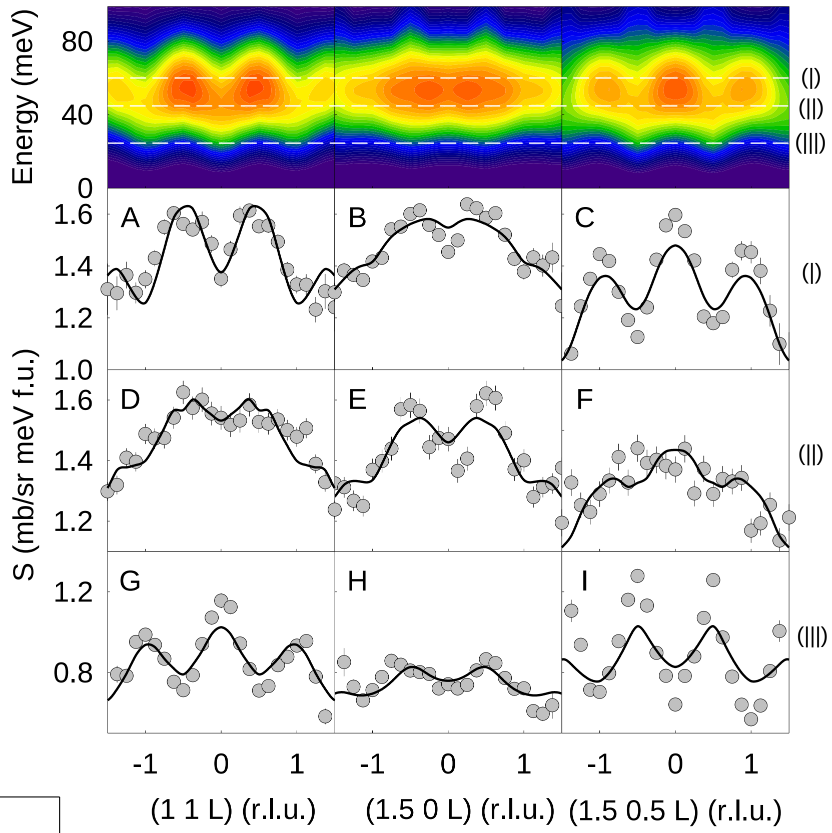
MERLIN, ISIS
$FeTe_{0.73}Se_{0.27}$

ARCS, SNS
$FeTe_{0.51}Se_{0.49}$

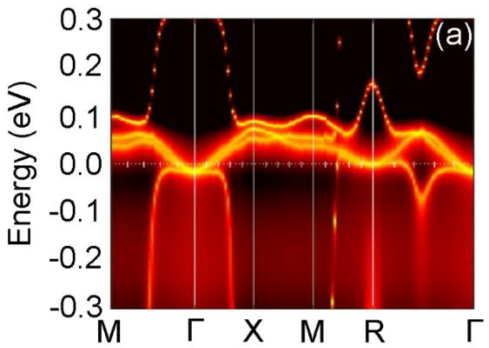
E. A. Goremychkin, H. Park, R. Osborn *et al.*,"Coherent band excitations in $CePd_3$: A comparison of neutron scattering and *ab initio* theory"
Science **359**, 186–191 (2018)



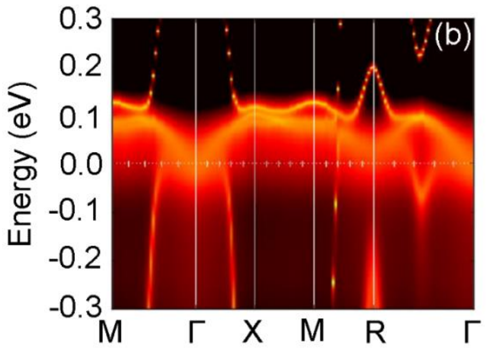




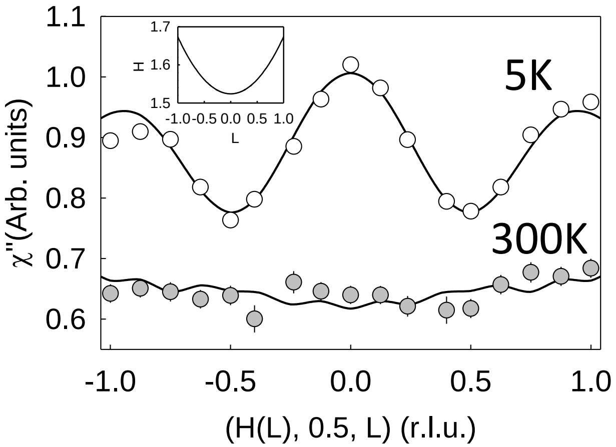
DFT+DMFT



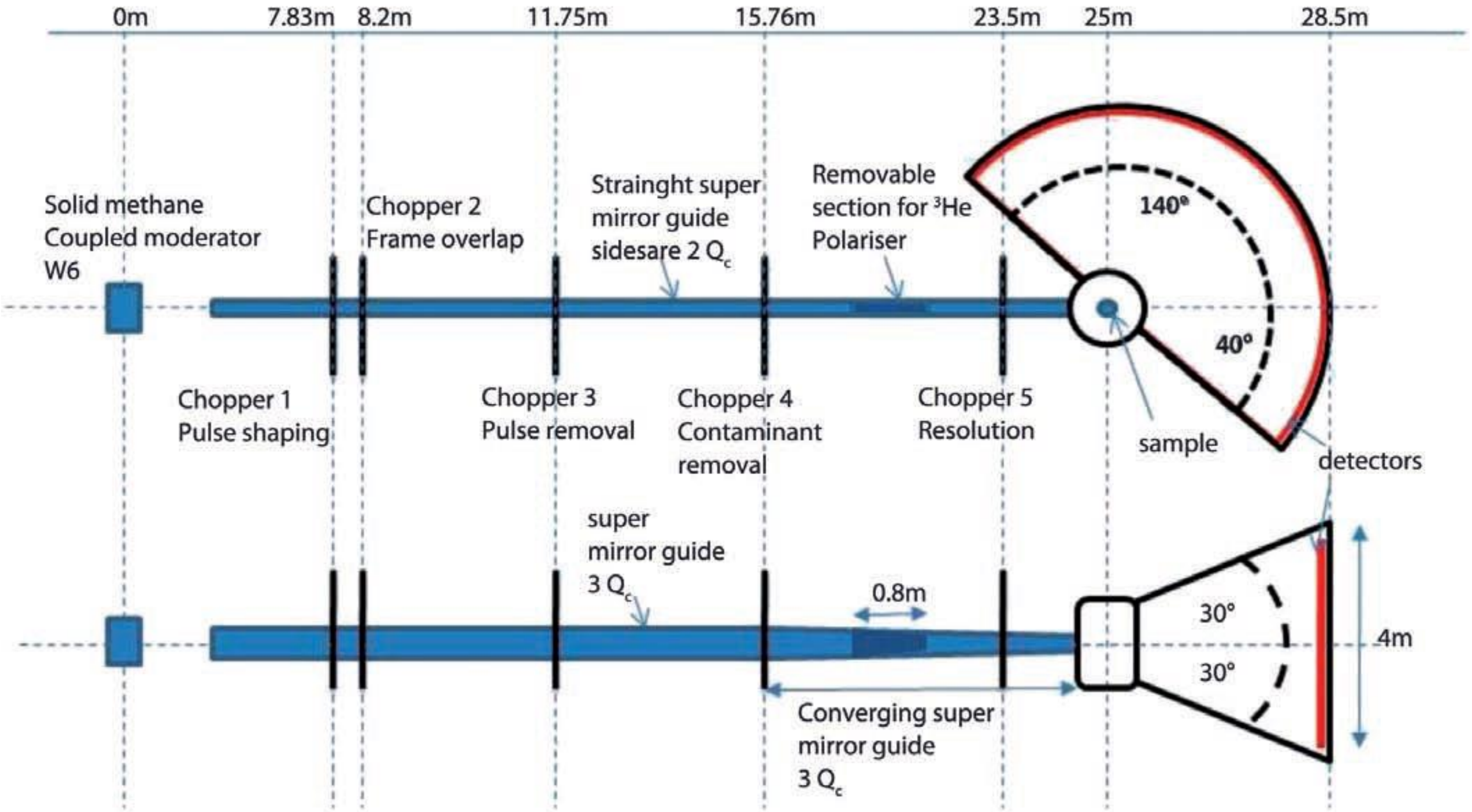
100K



400K



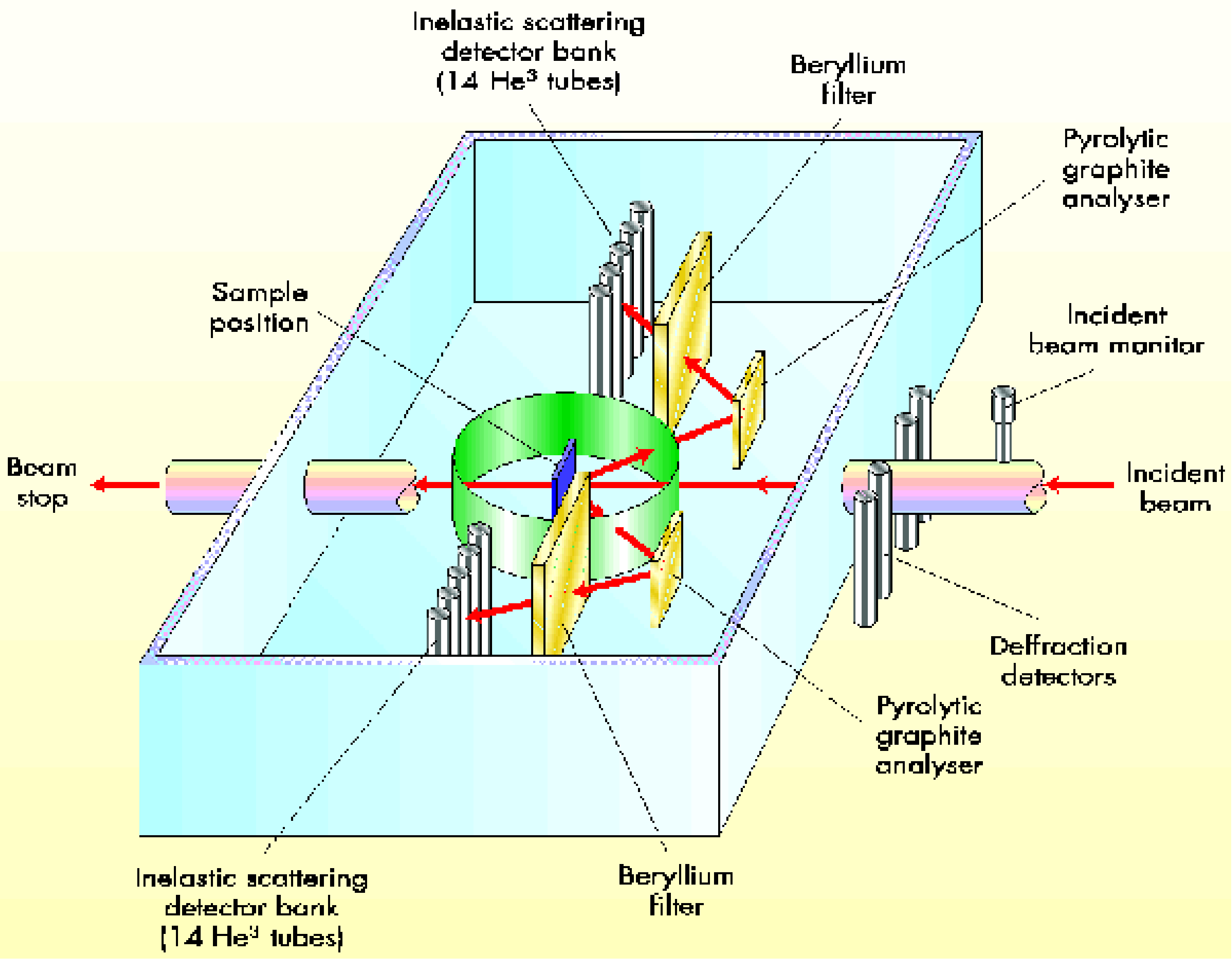
LET is a cold neutron multi-chopper spectrometer for the study of dynamics in condensed matter to understand the microscopic origin of material properties.

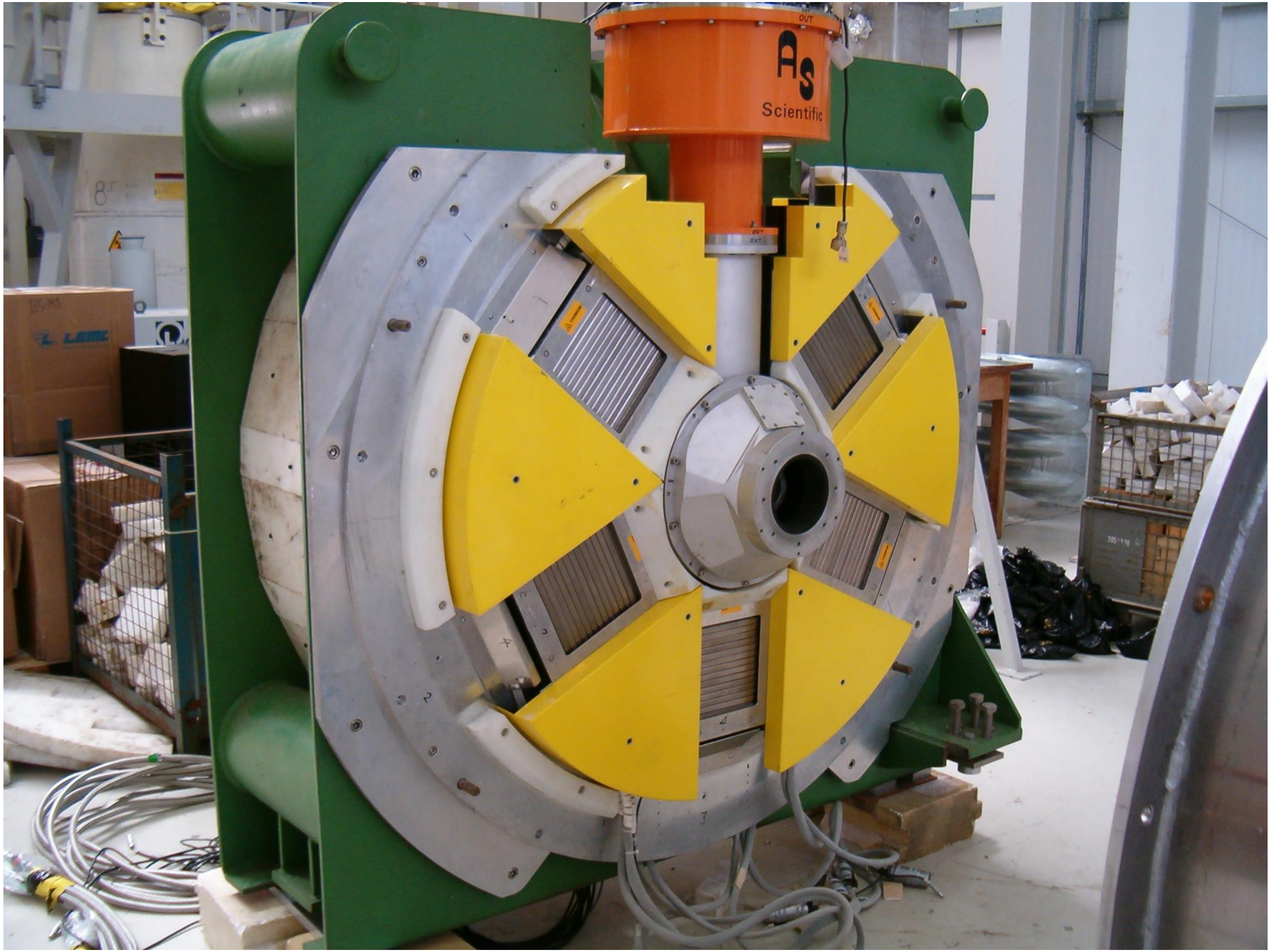


The Spectrometer	
Moderator	Coupled composite (solid CH4)
Primary flight paths L1	25 m
Secondary flight paths L2	3.5 m
Beam size (HxW) at sample	50 mmx40 mm
Scattering angles	Horizontal -40 to +140°, Vertical ±30°
Detector resolution	25 mmx25 mm or 0.4° x 0.4°
Incident energy	0.6–80 meV
Energy resolution	ΔE/Ei ≥ 1.5% at 20 meV, ΔE/Ei ≥ 0.8% at 1 meV
Qmax, Qmin	11.8/λ (Å-1), 0.32/λ (Å-1)
Sample environment	
CCR	5–600 K sample size 40 mmx50 mm
Orange cryostat	1.5–310 K sample size 40 mmx50 mm
Dilution fridge	50 mK–4 K sample size 35 mmx40 mm
Cryomagnet	9 T, 1.6–310 K sample size 25 mmx25 mm

440 PSD tubes S=15m^2

TOSCA is an indirect geometry spectrometer optimized for the study of molecular vibrations in the solid state.



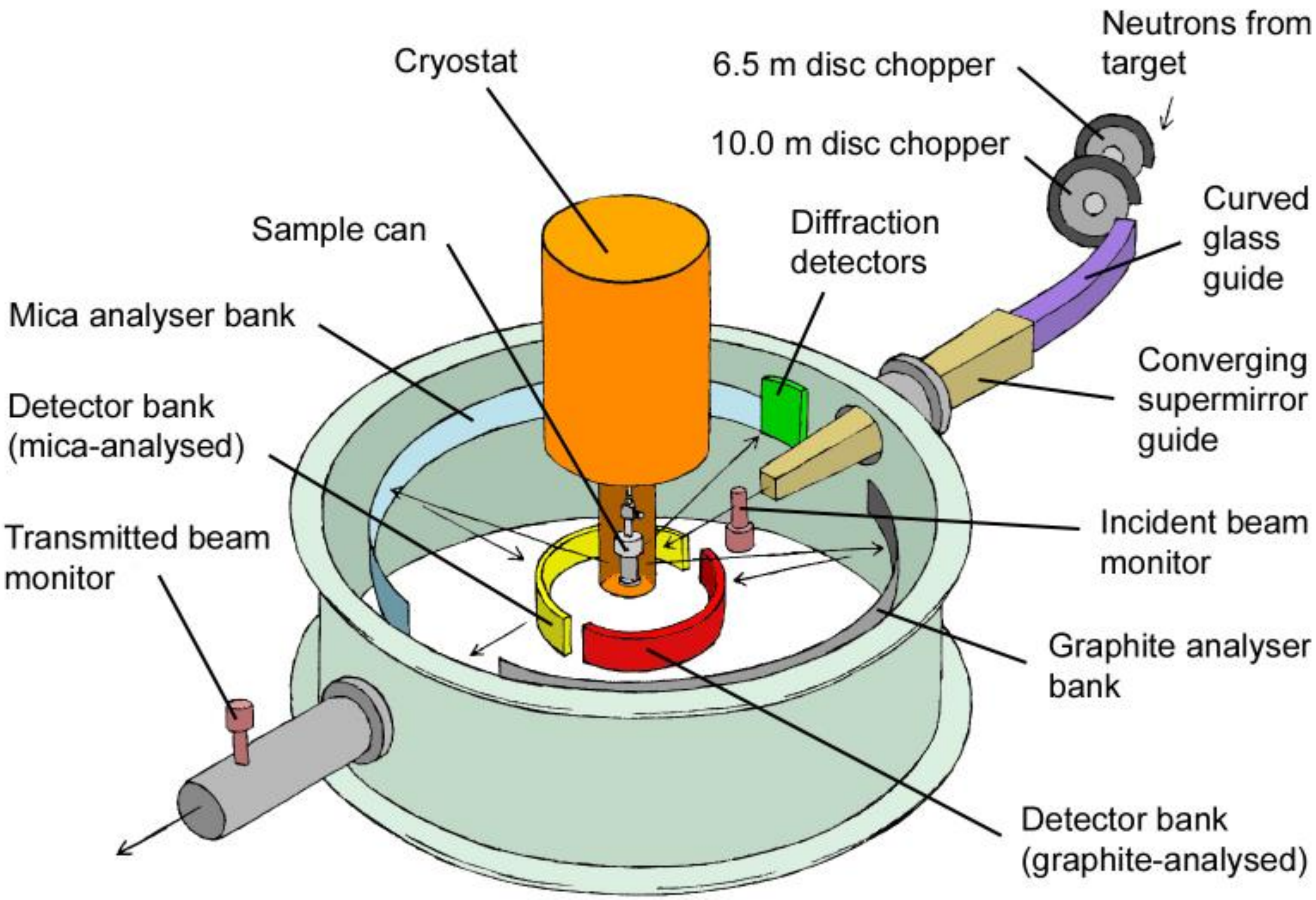


OUT
As
Scientific

TOSCA technical information

Beam line	N4
Moderator	300K water moderator poisoned at 1.5 cm
Energy resolution	~1% ΔE/E
Primary flight path	17 m
Chopper	4 blade chopper running at 10 Hz (operational February 2010)
Secondary flight path	0.6 m average
Beam size at sample	40 mm x 40 mm
Detectors	130 squashed ^3He tubes
Energy range	-20, 8000 cm^{-1} (-2.5, 1000 meV)
Temperature range	10 K (normal operational mode) up to 550 K
Sample changer	36 samples

IRIS is a time-of-flight inverted-geometry crystal analyzer spectrometer designed for quasi-elastic and low-energy high resolution inelastic spectroscopy.



Technical Summary

	PG 002	PG 004	Mica 002	Mica 004*	Mica 006
Analysing Energy (meV)	1.84	7.38	0.207	0.826	1.86
Dynamic Range (meV)	-0.4 to +0.4	-3.5 to +4.0	-0.02 to +0.02	-0.15 to +0.15	-0.4 to +0.4
Resolution (μeV)	17.5	54.5	1.0	4.5	11.0
Angular Coverage (deg)	25-160		25-155		
Q-range (Å-1)	0.42 to 1.85	0.84 to 3.70	0.13 to 0.62	0.26 to 1.24	0.40 to 1.87
Spectroscopy Detectors	51 Zn scintillators				
Diffraction Detectors	8 He3 tubes at $2\theta \approx 170°$ $\Delta d/d = 2.5 \times 10^{-3}$ d-range (Å) = 1-12				

* only available with muscovite Mica. Fluorinated mica should be used for Mica006 and Mica002

Instrument Parameters

Beam line	N6
Moderator	Hydrogen cooled to 25K
Wavelength limiting choppers	Disc choppers at 6.3m and 10m
Primary flight path	Curved neutron guide, 2.35 km radius; 65 mm (v) x 43mm (h) cross-section feeding a 2.5m focusing super mirror guide to the sample
Sample position	36.41m from the moderator

Beam size at sample	30 mm (v) x 20mm (h)
Intensity at sample	1×10^7 n/cm^2.s at 150uA ISIS power

FLNP inelastic instruments
NERA and DIN 2PI

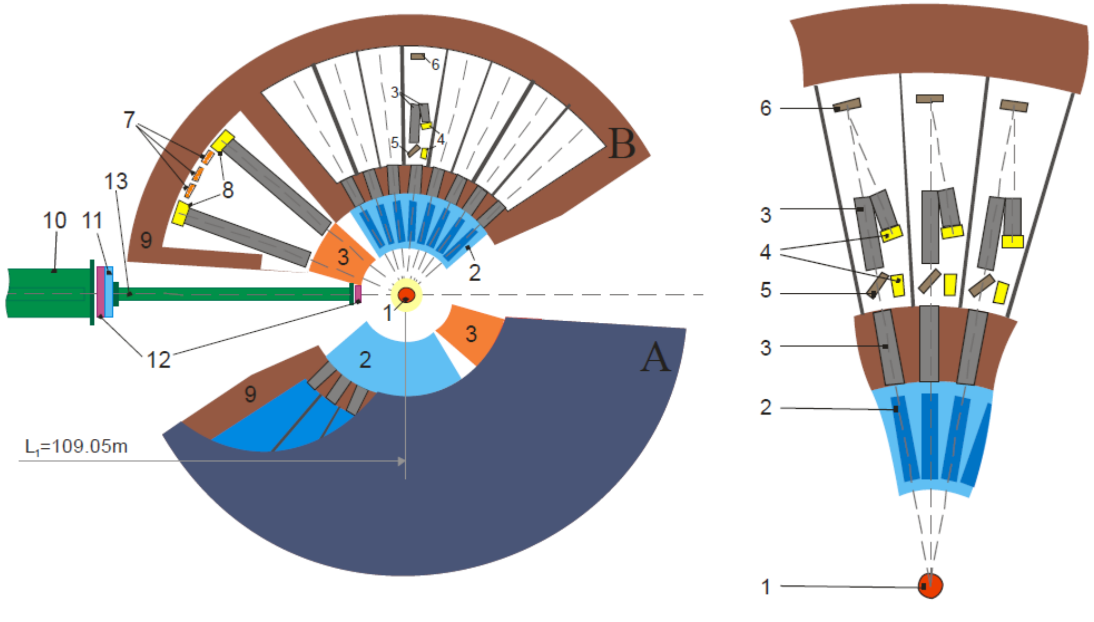
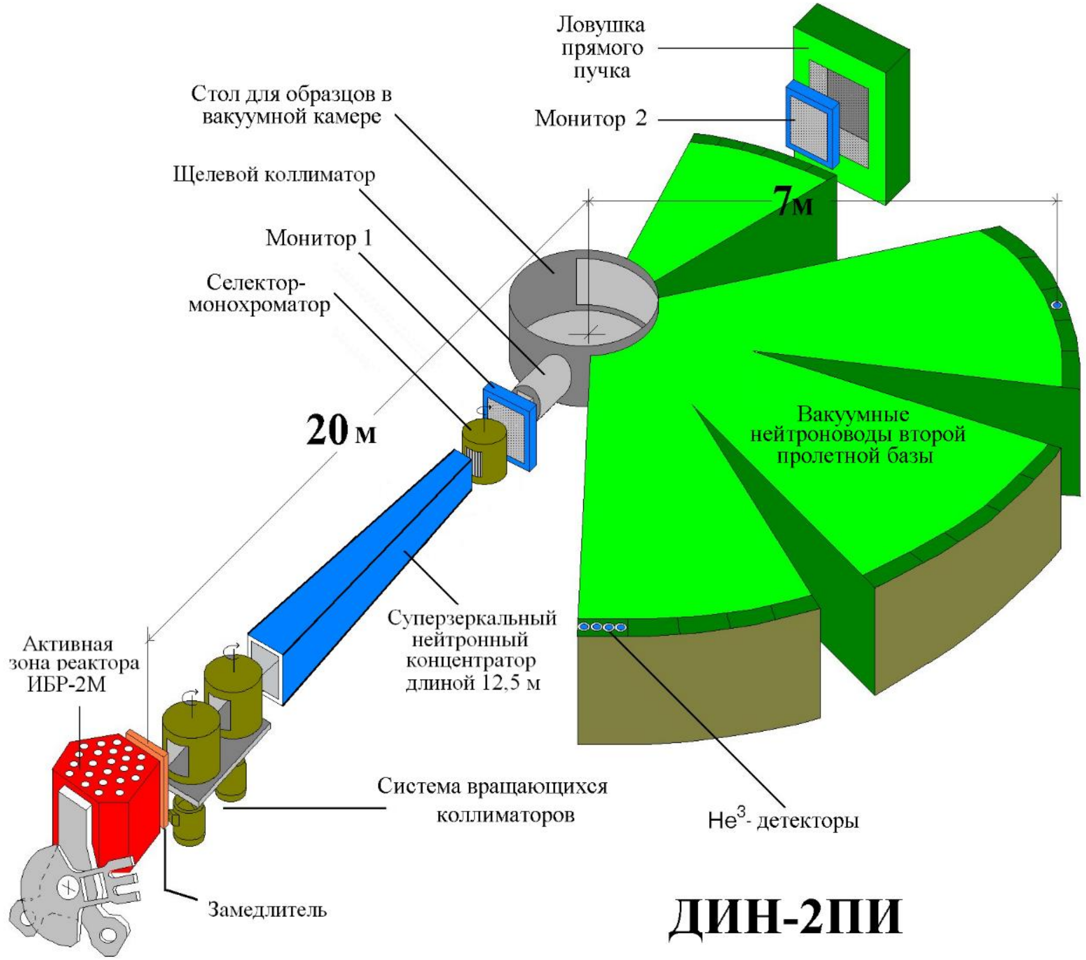


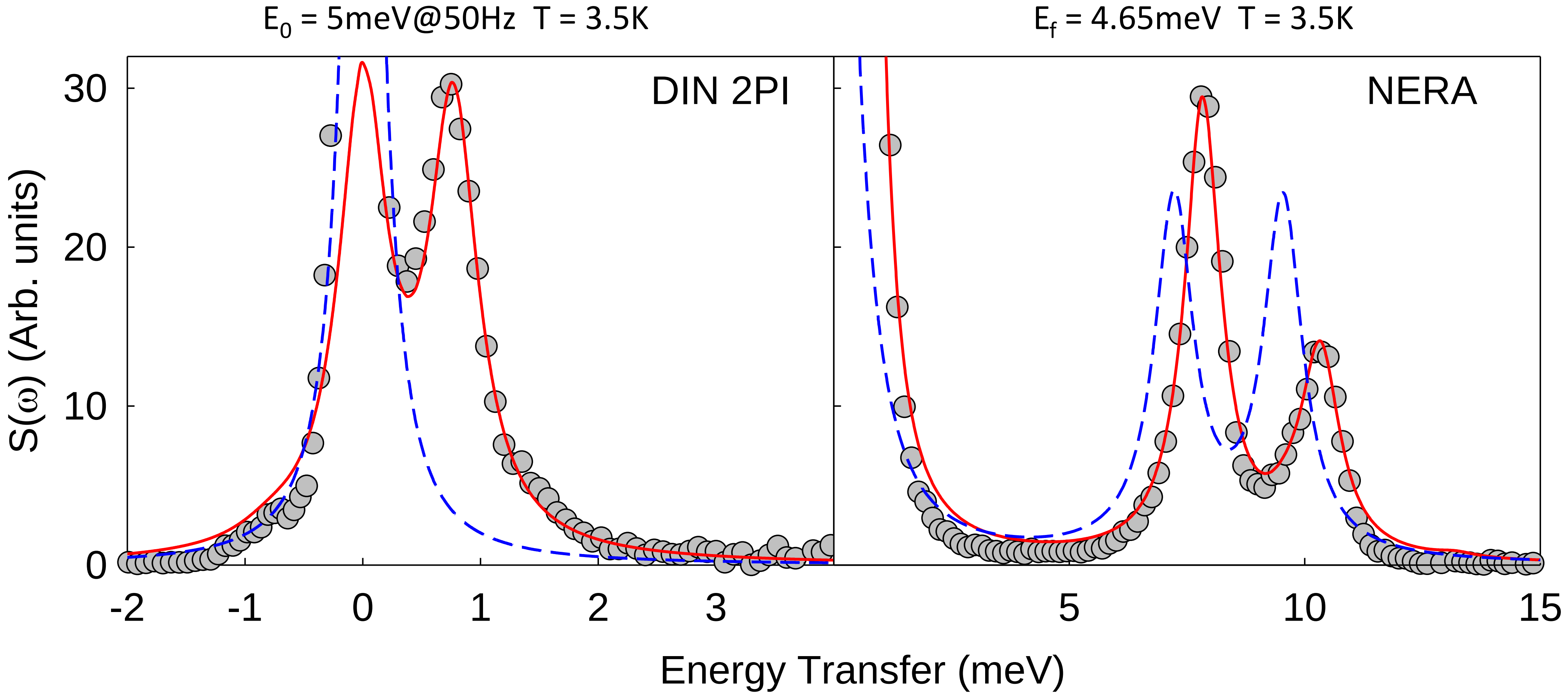
Figure 3. The main part of the NERA spectrometer: 1 - sample, 2 - Be-filters, 3 - collimators, 4 – He-3 detectors (INS and QENS), 5 - PG analysers (INS), 6 - single crystal analysers (QENS), 7 – detectors for high intensity diffraction, 8 – diffraction detectors with a good collimation, 9 - spectrometer shielding, 10 - Ni-coated mirror neutron guide in a vacuum tube, 11 - incident beam monitor, 12 – diaphragms, 13 - vacuum neutron guide.



$Ho^{11}B_{12}$

The blue dashed line is the CEF only response at 3.5K.

The red solid line is the CEF plus mean field due to AFM order



LLW CEF parameters: x = 0.0066 W = 0.03374meV (blue line) + Molecular Field: H_z = 0.18meV(2.1T) (red line)

DNS IV

1. INS spectrometer in direct geometry, fast Fermi chopper, medium resolution (~3-5%), large PSD detector, energy transfer range from 10meV up to 300-500meV, general purpose, single crystal and powder

2. INS spectrometer in direct geometry, disk choppers cascade, high resolution (~1.0-1.5%), large PSD detector, energy transfer range from ~0.1meV up to ~30meV, general purpose, single crystal and powder

3. Inverse geometry spectrometer for studies of vibrational dynamics in molecular systems, (chemistry, biology), large solid angle, high resolution (~1-2%)

Thanks a lot for your attention!