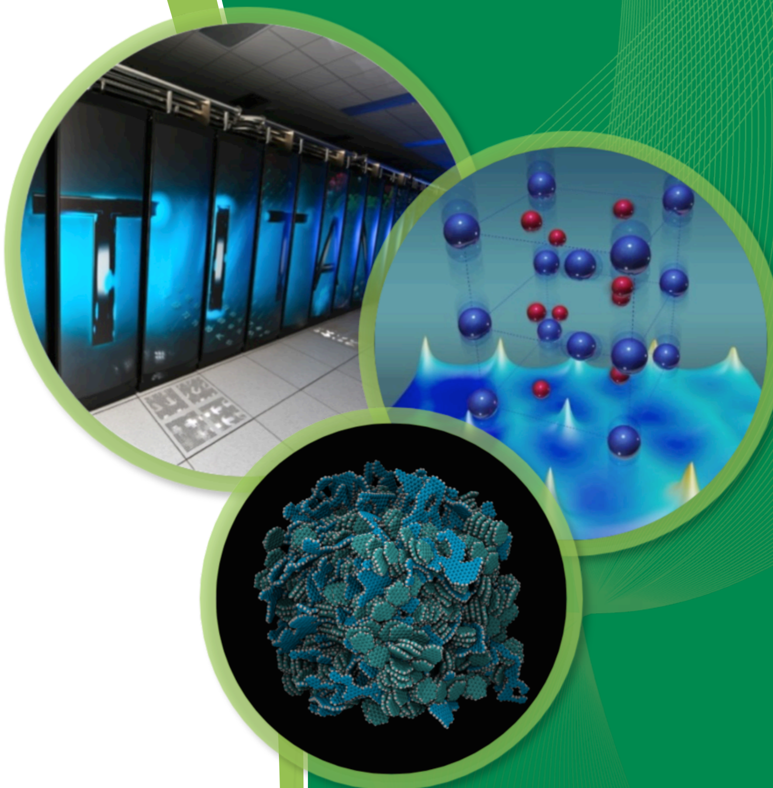
Energy/Wavelength selection methods



Georg Ehlers

Oak Ridge National Laboratory

ORNL is managed by UT-Battelle
for the US Department of Energy

Outline – By Technique

Neutrons show us where the atoms are and what they do.

- Introduction
- Elastic scattering
  - Diffraction
  - Other (Reflectometry, SANS)
- Monochromator Crystals & Choppers
- Inelastic scattering
  - Direct Geometry (TOF) vs Triple Axis
  - Indirect Geometry

Units commonly used

$$E = \frac{m}{2} \cdot v^2 = \frac{\hbar^2 \cdot k^2}{2m} = \frac{h^2}{2m \cdot \lambda^2}$$

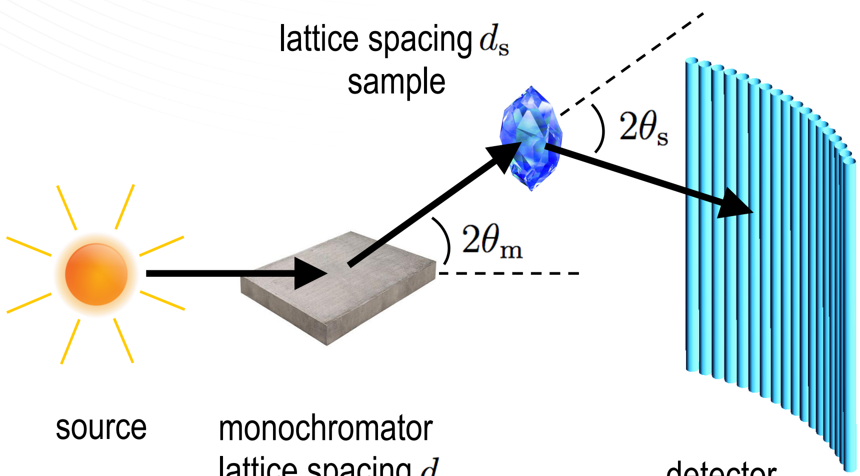
$$p = m \cdot v = \hbar \cdot k = \frac{h}{\lambda}$$

$$E\,[\mathrm{meV}] = \frac{81.8}{\lambda[\text{Å}]^2}$$

$$v\,[\mathrm{m/s}] = \frac{3956}{\lambda[\text{Å}]}$$

Methods for Elastic Scattering

crystal monochromator

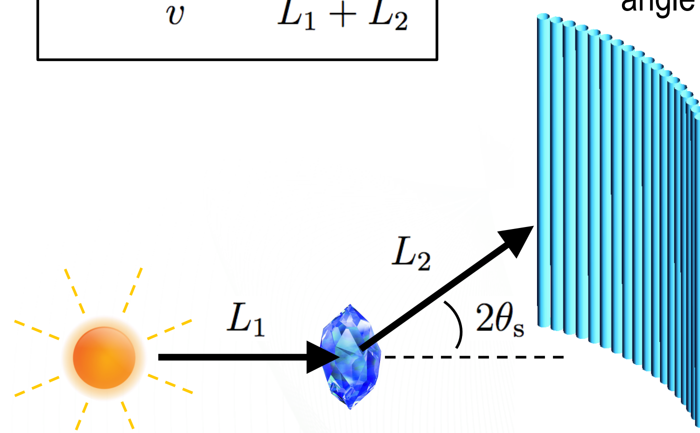


Bragg's law

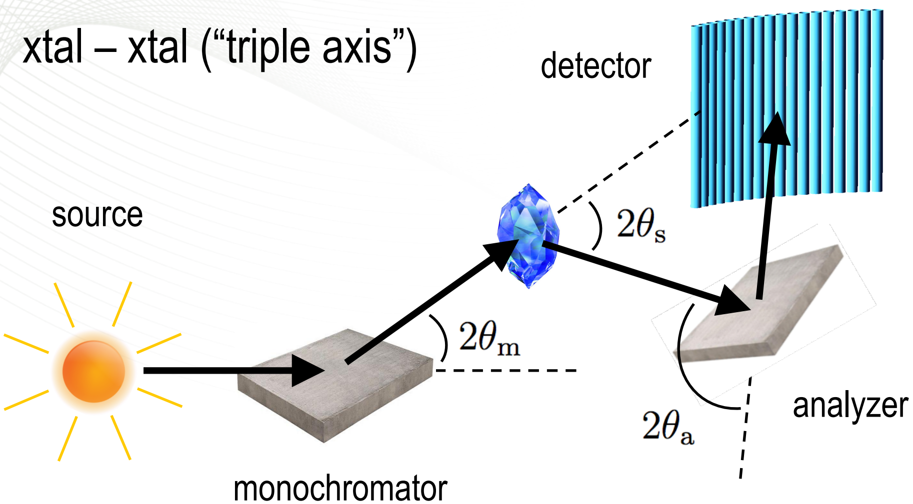
$$
\boxed{\begin{aligned} 2d_m \cdot \sin\theta_m &= \lambda \\ 2d_s \cdot \sin\theta_s &= \lambda \end{aligned}}
$$

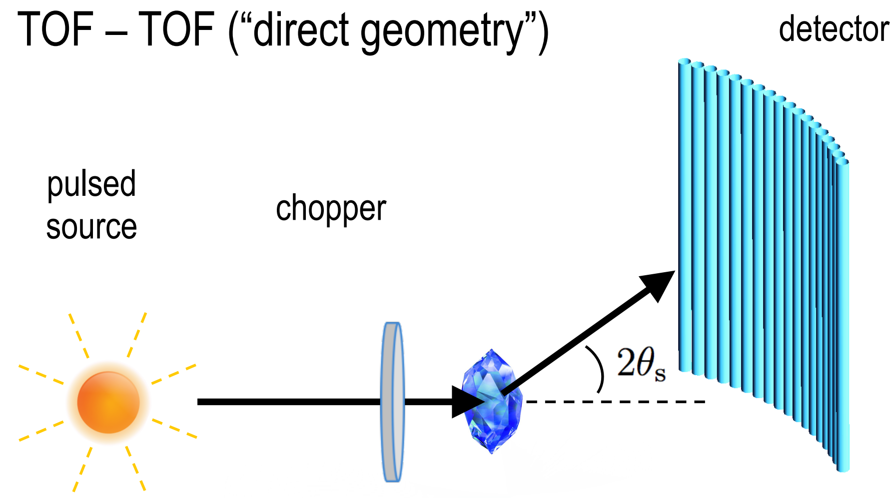
time-of-flight

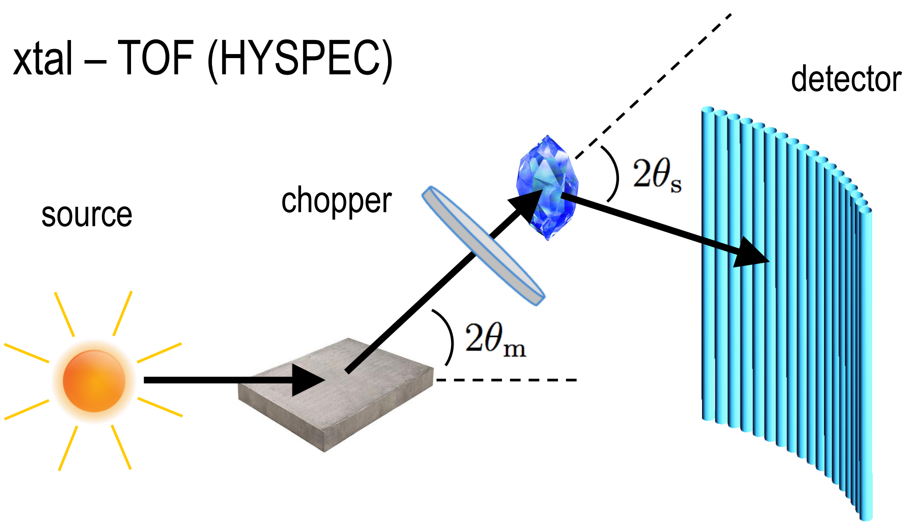
$$
\boxed{\lambda = \frac{3956}{v} = \frac{3956 \cdot t}{L_1 + L_2}}
$$

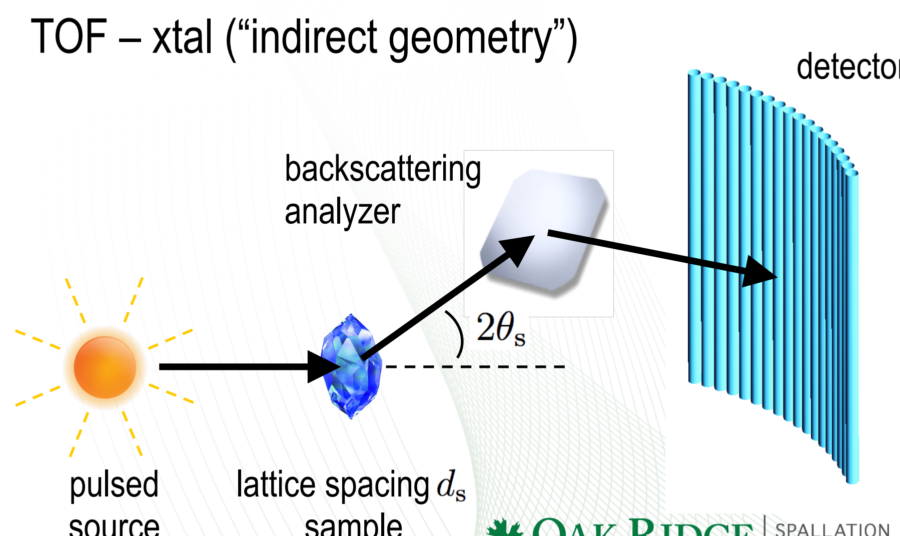


Methods for Inelastic Scattering





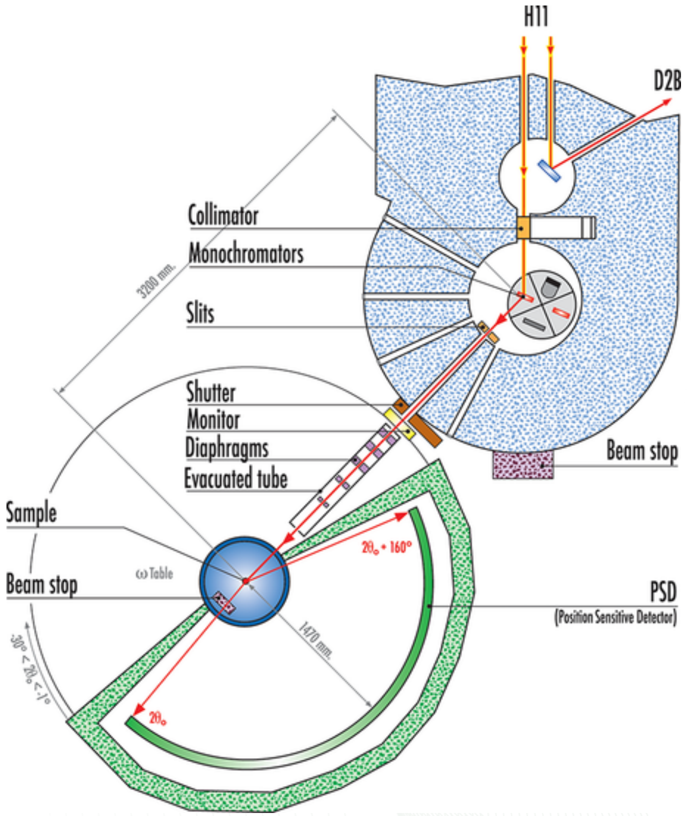




Diffraction

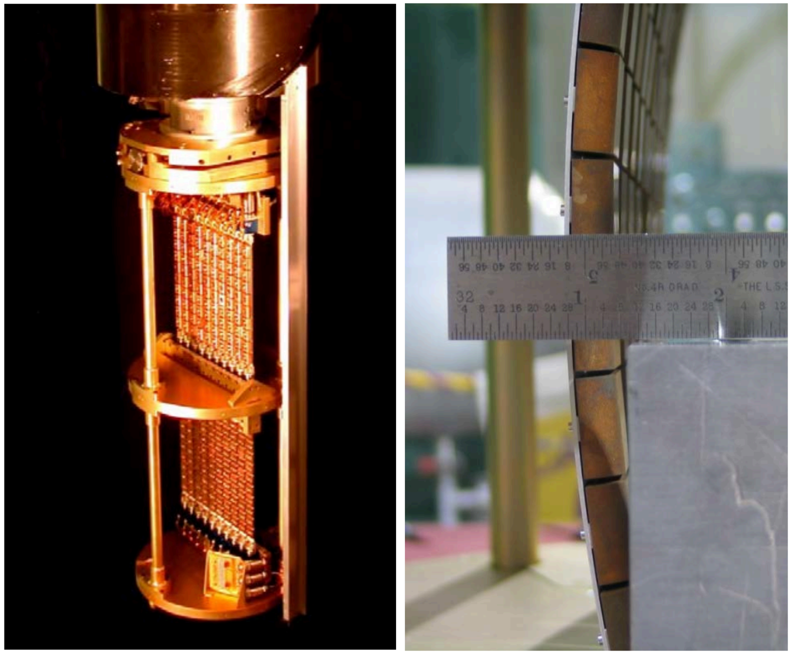
Bragg's law $2d \cdot \sin\theta = \lambda$

BT-1 (NIST website)

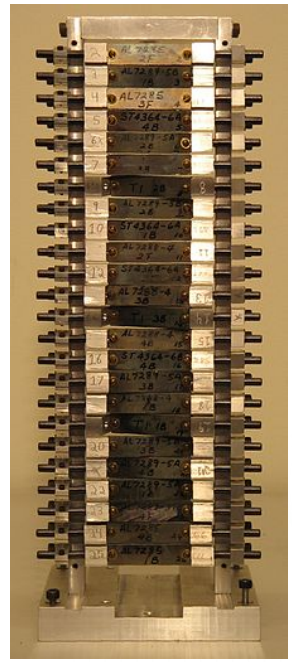


D20 (ILL website)

Key Component: Crystal Monochromator



Source: NIST (BT-7)

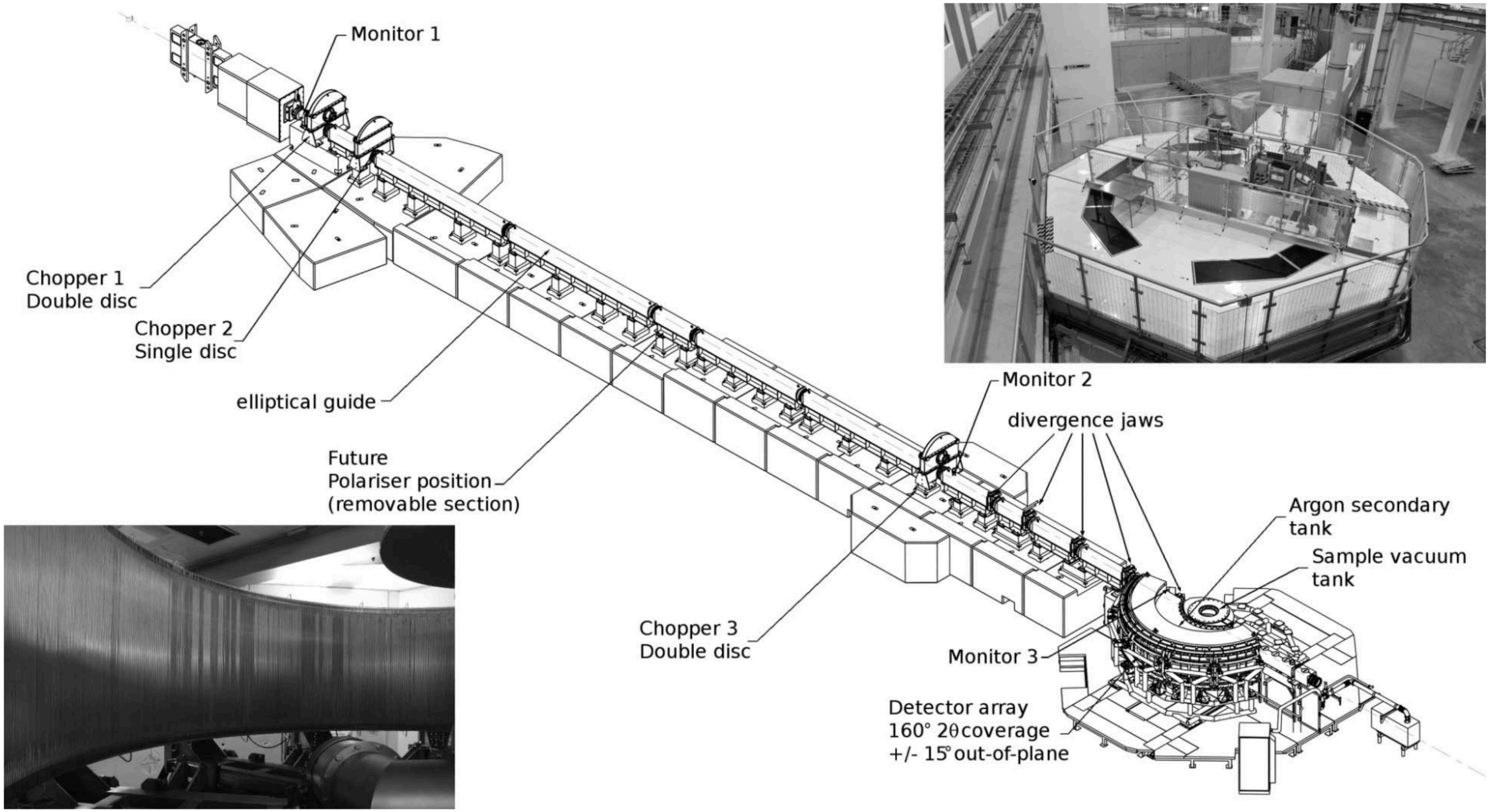


ANSTO (Echidna)

Materials: graphite, Si, Cu, Ge, Cu_2MnAl for polarized beam

To consider: reflectivity, mosaic

Diffraction using Time-Of-Flight

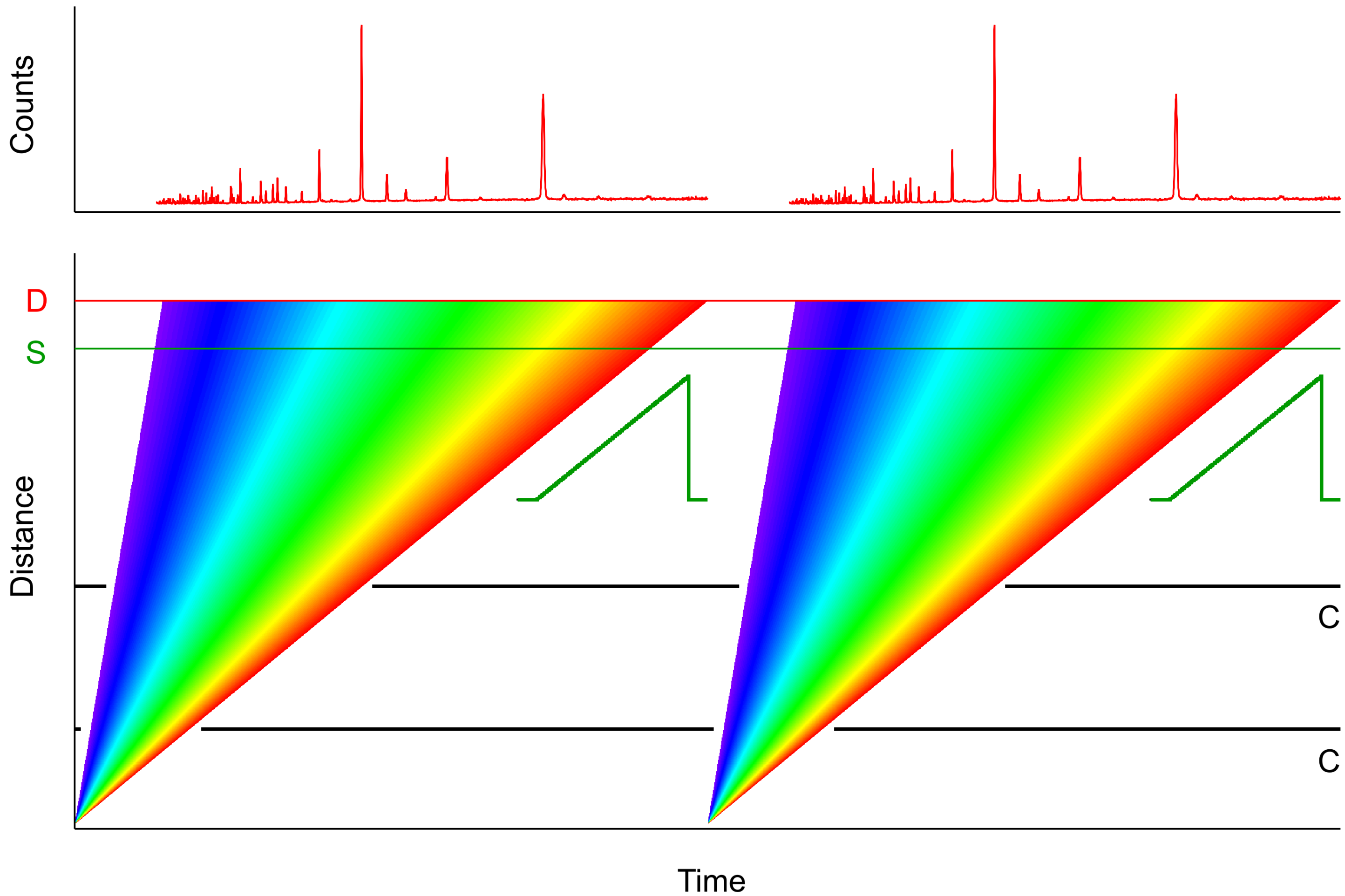


L. Chapon *et al.*, Neutron News **22** 22-25 (2011)

Bragg's law

$$2d \cdot \sin\theta = \lambda$$
$$d[\text{Å}] \cdot \sin\theta = 1.978 \cdot t[\text{ms}]/L[\text{m}]$$

Diffraction (elastic, no energy discrimination)



The first time-of-flight spectrum ever

Velocity of Slow Neutrons by Mechanical Velocity Selector

Four duraluminum disks were provided with sectors of sheet cadmium, the sectors subtending 3.7° with spacing of 3.5° between. Two of these disks were mounted 54 cm apart to rotate on the same shaft, while the other two disks were fixed within 5 mm of the rotating disks, respectively, as shown in Fig. 1. Since the cadmium is practically opaque to slow neutrons and the duraluminum transparent, the two pairs of disks form a mechanical velocity selector for slow neutrons. Speeds up to 5000 r.p.m. were used.

The Rn-Be source, about 600 millicuries, was placed in a Cd shielded paraffin cylinder 16 cm diameter and 22 cm long, and the neutrons were detected by an 8-cm diameter Li-lined ion chamber specially constructed to be insensitive to noise and connected to a linear amplifier-thyratron recording system.

Better resolution is desirable, but decreasing the ratio of width of spacing to width of Cd sectors not only reduces

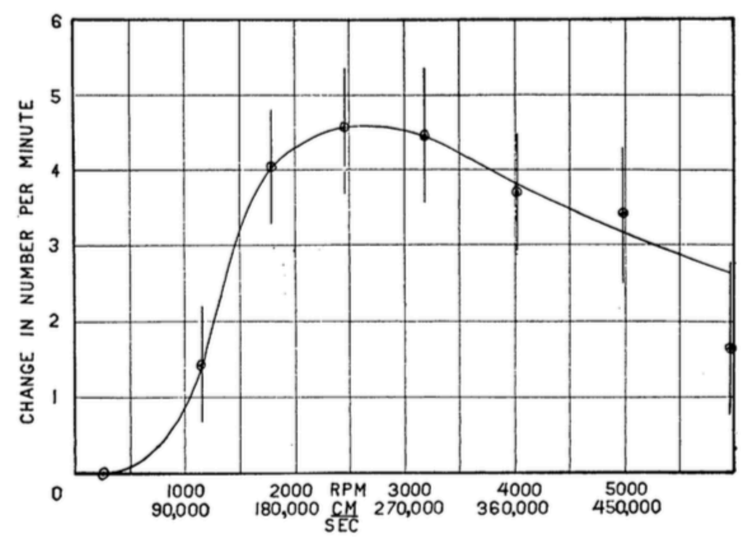
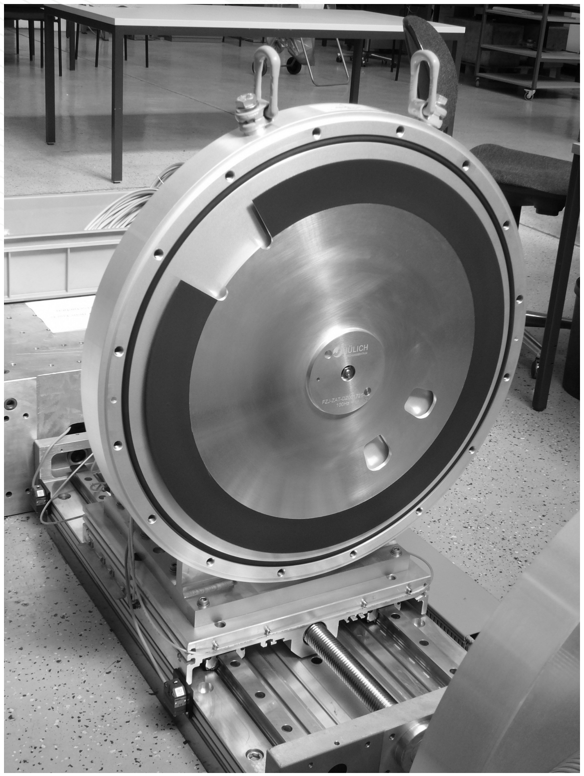


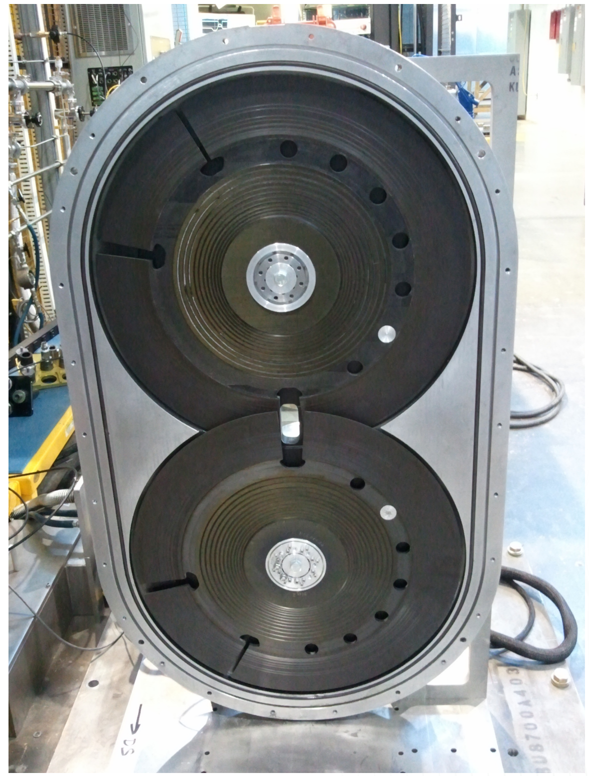
FIG. 2. Curve showing change (decrease) in number of slow neutrons detected after passing through the two shutter systems, as the speed of the sectors was changed. The speed of the sectors is indicated in revolutions per minute, and the neutron velocity for which the selector is most effective is also indicated.

J. R. Dunning et al., PR **48** 704 (1935)

OAK RIDGE National Laboratory | SPALLATION NEUTRON SOURCE

Key Component: Choppers – 1 – Disk Choppers



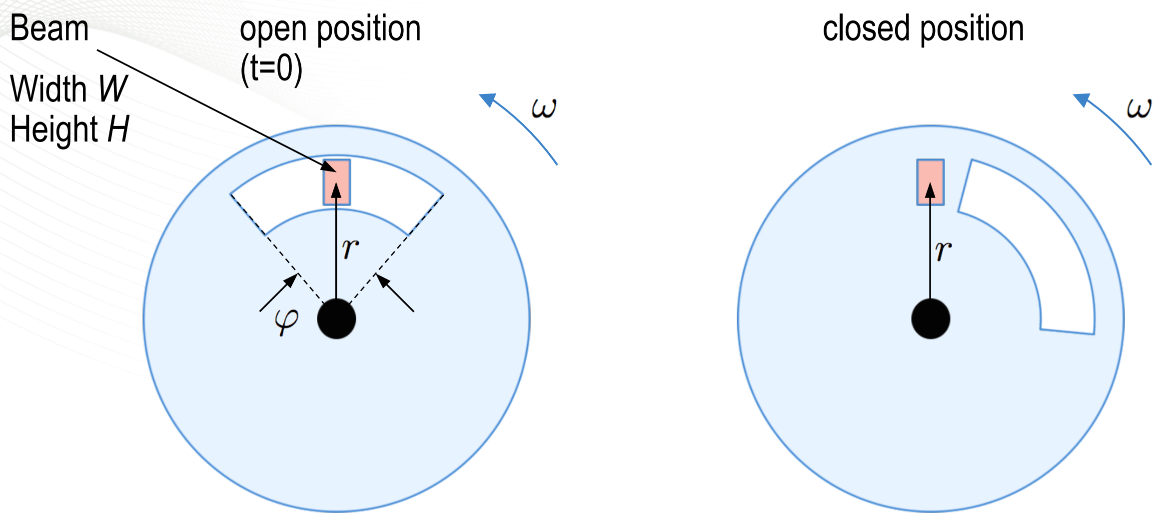


This type of chopper can be used as monochromating chopper or as bandwidth limiting chopper. The transmission is independent of wavelength

http://www.fz-juelich.de

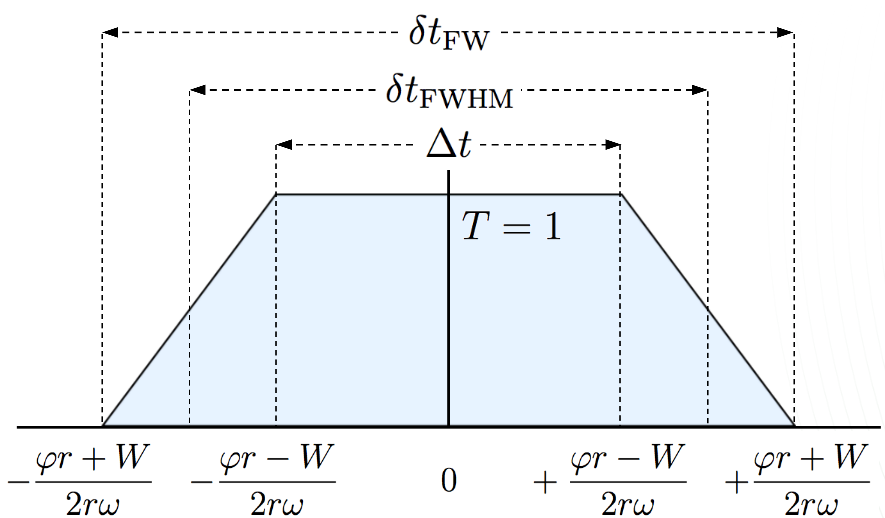
CNCS

Key Component: Choppers – 1 – Disk Choppers



Ian Anderson (ORNL)

$$\boxed{\varphi r \geq W}$$

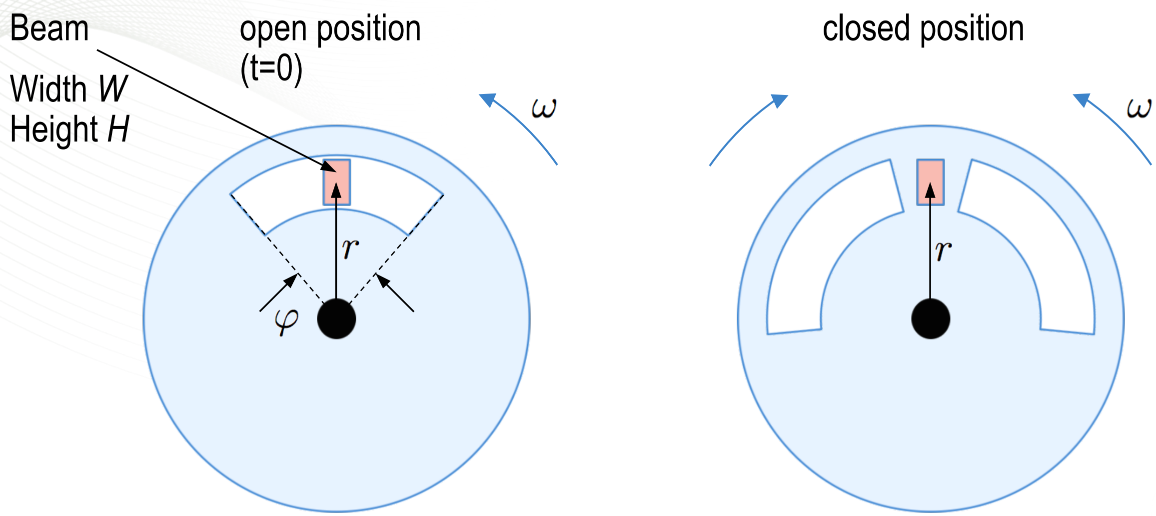


$$\delta t_{\mathrm{FW}} = \frac{\varphi r + W}{r\omega}$$

$$\delta t_{\mathrm{FWHM}} = \frac{\varphi}{\omega}$$

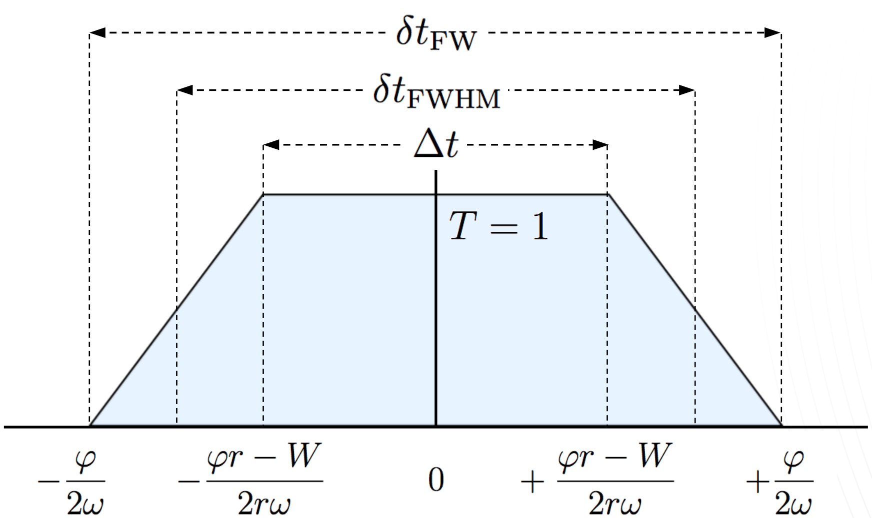
$$\Delta t = \frac{\varphi r - W}{r\omega}$$

Counter–rotating Disk Choppers



Ian Anderson (ORNL)

$$\varphi r \geq W$$



$$\delta t_{\mathrm{FW}} = \frac{\varphi}{\omega}$$

$$\delta t_{\mathrm{FWHM}} = \frac{2\varphi r - W}{2r\omega}$$

$$\Delta t = \frac{\varphi r - W}{r\omega}$$

Key Component: Choppers – 2 – Fermi Choppers

PHYSICAL REVIEW VOLUME 72, NUMBER 3 AUGUST 1, 1947

A Thermal Neutron Velocity Selector and Its Application to the Measurement of the Cross Section of Boron

E. Fermi, J. Marshall, and L. Marshall
Argonne National Laboratory, University of Chicago, Chicago,** Illinois*
(Received April 25, 1947)

A mechanical velocity selector for the study of monochromatic neutrons in the range of energies below 0.3 ev is described.
The instrument has been applied to the measurement of the cross section of boron, which is found to be 703×10^{-24} cm^2 for neutrons of 2200 meters per second velocity.

INTRODUCTION

Slow neutrons emerging from various moderators with different geometries usually have average velocities comparable, but by no means equal, to the thermal agitation velocity. Large differences, both positive and negative, are observed depending on the nature and the geometry of the moderating substance. This phenomenon has been observed by various experimenters.[1–4]

In this paper we have collected some typical examples of the variations of average velocity of slow neutrons using different moderators as 703×10^{-24} cm^2 per atom per neutrons of velocity 2200 meters per second.

TEMPERATURES OF NEUTRONS FROM VARIOUS SOURCES

With the thermal purification column of the graphite pile at the Argonne Laboratory as a primary neutron source, a number of measurements were made of the cross section of boron. In all cases the detector was a proportional counter filled with BF_3 gas. By the use of cadmium diaphragms a neutron beam was obtained with small angular dispersion.

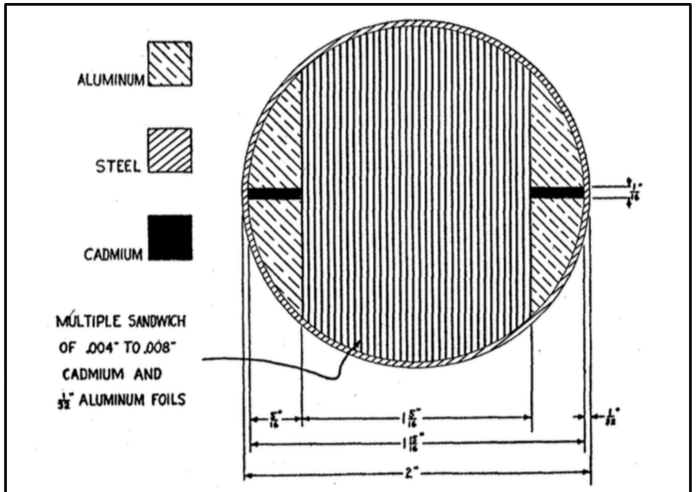


Fig. 1. Cross section of the shutter of the velocity selector.

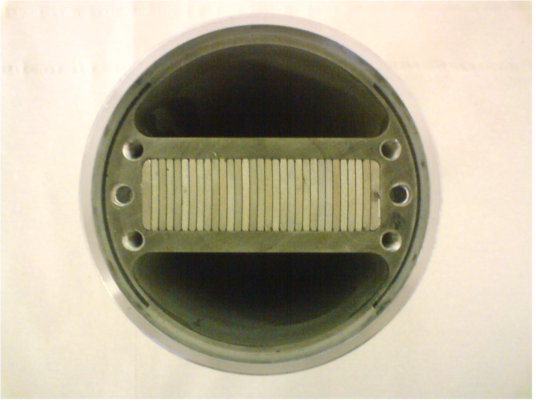
OAK RIDGE National Laboratory | SPALLATION NEUTRON SOURCE

Key Component: Choppers – 2 – Fermi Choppers

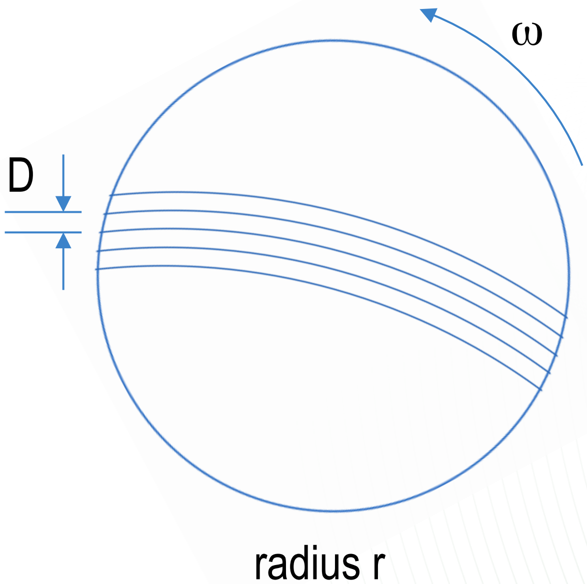
ARCS

The transmission is wavelength dependent and has approx. triangular shape.

$\Delta t = D/2r\omega$



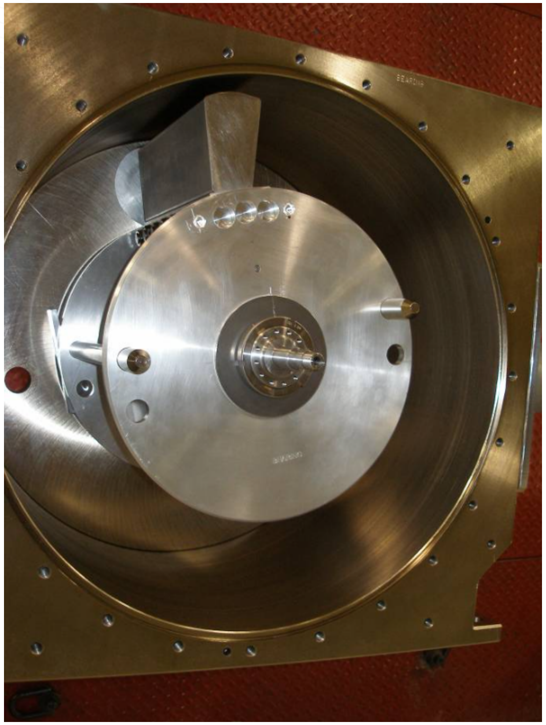
CNCS

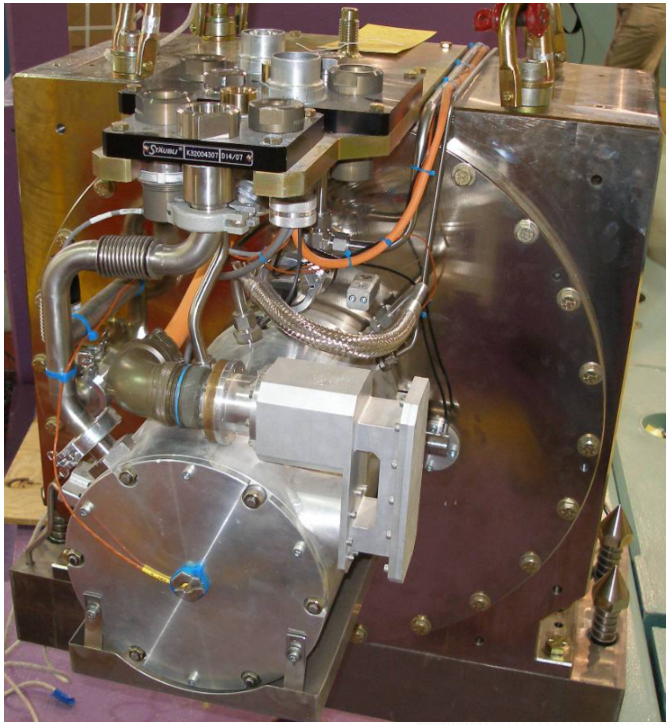


Disk vs Fermi Choppers

Disk Chopper	Fermi Chopper
Line shape (width) is *flexible* but pulses cannot be very short unless the beam is narrow	Pulses can be nearly arbitrarily sharp even when the beam is wide (especially important for thermal neutrons)
Monochromator or bandwidth limiter	Monochromator or pulse-shaping
Does not need much space along the beam (≤5 cm)	Rotor is more compact, rotational speed can be higher, needs ≥15 cm of beam
Can have 1, 2, 3 or more slits	Opens twice per revolution
Transmission is wavelength-independent and approaches 1 in open position	

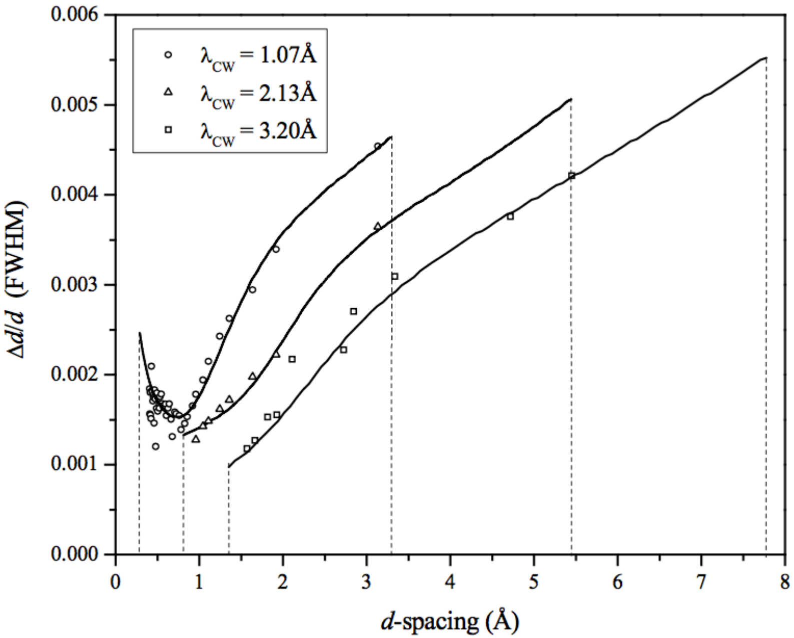
Horizontal axis T_0 chopper



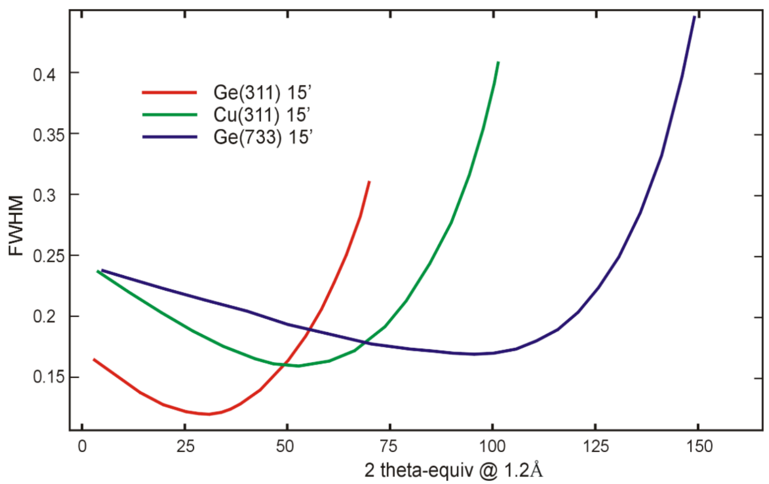


Comparison TOF – monochromator instrument

POWGEN (TOF) @ SNS



BT-1 (Mono.) @ NIST

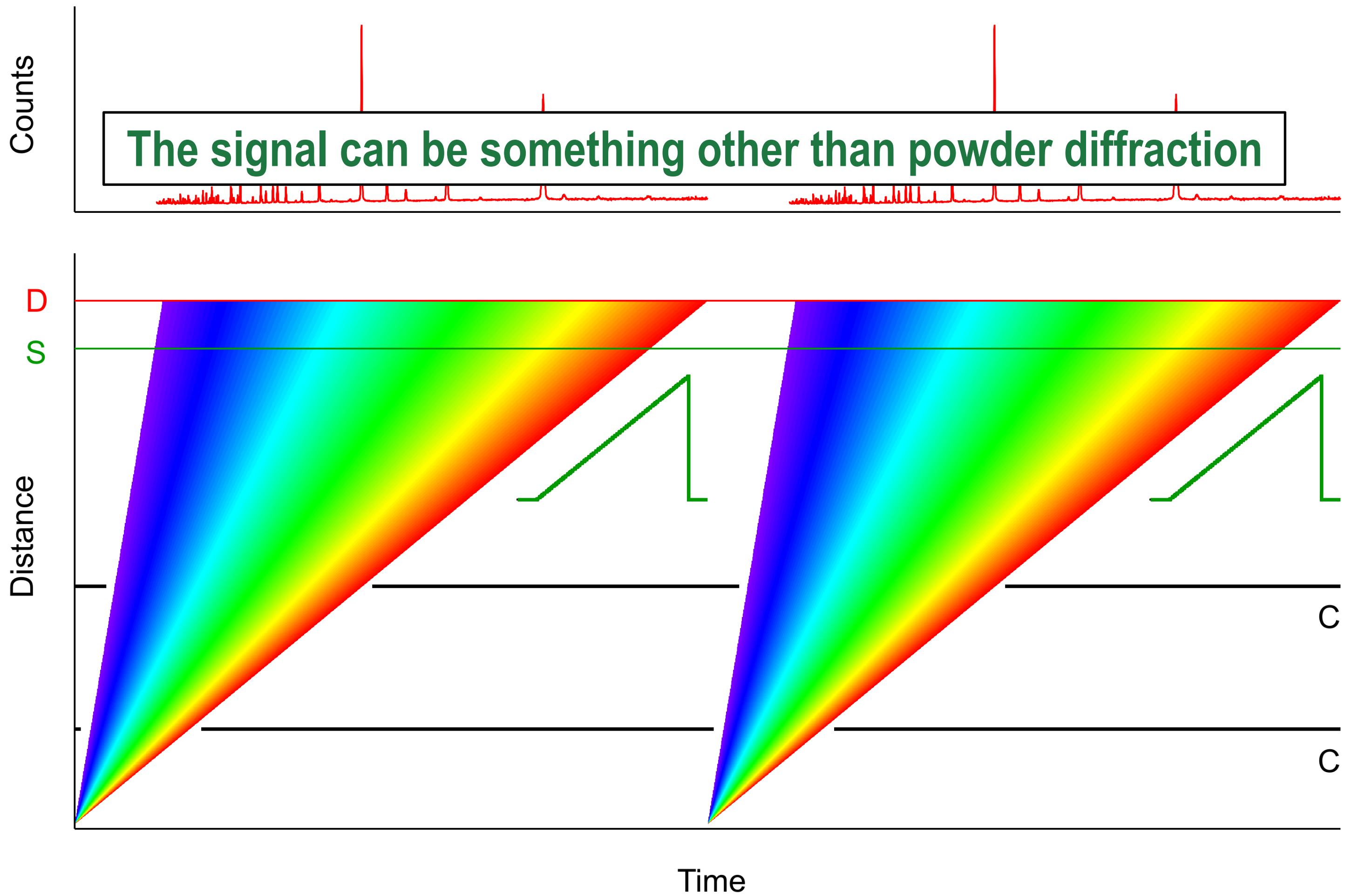


Resolution as FWHM (degrees) as a function of 2theta (degrees), for BT-1 using each of the three monochromators and 15' collimation. For comparison purposes, angles for the Ge(311) and Cu(311) monochromators are extrapolated to the wavelength of the Ge(733) monochromators.

A. Huq *et al*., Z. Krist. Proc. **1** 127-135 (2011)

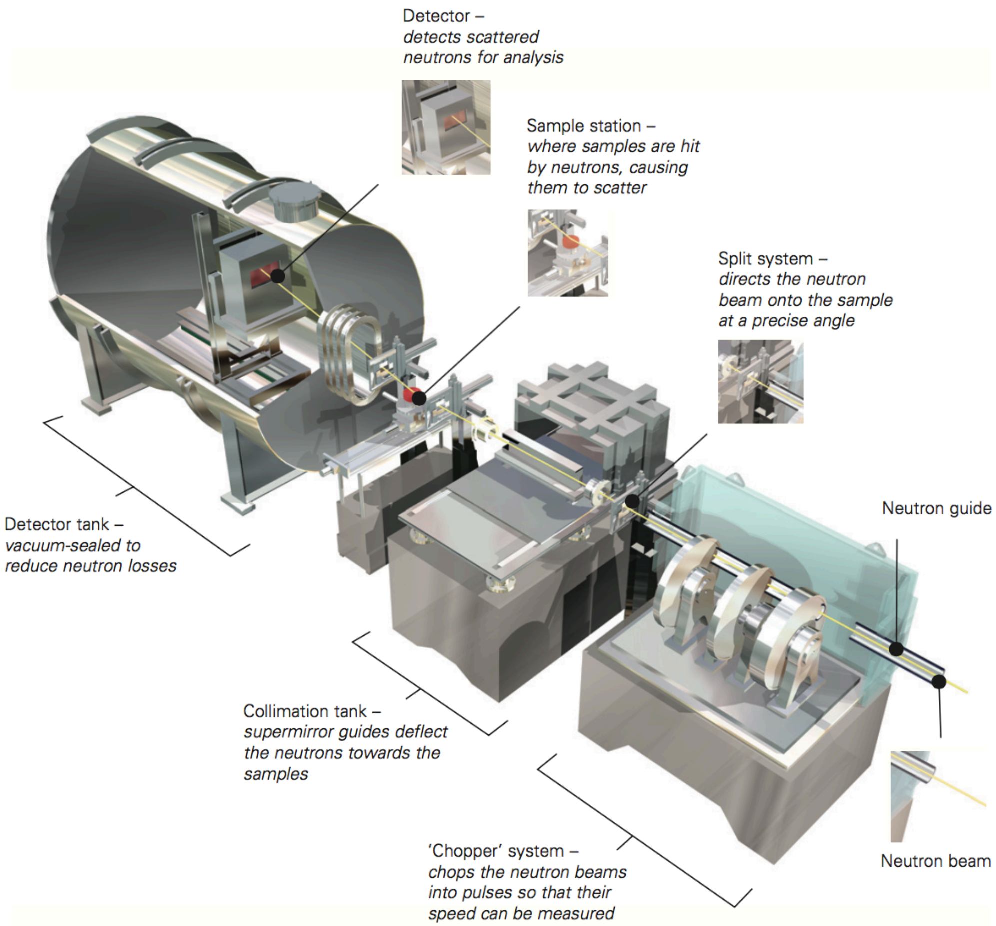
NIST website

Elastic scattering (again)



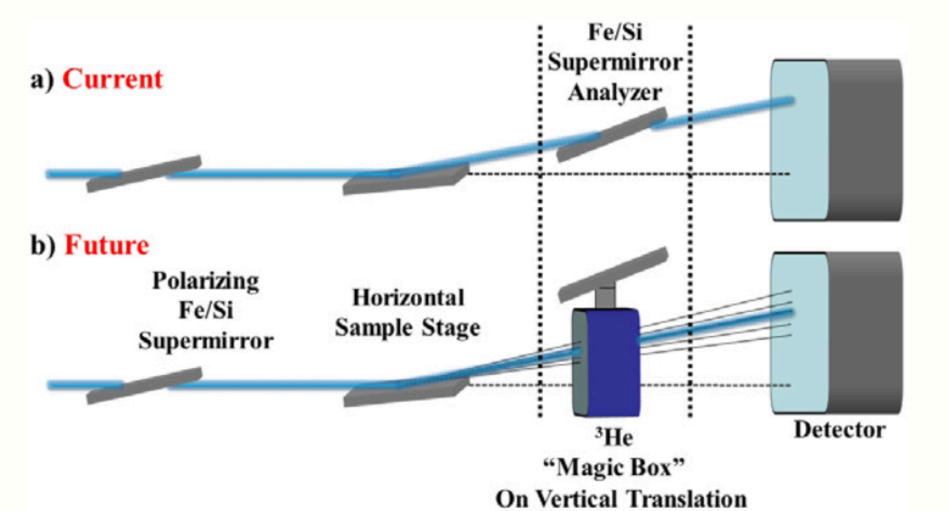
OAK RIDGE National Laboratory | SPALLATION NEUTRON SOURCE

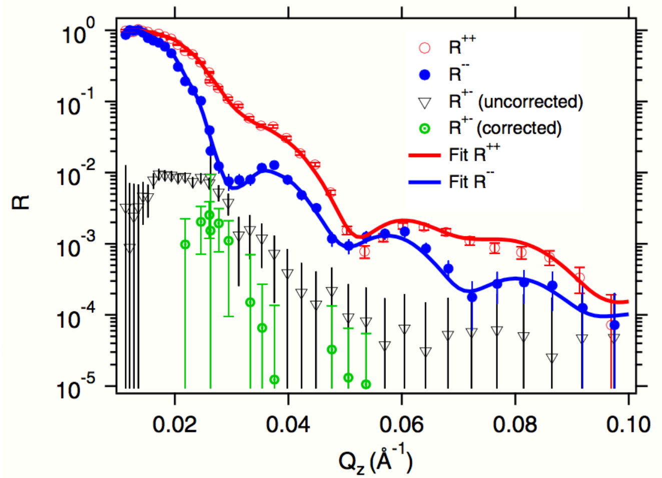
TOF – Reflectometer



ANSTO website

TOF – Reflectometer



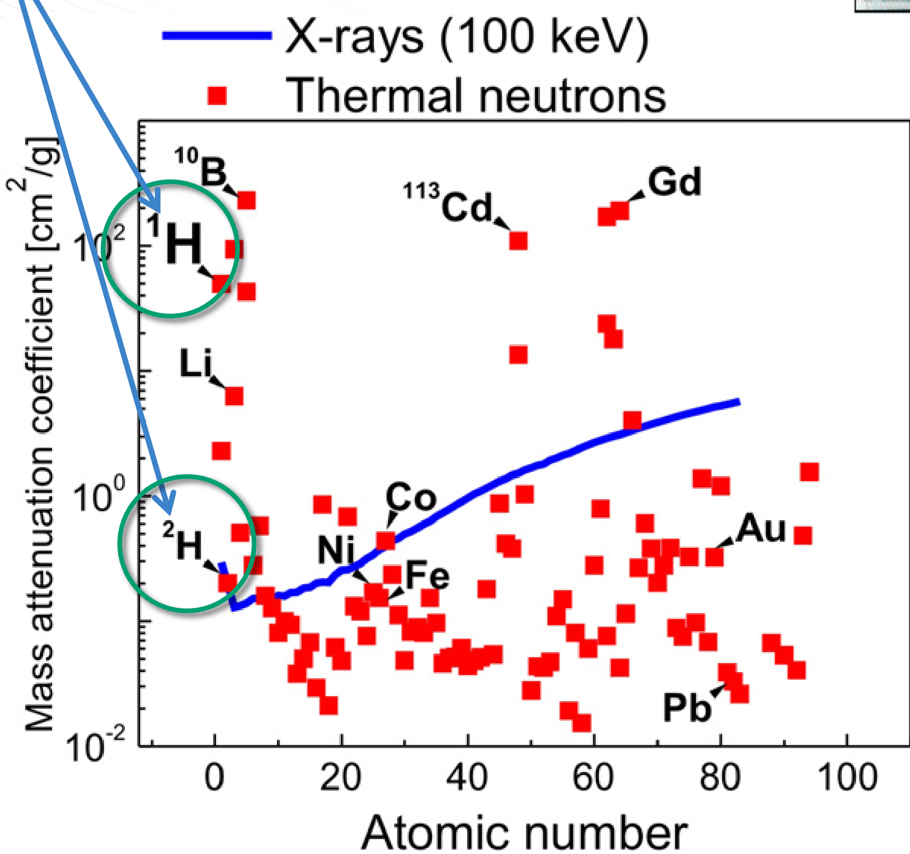


T. Saerbeck *et al*., Physics Procedia **42** 213-217 (2013)

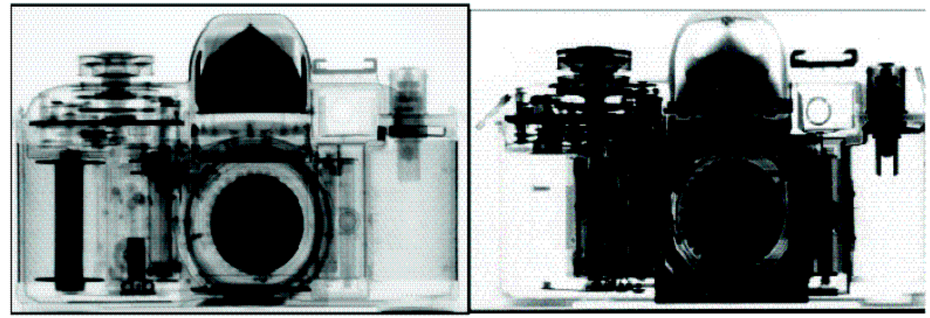
OAK RIDGE National Laboratory | SPALLATION NEUTRON SOURCE

TOF – Imaging

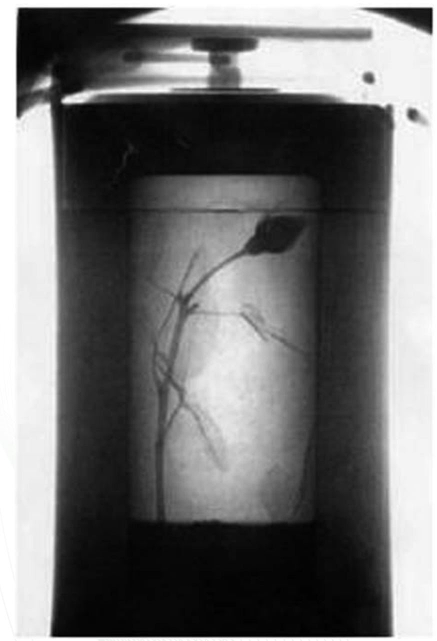
Isotope Sensitivity (important for soft matter studies)



M. Strobl *et al*., J. Phys. D: Appl. Phys. **42** (2009) 243001



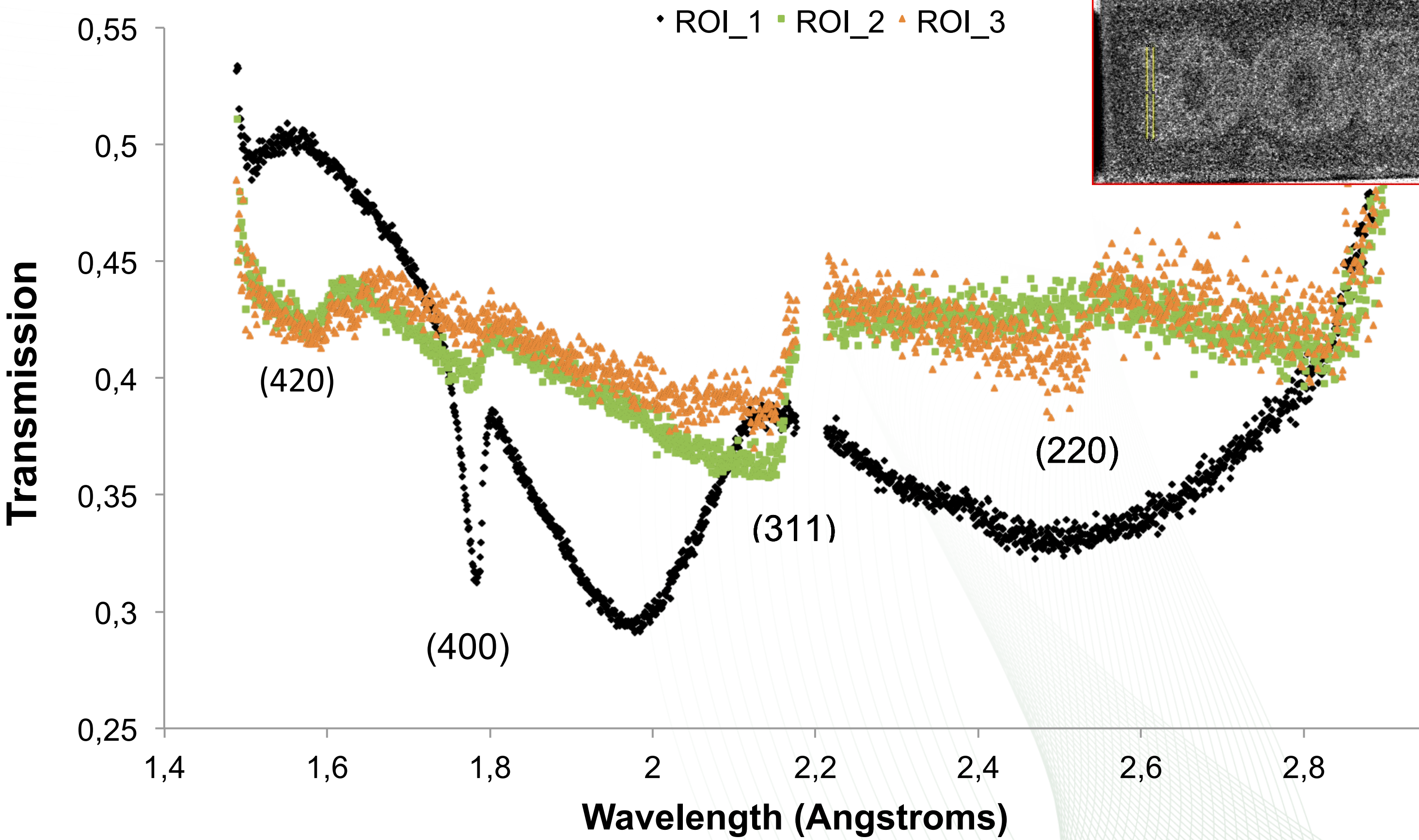
courtesy of E. Lehmann, PSI

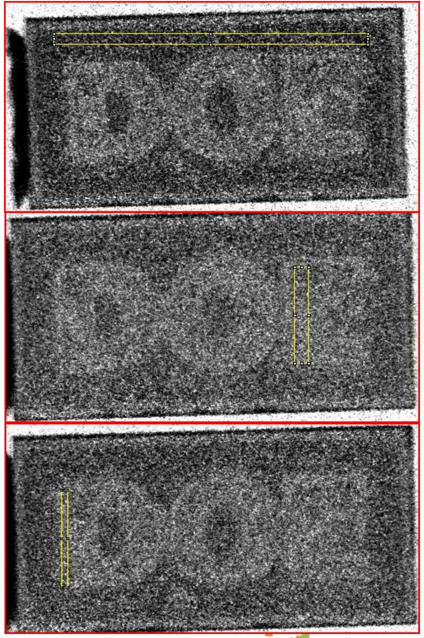


***Neutron** Radiograph of Rose in Lead Flask*

TOF – Imaging

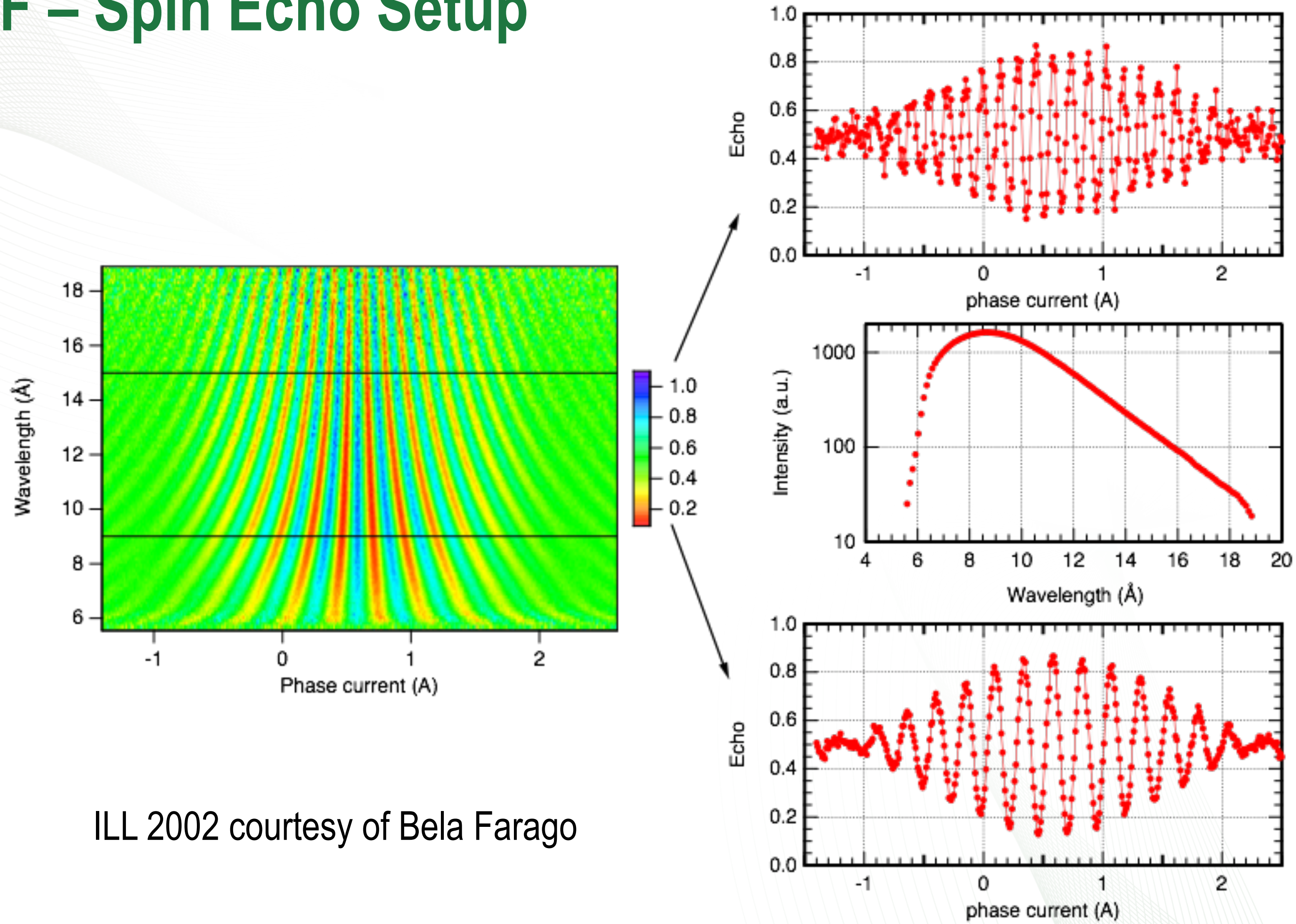
	Ni	Inconel	High textured ROI_1	Polycrystal ROI_2	Mixed ROI_3
220	2.492	2.542	/	/	2.509
311	2.125	2.168	1.969	2.146	2.128
400	1.762	1.797	1.781	1.779	/





courtesy of H. Bilheux, SNS

TOF – Spin Echo Setup



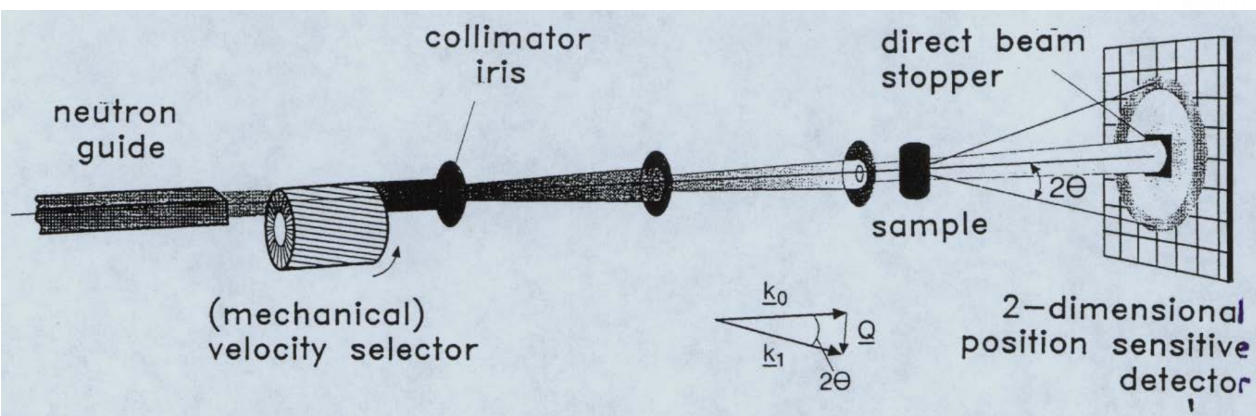
ILL 2002 courtesy of Bela Farago

Velocity Selector

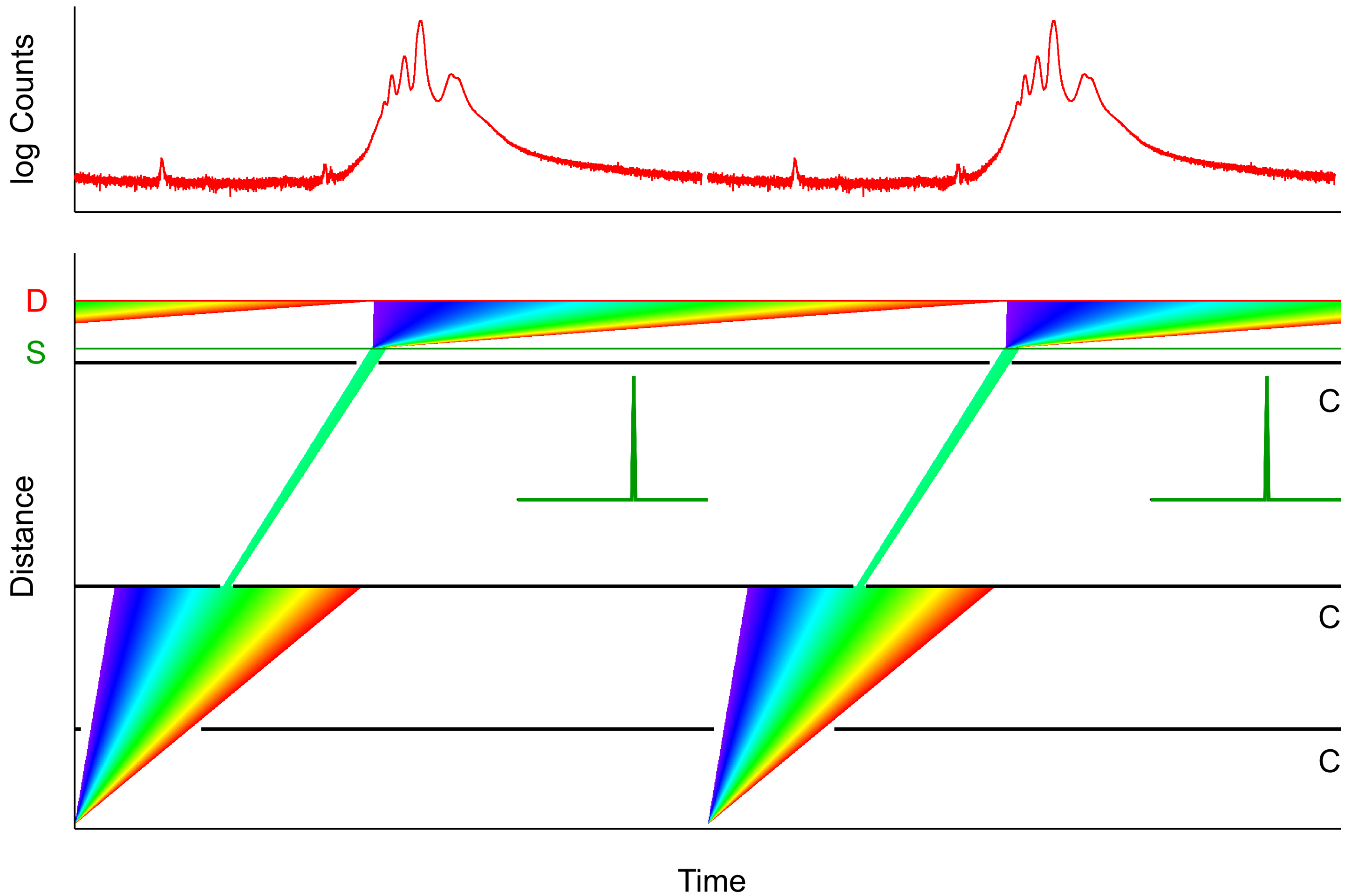
https://www.ph.tum.de

Competes with TOF for use with reflectometers, SANS instruments, and spin echo spectrometers at a reactor source. Essentially a rotating collimator. Triple-axis spectrometers may use it for background suppression.

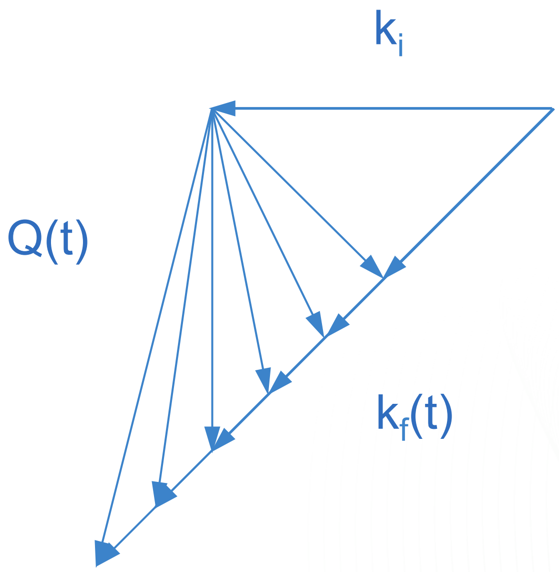
The resulting wavelength spectrum is triangular.



Direct Geometry Spectroscopy



Momentum Space Representation

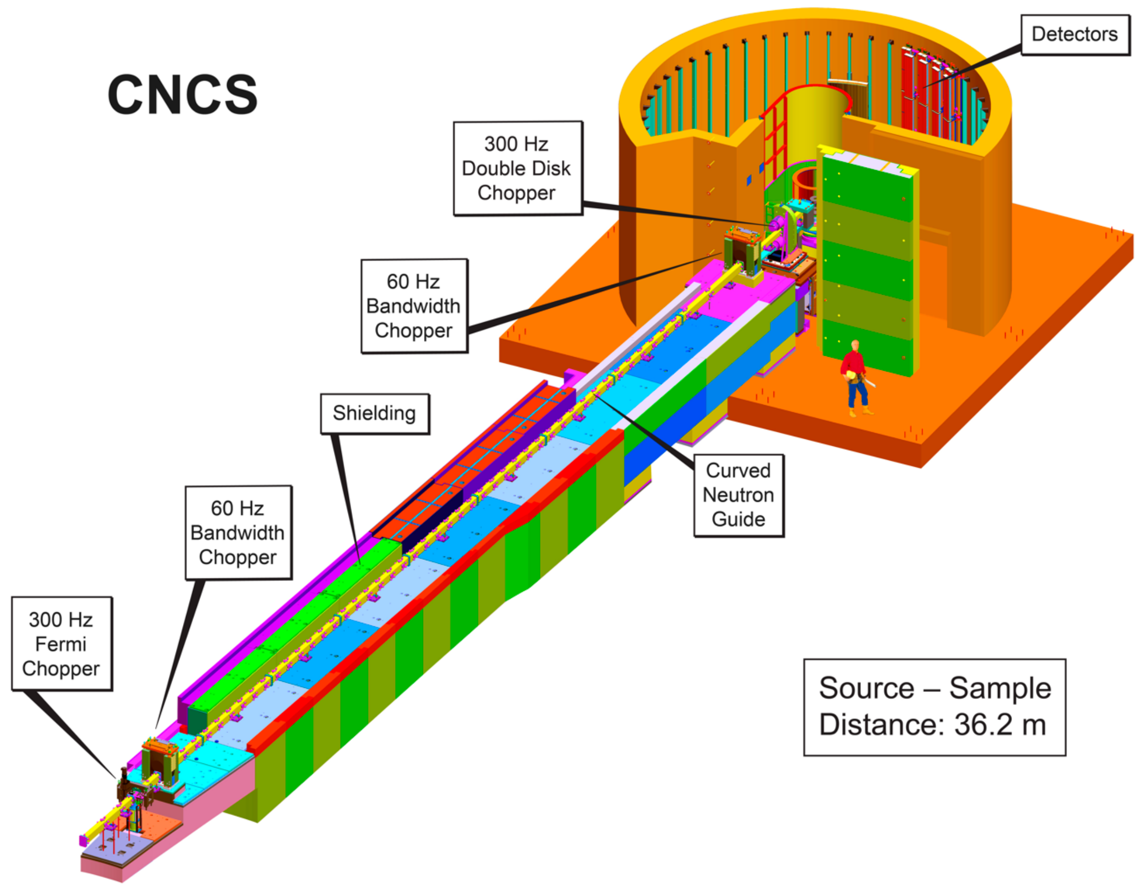


Direct Geometry Spectroscopy

Time of flight now encodes energy transfer

$$
\begin{aligned}
t_0 &= L/v_i \\
t &= L/v_f \\
\hbar\omega(t) &= \frac{m}{2}L^2 \cdot \left(\frac{1}{t_i^2} - \frac{1}{t_f^2}\right) \\
|Q| &= \frac{m}{\hbar}L \cdot \sqrt{\frac{t_i^2 + t_f^2 - 2t_i t_f \cos 2\theta}{t_i^2 t_f^2}}
\end{aligned}
$$

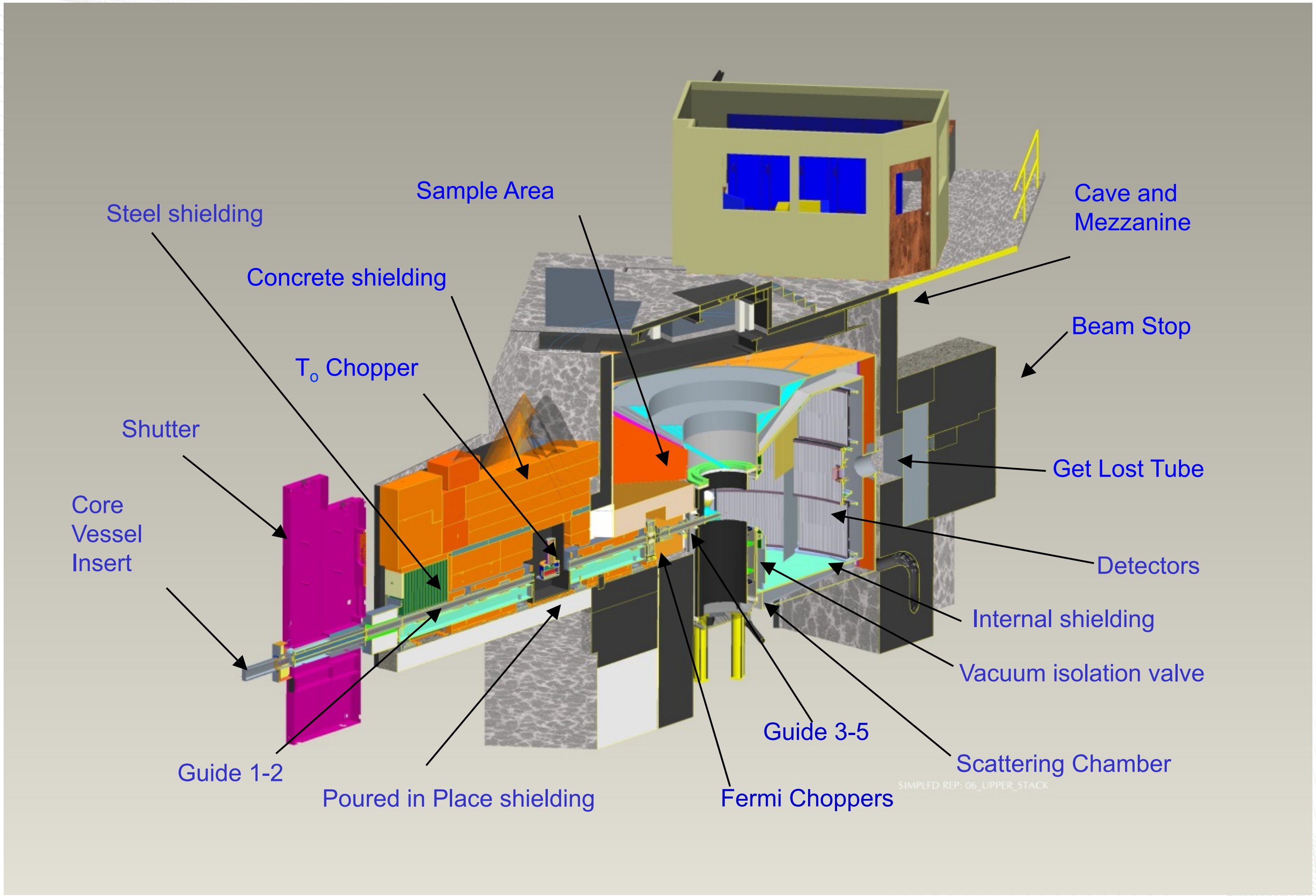
Direct Geometry Spectroscopy – Cold Range



Source – Sample
Distance: 36.2 m

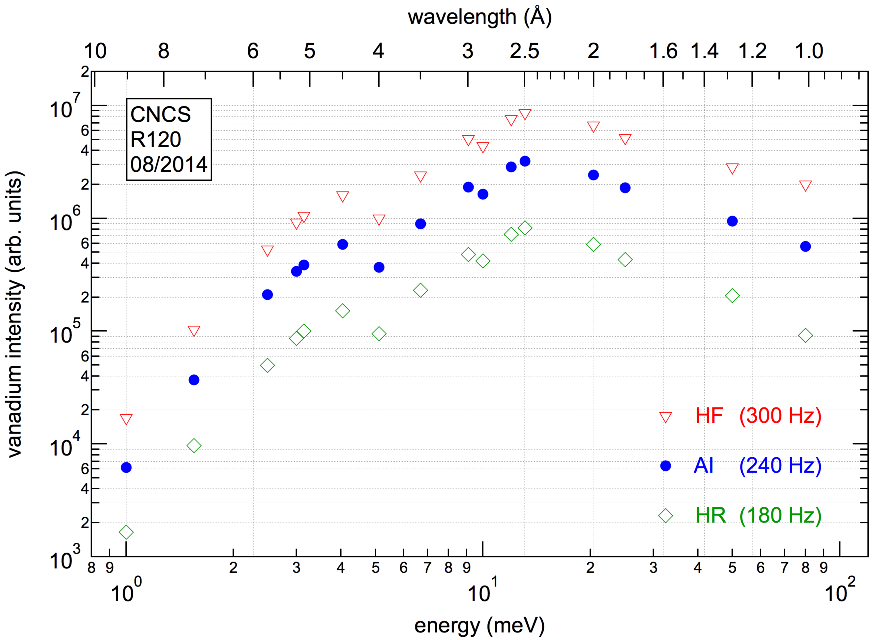
CNCS

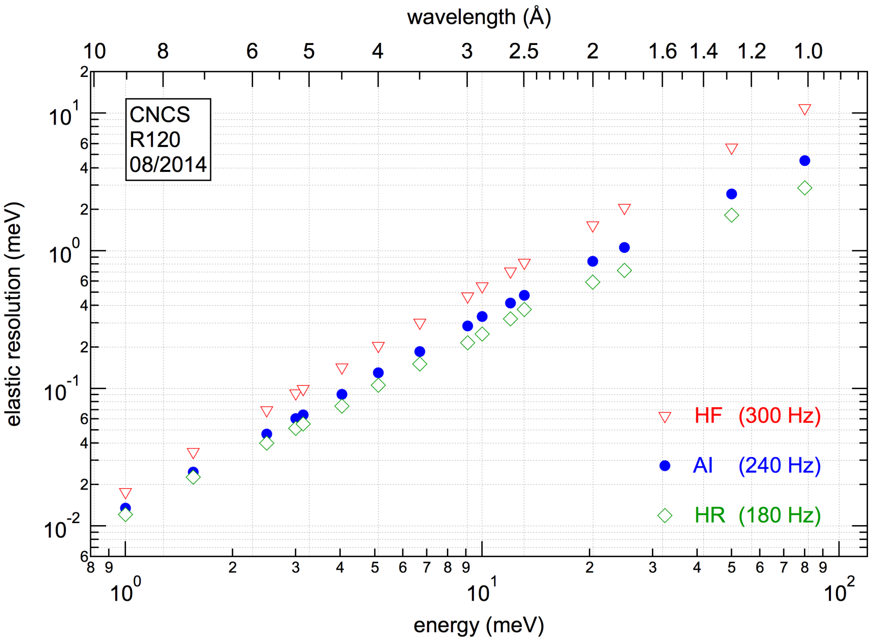
Direct Geometry Spectroscopy – Thermal Range



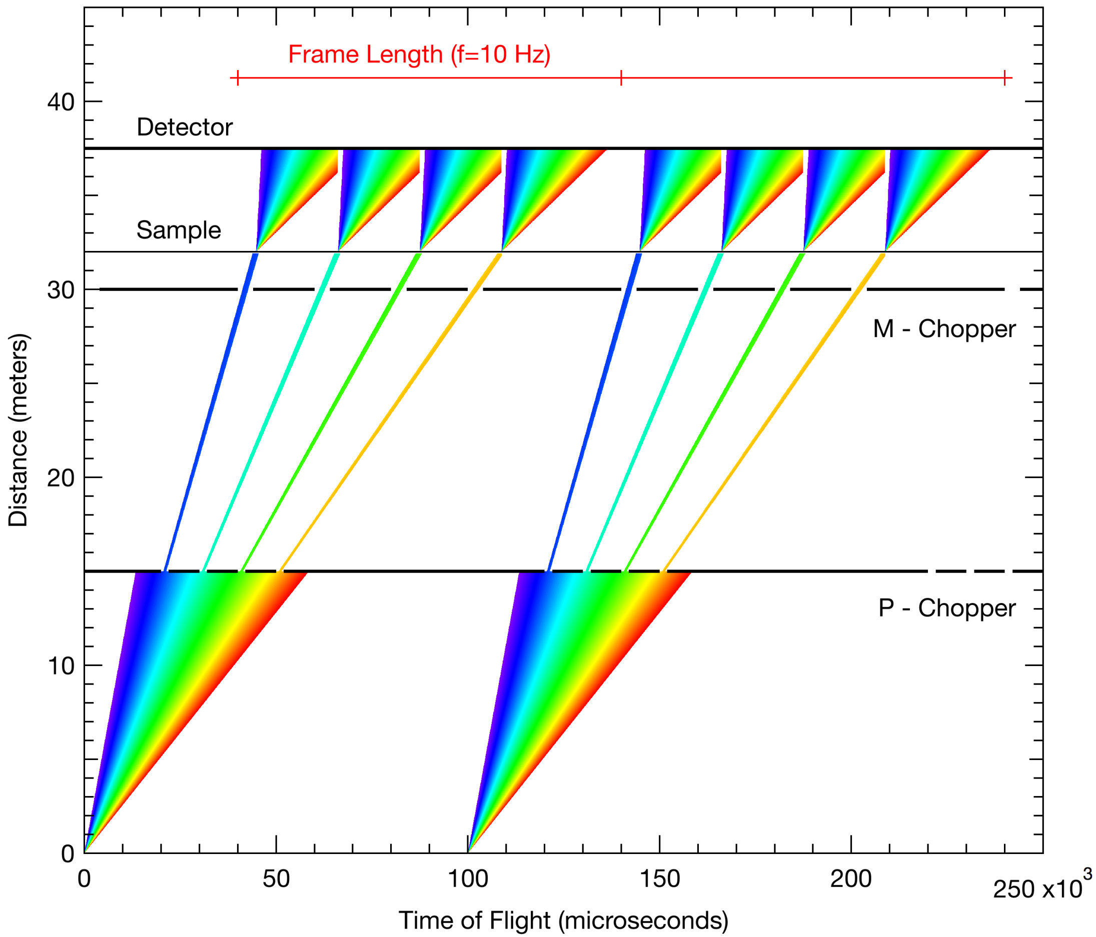
ARCS

Intensity vs Resolution

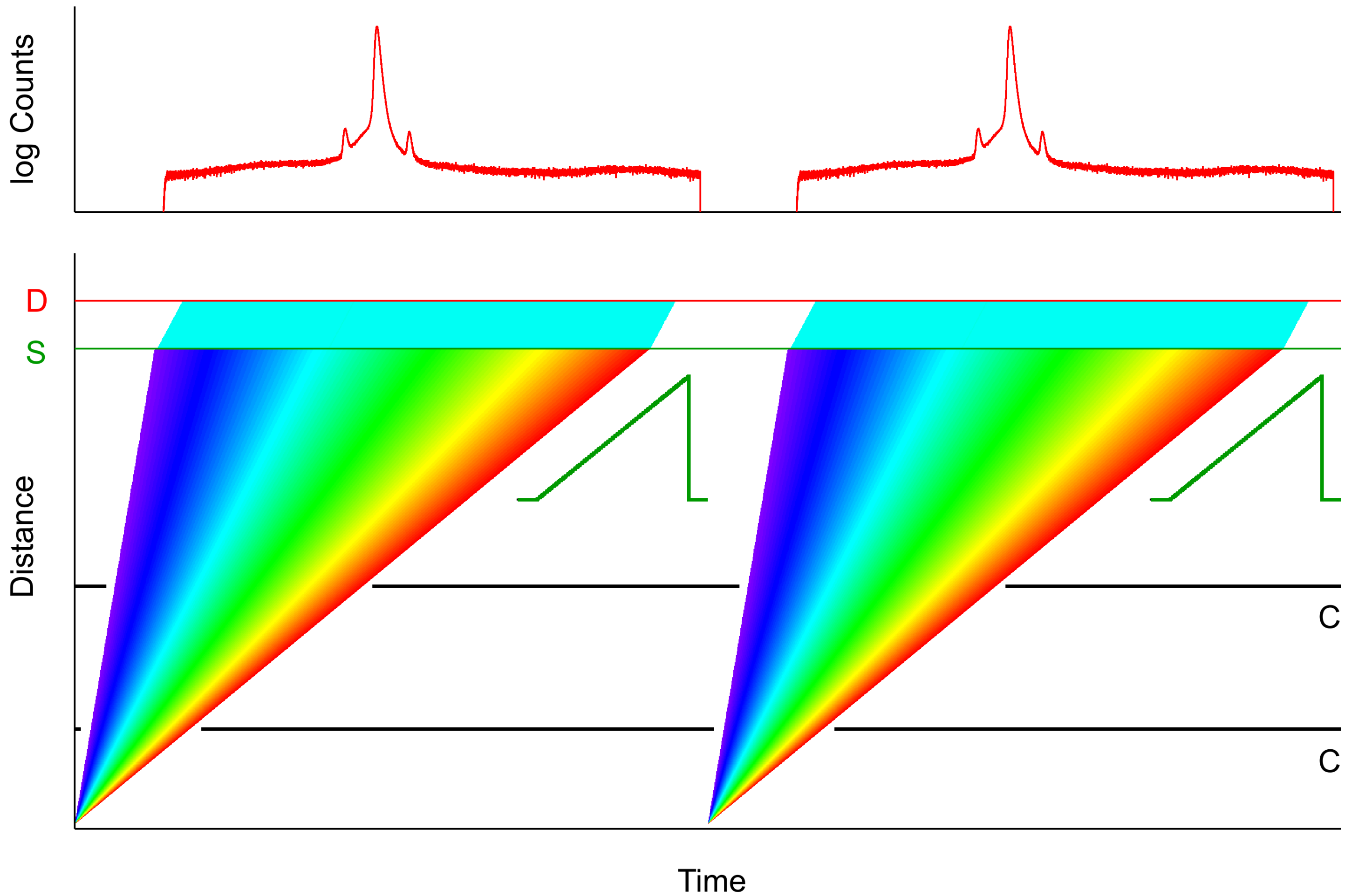




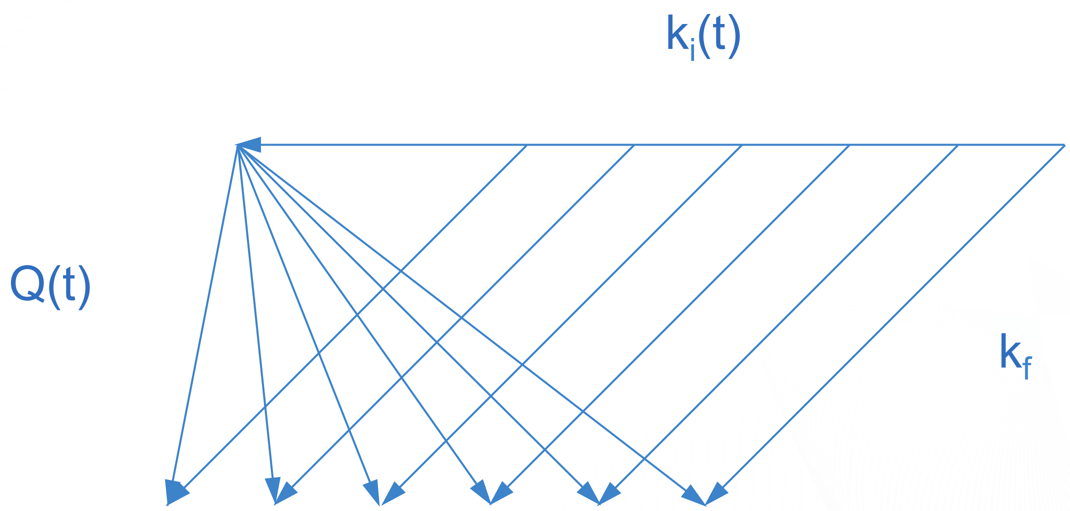
Repetition Rate Multiplication



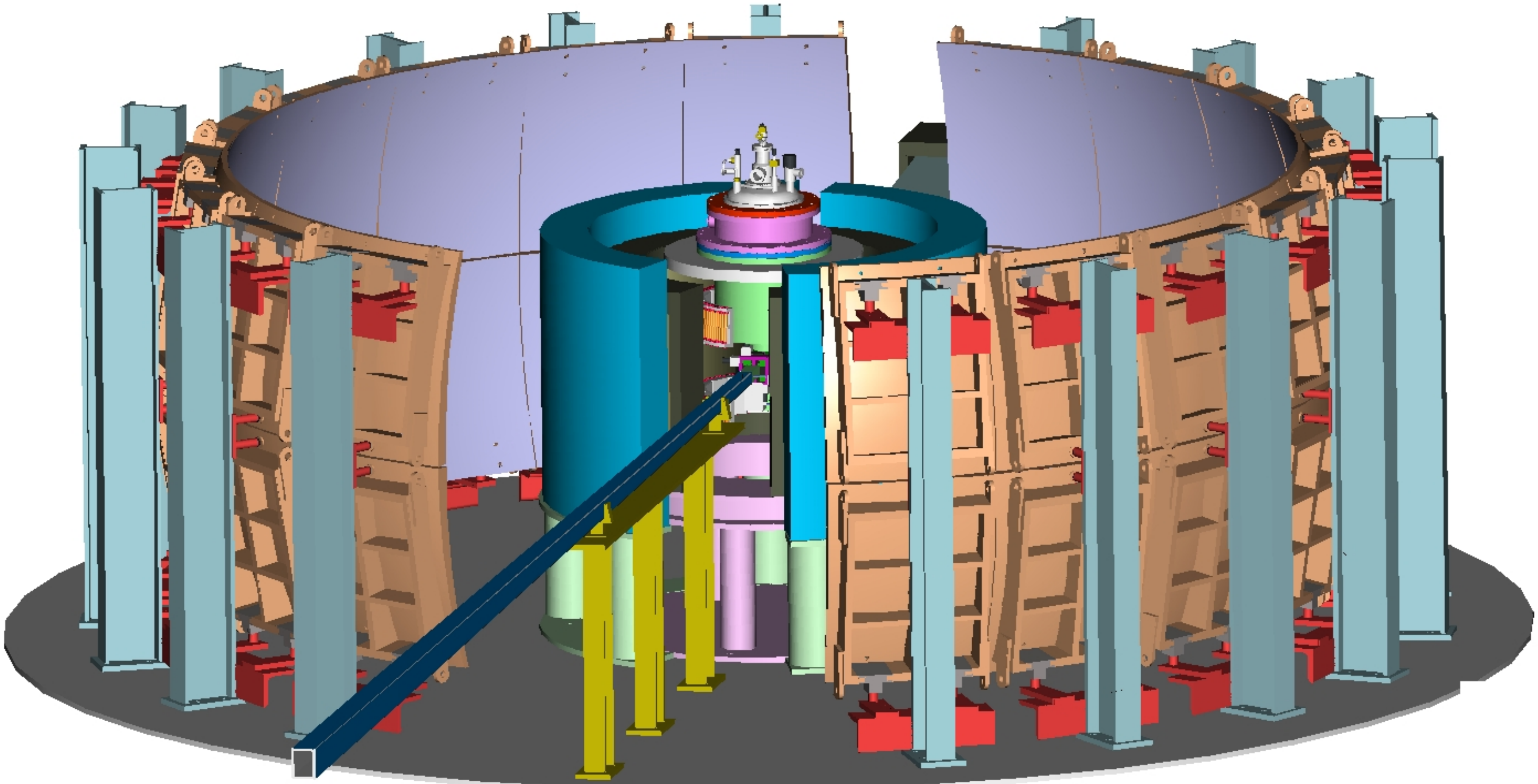
Indirect Geometry Spectroscopy



Momentum Space Representation



Indirect Geometry Spectroscopy – Cold Range



BASIS

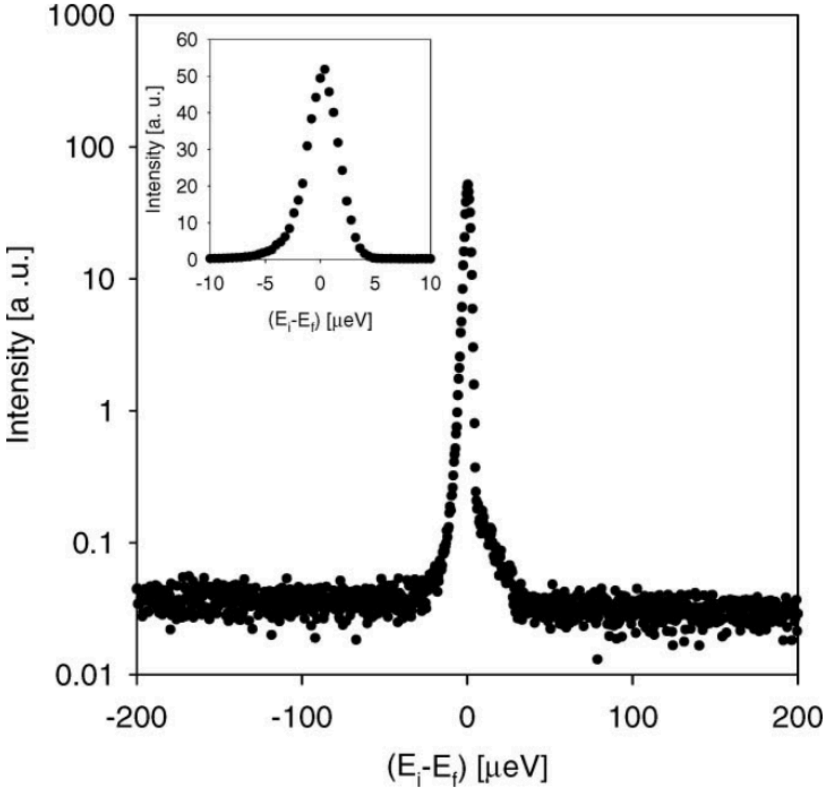
E. Mamontov *et al*., Rev. Sci. Instrum. Phys. **82** 085109 (2011)

Indirect Geometry Spectroscopy – Cold Range

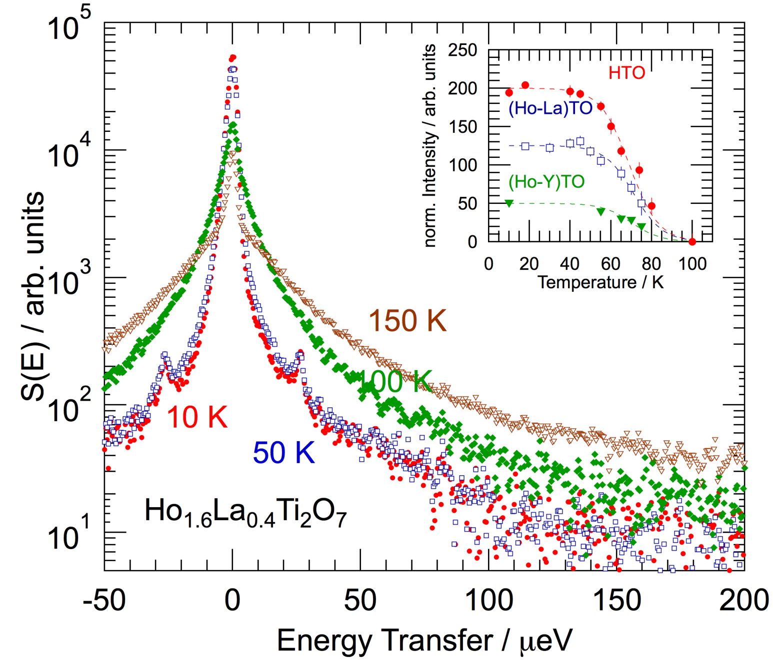
- high flux (~2.5×10^7 neutrons/cm^2/s)
- Si-(111) and Si-(311) crystals (the latter is an upgrade)
- bandwidth ±300 μeV at 30 Hz, ±150 μeV at 60 Hz

E. Mamontov *et al*., Rev. Sci. Instrum. Phys. **82** 085109 (2011)

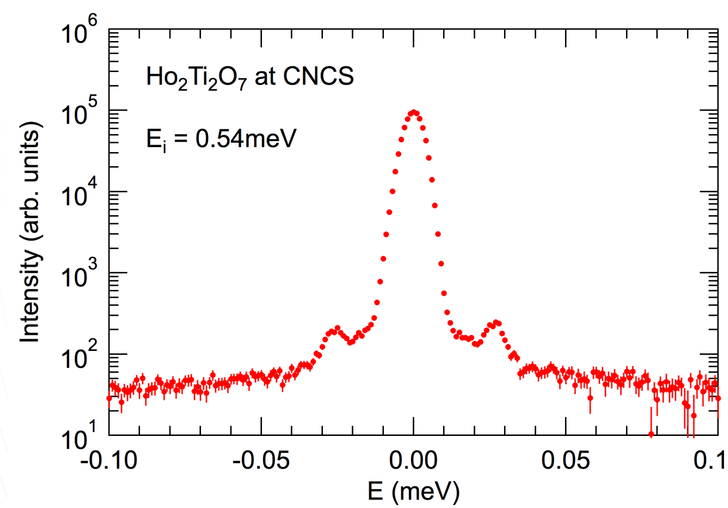
Energy Resolution



Resolution is flat ~3 μeV

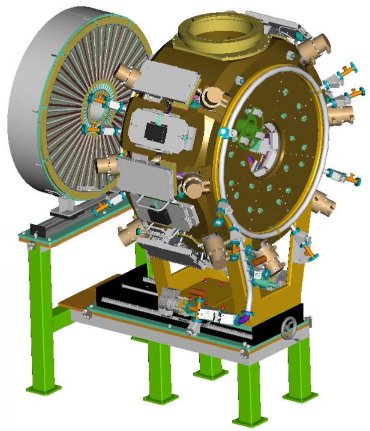


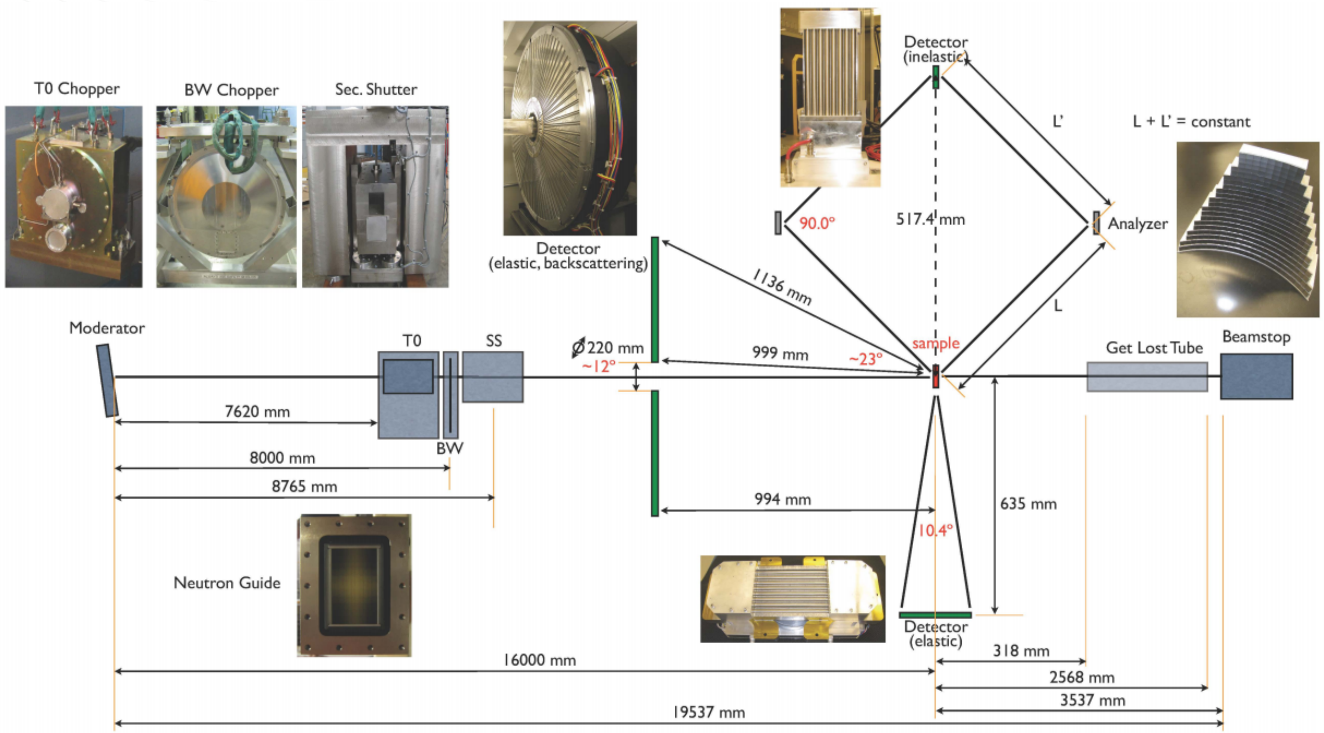
G. Ehlers *et al.*, PRL **102** 016405 (2009)



Indirect Geometry Spectroscopy – Thermal Range

- high flux (~$5x10^7$ neutrons/cm^2/s) and double-focusing
- Broad band (-2 to 1000 meV at 30 Hz, 5 to 500 meV at 60 Hz)
- Elastic line HMFW ~150 μs
- backward and 90° diffraction banks





VISION

Courtesy of Luke Daemen (SNS)

Resolution

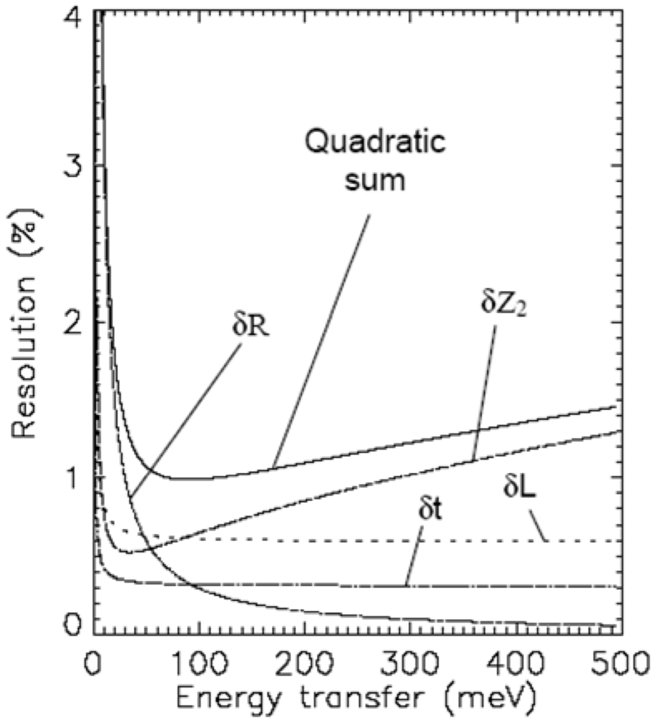
Instrument Resolution again flat

$$\frac{\partial\hbar\omega}{\partial L_1} = 2\frac{E_1}{L_1}$$

$$\frac{\partial\hbar\omega}{\partial Z_2} = \frac{4md}{\hbar\pi}\frac{E_1}{(t-t_2)} + \frac{\hbar^2}{4m}\left(\frac{\pi}{d}\right)^2\left(\frac{R_2^2}{Z_2^3}\right)$$

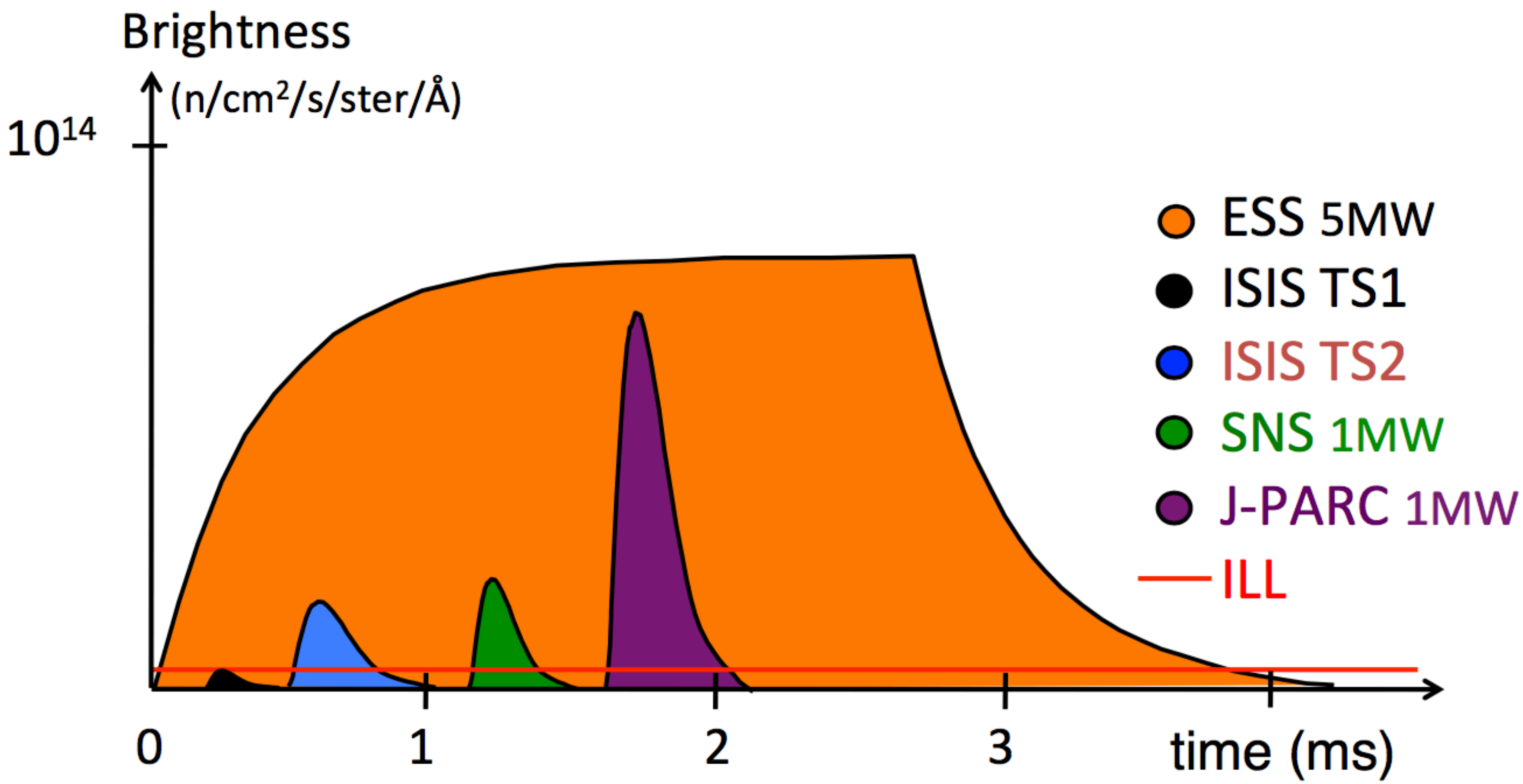
$$\frac{\partial\hbar\omega}{\partial t} = -2\frac{E_1}{t-t_2}$$

$$\frac{\partial\hbar\omega}{\partial R_2} = -\frac{\hbar^2}{2m}\left(\frac{\pi}{d}\right)^2\left(\frac{R_2}{2Z_2^2}\right)$$



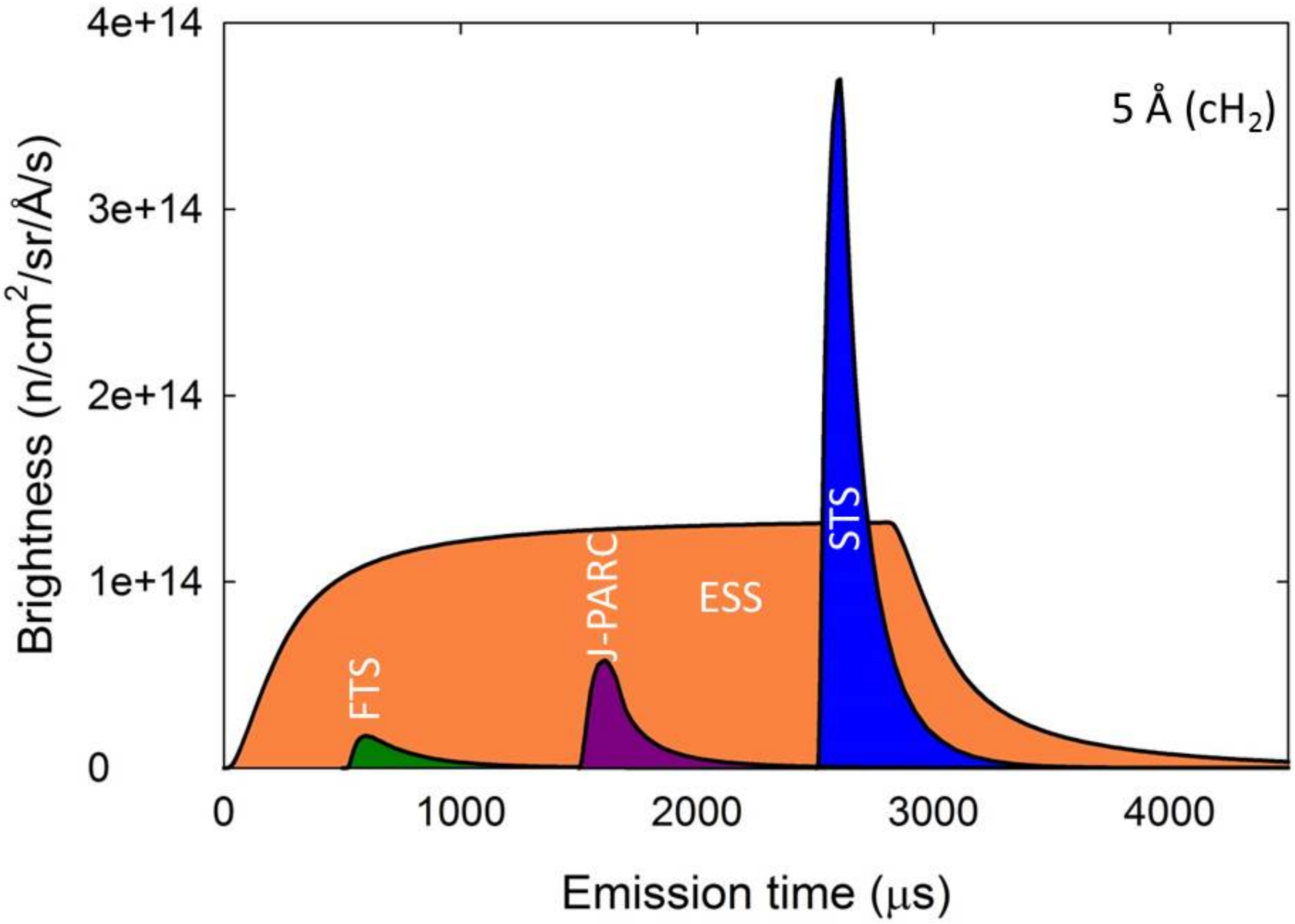
Courtesy of Uli Wildgruber (SNS)

TOF spectrometer at a reactor source?



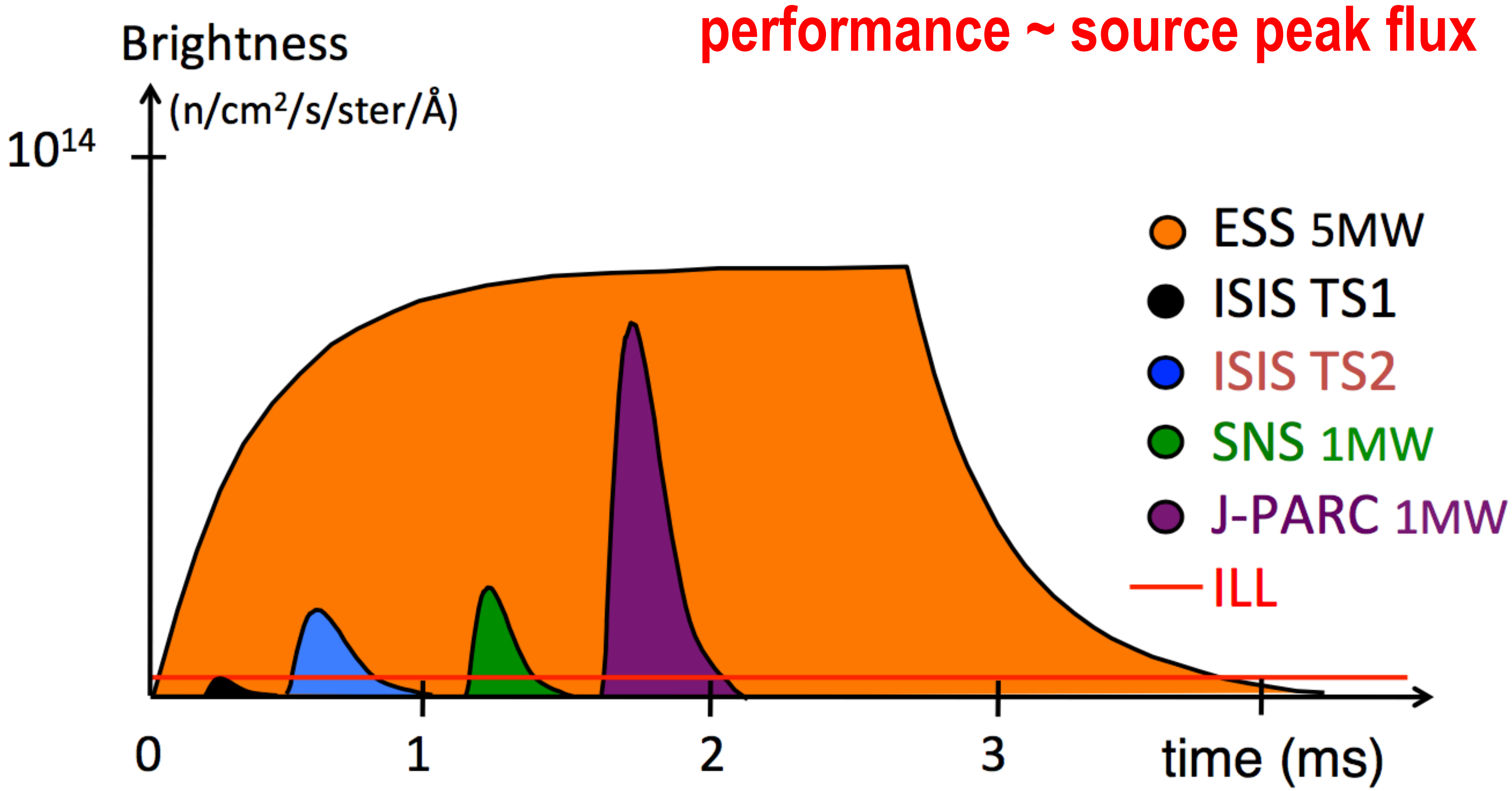
ESS TDR (2012)

Updated Slide 😉



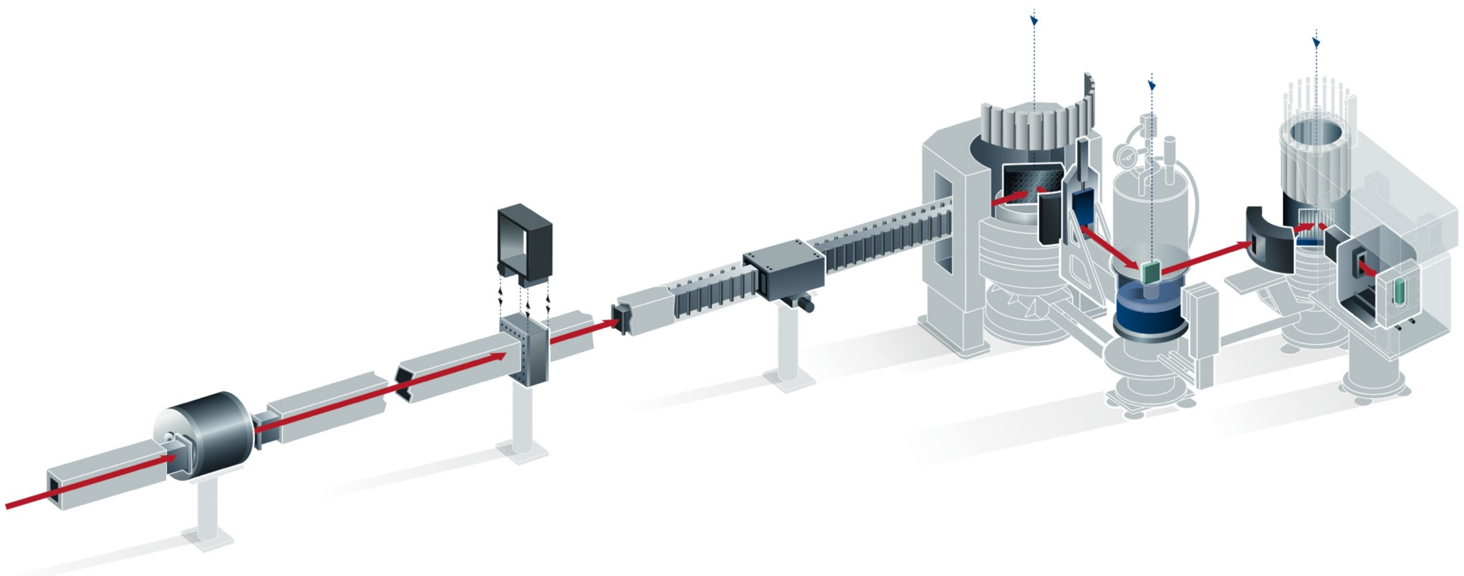
Franz Gallmeier (SNS)

TOF spectrometer at a reactor source?



ESS TDR (2012)

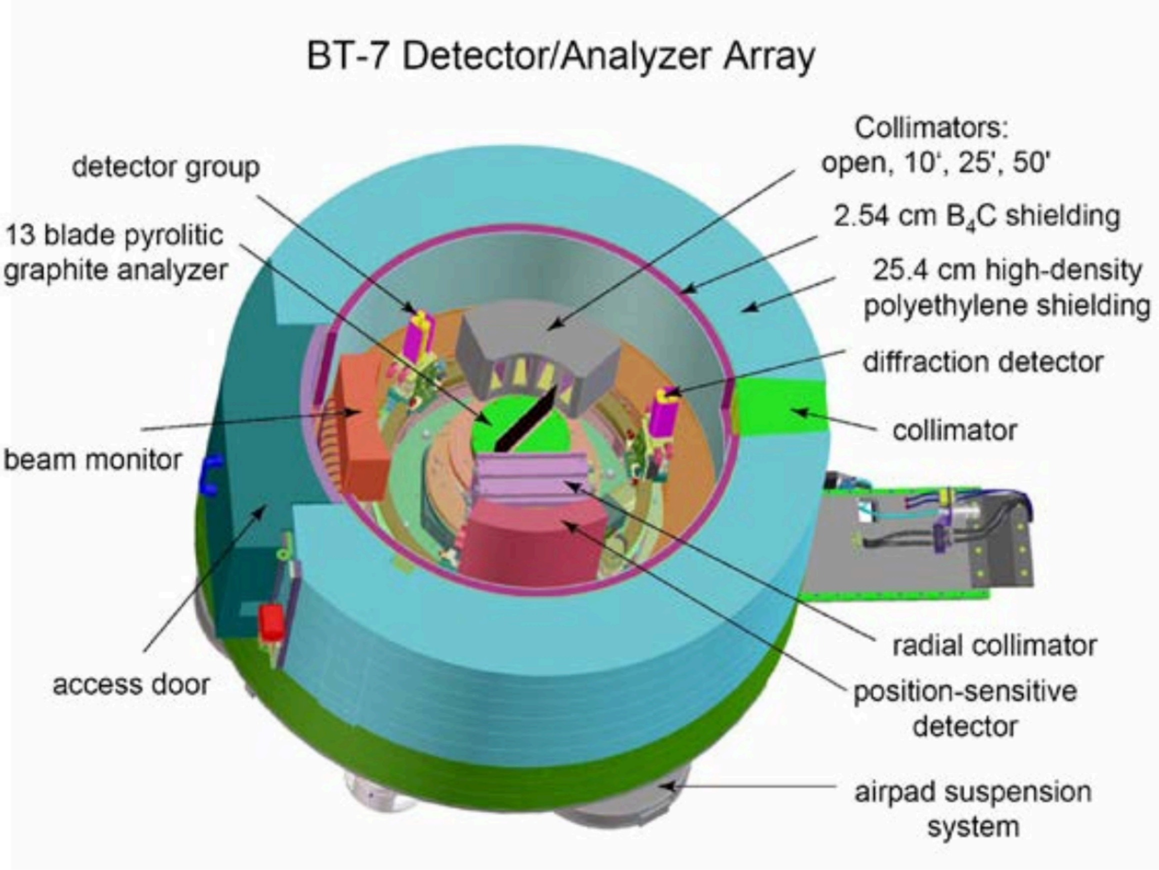
Spectroscopy at a reactor source



https://www.helmholtz-berlin.de/forschung/oe/em/transport-phenomena/flex/index_en.html

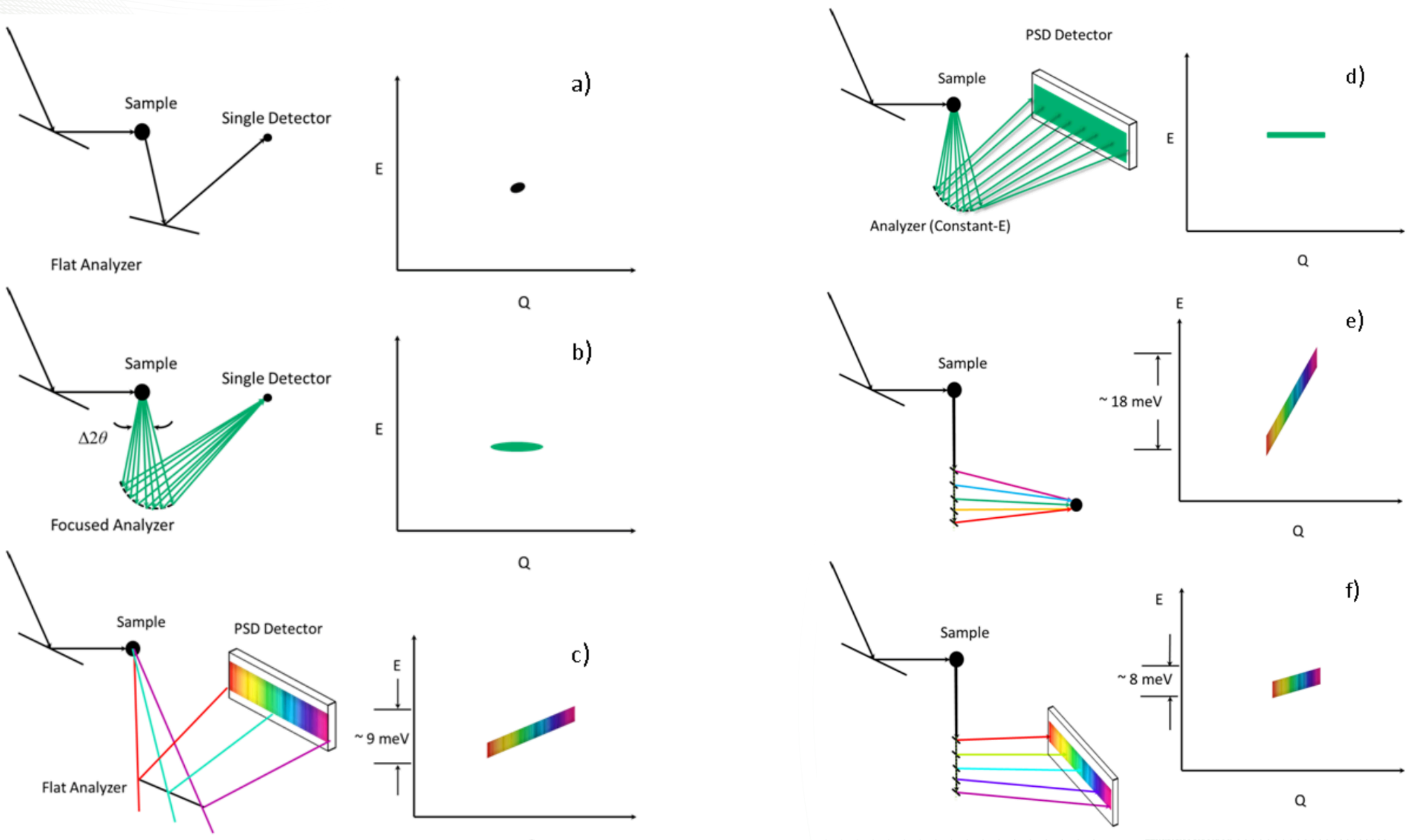
OAK RIDGE National Laboratory | SPALLATION NEUTRON SOURCE

Crystal Analyzer



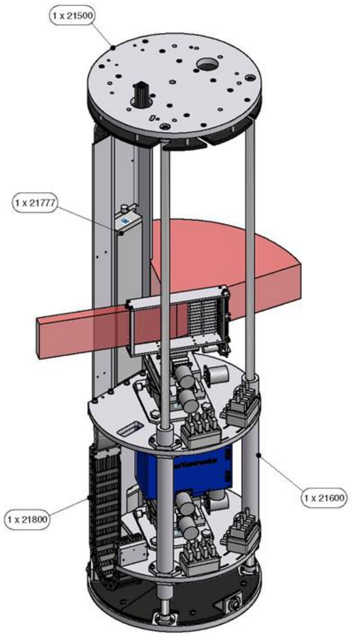
http://nvlpubs.nist.gov/nistpubs/jres/117/jres.117.002.pdf

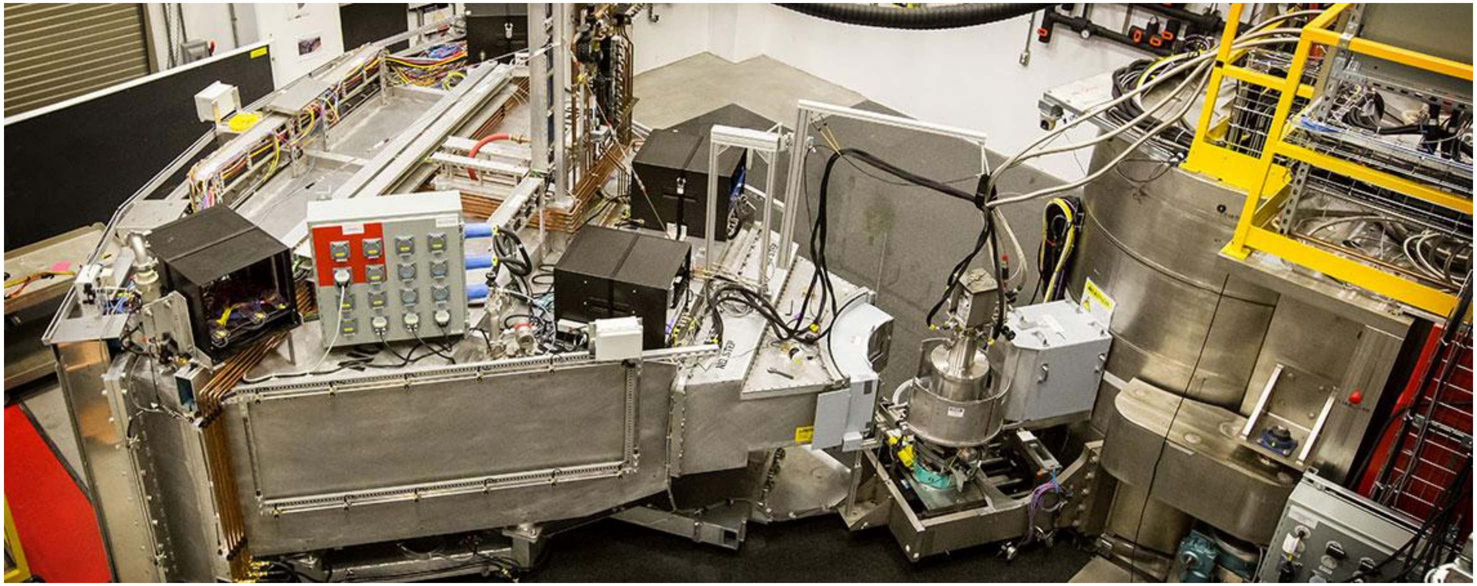
Ultimate Flexibility

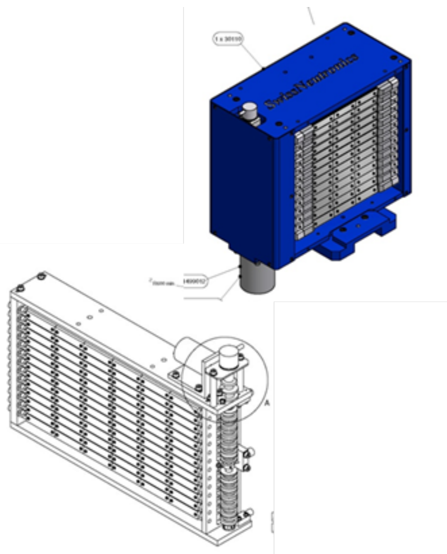


http://nvlpubs.nist.gov/nistpubs/jres/117/jres.117.002.pdf

Crystal monochromator at a pulsed source – HYSPEC







http://neutrons.ornl.gov/hyspec

They call their crystal array a "focusing" device as the beam is already monochromatic at this point by using choppers and time-of-flight.

Diffraction by Time-of-Flight

151

Acta Cryst. (1956). 9, 151

A New Rationale of Structure-Factor Measurement in Neutron-Diffraction Analysis

By R. D. Lowde

Atomic Energy Research Establishment, Harwell, Berkshire, England

(*Received 8 August* 1955)

The Laue method of recording integrated intensities, with certain adjuncts, appears to be in many ways simpler than the rotating-crystal method for single-crystal neutron diffraction analysis, at the same time as offering increased intensities. A proposed technique is discussed, which is particularly suitable for use with pulsed neutron sources such as electron accelerators.

Bragg's law

$$2d \cdot \sin\theta = \lambda$$
$$d[\text{Å}] \cdot \sin\theta = 1.978 \cdot t[\text{ms}]/L[\text{m}]$$

Phonons in Be by Time-of-Flight

NEUTRON
TIME-OF-FLIGHT METHODS

PROCEEDINGS OF A SYMPOSIUM
ORGANIZED BY
EUROPEAN-AMERICAN NUCLEAR DATA COMMITTEE
IN COLLABORATION WITH
CENTRE D'ETUDES NUCLEAIRES DE SACLAY (FRANCE)
AND
INSTITUT NATIONAL DES SCIENCES ET TECHNIQUES NUCLEAIRES
SACLAY, 24—27 JULY, 1961

THERMAL NEUTRON INELASTIC SCATTERING MEASUREMENT WITH THE CHALK RIVER PHASED ROTOR APPARATUS

S.J. COCKING
Atomic Energy Research Establishment, Harwell, U.K.

Abstract

This paper presents experimental details of this apparatus (briefly described in Proc. Conf. on Inelastic Neutron Scattering, Vienna (1960) IS/P/9) together with some results obtained during two years operation.

The object of measurements has been to obtain absolute values of the scattering cross sections ($d^2\sigma/d\Omega \,.\, dE$) over as wide as possible a range of energy transfer and momentum transfer. Results are presented to illustrate the range of these parameters covered in experiments completed.

Intensities of the monokinetic beam (e.g. 8×10^5 neutrons/min at .07 eV) and time-of-flight resolution ($\Delta\tau/\tau$) are given together with the methods used for normalizing data to absolute cross section scale.

Experimental results are illustrated with examples of scattering by water, vanadium and beryllium.

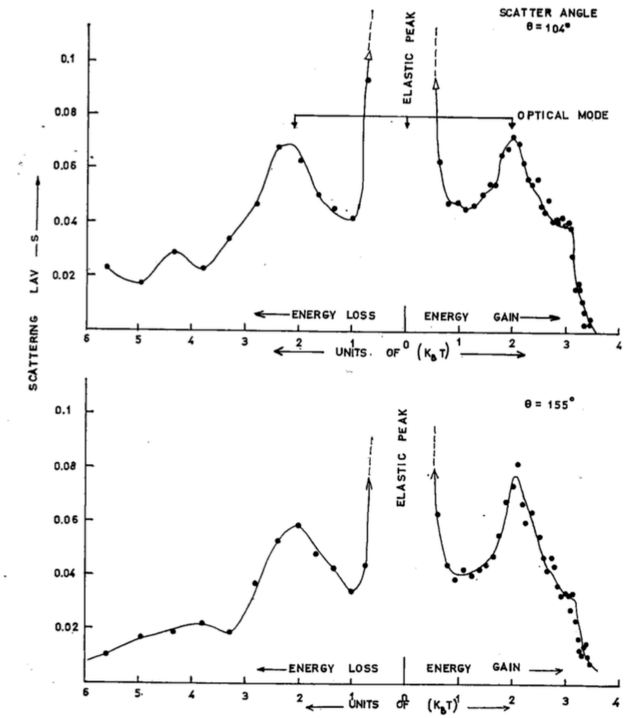


Figure 3
Inelastic scattering from polycrystalline beryllium (at room temperature). Incident neutron energy ~ 0.12 eV.

Edited by J. Spaepen (1961)

Diffraction by Time-of-Flight

phys. stat. sol. 4, 349 (1964)

Laboratory II for Nuclear Physics, Institute for Nuclear Research, Świerk

A New Method for Neutron Diffraction Crystal Structure Investigations

By

B. Buras and J. Leciejewicz

A new neutron method for structure investigations of powdered crystals using time-of-flight techniques is described, and results presented for aluminium and silicon powders. The measured and calculated structure factors are in good agreement. The value of the method and its possible applications are discussed.

Es werden eine neue Methode für neutronographische Untersuchungen von Kristallpulvern unter Anwendung der „time-of-flight"-Technik beschrieben und die Ergebnisse für Aluminium- und Siliziumpulver angegeben. Die gemessenen Strukturfaktoren stimmen gut mit den berechneten überein. Die Methode und ihre Anwendungsmöglichkeiten werden diskutiert.

1. Introduction

In the case of powdered crystals the conventional method of X-ray and neutron diffraction structure investigations uses X-rays or neutrons of a fixed wavelength and the measured quantity is the intensity I of the diffracted beam as a function of the variable angle θ (Fig. 1a). Whenever the Bragg equation $\lambda = 2\,d \sin\theta$ (d is the interplanar spacing) is satisfied, the function I vs. θ shows a maximum. From the intensities and positions of these peaks the structure of the crystal under investigation can be determined. In the case of neutrons, however, as

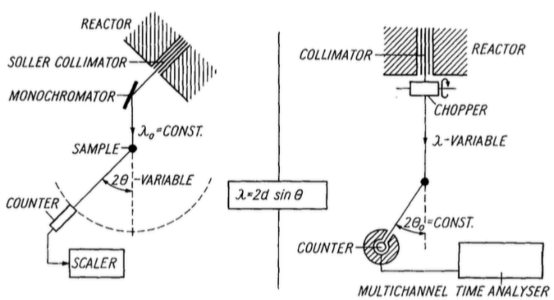


Fig. 1. The principles of neutron spectrometer method (a) and time-of-flight method (b) for crystallographic investigations

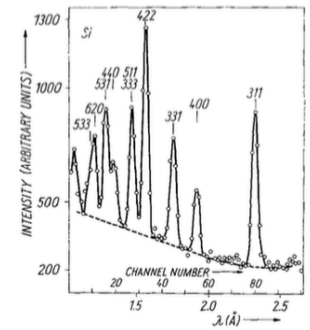


Fig. 8. A diffraction pattern of silicon powder taken at 3000 rpm ($2\theta = 90°$)

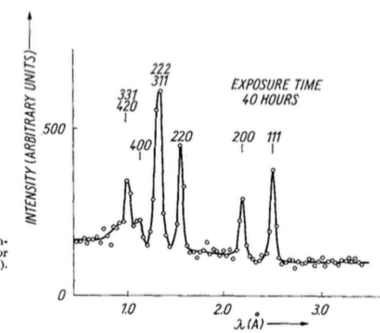


Fig. 3. A neutron diffraction pattern obtained using the time-of-flight technique for aluminium powder (λ neutron wavelength). The exposure time was 40 hours [1]

Phonons in Mg by Time-of-Flight

Proc. R. Soc. Lond. A. **326**, 347–360 (1972)
Printed in Great Britain

Measurements of the normal-mode frequencies of magnesium

By R. Pynn† and G. L. Squires
Cavendish Laboratory, University of Cambridge, England

(*Communicated by W. Cochran, F.R.S. – Received 26 April* 1971)

The normal-mode frequencies of magnesium at 290 K have been determined by the inelastic scattering of slow neutrons. The frequencies of about 3500 phonons with wavevectors in the (0001) and (01$\bar{1}$0) planes have been measured with a time-of-flight apparatus, and an

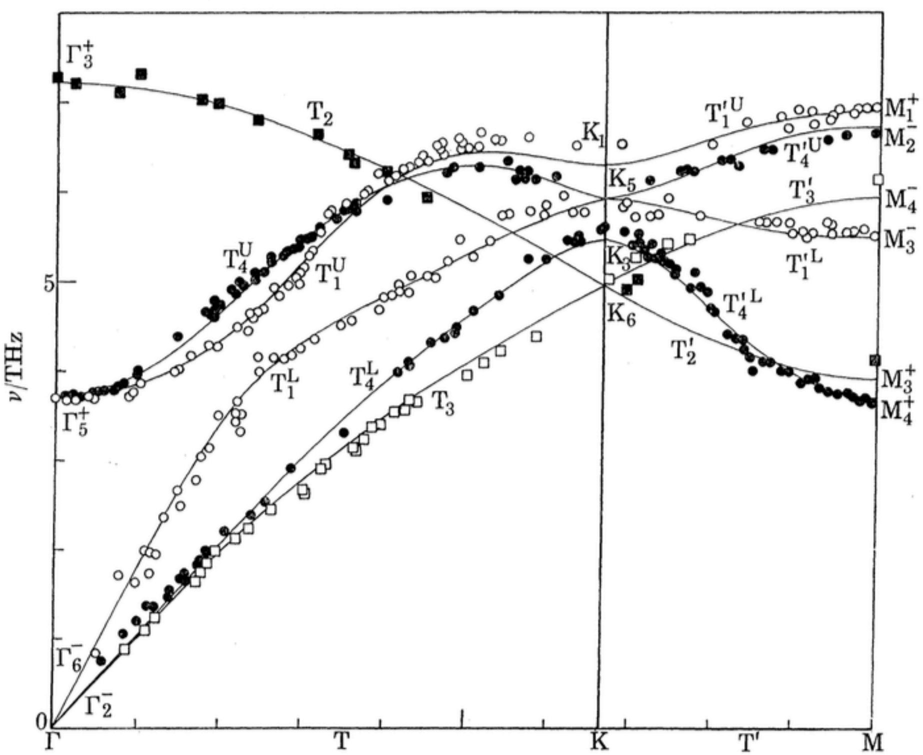
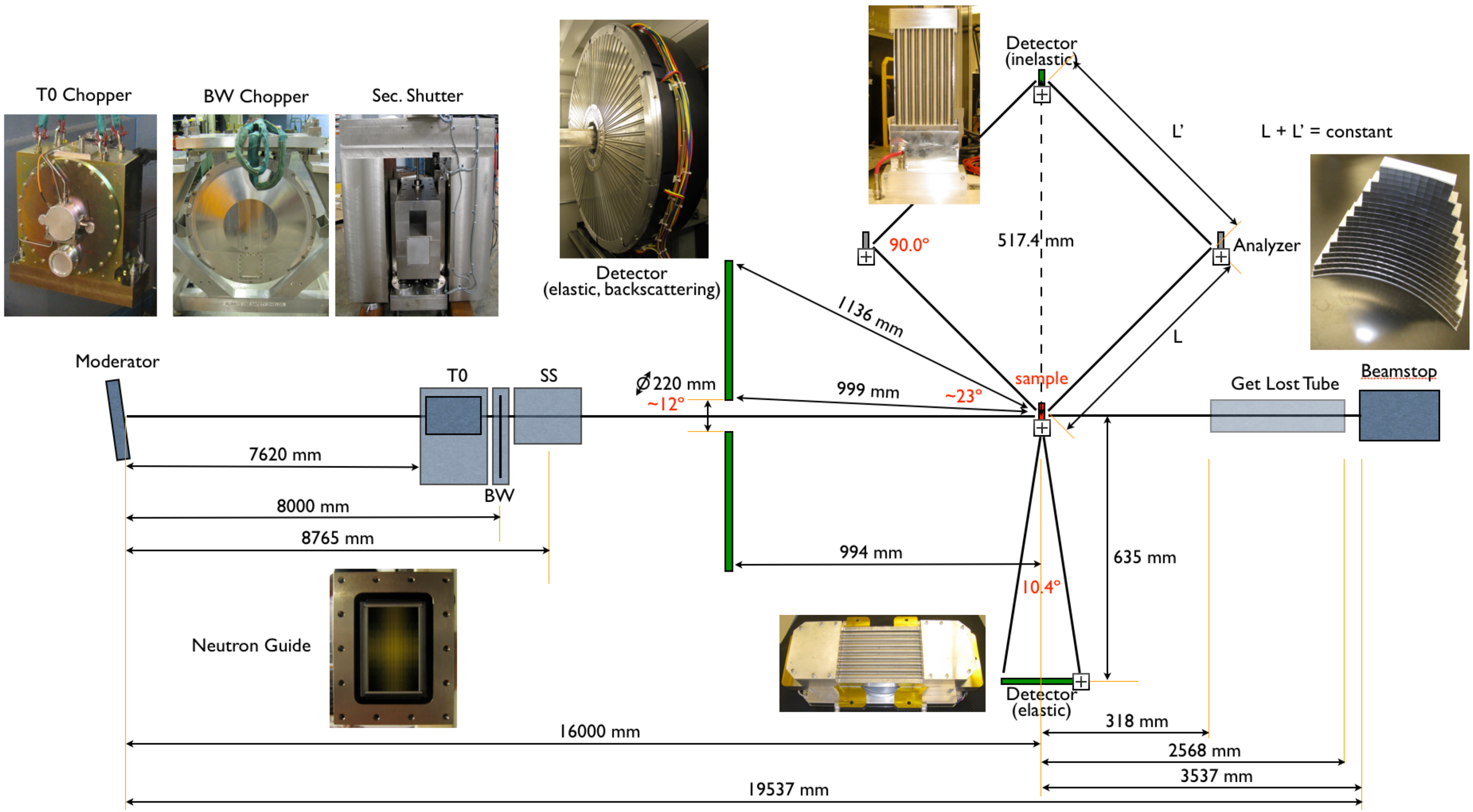


FIGURE 2. Phonon wavevector along the T and T′ directions.

DONE!

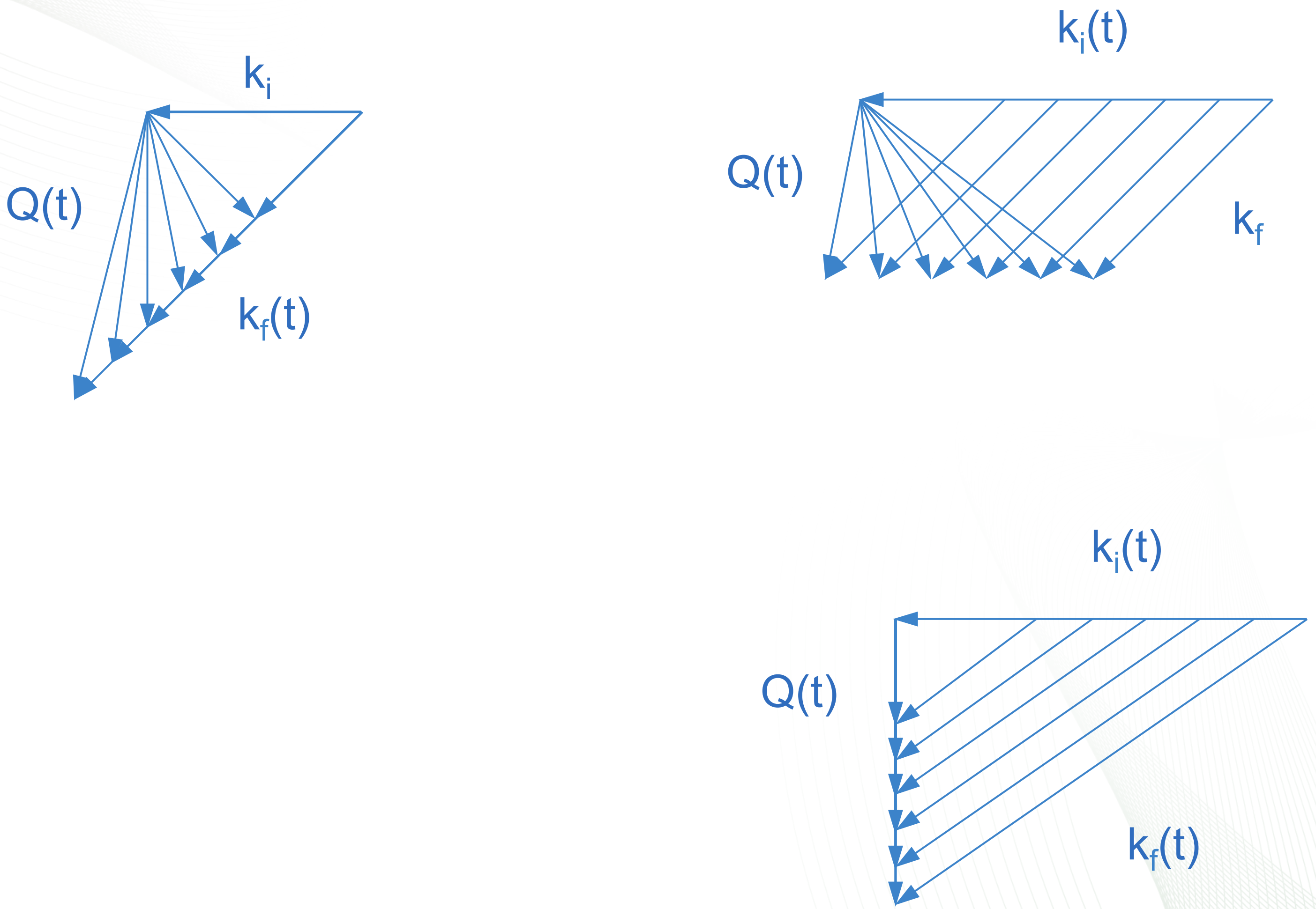
Questions ?

Indirect Geometry Spectroscopy – Thermal Range



Courtesy of Uli Wildgruber

Momentum Space Representation



OAK RIDGE National Laboratory | SPALLATION NEUTRON SOURCE