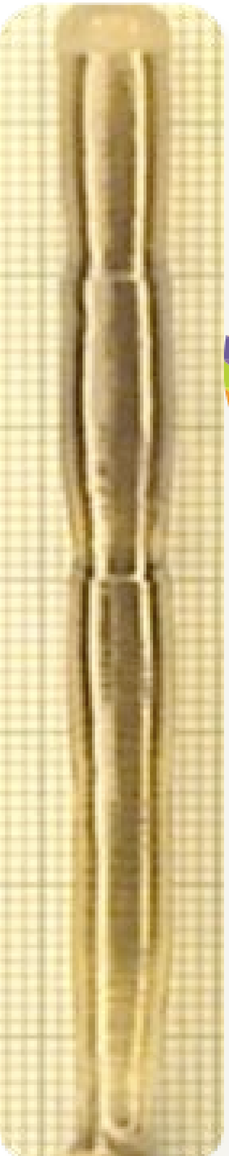
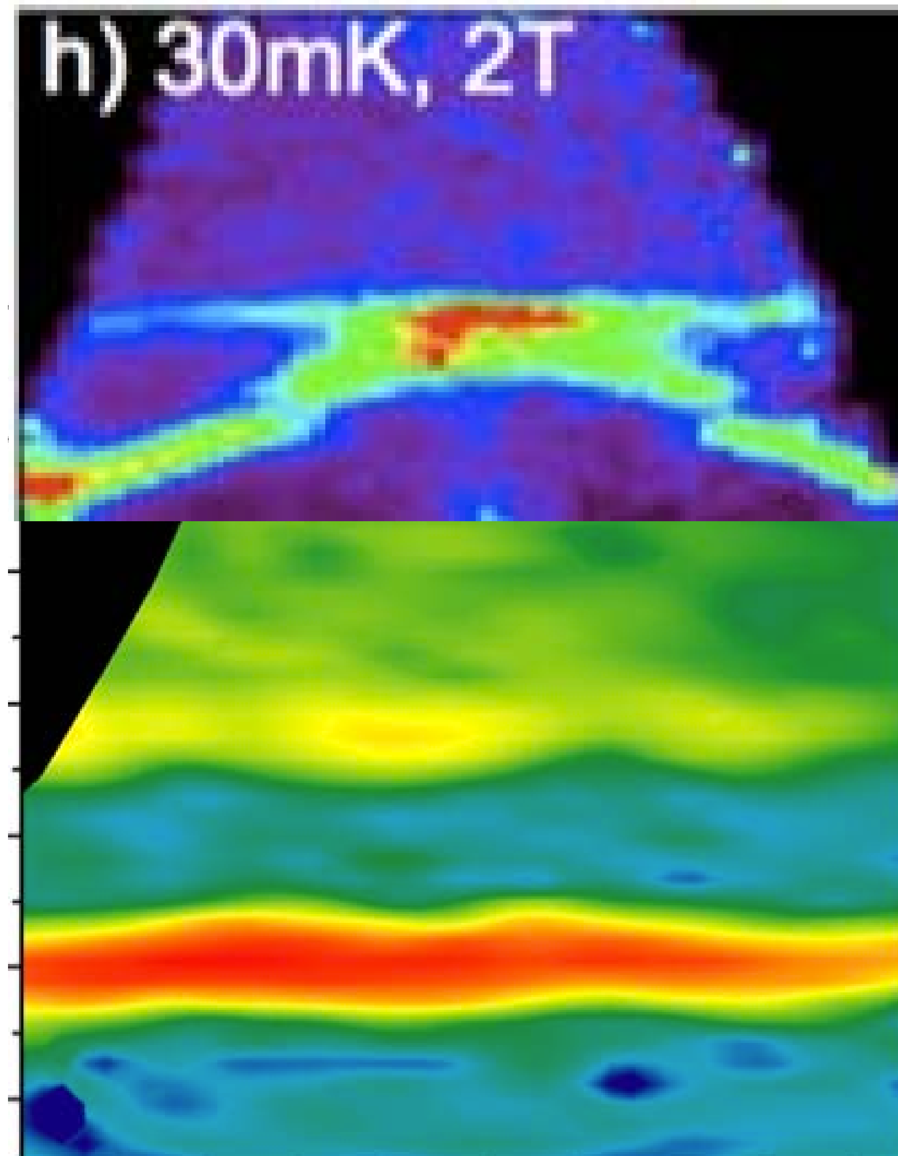
Introduction to Inelastic Neutron Scattering

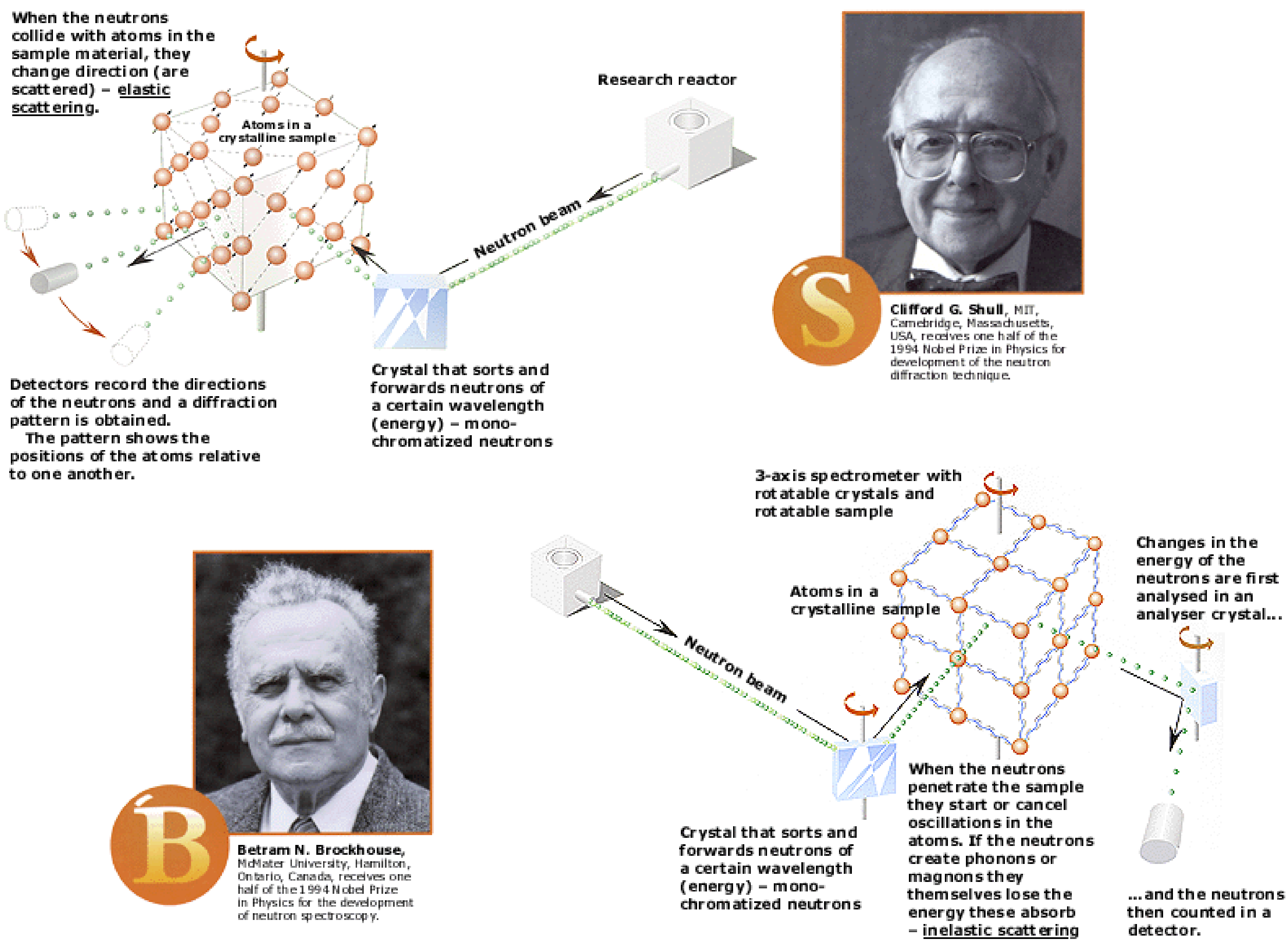


Bruce D Gaulin
McMaster University

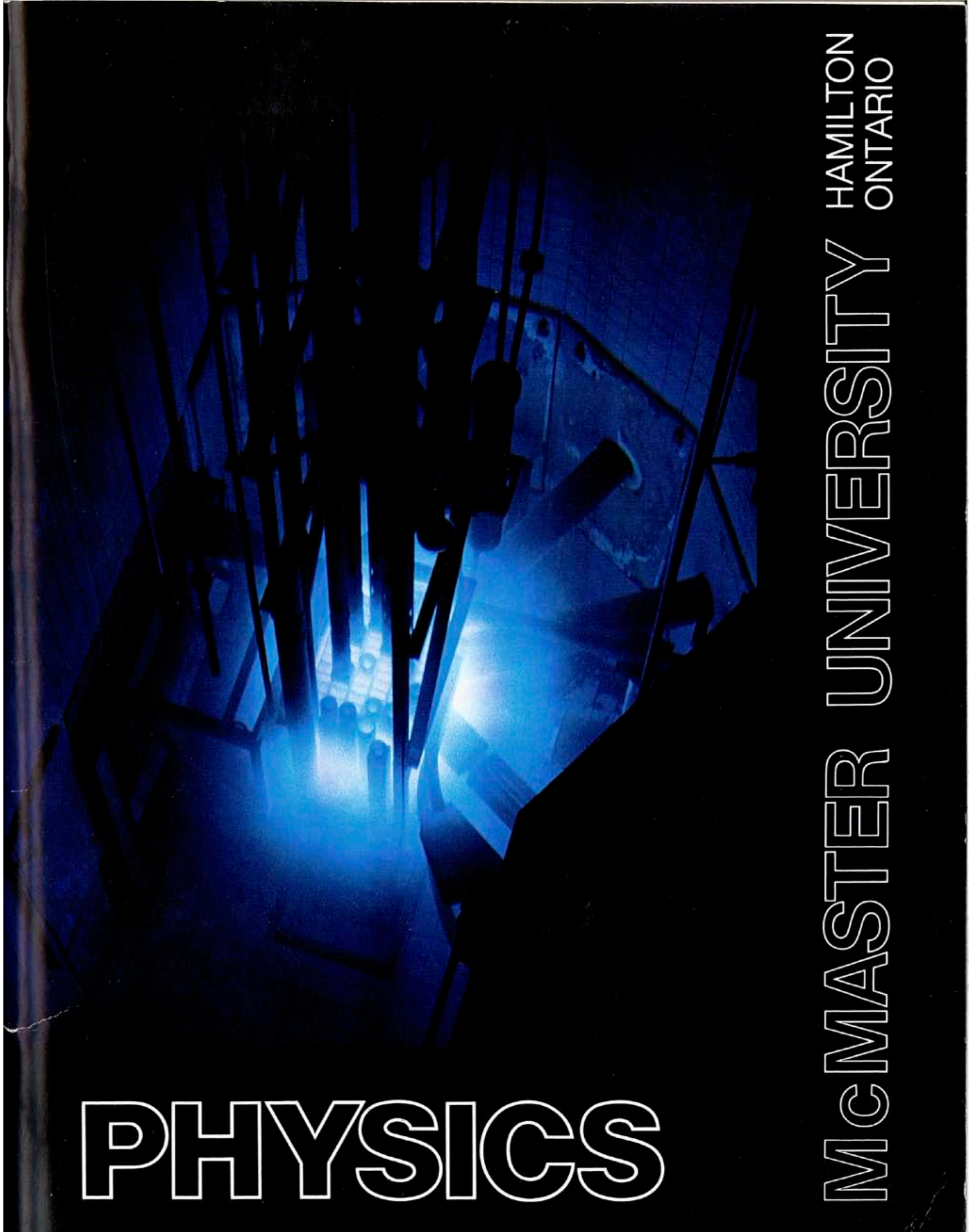
Brockhouse Institute for Materials Research

- ***Neutrons: Properties and Cross Sections***
- ***Excitations in solids***
- ***Triple Axis and Chopper TOF Techniques***
- ***Practical concerns***





When the neutrons collide with atoms in the sample material, they change direction (are scattered) – elastic scattering.
Atoms in a crystalline sample
Research reactor
Neutron beam
Detectors record the directions of the neutrons and a diffraction pattern is obtained.
The pattern shows the positions of the atoms relative to one another.
Crystal that sorts and forwards neutrons of a certain wavelength (energy) – monochromatized neutrons
S
Clifford G. Shull, MIT, Camebridge, Massachusetts, USA, receives one half of the 1994 Nobel Prize in Physics for development of the neutron diffraction technique.
3-axis spectrometer with rotatable crystals and rotatable sample
Atoms in a crystalline sample
Changes in the energy of the neutrons are first analysed in an analyser crystal...
Neutron beam
B
Betram N. Brockhouse, McMater University, Hamilton, Ontario, Canada, receives one half of the 1994 Nobel Prize in Physics for the development of neutron spectroscopy.
Crystal that sorts and forwards neutrons of a certain wavelength (energy) – monochromatized neutrons
When the neutrons penetrate the sample they start or cancel oscillations in the atoms. If the neutrons create phonons or magnons they themselves lose the energy these absorb – inelastic scattering
...and the neutrons then counted in a detector.



$^{235}U + n$

$\rightarrow$

daughter nuclei +

2-3 n + gammas

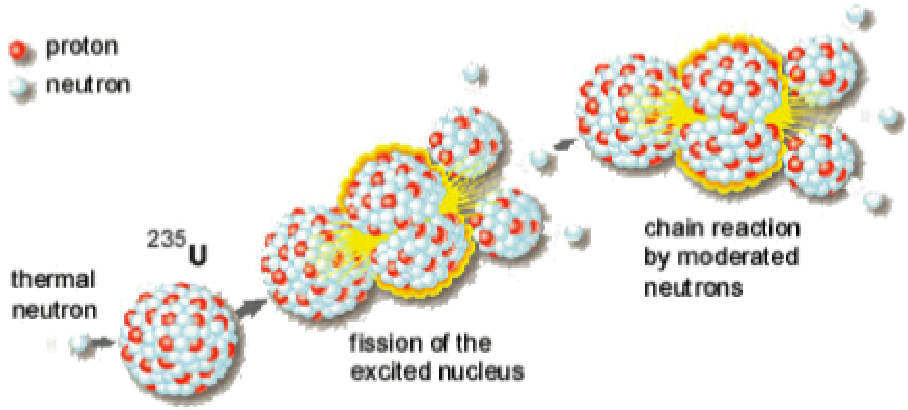
neutrons:

no charge

s=1/2

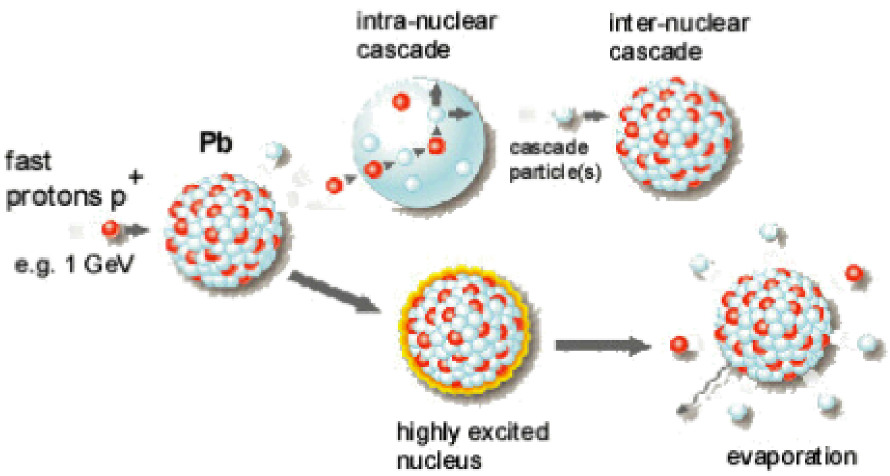
massive: mc^2~1 GeV

How do we produce neutrons



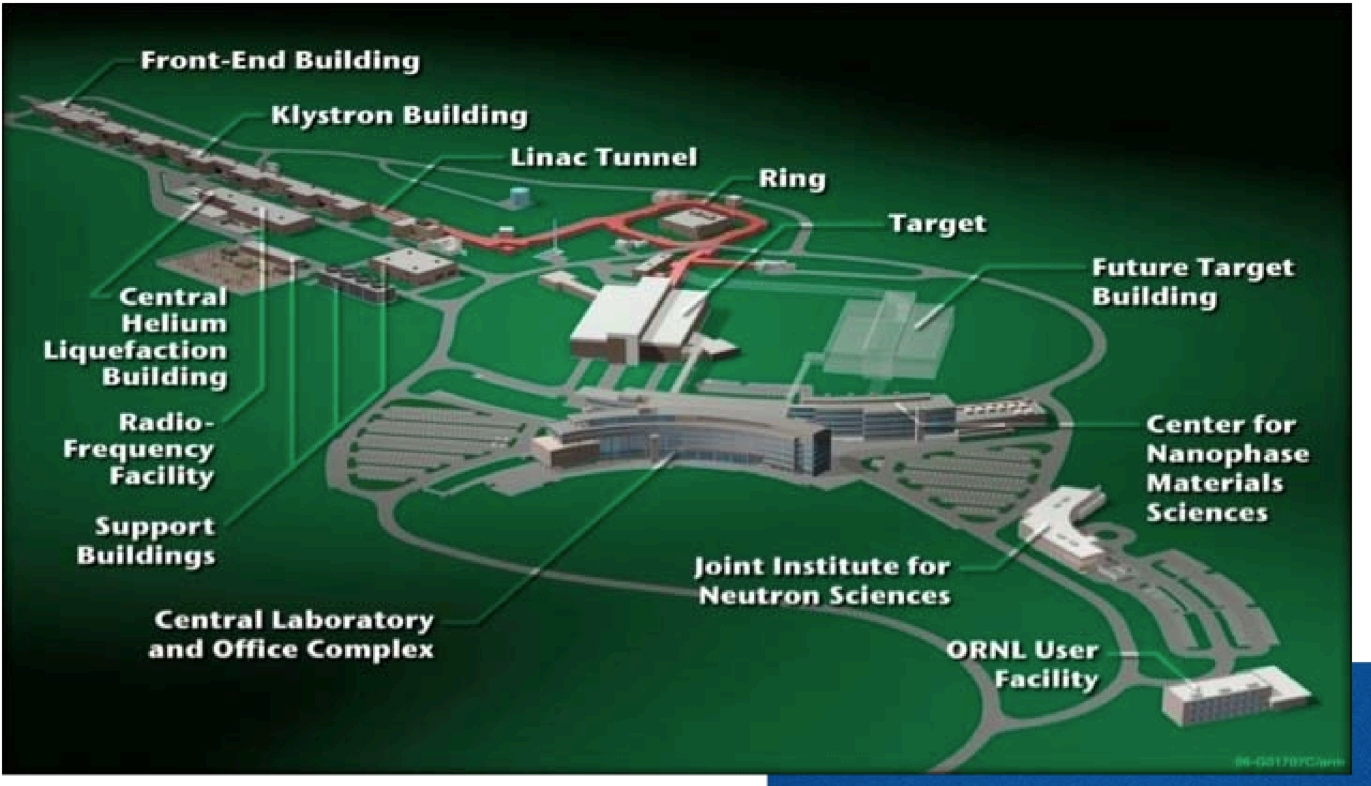
Fission

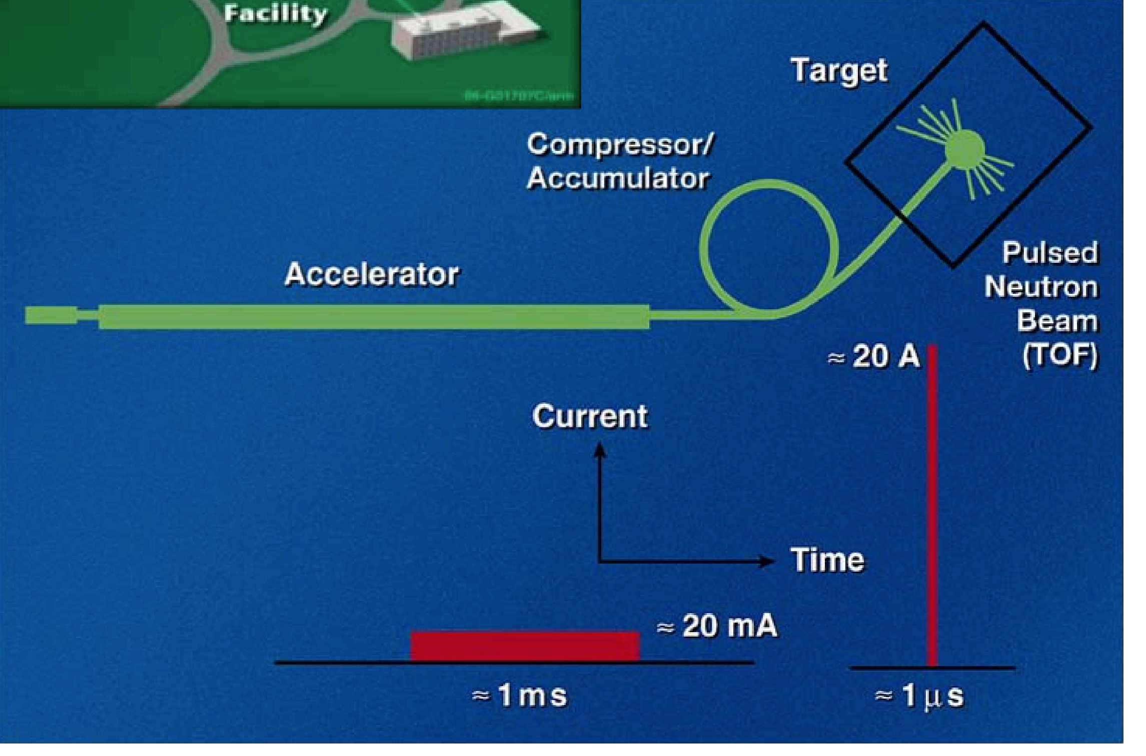
- chain reaction
- continuous flow
- 1 neutron/fission



Spallation

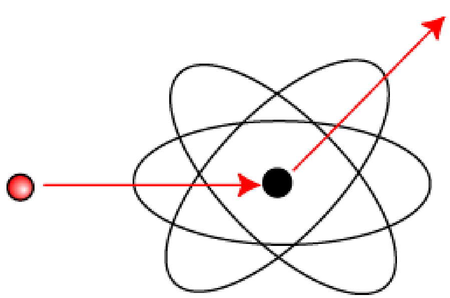
- no chain reaction
- pulsed operation
- 30 neutrons/proton


Front-End Building
Klystron Building
Linac Tunnel
Ring
Target
Future Target Building
Central Helium Liquefaction Building
Radio-Frequency Facility
Support Buildings
Central Laboratory and Office Complex
Joint Institute for Neutron Sciences
Center for Nanophase Materials Sciences
ORNL User Facility

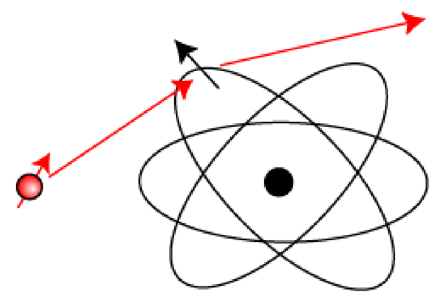

Target
Compressor/ Accumulator
Accelerator
Pulsed Neutron Beam (TOF)
≈ 20 A
Current
Time
≈ 20 mA
≈ 1 ms
≈ 1 μs

Neutron interaction with matter

- **Properties of the neutron**
  - Mass m_n =1.675 x 10^{-27} kg
  - Charge   0
  - Spin-1/2, magnetic moment μ_n = -1.913 μ_N
- **Neutrons interact with…**
  - Nucleus
    - Crystal structure/excitations (eg. phonons)
  - Unpaired e^- via dipole scattering
    - Magnetic structure/excitations (eg. spin waves)



Nuclear scattering



Magnetic dipole scattering

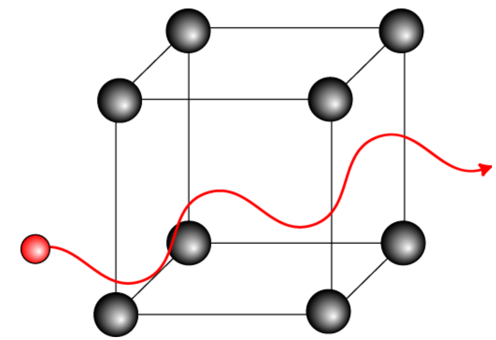
Wavelength-energy relations

- **Neutron as a wave …**
  - Energy (E), velocity (v), wavenumber (k), wavelength (λ)

$$k = \frac{m_n \mathrm{v}}{\mathrm{h}} = \frac{2\pi}{\lambda}$$

$$E = \frac{\mathrm{h}^2 k^2}{2m_n} = \frac{\mathrm{h}^2}{2m_n}\left(\frac{2\pi}{\lambda}\right)^2 = \frac{81.81\,\mathrm{meV}\cdot\mathrm{Å}^2}{\lambda^2}$$

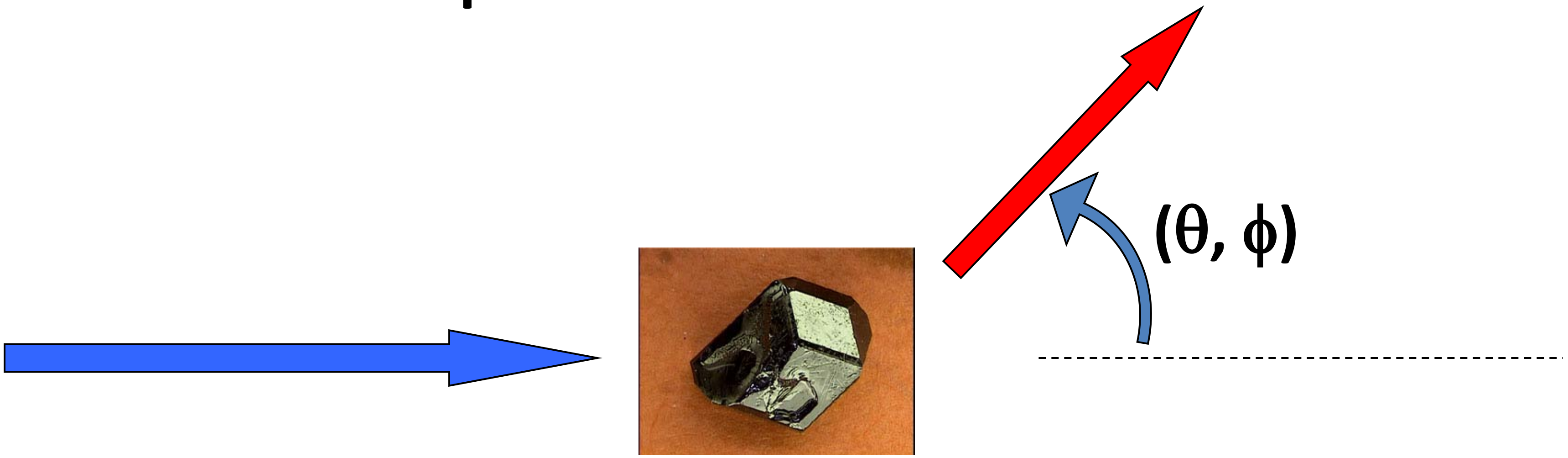
$$E = k_B T = \left(0.08617\,\mathrm{meV}\cdot\mathrm{K}^{-1}\right)T$$



λ ~ interatomic spacing → E ~ excitations in condensed matter

	Energy (meV)	Temperature (K)	Wavelength (Å)
Cold	0.1 – 10	1 – 120	4 – 30
Thermal	5 – 100	60 – 1000	1 – 4
Hot	100 – 500	1000 – 6000	0.4 – 1

The Basic Experiment:



Incident Beam:

- monochromatic
- "white"
- "pink"

Scattered Beam:

- Resolve its energy
- Don't resolve its energy
- Filter its energy

Fermi's Golden Rule within the 1st Born Approximation

$$W = 2\pi / h \quad |\langle f \mid V \mid i \rangle|^2 \quad \rho\,(E_f)$$

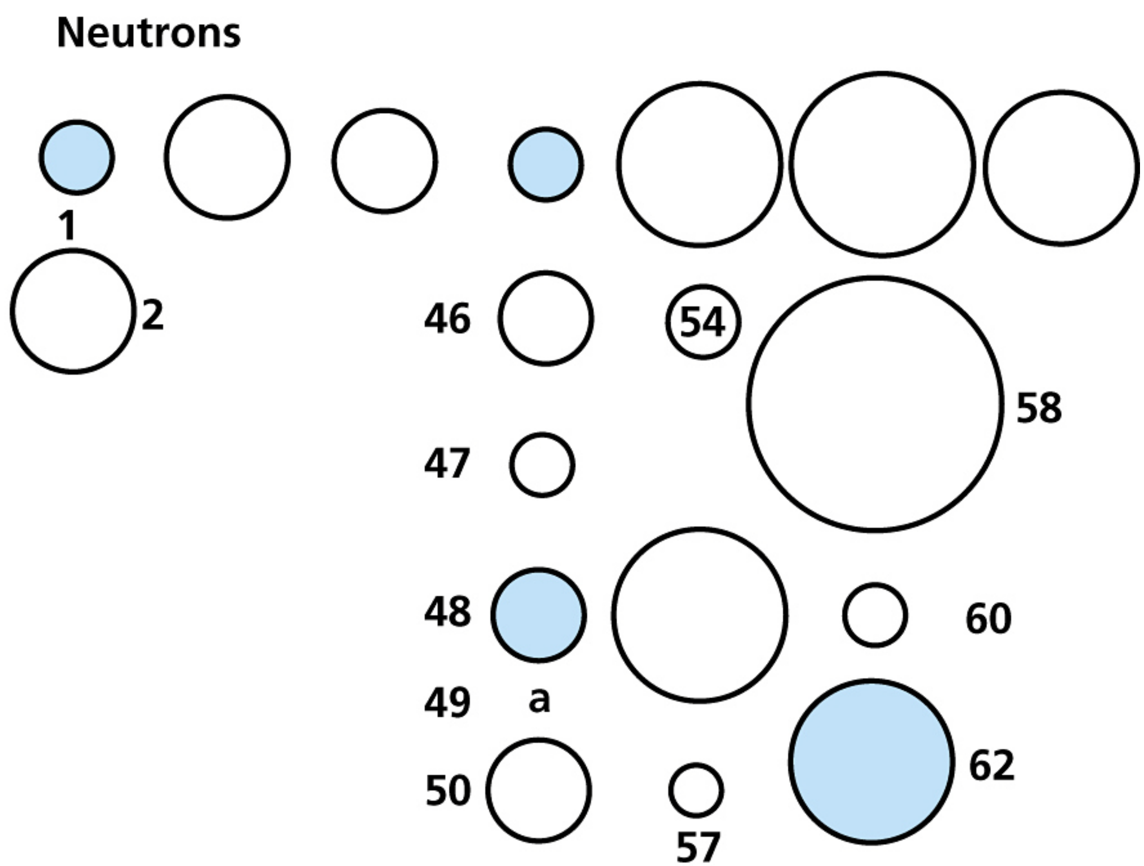
$$\delta\sigma = W / \Phi \;=\; (m/2\pi h^2)^2 \;\; k_f / k_i \quad |\langle f \mid V \mid i \rangle|^2 \;\; \delta\Omega$$

$$\delta^2\sigma / \delta\Omega\, \delta E_f \;=\; k_f/k_i \;\; \sigma_{coh}/4\pi \;\; N \;\; S_{coh}(\mathbf{Q}, \omega)$$

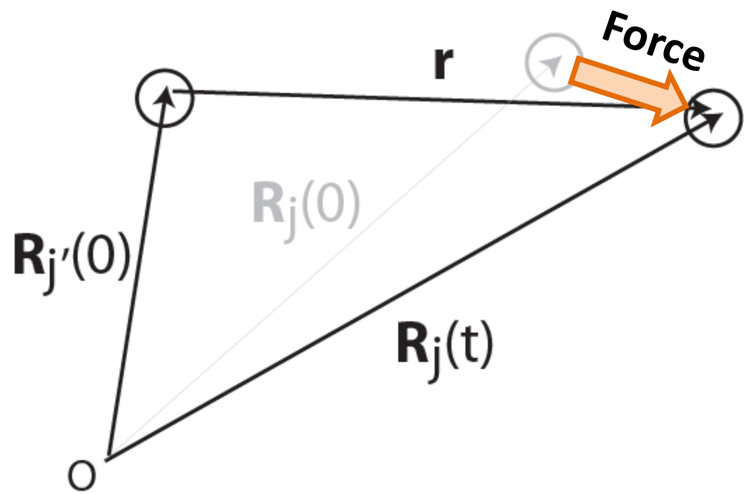
$$+\; k_f/k_i \;\sigma_{incoh}/4\pi \;\; N \;\; S_{incoh}(\mathbf{Q}, \omega)$$

σ_{coh} and σ_{incoh}

parametrize the strength of the scattering from the nuclei



Nuclear correlation functions



Pair correlation function

$$G(\mathbf{r},t)=\frac{1}{N}\int\sum_{jj'}\delta\left(\mathbf{r}'-\mathbf{R}_{j'}(0)\right)\delta\left(\mathbf{r}'+\mathbf{r}-\mathbf{R}_j(t)\right)d\mathbf{r}'$$

Intermediate function

$$I(\mathbf{Q},t)=\int G(\mathbf{r},t)e^{i\mathbf{Q}\cdot\mathbf{r}}d\mathbf{r}=\frac{1}{N}\sum_{jj'}\exp\left(-i\mathbf{Q}\cdot\mathbf{R}_{j'}(0)\right)\exp\left(i\mathbf{Q}\cdot\mathbf{R}_j(t)\right)$$

Scattering function

$$S(\mathbf{Q},\omega)=\frac{1}{2\pi\hbar}\int I(\mathbf{Q},t)e^{-i\omega t}dt$$

Differential scattering cross-section

$$\frac{d^2\sigma}{d\Omega dE_f}=\frac{\sigma_{scat}}{4\pi}\frac{k_f}{k_i}NS(\mathbf{Q},\omega)$$

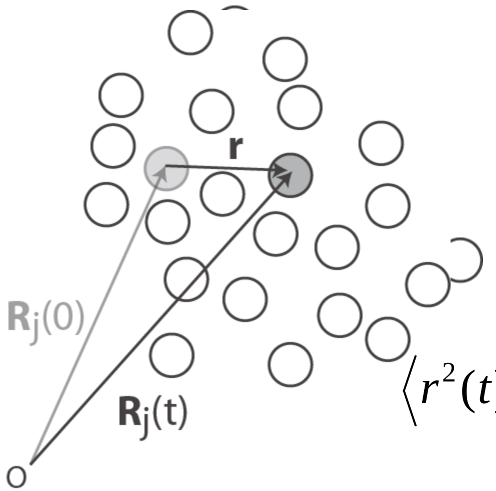
Nuclear (lattice) excitations

Neutron scattering measures simultaneously the wavevector and energy of **collective excitations** → dispersion relation, $\omega(\mathbf{q})$
In addition, **local excitations** can of course be observed

- **Commonly studied excitations**
  - Phonons
  - Librations and vibrations in molecules
  - Diffusion
  - Collective modes in glasses and liquids
- **Excitations can tell us about**
  - Interatomic potentials & bonding
  - Phase transitions & critical phenomena (soft modes)
  - Fluid dynamics
  - Momentum distributions & superfluids (eg. He)
  - Interactions (eg. electron-phonon coupling)

Atomic diffusion

For long times compared to the collision time, atom diffuses



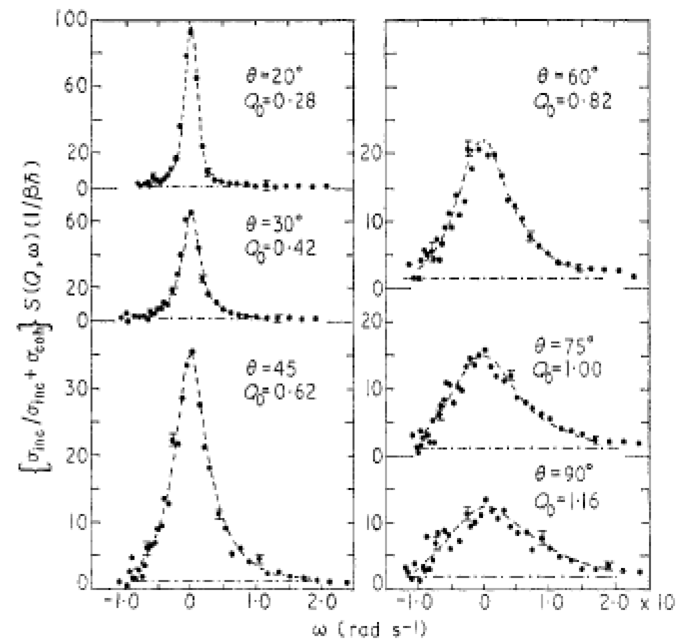
$$\left\langle r^2(t) \right\rangle \approx 6Dt$$

Auto-correlation function

$$G_s(r,t) = \left\{ 6\pi \left\langle r^2(t) \right\rangle \right\}^{-3/2} \exp\left(-\frac{r^2}{6\left\langle r^2(t) \right\rangle} \right)$$

$$S(Q,\omega) = \frac{1}{\pi\hbar} \exp\left(\frac{\hbar\omega}{2k_B T} \right) \frac{DQ^2}{\omega^2 + (DQ^2)^2}$$

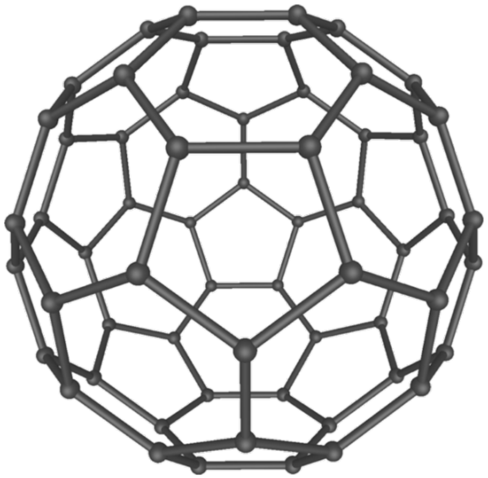
Liquid Na



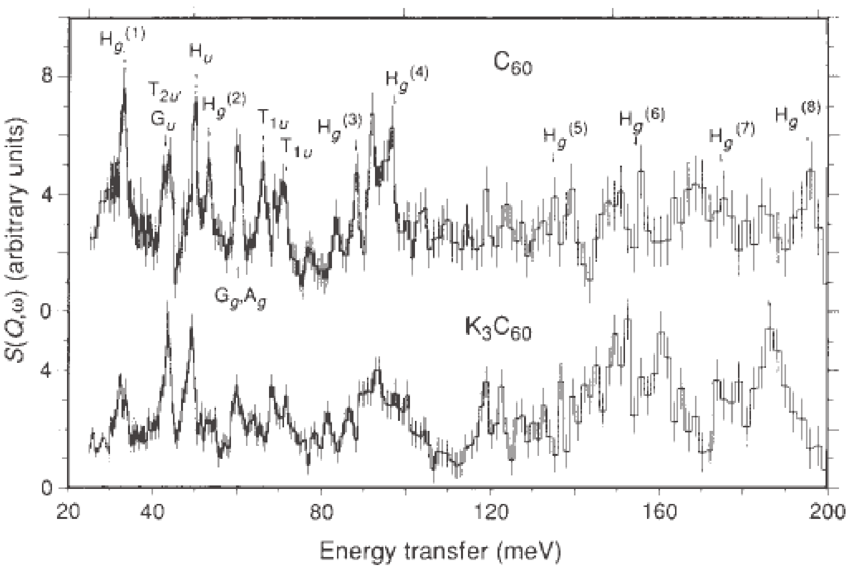
Cocking, *J. Phys. C* **2**, 2047 (1969)..

Molecular vibrations

- Large molecule, many normal modes
- Harmonic vibrations can determine interatomic potentials



C60 molecule



Prassides *et al., Nature* **354**, 462 (1991).

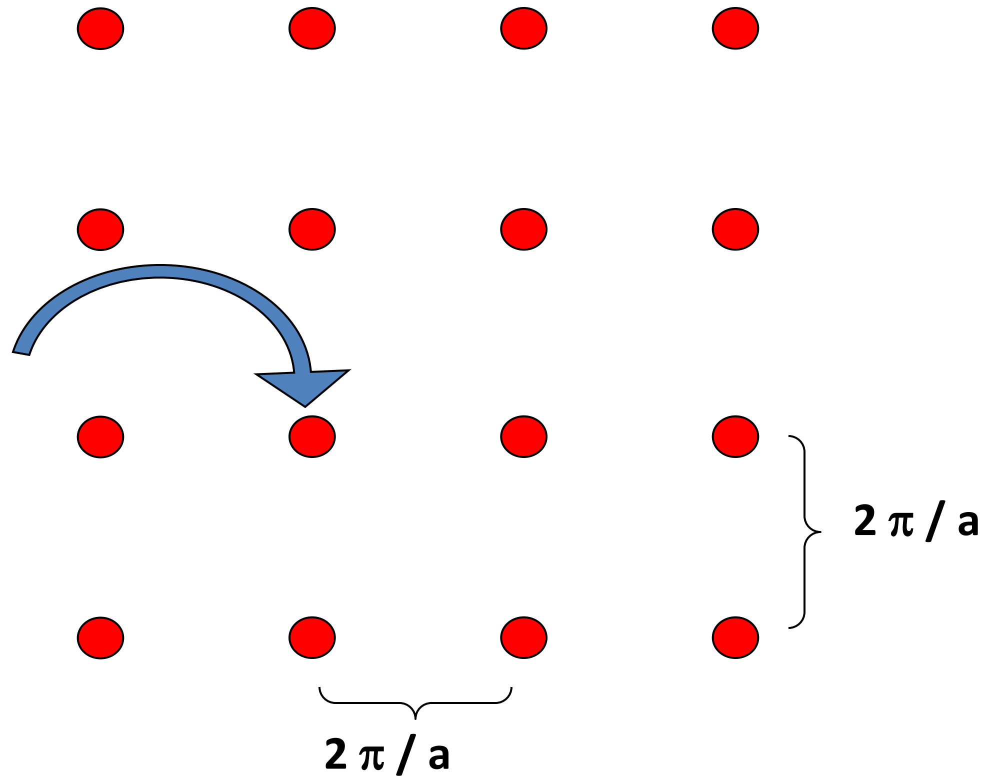
Crystalline Materials: Structure is Periodic with Period a

Work in Reciprocal Space – Momentum space, most natural for understanding diffraction and scattering

Mapping Momentum – Energy (Q-E) space

Origin of reciprocal space;

Remains fixed for any sample rotation

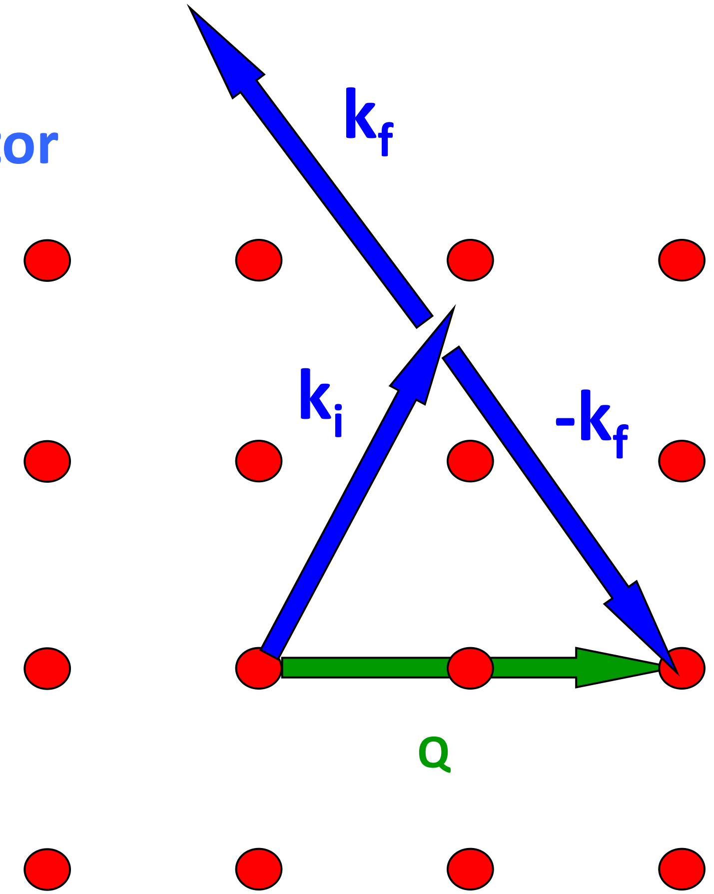


Bragg diffraction:

Constructive Interference

Q = Reciprocal Lattice Vector

Elastic scattering : $| k_i | = | k_f |$



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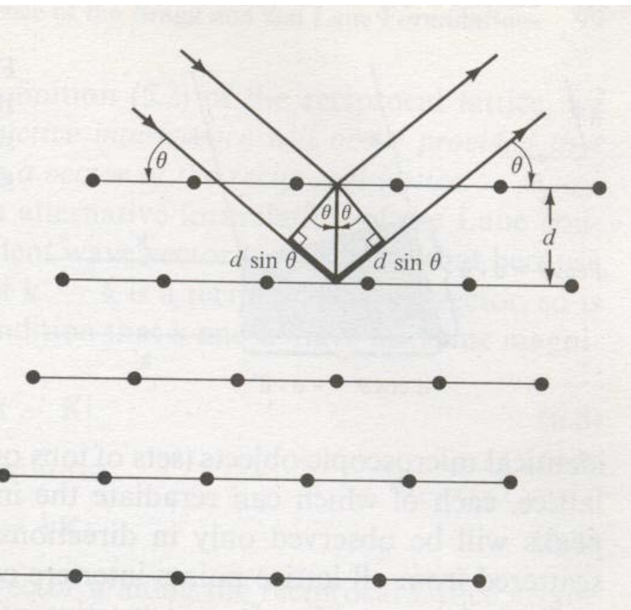

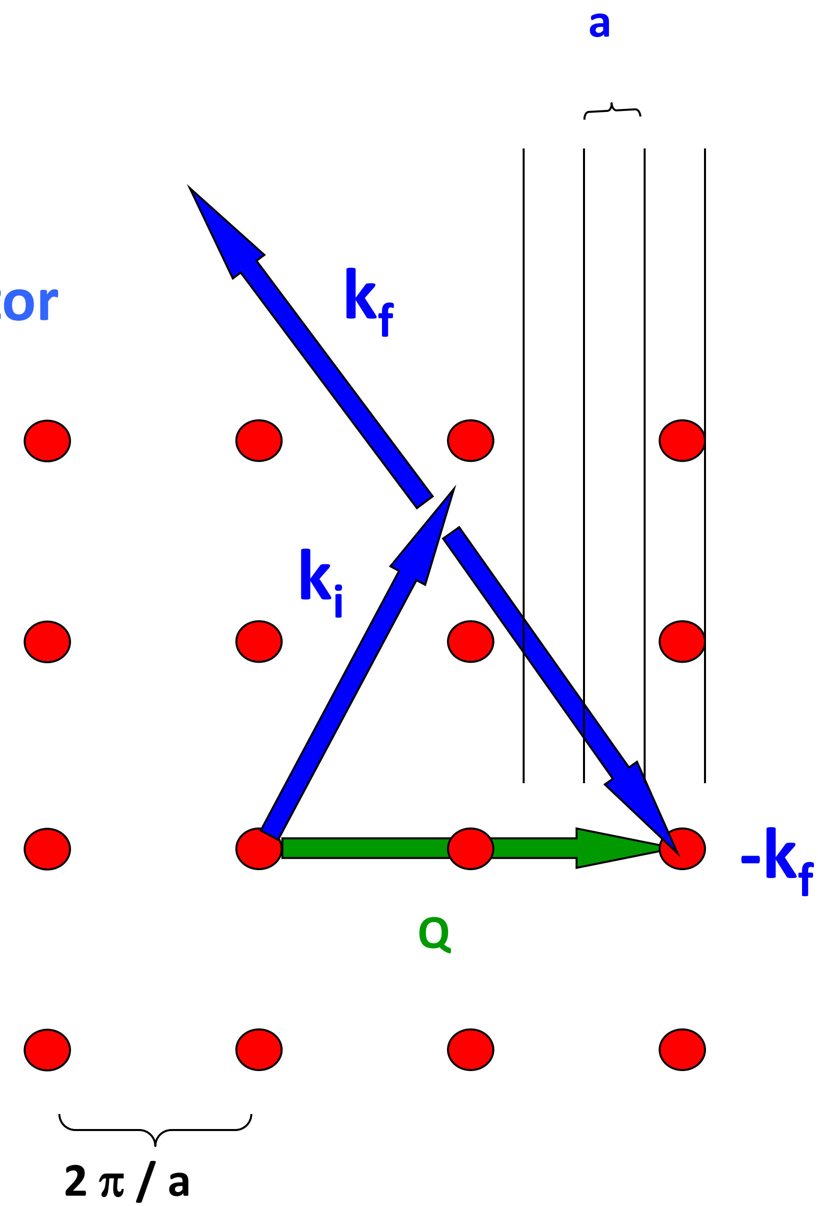

Elastic scattering : $| k_i | = | k_f |$

Bragg diffraction:

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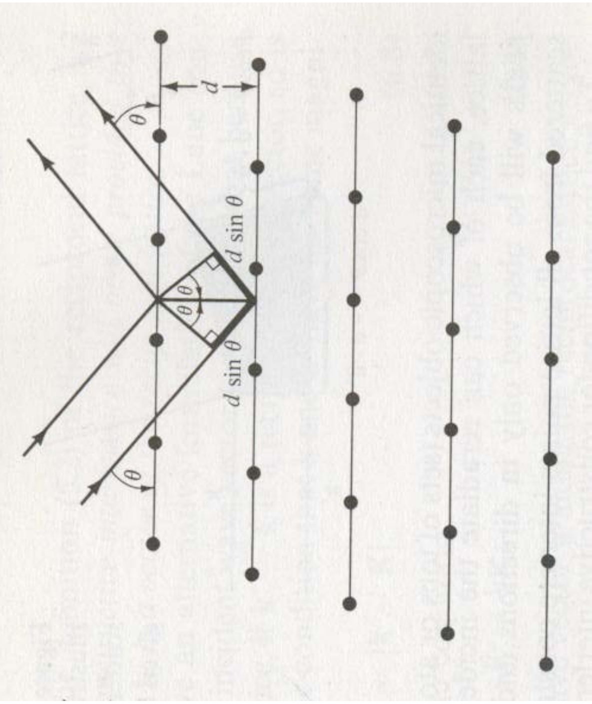
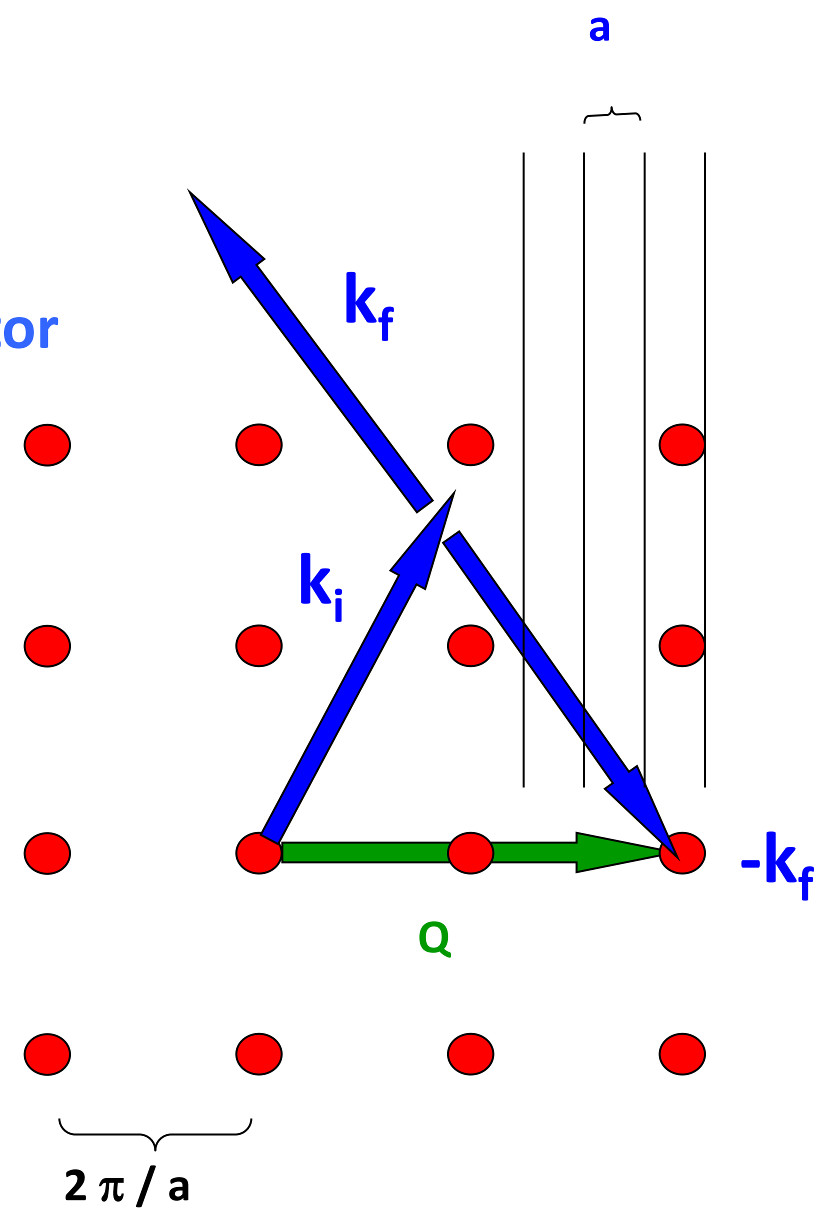
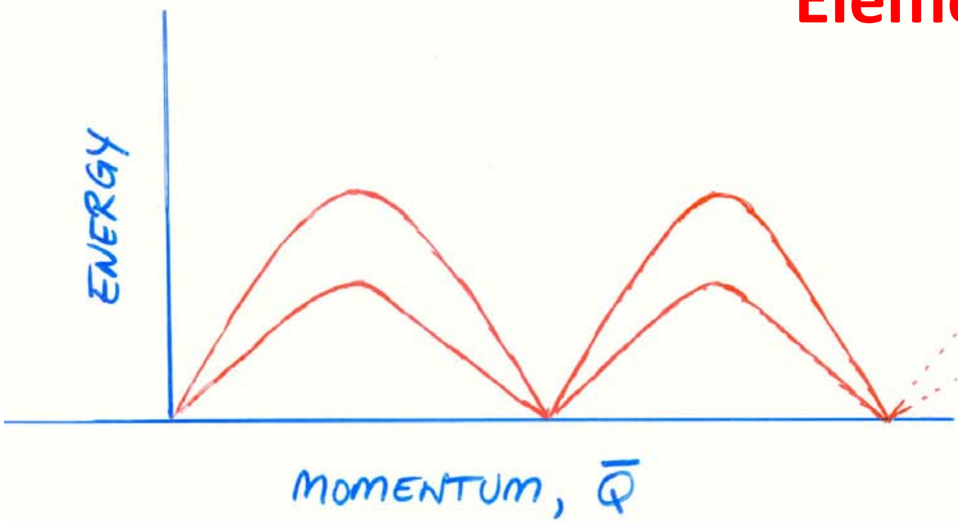


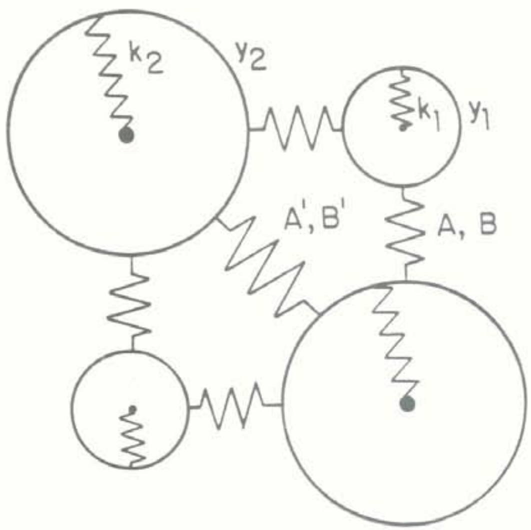


Elastic scattering : $| k_i | = | k_f |$

Elementary Excitations in Solids



- Lattice Vibrations (Phonons)
- Spin Fluctuations (Magnons)



Energy vs Momentum

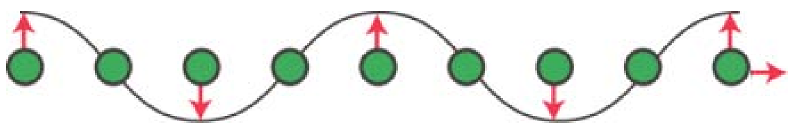
- Forces which bind atoms together in solids

Phonons

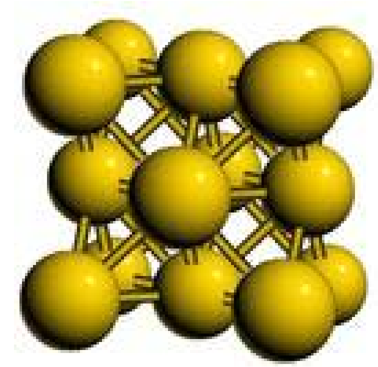
- Normal modes in periodic crystal → wavevector

$$\mathbf{u}(l,t) = \frac{1}{\sqrt{NM}} \sum_{j\mathbf{q}} \boldsymbol{\varepsilon}_j(\mathbf{q}) \exp(i\mathbf{q}\cdot\mathbf{l}) \hat{B}(\mathbf{q}j,t)$$

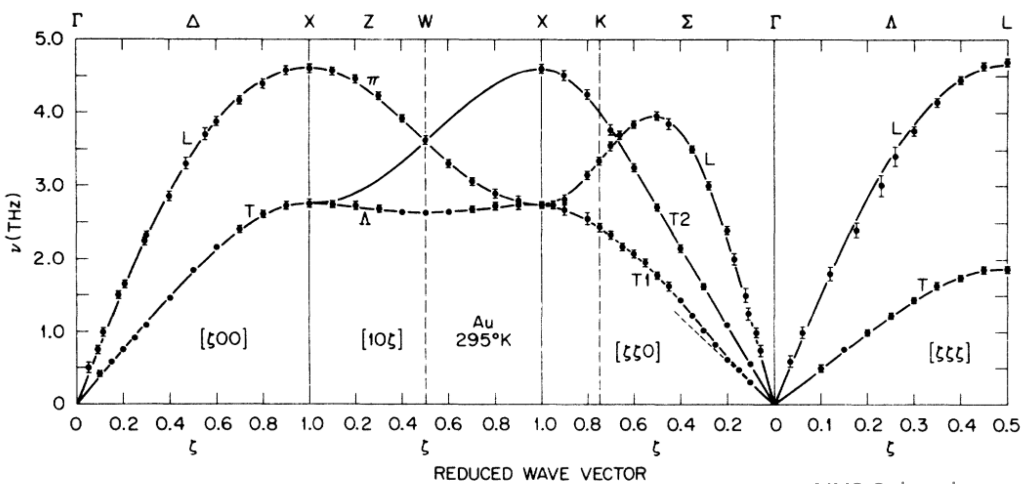
- Energy of phonon depends on **q** and polarization



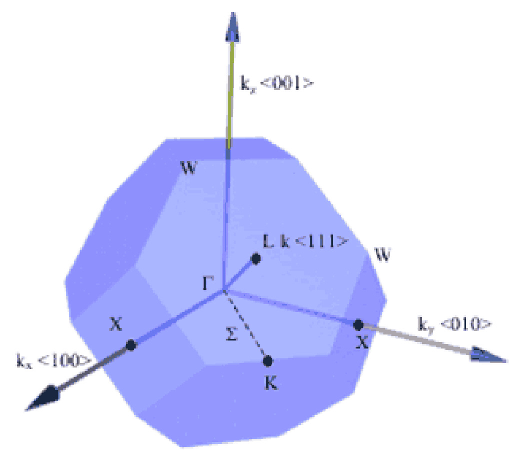
Longitudinal mode
Transverse mode



FCC structure



Lynn, *et al.*, *Phys. Rev. B* **8**, 3493 (1973).

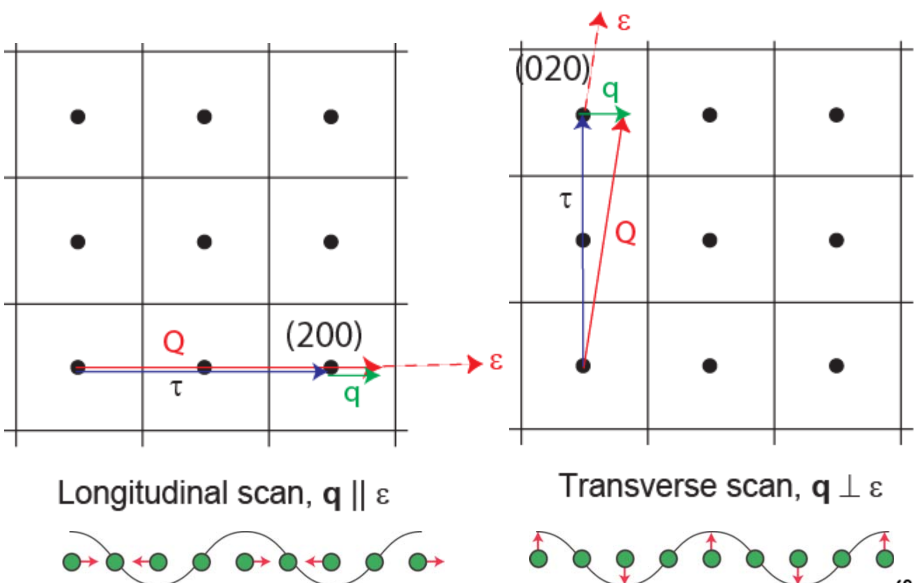


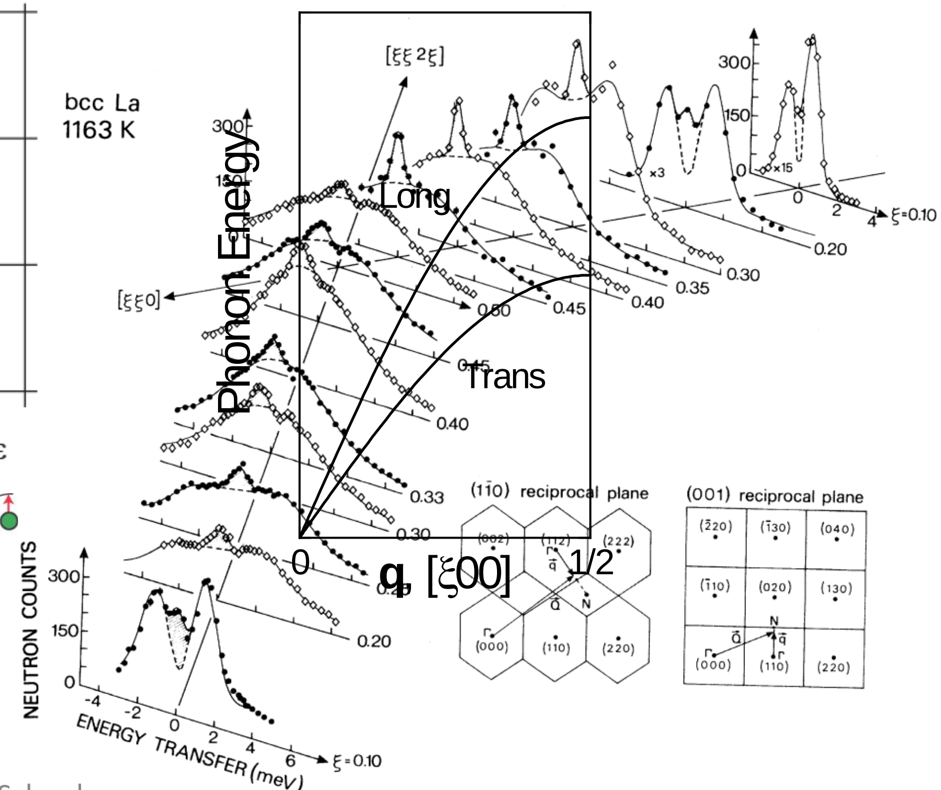
FCC Brillouin zone

Phonon intensities

Structure (polarization) factor

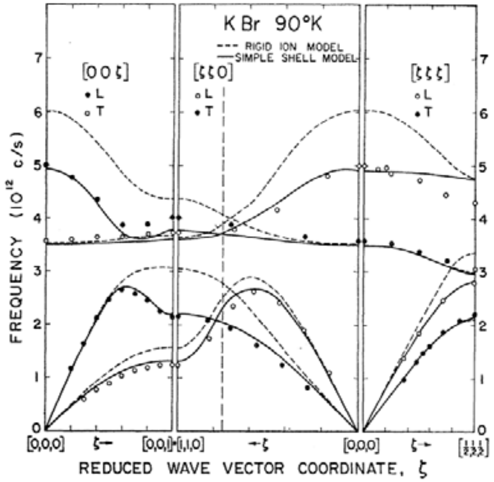
$$S_{1+}(\mathbf{Q},\omega)=\frac{1}{2NM}e^{-Q^2\langle u^2\rangle}\sum_{j\mathbf{q}}\frac{\left|\mathbf{Q}\cdot\boldsymbol{\varepsilon}_j(\mathbf{q})\right|^2}{\omega_j(\mathbf{q})}(1+n(\omega))\delta(\mathbf{Q}-\mathbf{q}-\boldsymbol{\tau})\delta(\omega-\omega_j(\mathbf{q}))$$



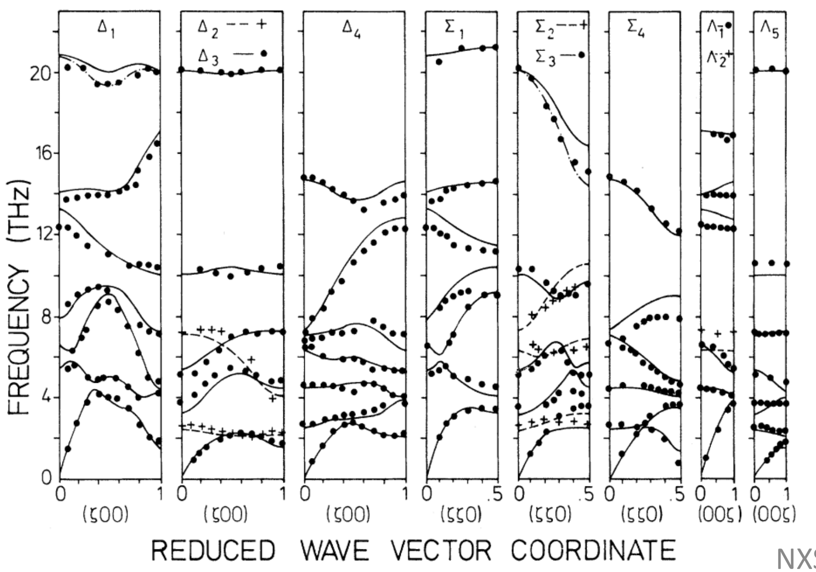


Guthoff *et al., Phys. Rev. B* **47**, 2563 (1993).

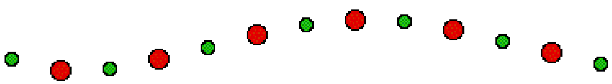
More complicated structures



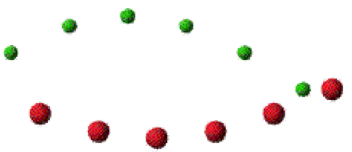
Woods, *et al., Phys. Rev*. **131**, 1025 (1963).



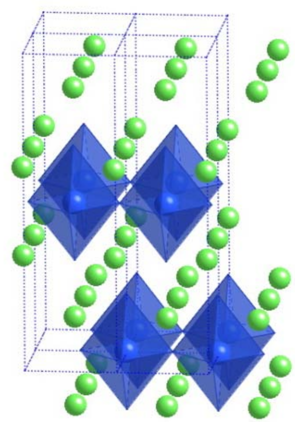
Chaplot, *et al., Phys. Rev*. B **52**, 7230(1995).



Acoustic phonon



Optical phonon



La_2CuO_4

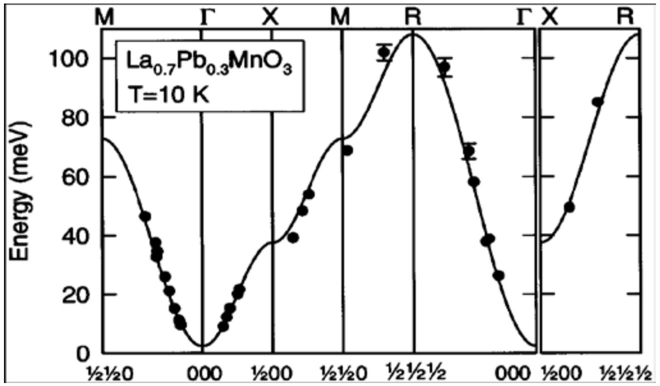
Spin excitations

- **Spin excitations**
  - Spin waves in ordered magnets
  - Paramagnetic & quantum spin fluctuations
  - Crystal-field & spin-orbit excitations

- **Magnetic inelastic scattering can tell us about**
  - Exchange interactions
  - Single-ion and exchange anisotropy (determine Hamiltonian)
  - Phase transitions & critical phenomena
  - Quantum critical scaling of magnetic fluctuations
  - Other electronic energy scales (eg. CF & SO)
  - Interactions (eg. spin-phonon coupling)

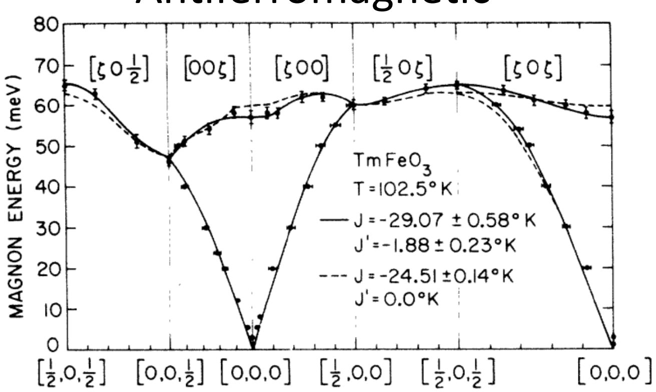
Spin waves

Ferromagnetic



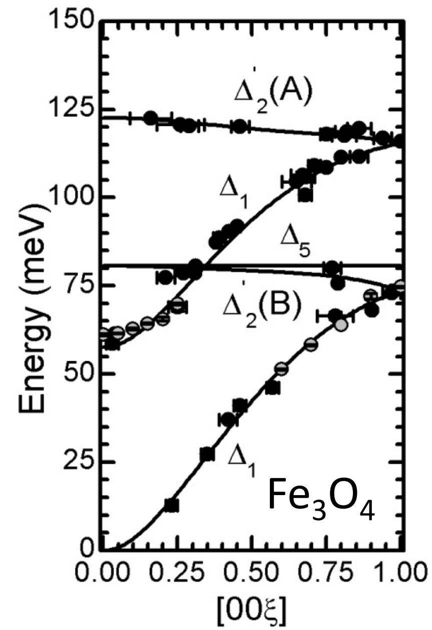
Perring *et al., Phys. Rev*. Lett. **77**, 711 (1996).

Antiferromagnetic



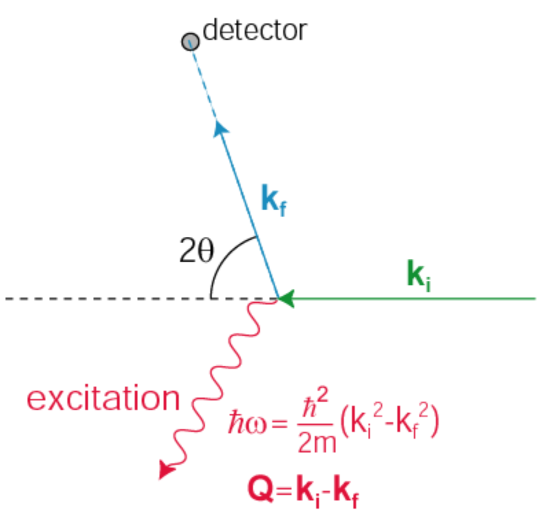
Shapiro *et al., Phys. Rev*. B **10**, 2014 (1974).

Ferrimagnetic

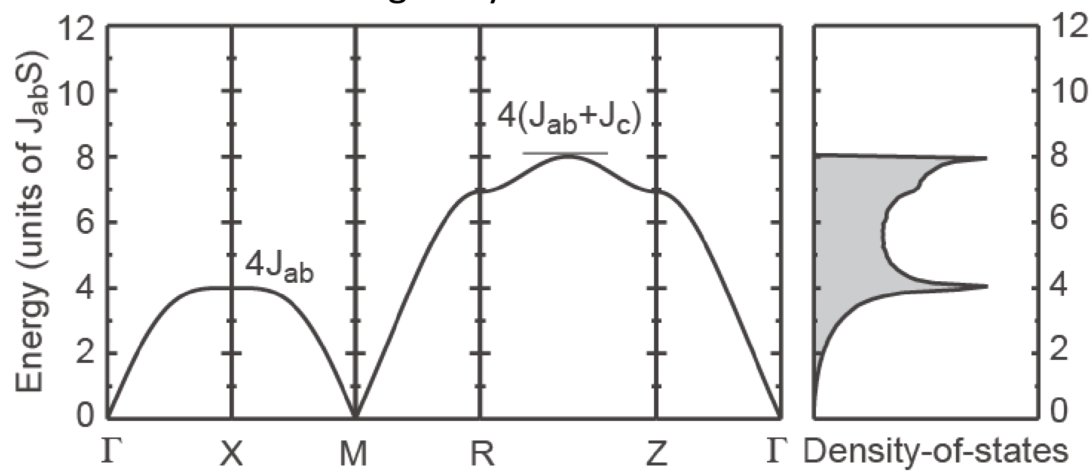


McQueeney *et al., Phys. Rev*. Lett. **99**, 246401 (2007).

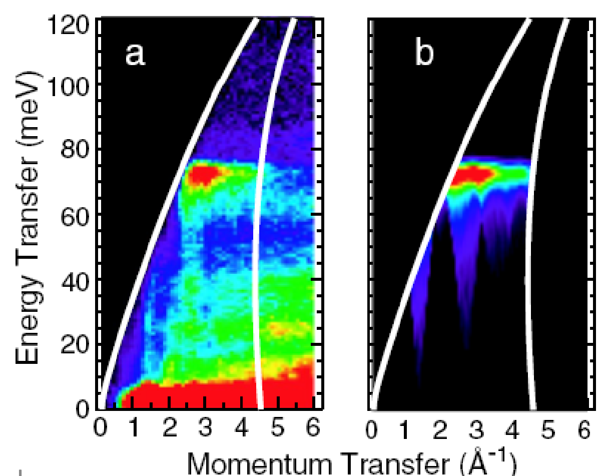
Scattering experiments



Single-crystal



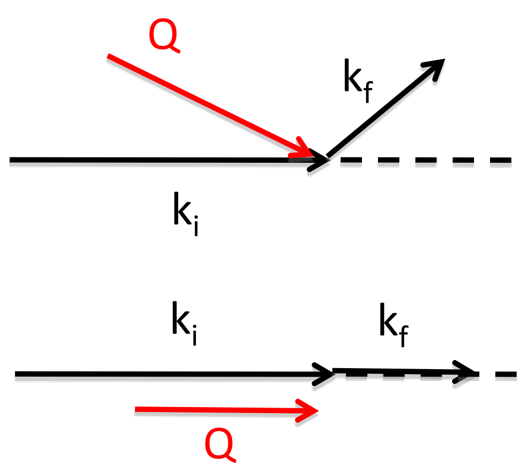
Powder $S(|\mathbf{Q}|,\omega)$



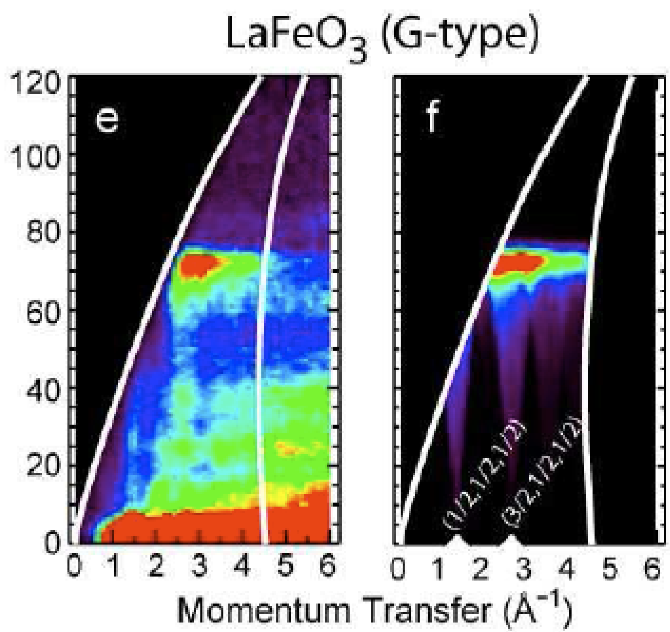
Instrument and sample (powder or single-crystal) determine how ($\mathbf{Q}$,ω) space is sampled

Kinematic limitations

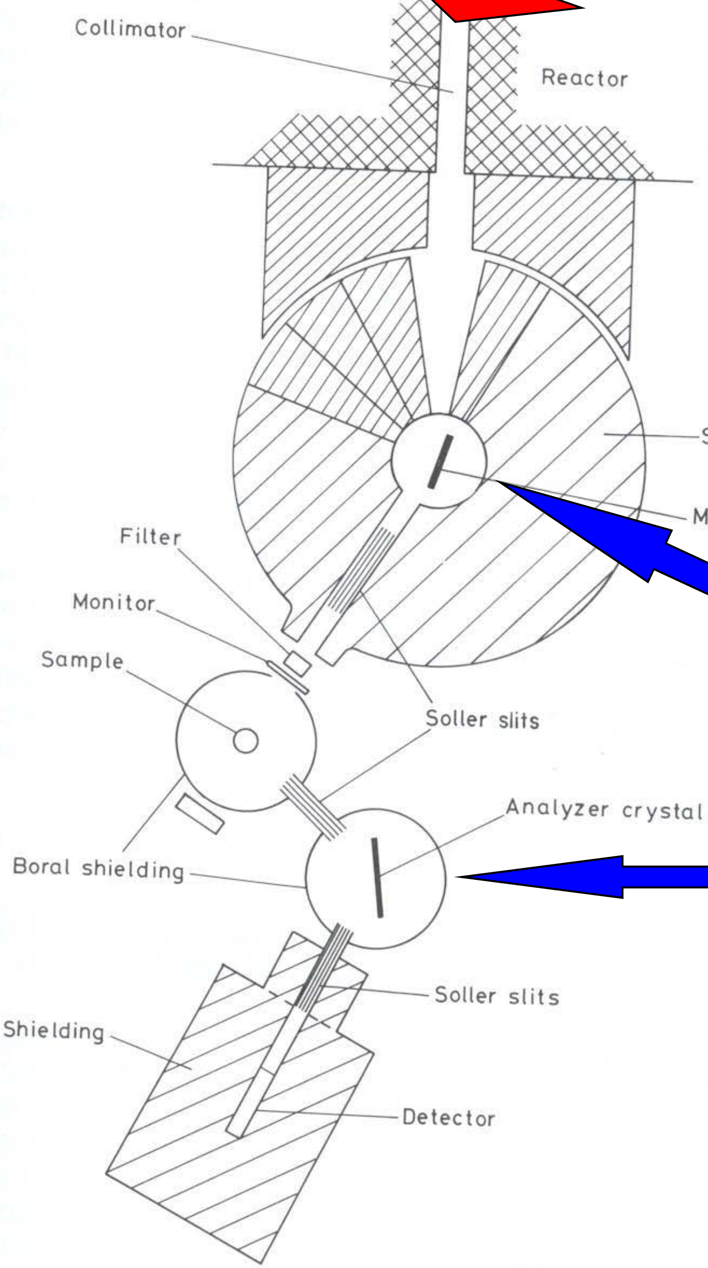
- **Many combinations of k_i,k_f for same Q,ω**
  - Only certain configurations are used (eg. E_f-fixed)
- **Cannot "close triangle" for certain Q,ω due to kinematics**

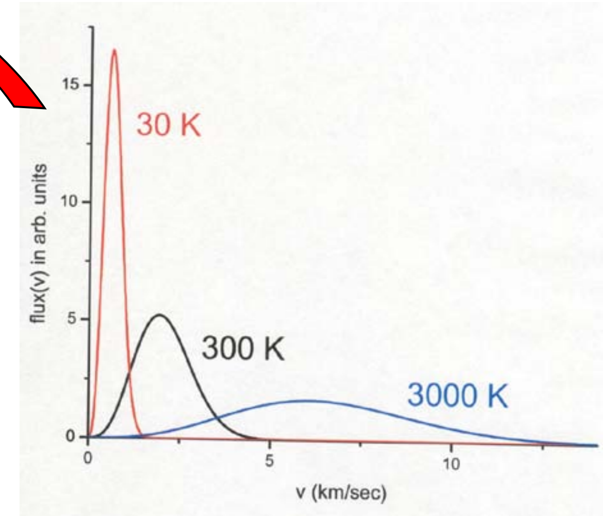


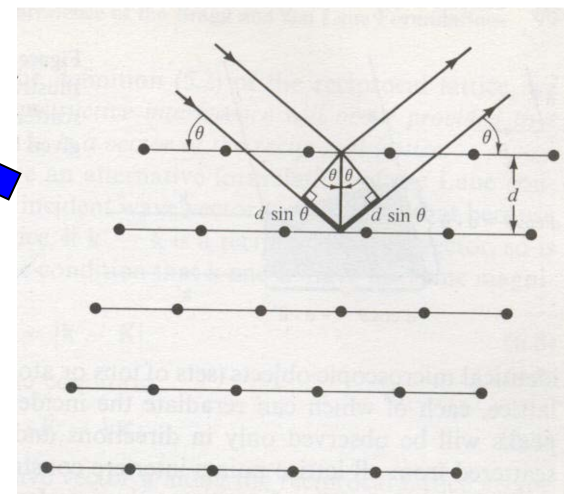
Minimum accessible Q



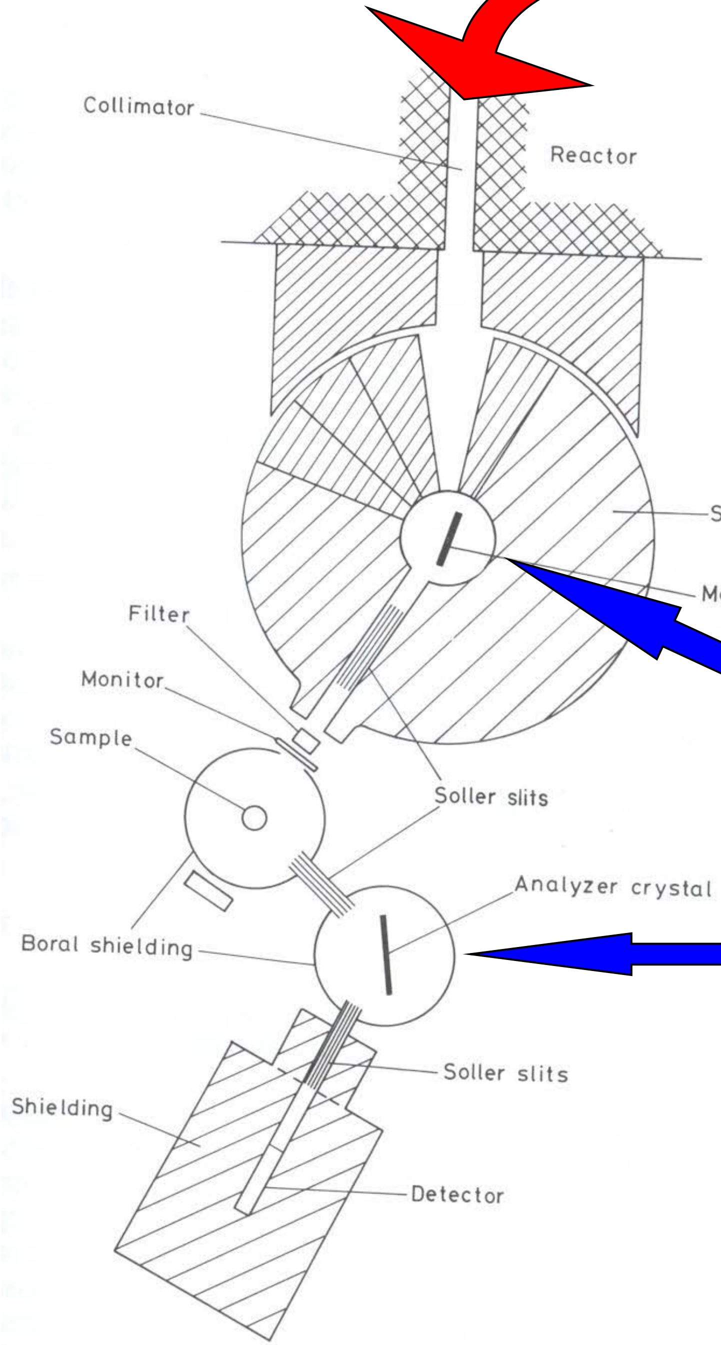
Kinematic limits, E_i=160 meV

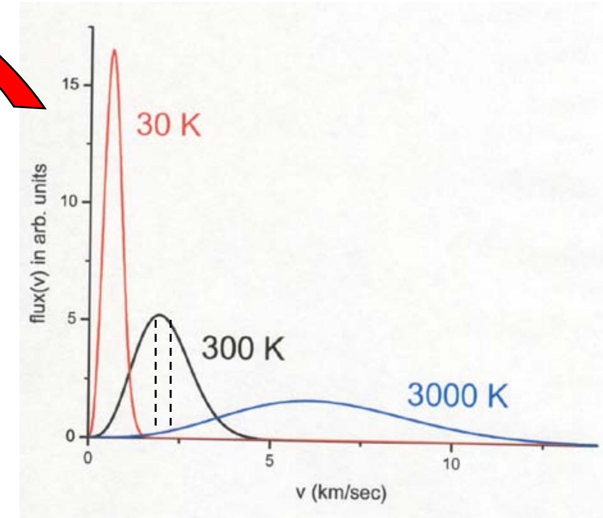


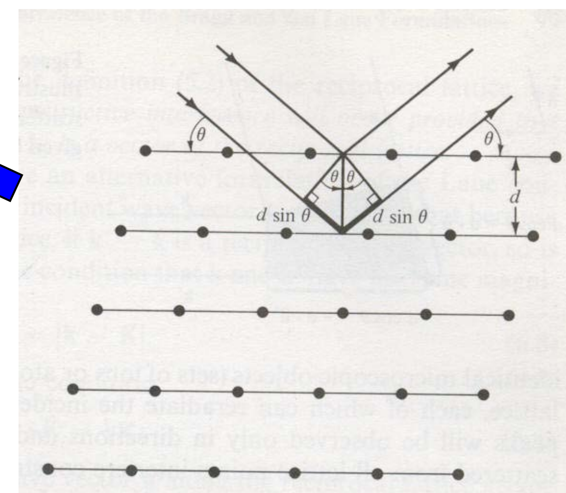




Bragg's Law: nλ = 2d sin(θ)



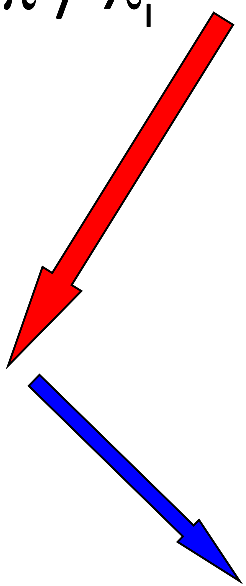




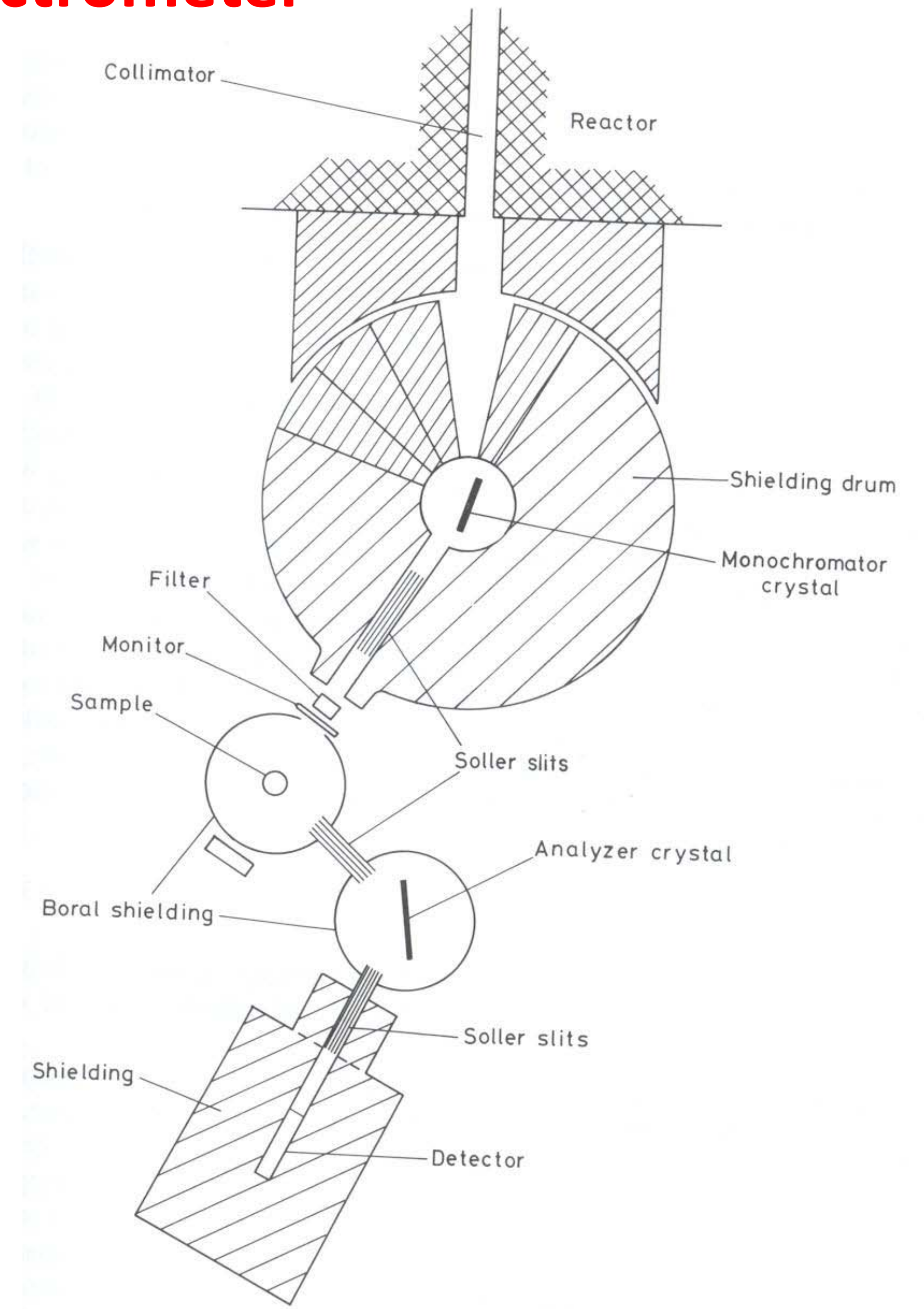
Bragg's Law: nλ = 2d sin(θ)

Brockhouse's Triple Axis Spectrometer

$|\,\mathbf{k_i}\,| = 2\,\pi\,/\,\lambda_i$

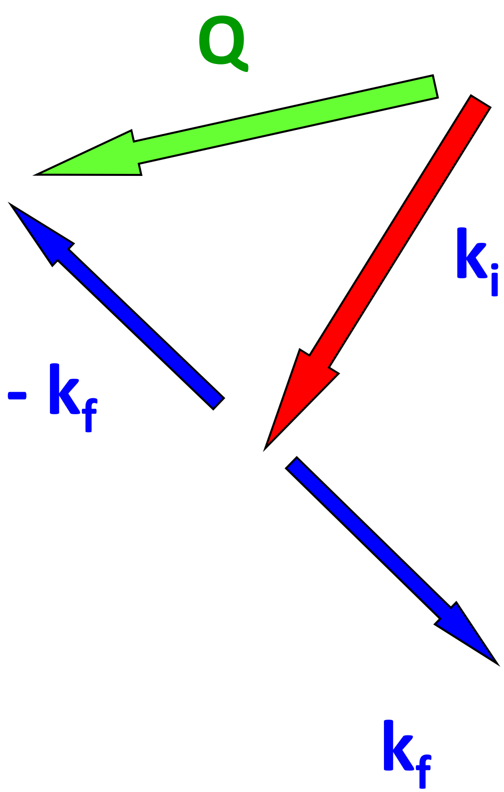


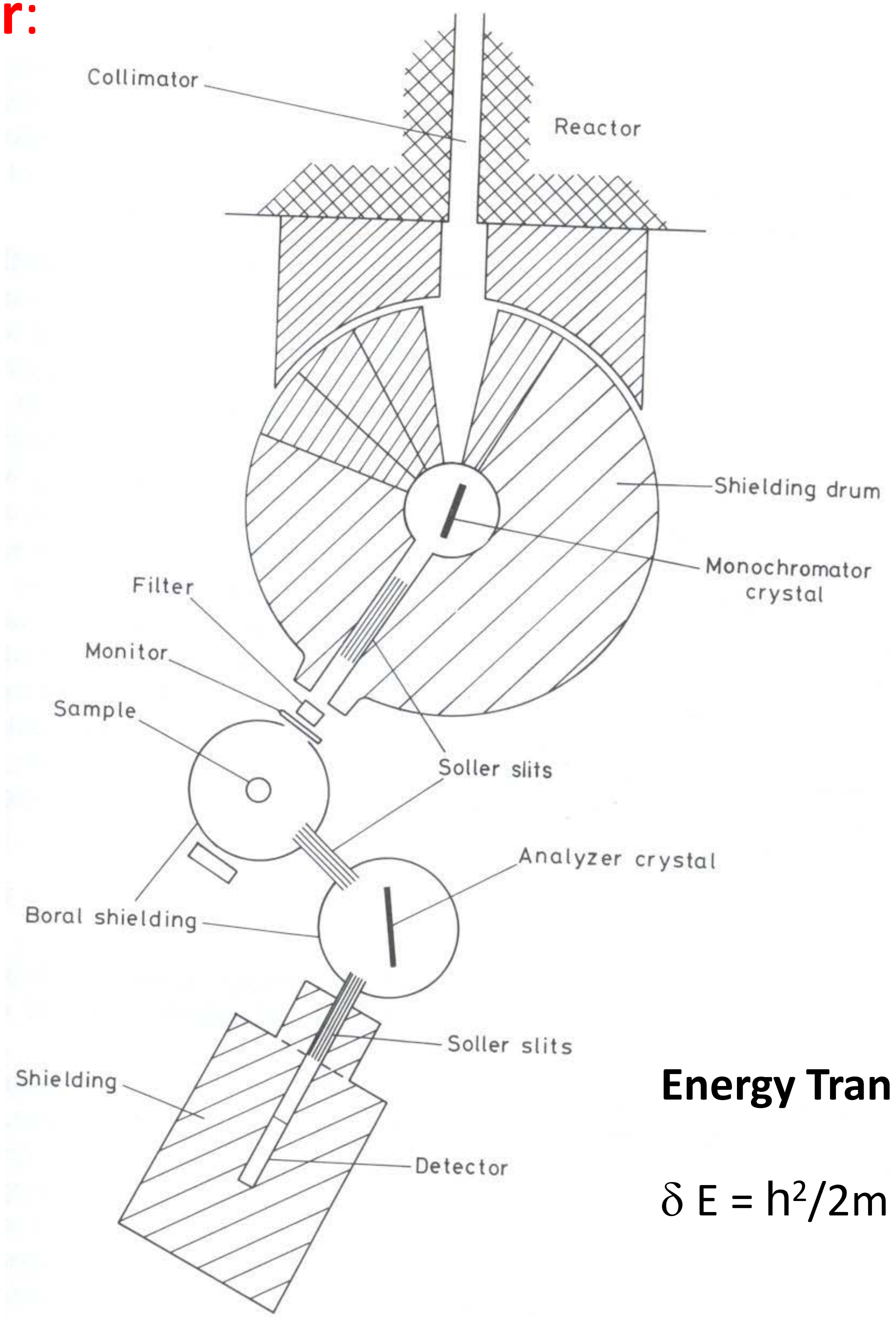
$|\,\mathbf{k_f}\,| = 2\,\pi\,/\,\lambda_f$



Momentum Transfer:

$Q = k_i - k_f$





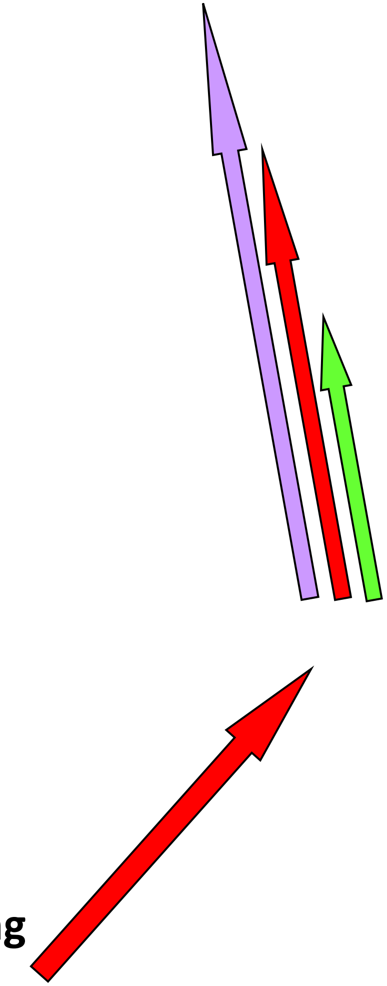
Energy Transfer:

$\delta E = h^2/2m\,(k_i^2 - k_f^2)$

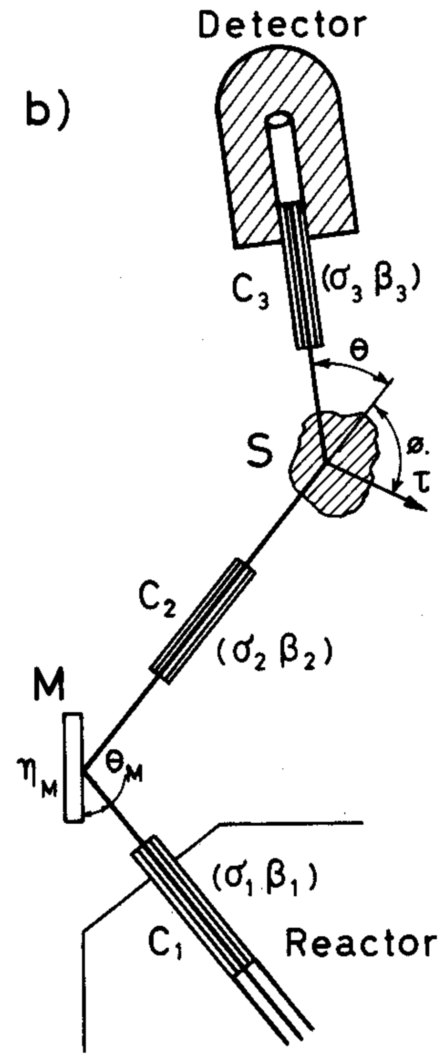
Two Axis Spectrometer:

- 3-axis with analyser removed

- Powder diffractometer
- Small angle diffractometer
- Reflectometers

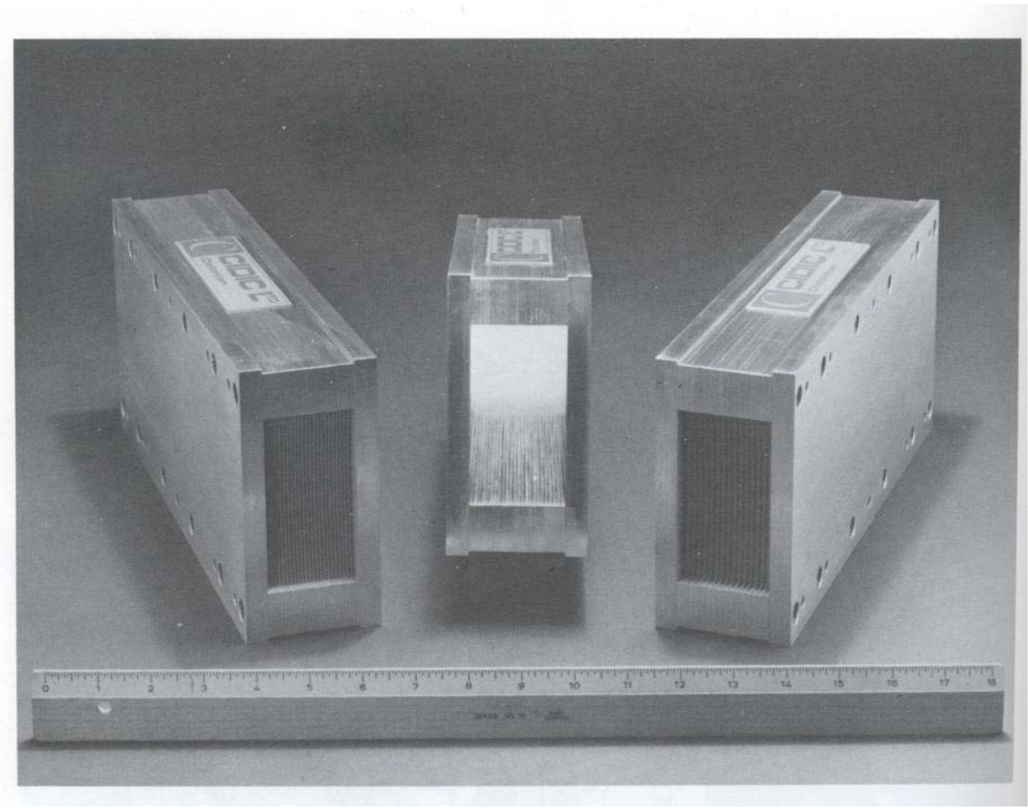


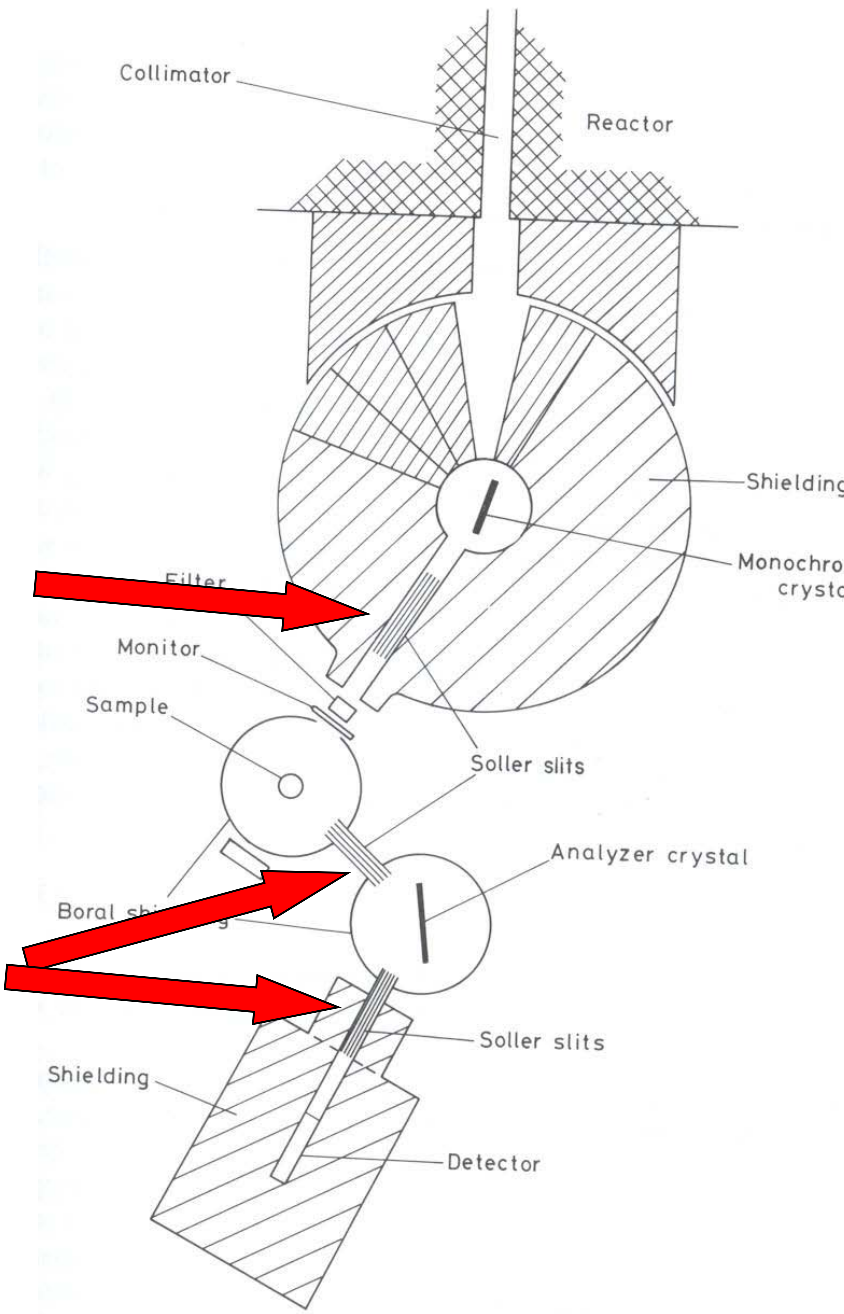
Diffractometers often employ working assumption that all scattering is *elastic.*



Soller Slits: Collimators

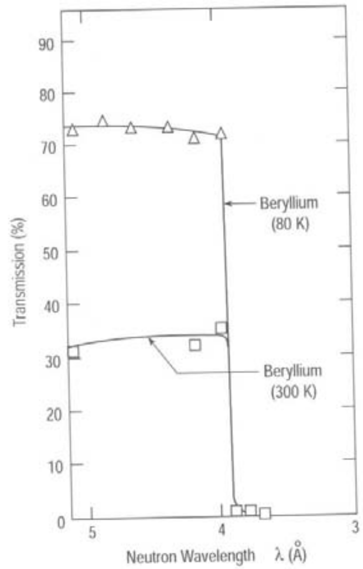
Define beam direction to +/- 0.5, 0.75 etc. degrees

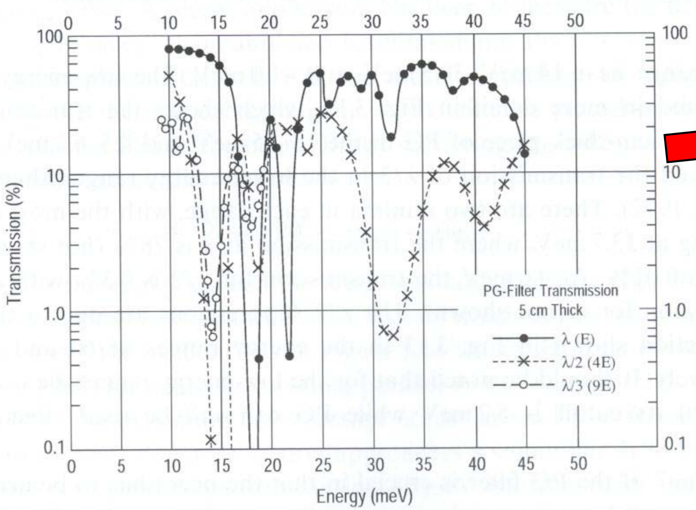


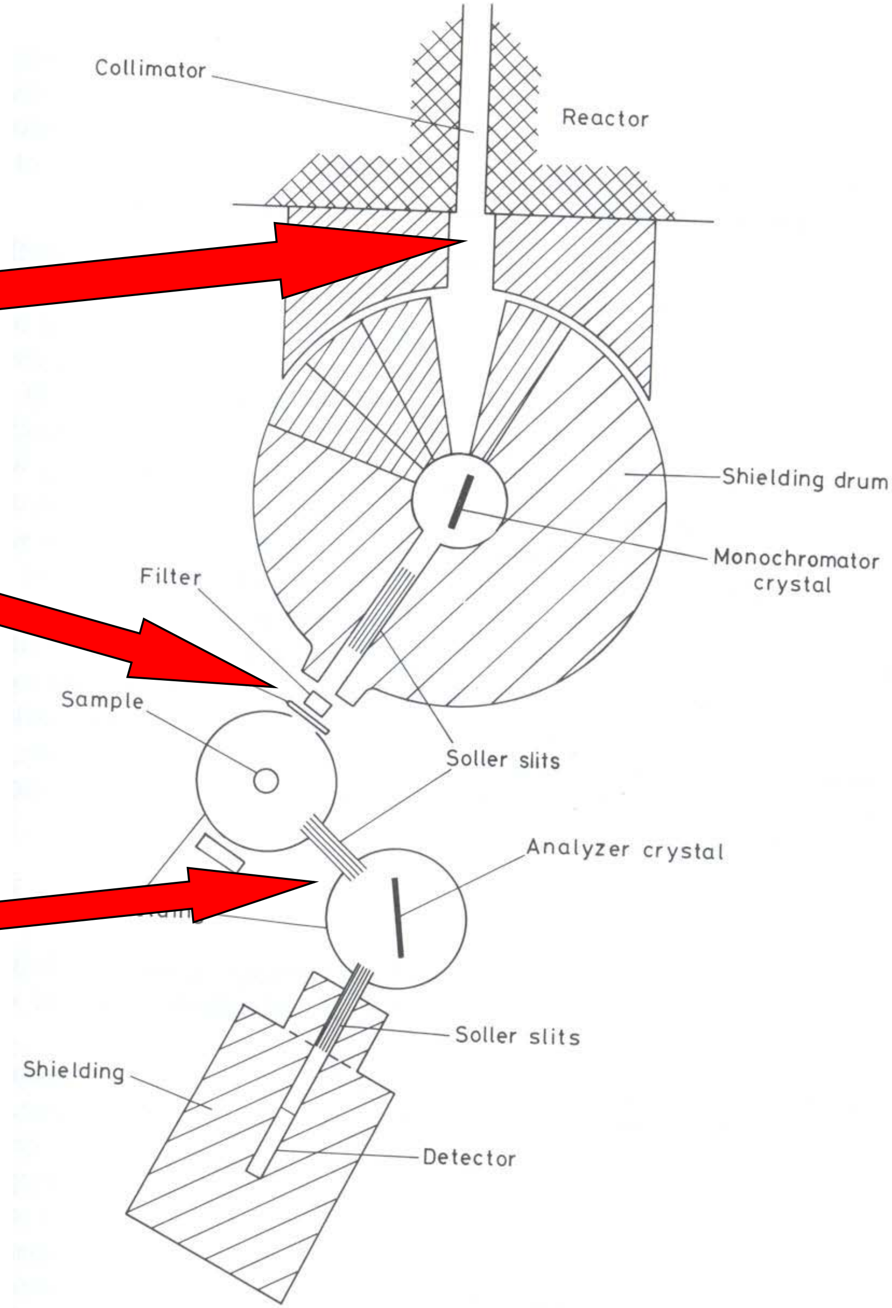


Filters:

Remove λ /n from incident or scattered beam, or both

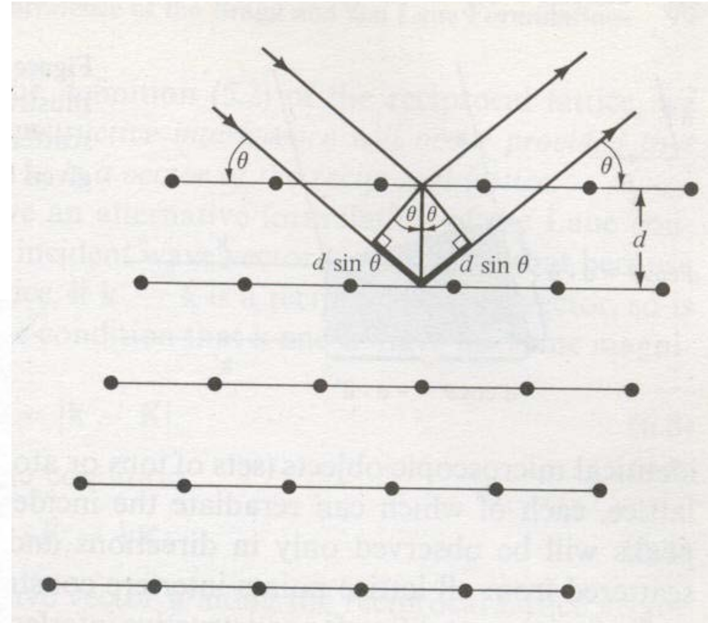


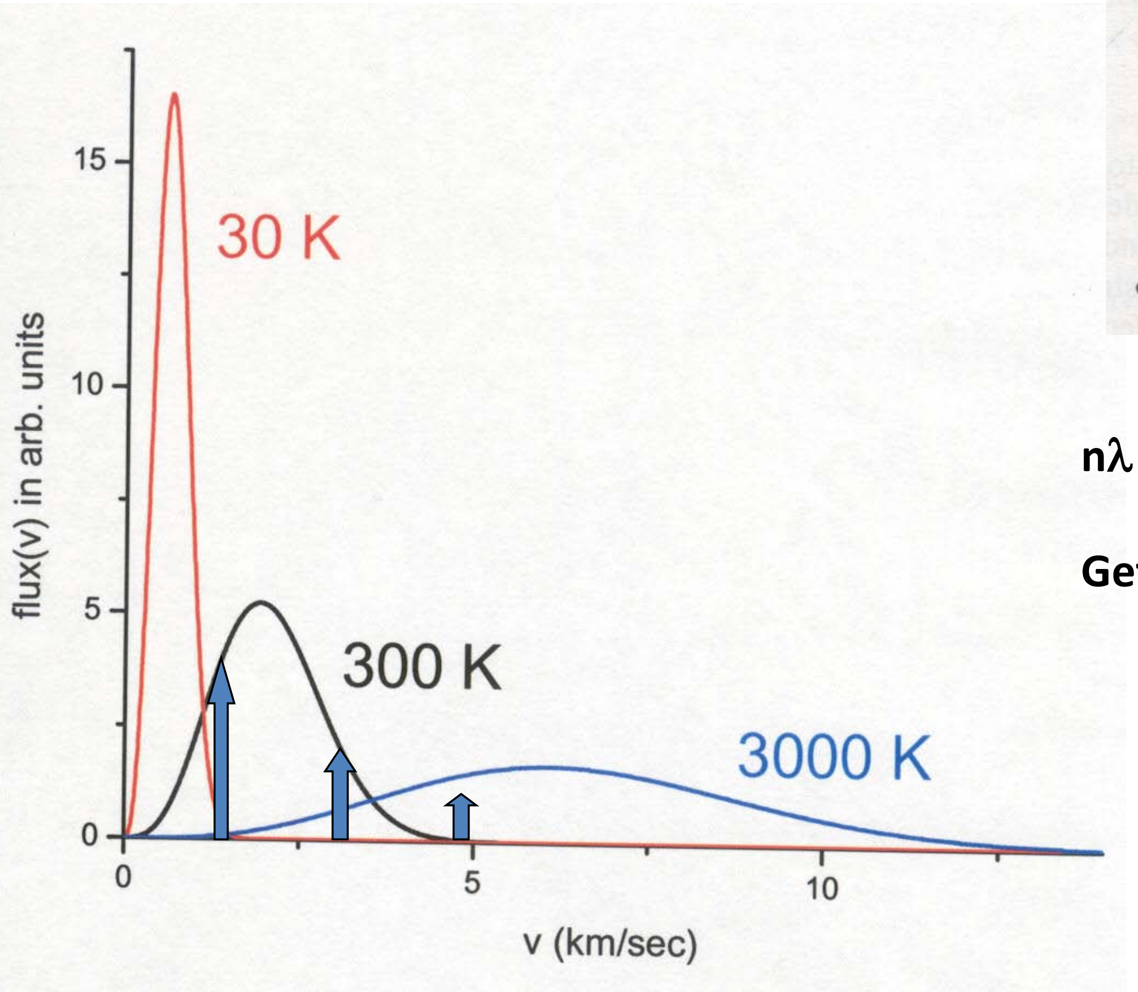




Single crystal monochromators:

Bragg reflection and harmonic contamination

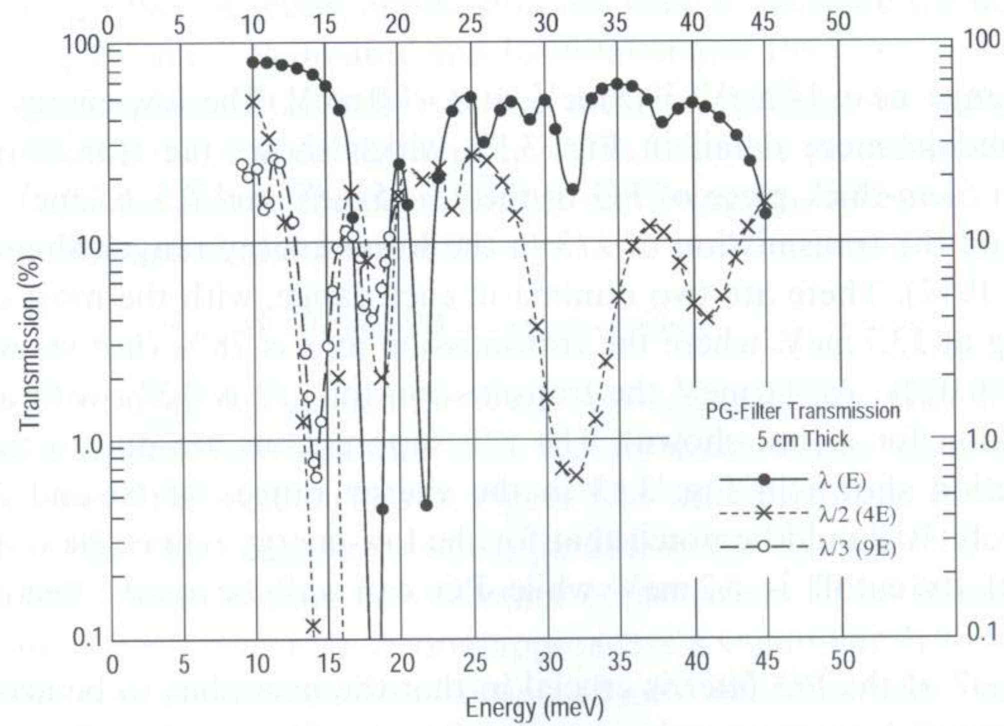


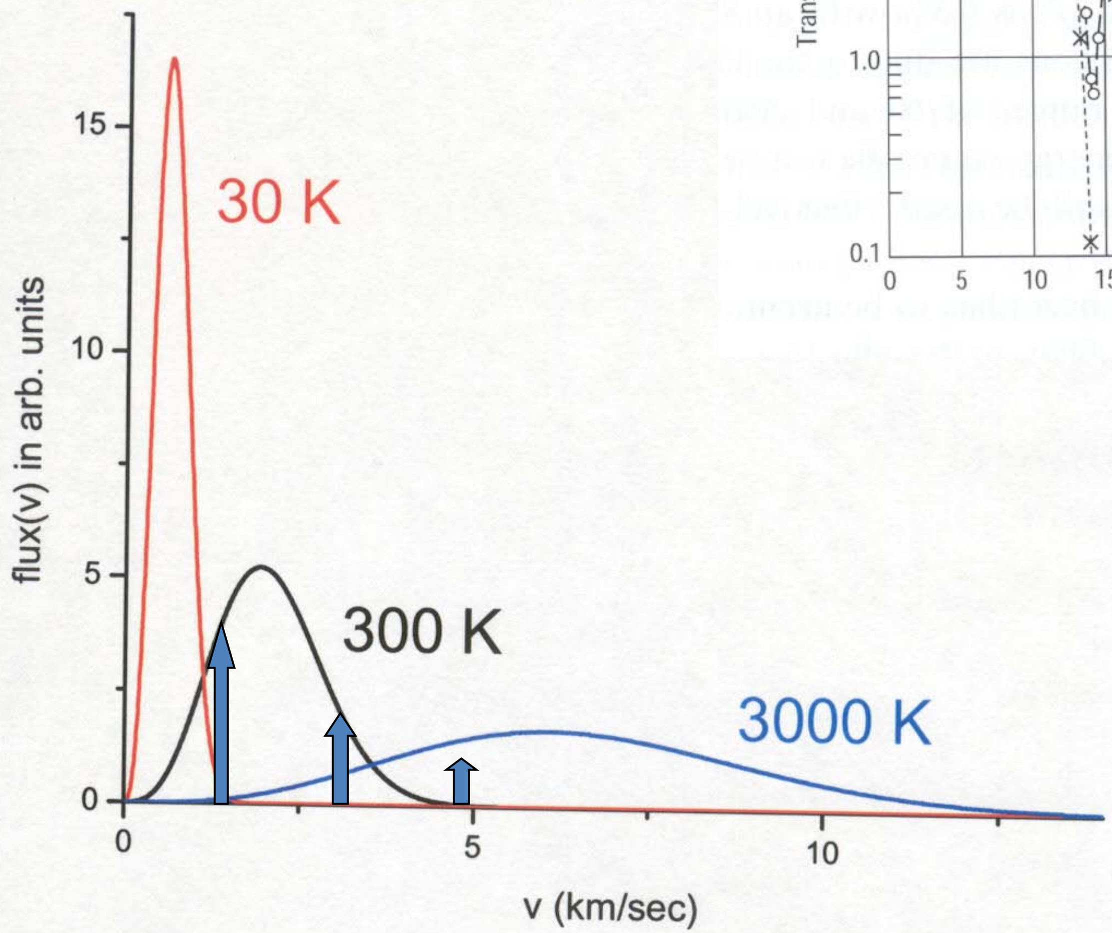


nλ = 2d sin(θ)

Get: λ , λ/2 , λ/3 , etc.

Pyrolitic graphite filter:





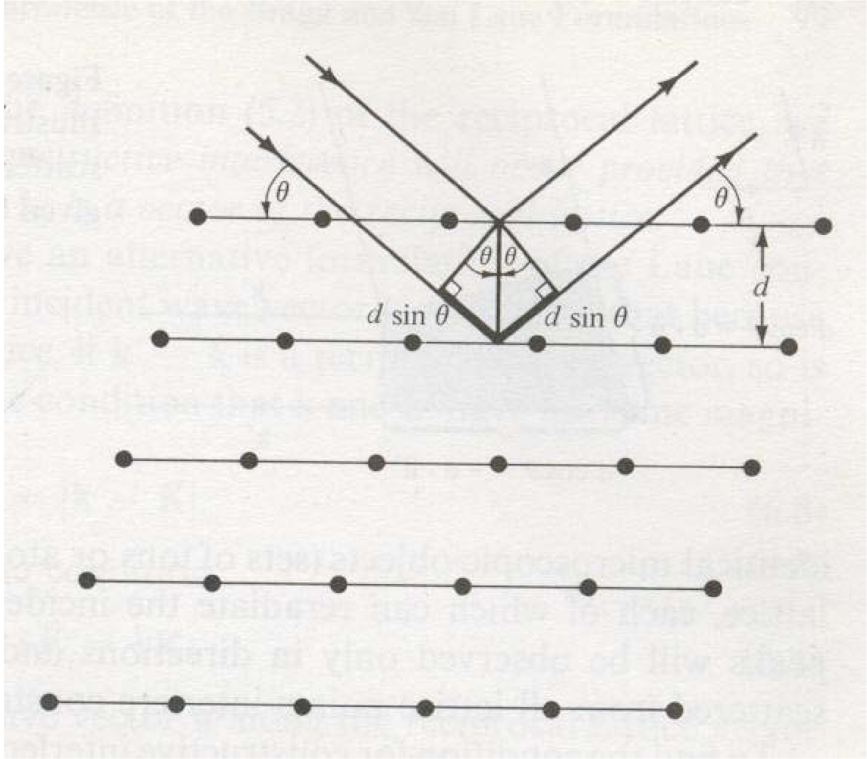
E = 14.7 meV

λ = 2.37 A

v = 1.6 km/s

2 x v = 3.2 km/s

3 x v = 4.8 km/s



Bragg's Law: nλ = 2d sin(θ)

$| k | = 2 \pi / \lambda$

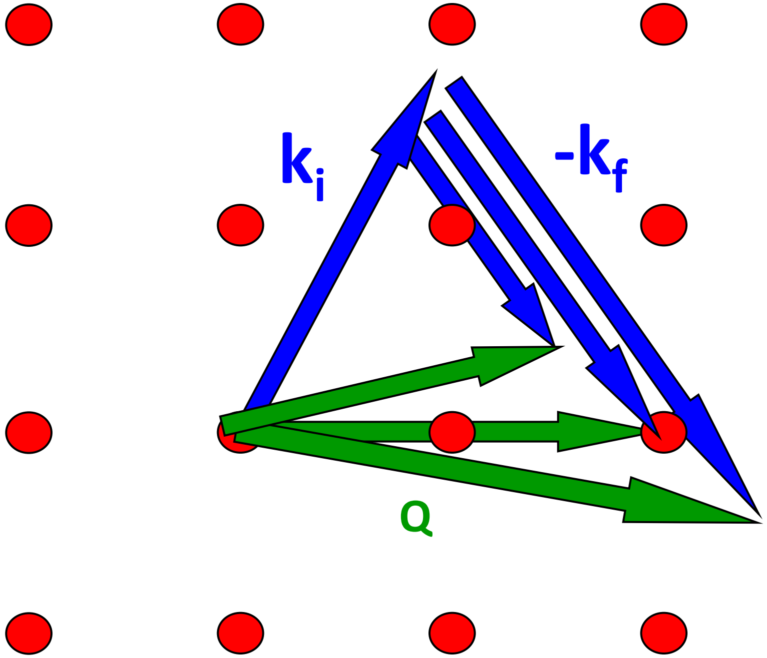
Volume of Q – E space sampled

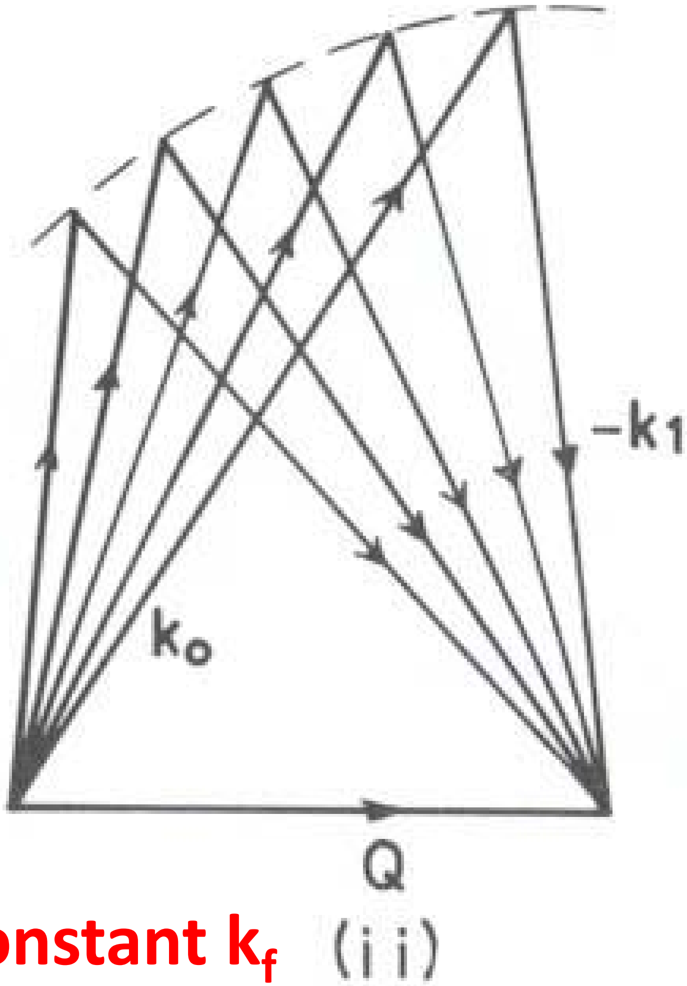
~ $k^3 \cot(\theta)$

"Efficiency" of monochromator / analyser varies strongly with k, θ

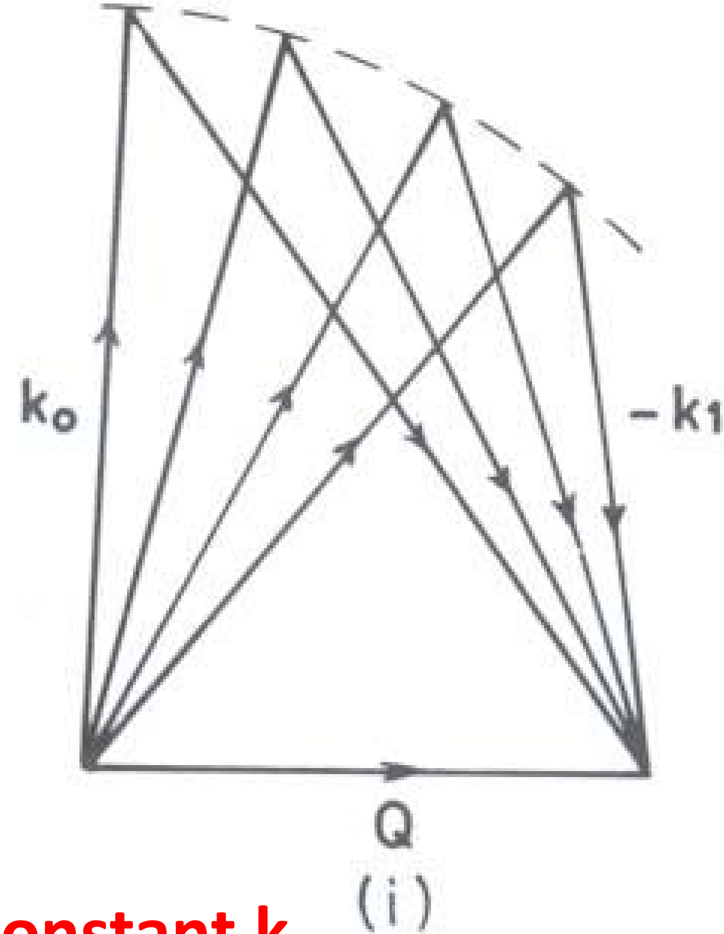
Bragg Diffraction:

Two Axis Diffraction: No E_f discrimination





Constant k_f



Constant k_i

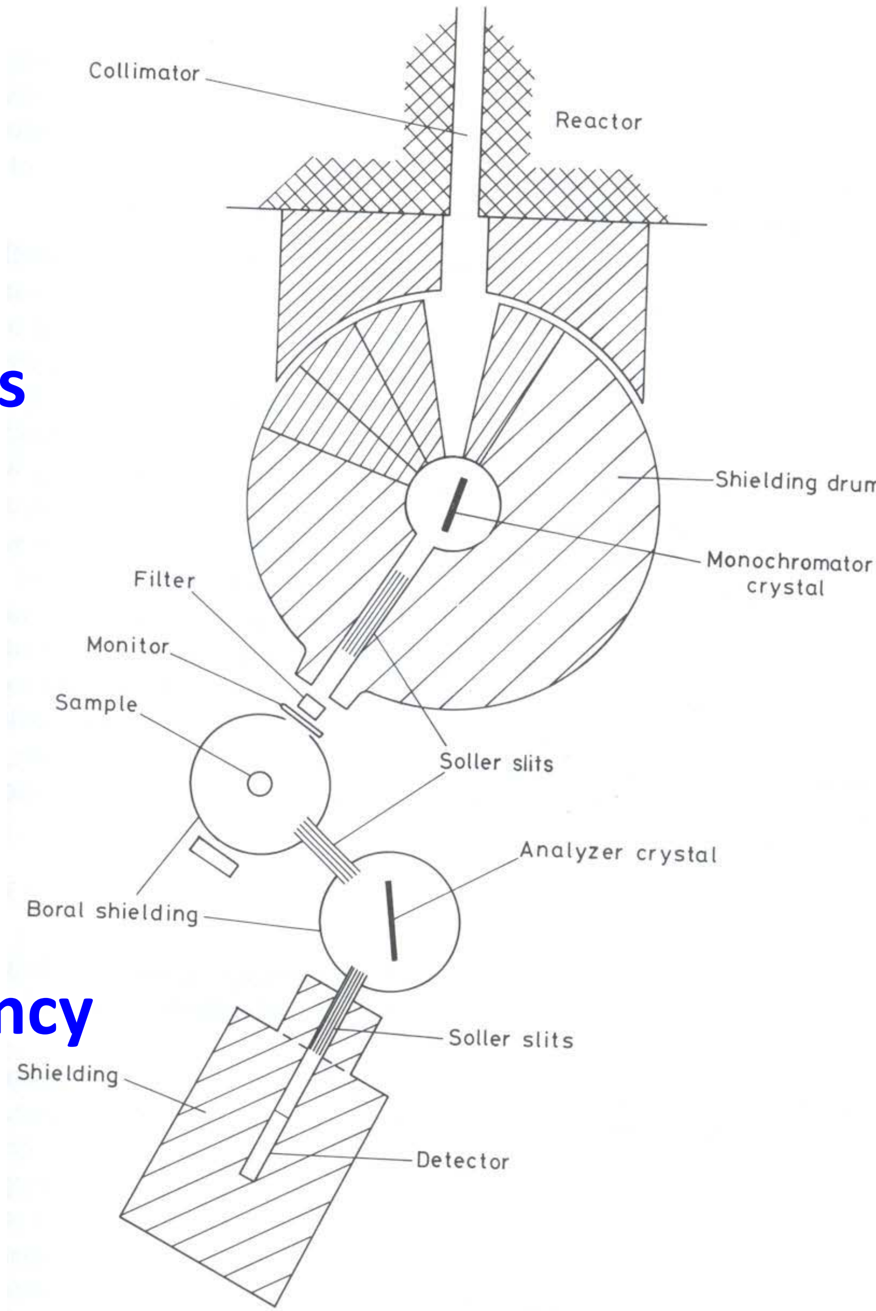
Two different ways of performing constant-Q scans

Constant k_f:

- k_f , θ_A do not change;
therefore analyser "efficiency" is constant

- k_i, θ_M do change, but
monitor detector normalizes to incident neutron flux

- Monitor detector (low) efficiency goes like ~ $1/v$ ~ $1/k_i$



Recall that our cross-section was:

$$\delta\sigma = W / \Phi = (m/2\pi h^2)^2 \; k_f / k_i \; |< f \mid V \mid i>|^2 \; \delta\Omega$$

Which gave us (keeping only the coherent scattering)

$$\delta^2\sigma / \delta\Omega \, \delta E_f = k_f / k_i \; \sigma_{coh}/4\pi \; N \; S_{coh}(\mathbf{Q}, \omega)$$

However, we are measuring the incident flux with an efficiency of $1/k_i$

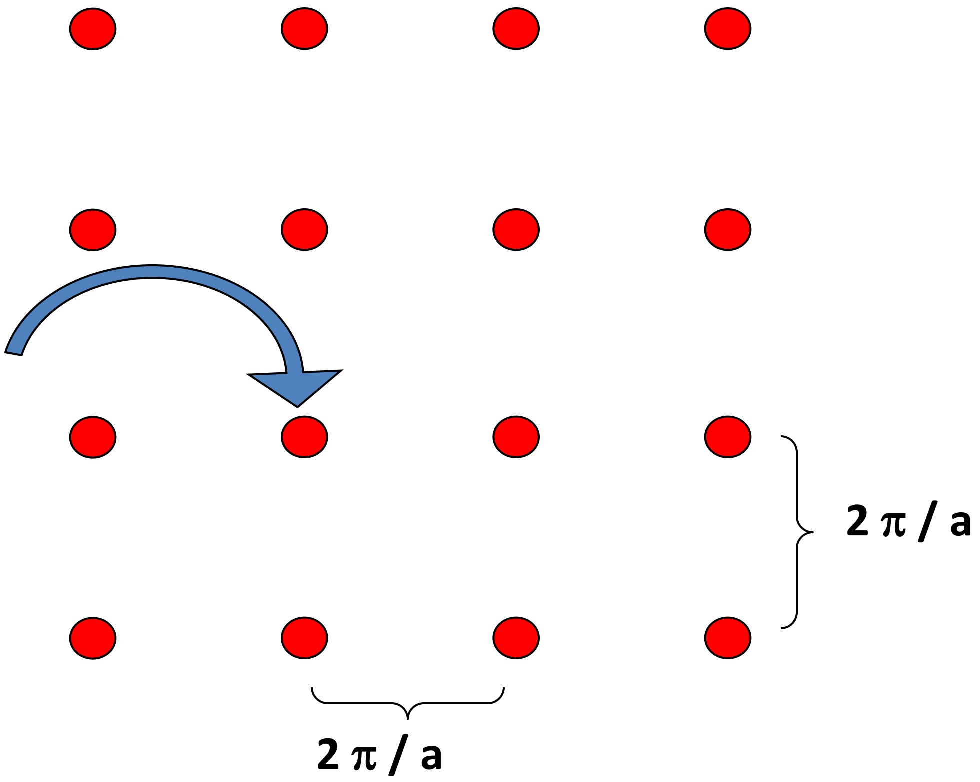
So, for constant k_f, this means we measure:

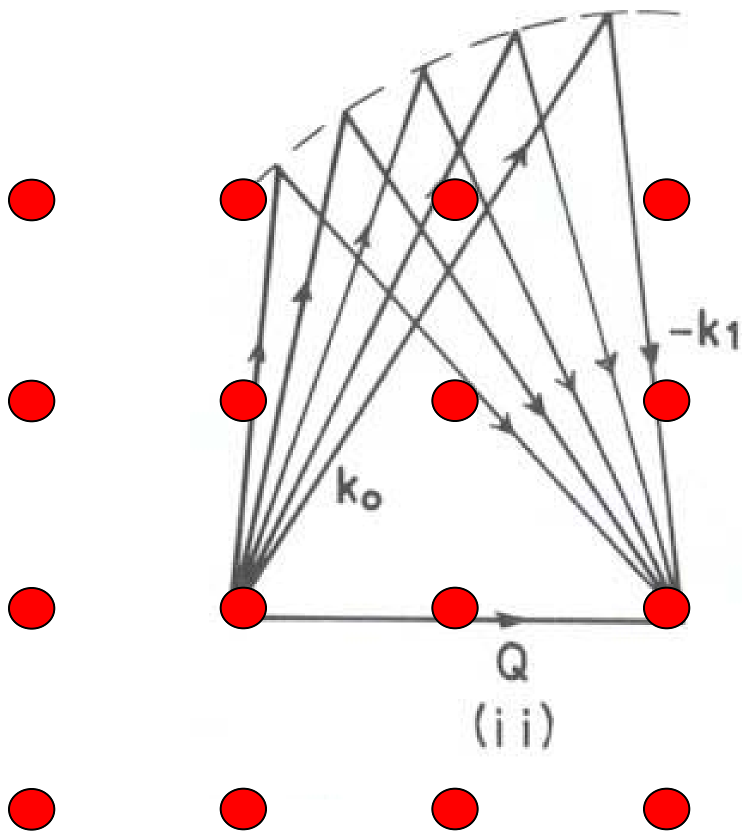
$$\delta^2\sigma / \delta\Omega \, \delta E_f = k_f/k_i \; \sigma_{coh}/4\pi \; N \; S_{coh}(\mathbf{Q}, \omega) / 1/k_i \sim S_{coh}(\mathbf{Q}, \omega)$$

Mapping Momentum – Energy (Q-E) space

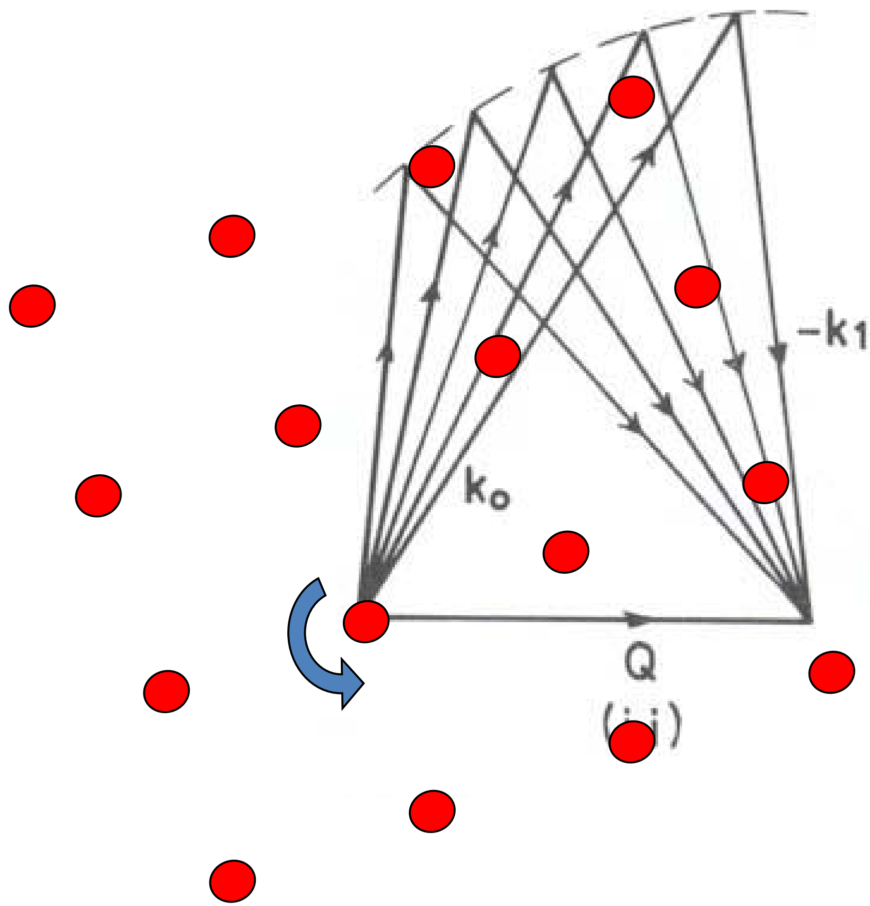
Origin of reciprocal space;

Remains fixed for any sample rotation

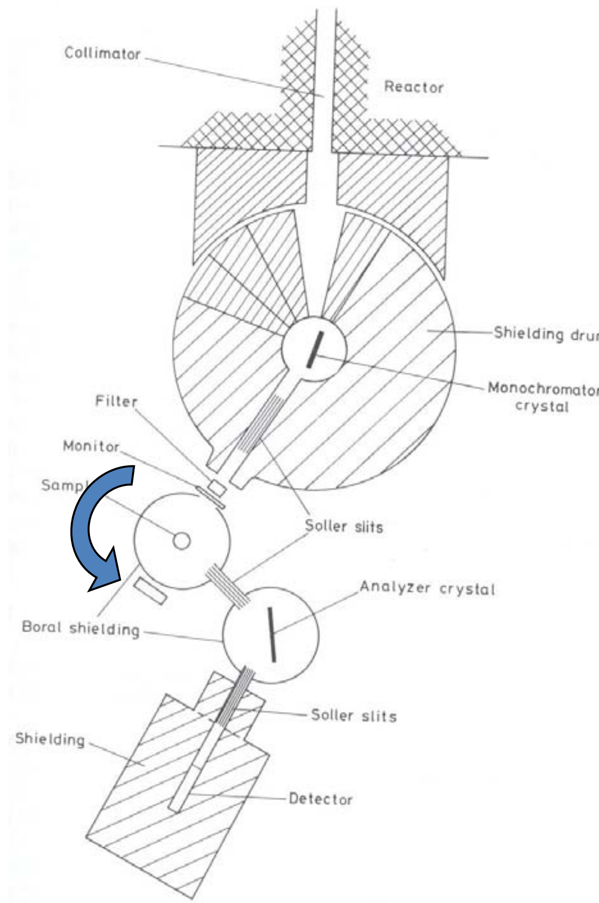




-k1
ko
Q
(i i)

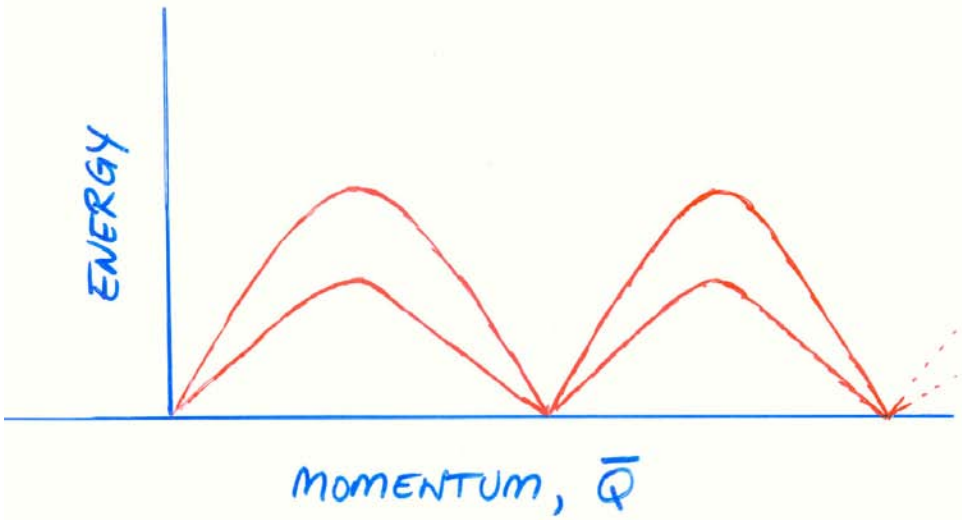


-k1
ko
Q
(i,j)

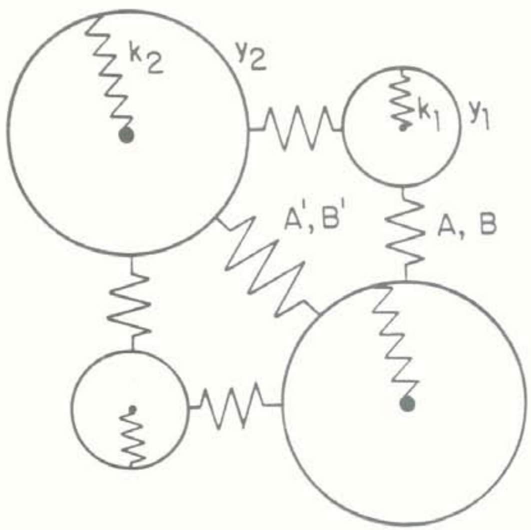


Collimator
Reactor
Shielding drum
Monochromator crystal
Filter
Monitor
Sampl
Soller slits
Analyzer crystal
Boral shielding
Soller slits
Shielding
Detector

Elementary Excitations in Solids

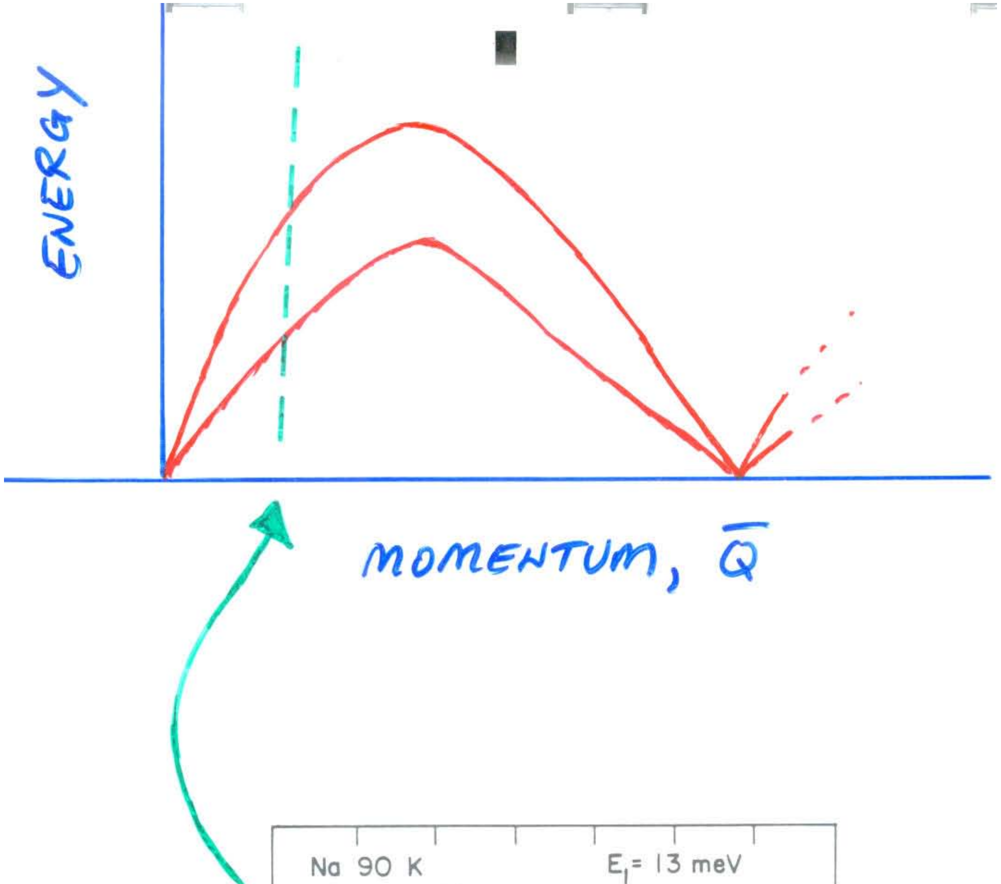


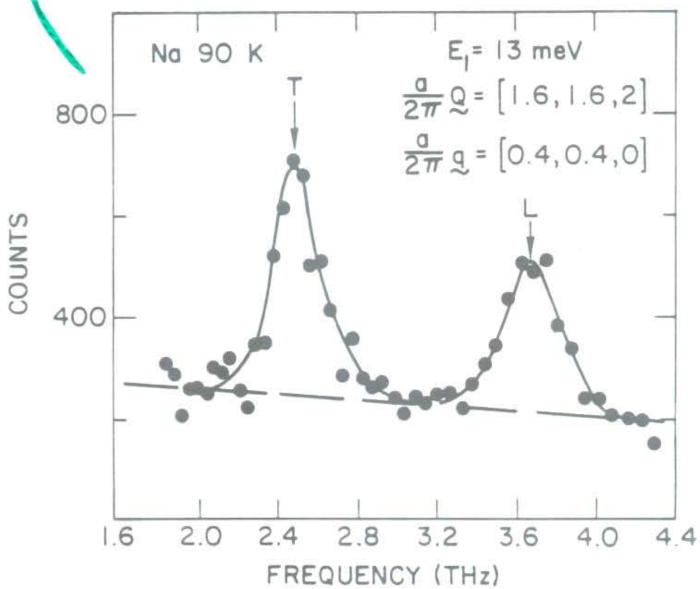
- Lattice Vibrations (Phonons)
- Spin Fluctuations (Magnons)



Energy vs Momentum

- Forces which bind atoms together in solids



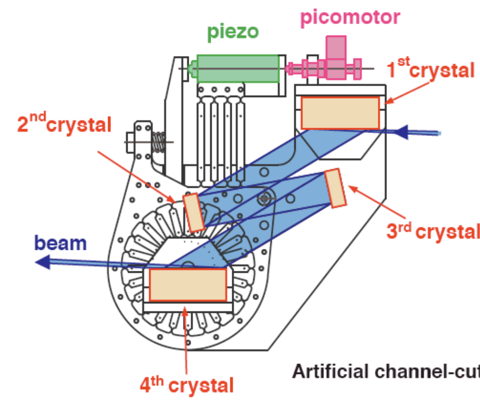


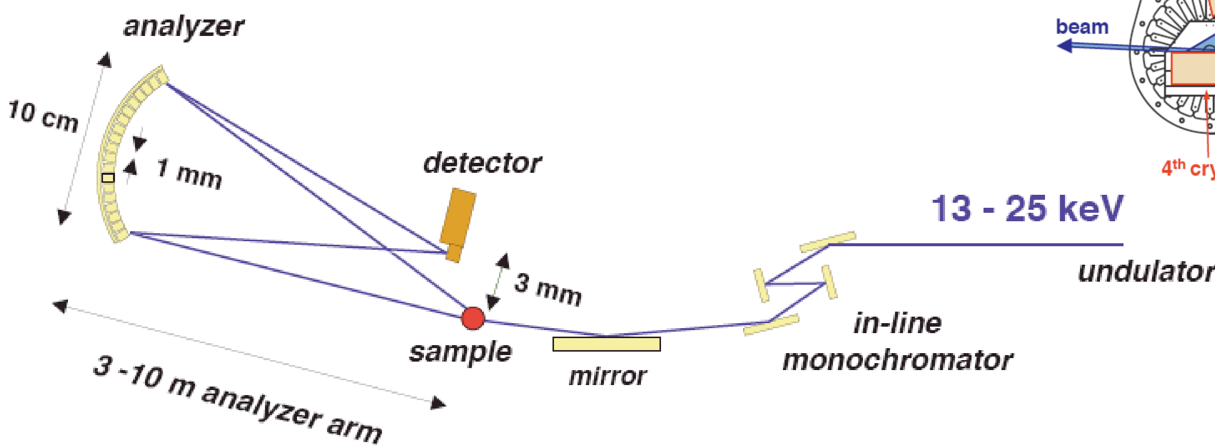
Constant Q, Constant E
3-axis technique allow us to
Put Q-Energy space on a grid,
And scan through as we wish

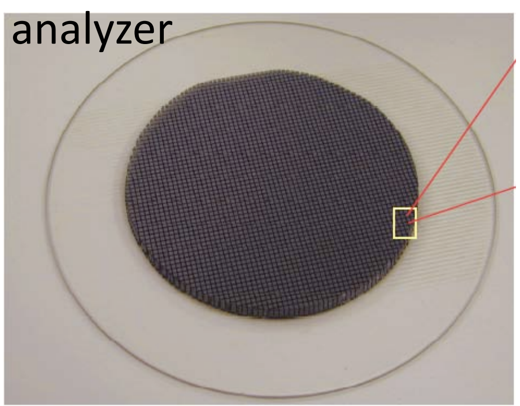
Map out elementary excitations
In Q-energy space (dispersion
Surface)

Inelastic x-ray scattering

- Ei=20 keV, need 1 meV resolution
- $\Delta E/E_i \sim 10^{-7}$!!!







ϕ-scan of monochromator
1 meV $\Rightarrow$ μrad

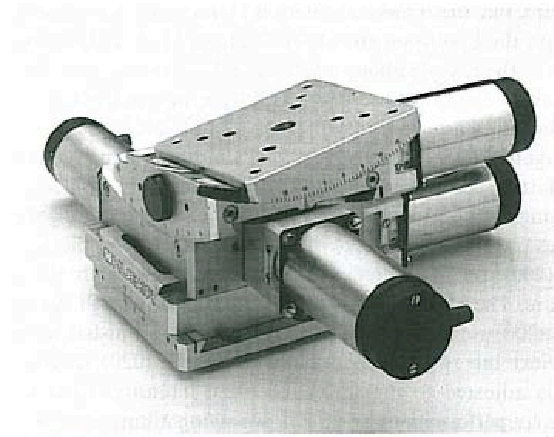
T-scan of monochromator
1 meV $\Rightarrow$ 0.02 K

Sector-3, APS

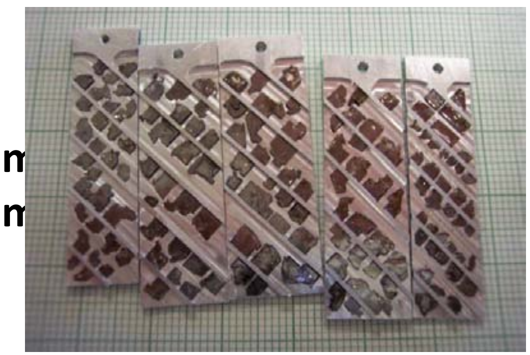
McMaster University

Samples

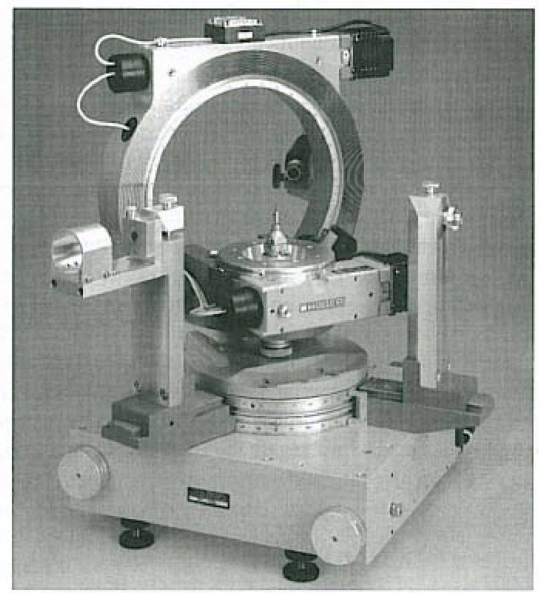
- **Samples need to be BIG**
  - ~ gram or cc
  - Counting times are long (mins/pt)



- **Sam**
- **Sam**

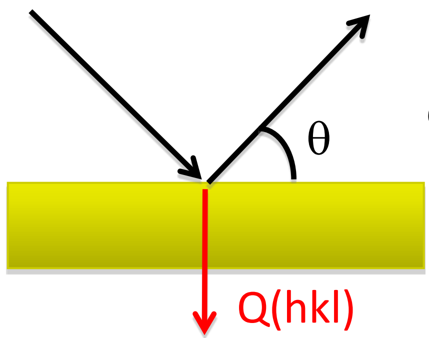


Co-aligned $CaFe_2As_2$ crystals

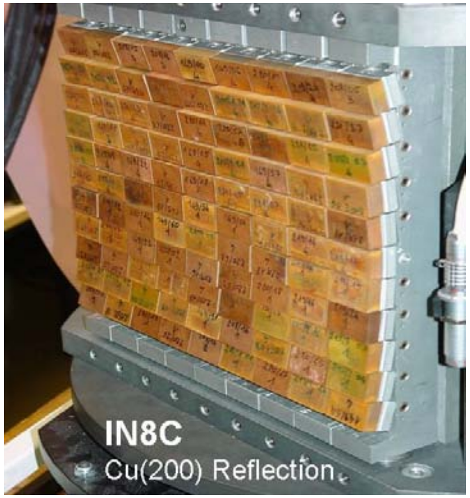


Monochromators

- **Selects the incident wavevector**



$$Q(hkl) = \frac{2\pi}{d(hkl)} = 2k_i \sin\theta$$

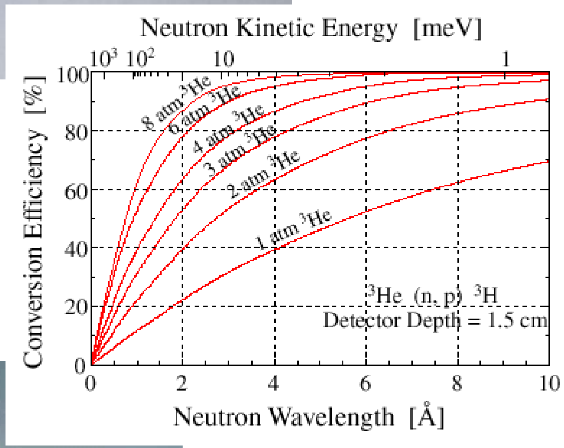


- Reflectivity
- focusing
- high-order contamination
  eg. $\lambda/2$ PG(004)

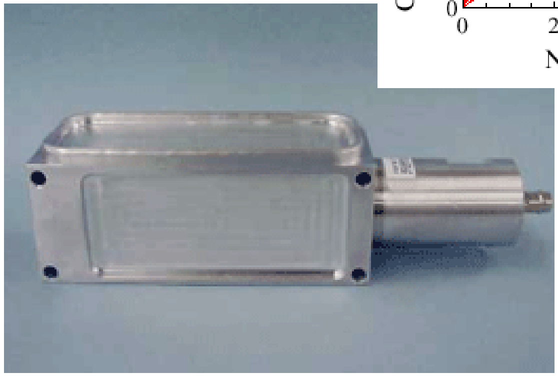
Mono	d(hkl)	uses
PG(002)	3.353	General
Be(002)	1.790	High k_i
Si(111)	3.135	No $\lambda/2$

Detectors

- **Gas Detectors**
- $n + {}^3He \rightarrow {}^3H + p + 0.764$ MeV
- Ionization of gas
- e^- drift to high voltage anode
- High efficiency

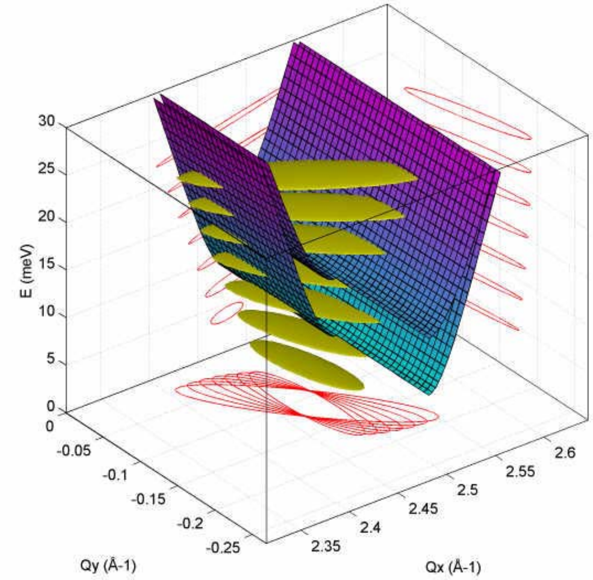


- **Beam monitors**
- Low efficiency detectors for measuring beam flux



Resolution

- **Resolution ellipsoid**
  - Beam divergences
  - Collimations/distances
  - Crystal mosaics/sizes/angles

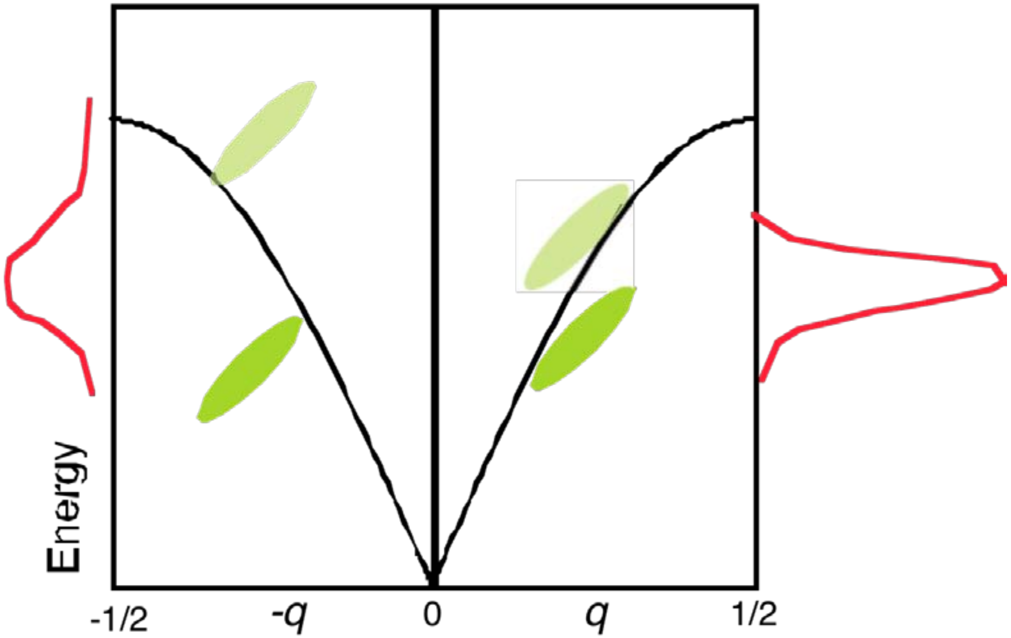


- **Resolution convolutions**

$$I(\mathbf{Q}_0,\omega_0) = \int S(\mathbf{Q}_0,\omega_0)R(\mathbf{Q}-\mathbf{Q}_0,\omega-\omega_0)d\mathbf{Q}d\omega$$

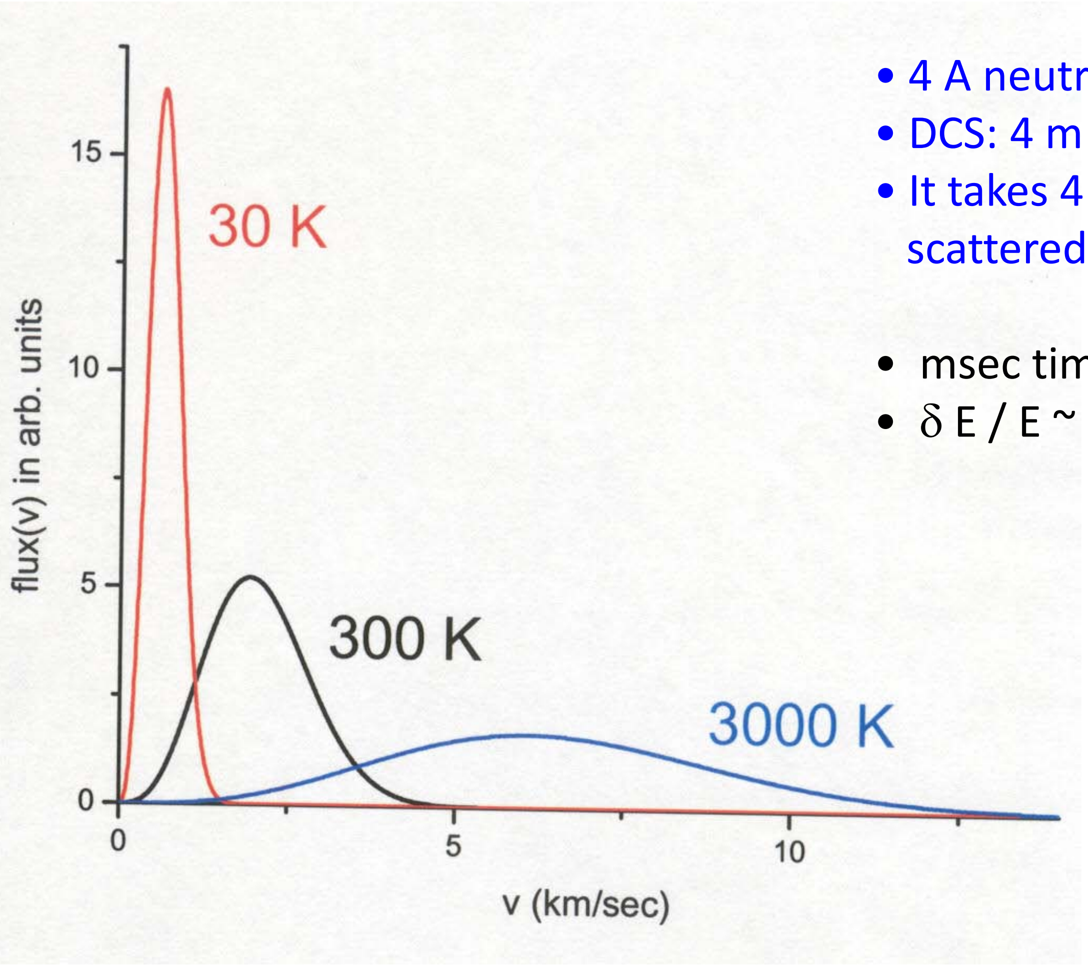
Resolution focusing

- **Optimizing peak intensity**
- **Match slope of resolution to dispersion**



Neutrons have mass
so higher energy means faster – lower energy means slower

v (km/sec) = 3.96 / λ (A)



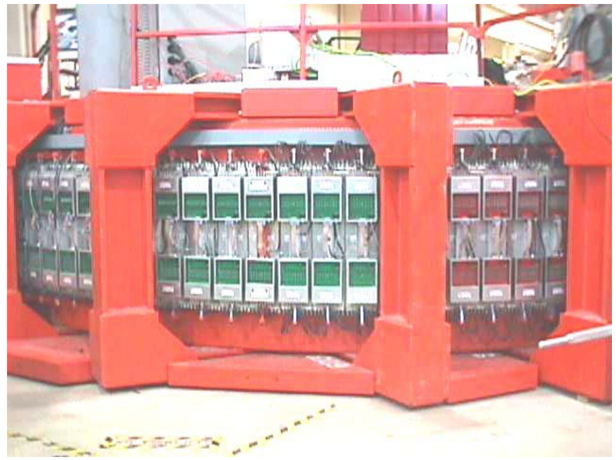
- 4 A neutrons move at ~ 1 km/sec
- DCS: 4 m from sample to detector
- It takes 4 msec for elastically scattered 4 A neutrons to travel 4 m

- msec timing of neutrons is easy
- δ E / E ~ 1-3 % - very good !

We can measure a neutron's energy, wavelength by measuring its *speed*

Time-of-flight methods

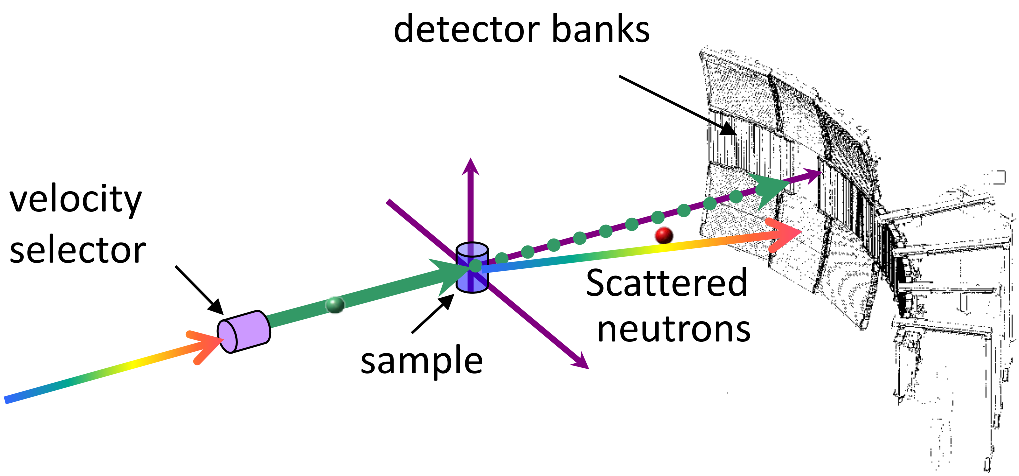
Spallation neutron source

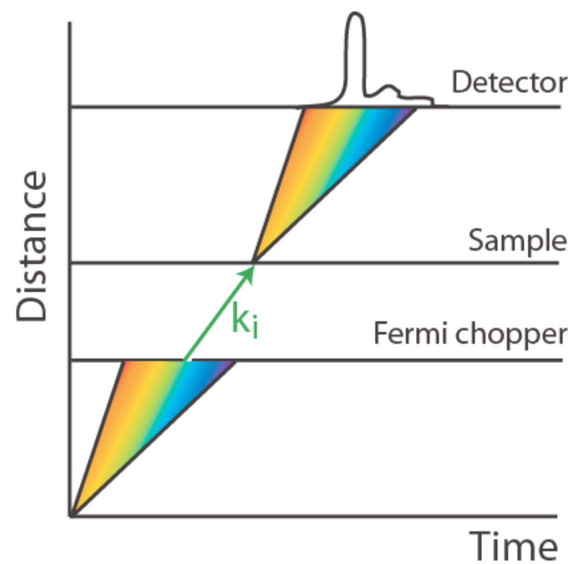


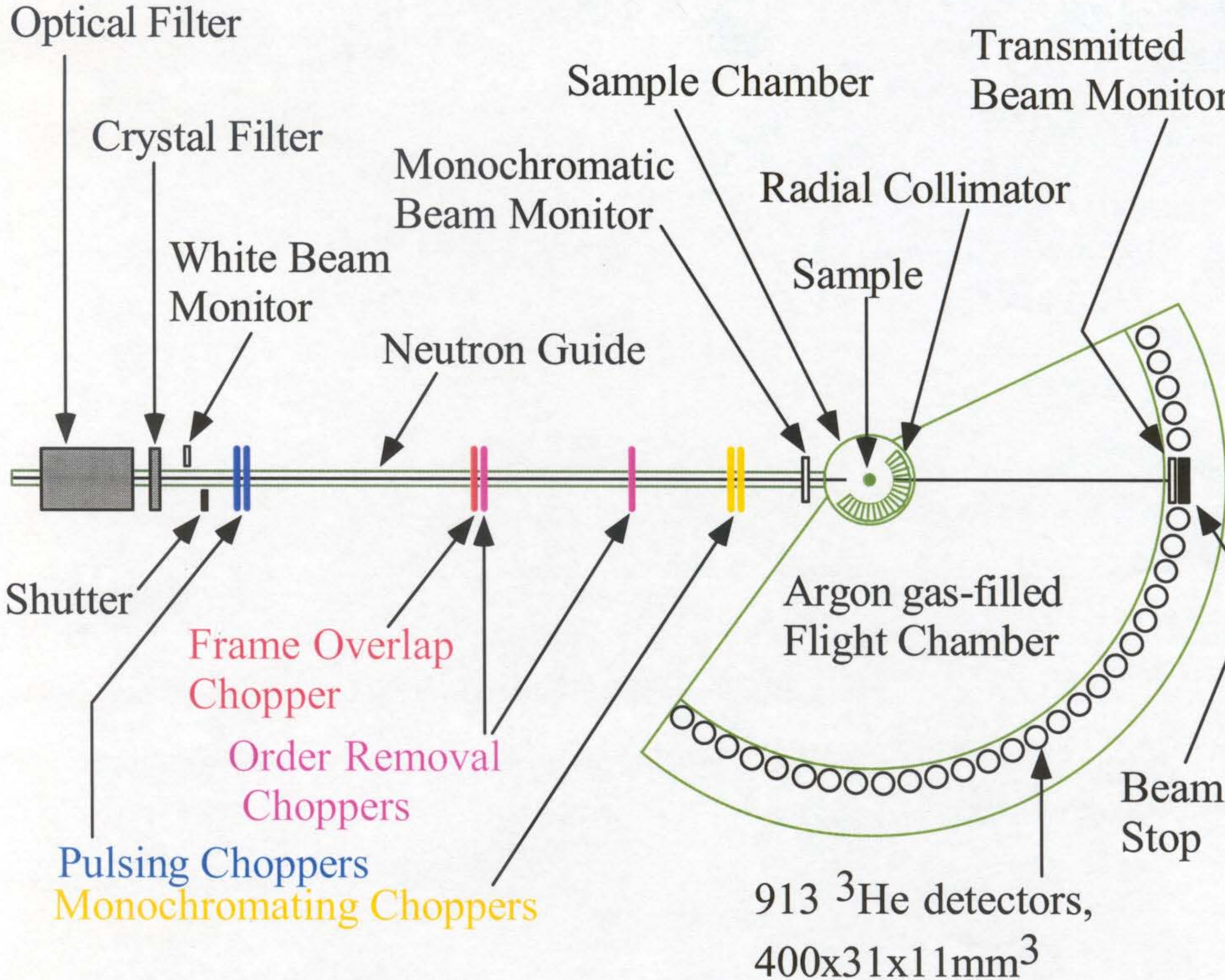
Pharos – Lujan Center

- Effectively utilizes time structure of pulsed neutron groups

$$t = \frac{d}{v} = \left(\frac{m}{h} d \right) \lambda$$

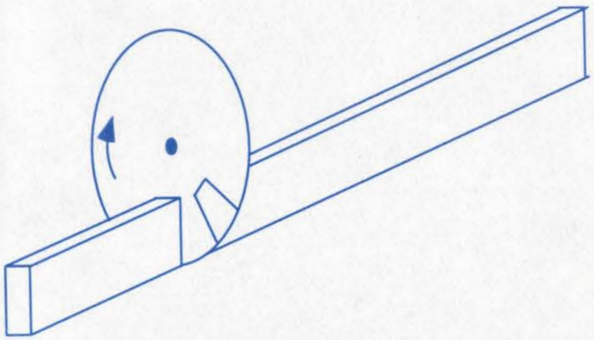


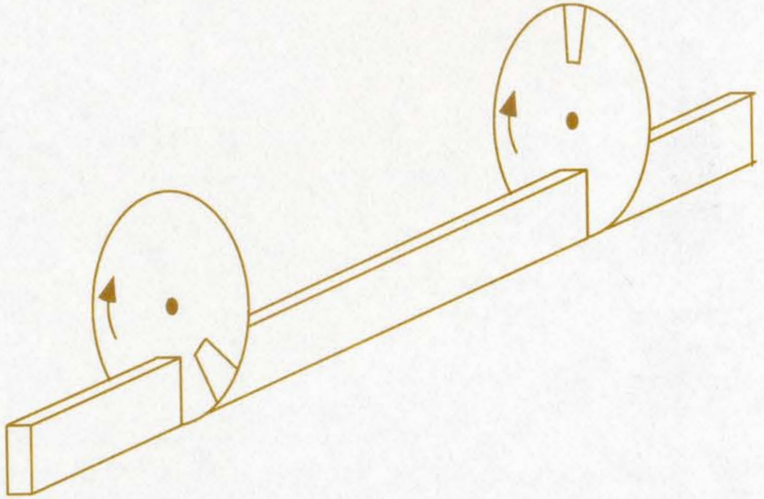



Optical Filter
Crystal Filter
White Beam Monitor
Neutron Guide
Monochromatic Beam Monitor
Sample Chamber
Transmitted Beam Monitor
Radial Collimator
Sample
Shutter
Frame Overlap Chopper
Order Removal Choppers
Pulsing Choppers
Monochromating Choppers
Argon gas-filled Flight Chamber
Beam Stop
913 ³He detectors, 400x31x11mm³

A single (disk) chopper pulses the neutron beam.

A second chopper selects neutrons within a narrow range of speeds.

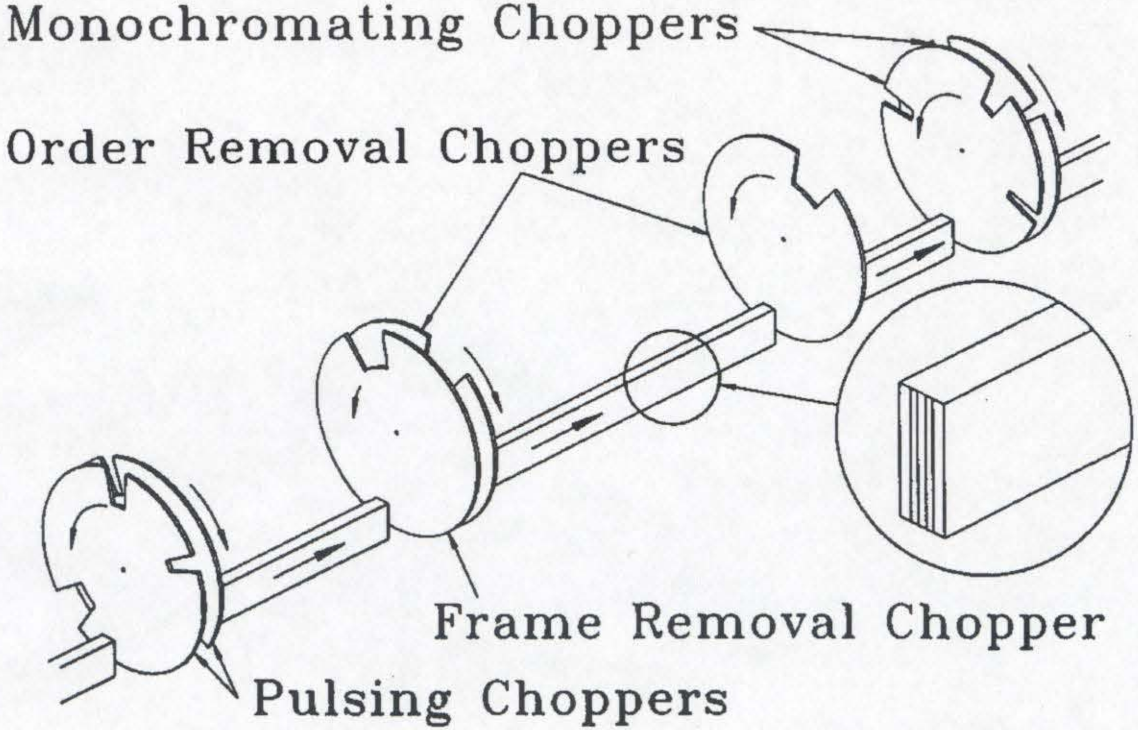




Counter-rotating choppers (close together), with speed ◆, behave like single choppers with speed 2◆. They can also permit a choice of pulse widths.

Additional choppers remove "contaminant" wavelengths and reduce the pulse frequency at the sample position.

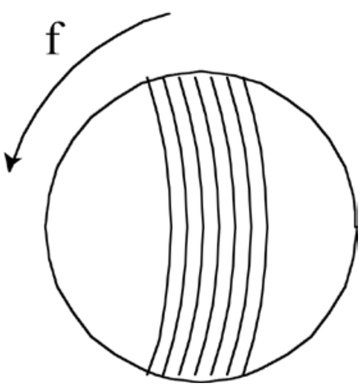
The DCS has seven choppers, 4 of which have 3 "slots"



Disk 4B

Fermi Choppers

- Body radius ~ 5 cm
- Curved absorbing slats
  - B or Gd coated
  - ~mm slit size
- f = 600 Hz (max)
- Acts like shutter, Δt ~ μs



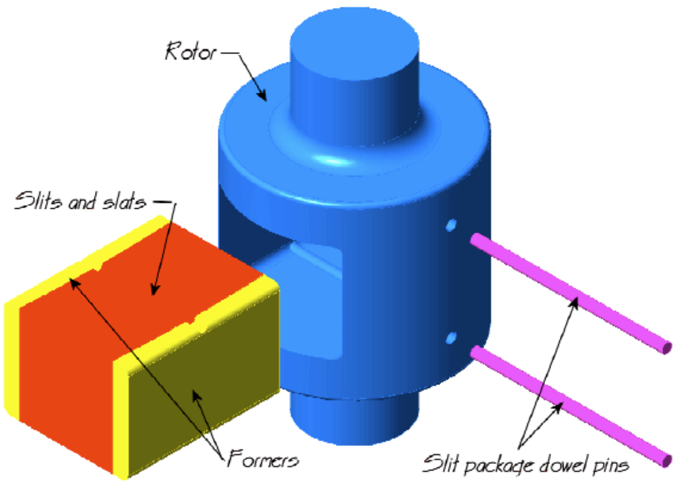
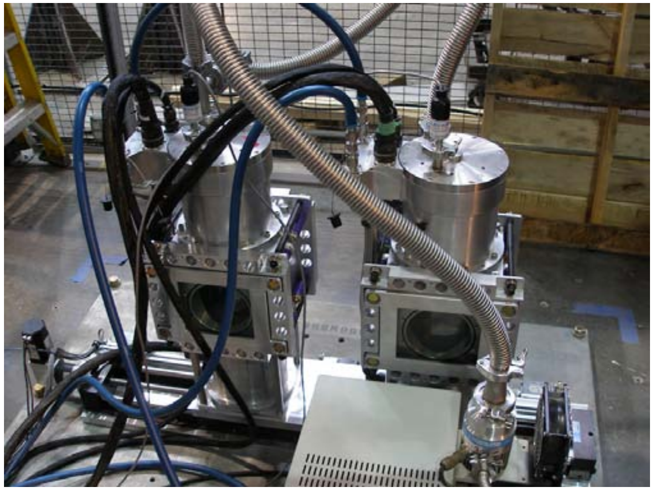
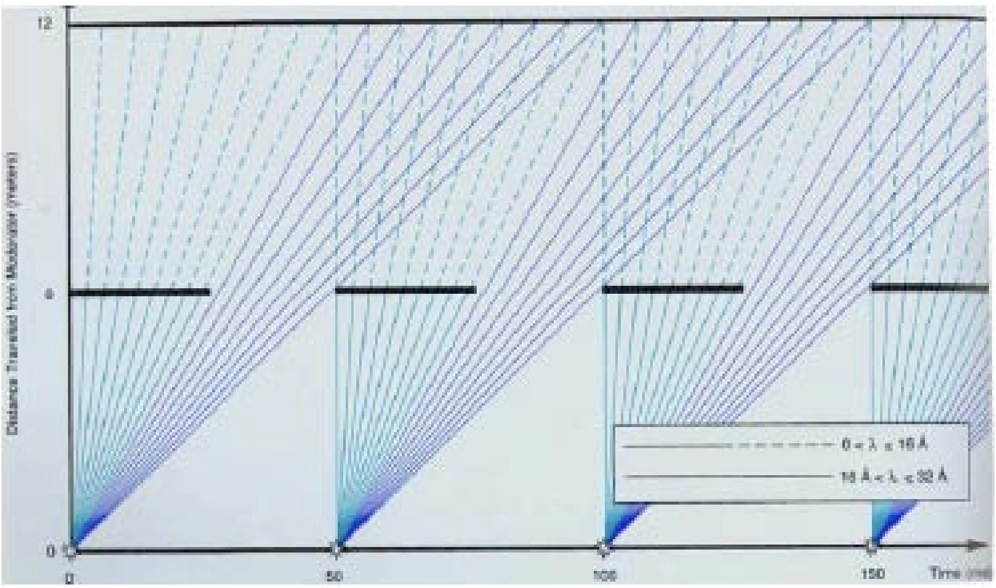


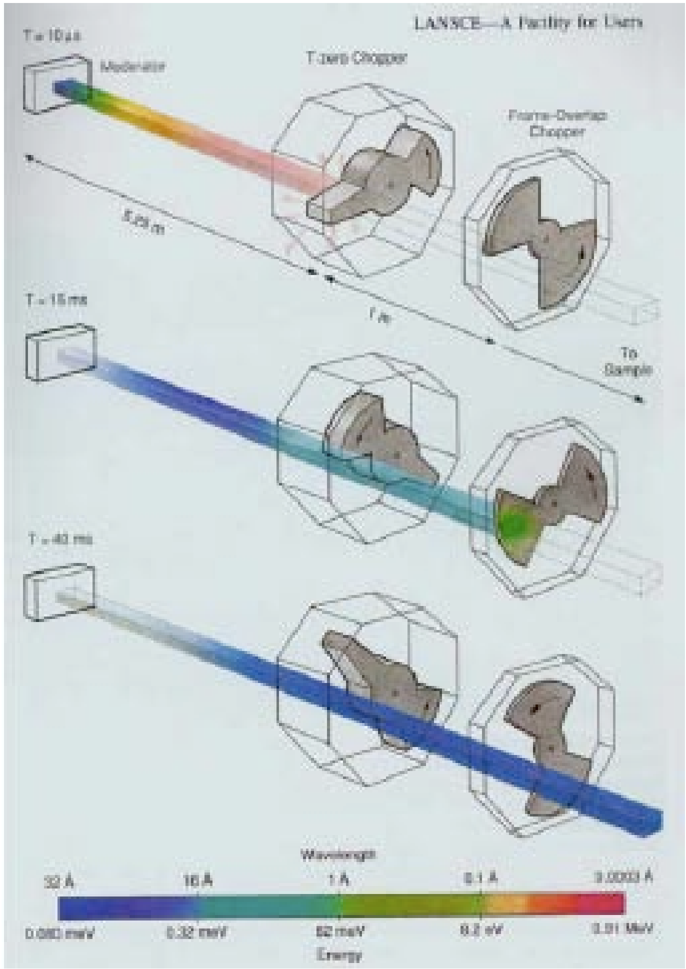
Figure 1. ISIS MAPS chopper and slit package assembly – exploded view



T-zero chopper

- **Background suppression**
- **Blocks fast neutron flash**

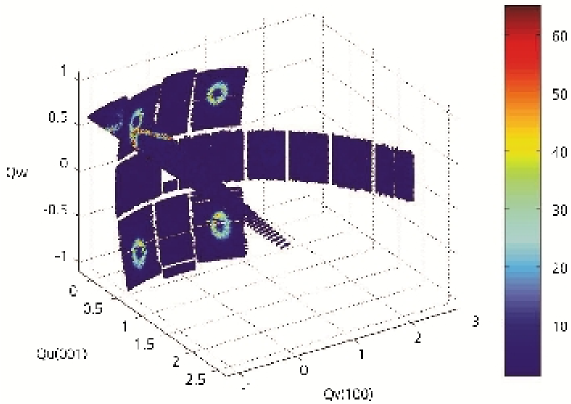




Position sensitive detectors

- ^{3}He tubes (usu. 1 meter)
- Charge division
- Position resolution ~ cm
- Time resolution ~ 10 ns

MAPS detector bank

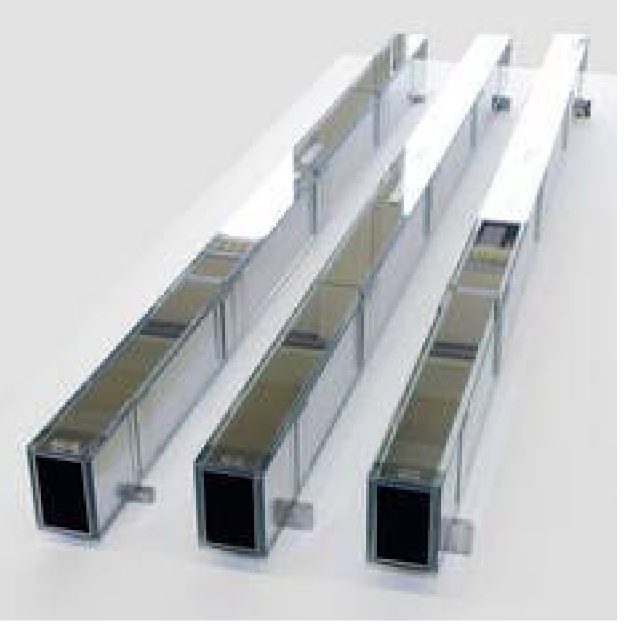


Sample environment

- **Temperature, field, pressure**
- **Heavy duty for large sample environment**
  - CCR
  - He cryostats
  - SC magnets
  - …

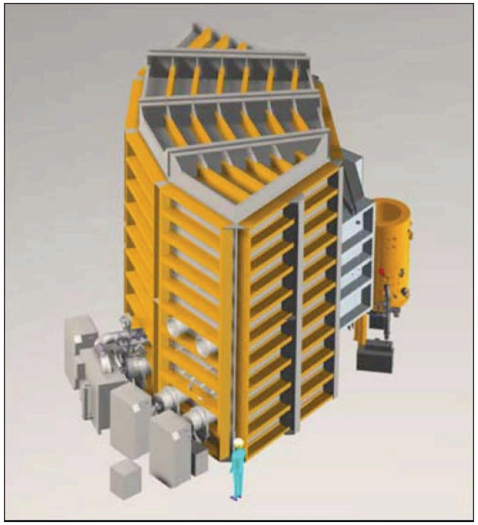
Guides

- **Transport beam over long distances**
- **Background reduction**
- **Total external reflection**
  - Ni coated glass
  - Ni/Ti multilayers (supermirror)



Size matters

- **Length = resolution**
  - Instruments ~ 20 – 40 m long
  - E-resolution ~ 2-4% E_i
- **More detectors**
  - SEQUOIA – 1600 tubes, 144000 pixels
  - Solid angle coverage 1.6 steradians
- **Huge data sets**
- 0.1 – 1 GB

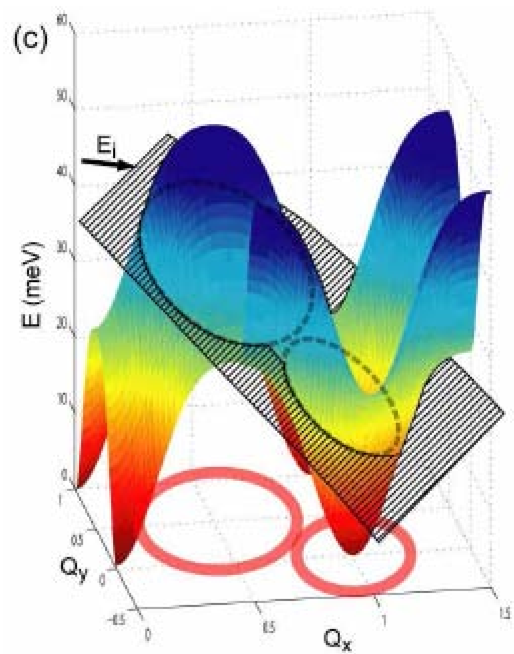


SEQUOIA detector vacuum vessel

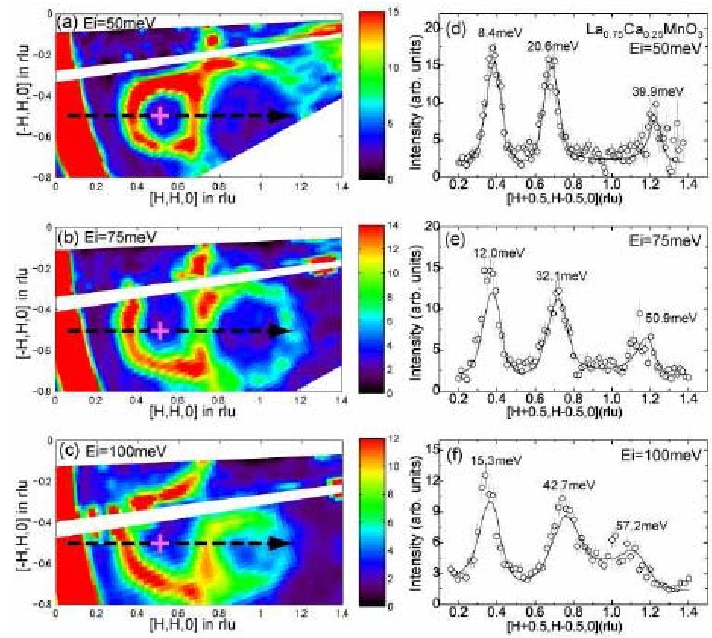
Data visualization

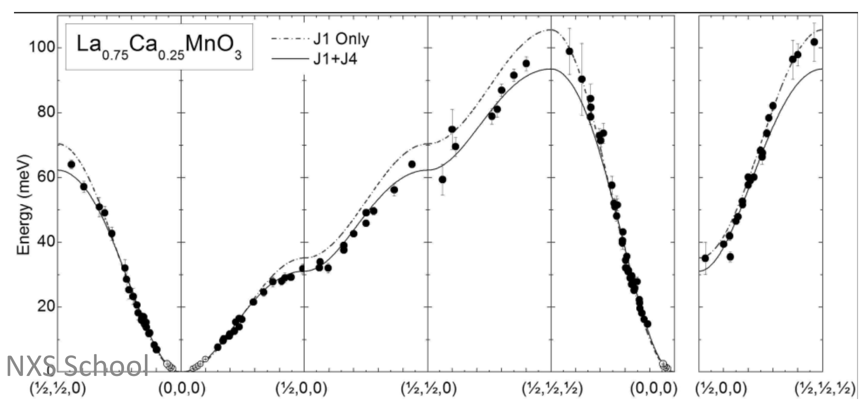
- Large, complex data from spallation sources
- Measure $S(\mathbf{Q},\omega)$ – 4D function

$La_{1-x}Ca_xMnO_3$

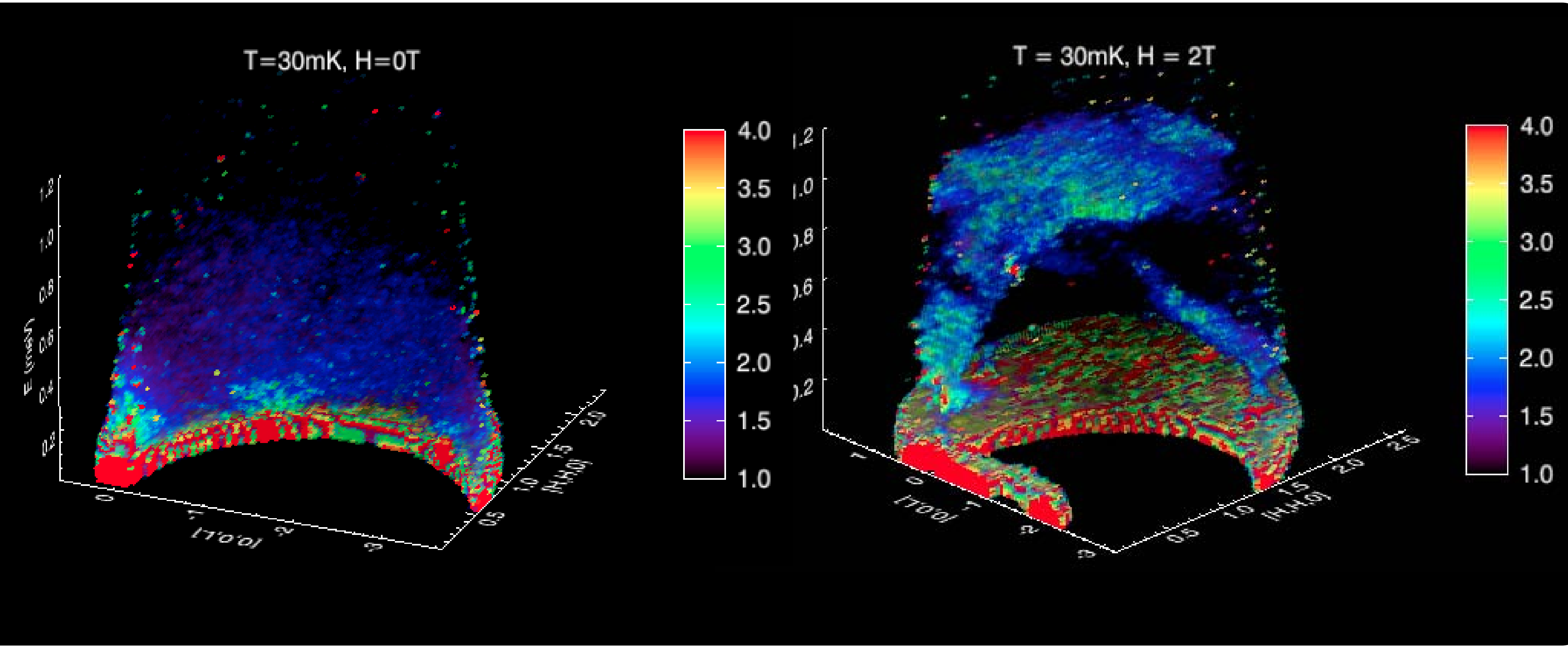


Ye *et al., Phys. Rev. B*, **75** 144408 (2007).





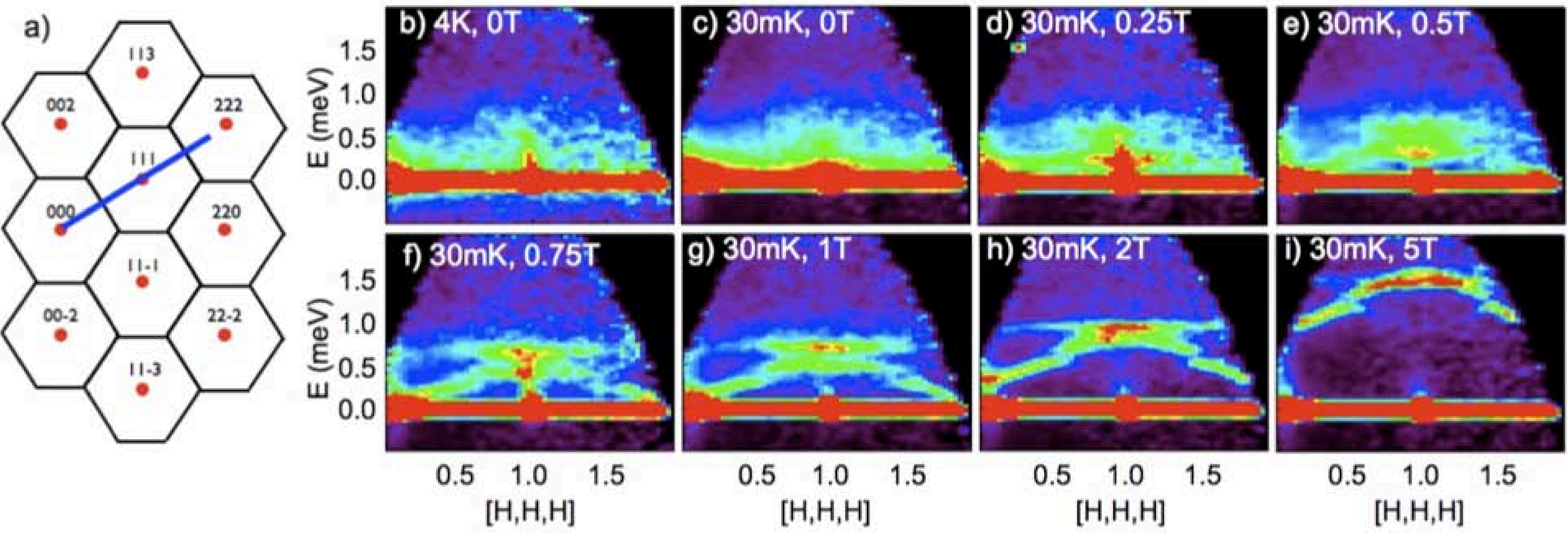
Development of Long Range Order



The appearance of spin waves indicates that the field-induced state is long range ordered

Weak magnetic field // [110] induces LRO:

appearance of long-lived spin waves at low T and moderate H



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General neutron scattering

G. Squires, “Intro to theory of thermal neutron scattering”, Dover, 1978.
S. Lovesey, “Theory of neutron scattering from condensed matter”, Oxford, 1984.
R. Pynn, http://www.mrl.ucsb.edu/~pynn/.

Polarized neutron scattering

Moon, Koehler, Riste, Phys. Rev **181**, 920 (1969).

Triple-axis techniques

Shirane, Shapiro, Tranquada, “Neutron scattering with a triple-axis spectrometer”, Cambridge, 2002.

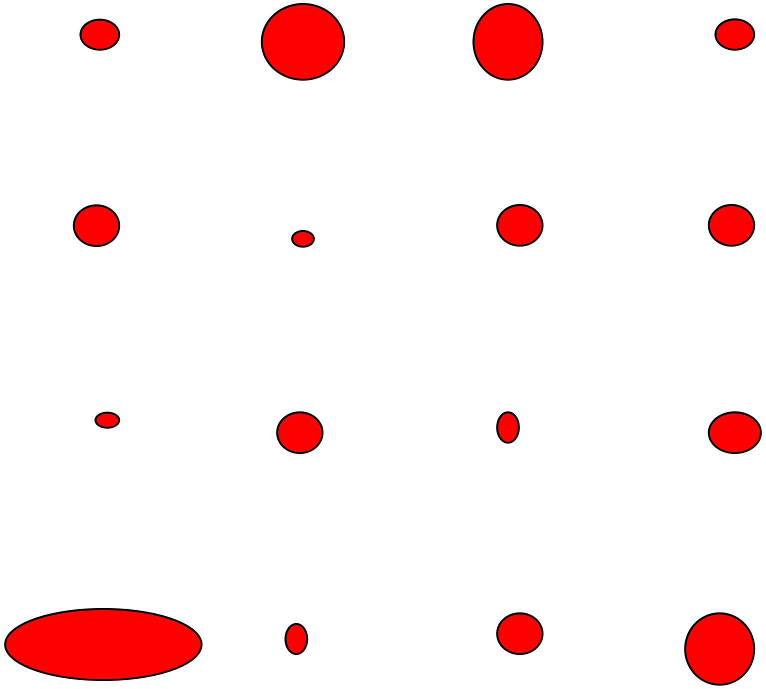
Time-of-flight techniques

B. Fultz, http://www.cacr.caltech.edu/projects/danse/ARCS_Book_16x.pdf

Why map reciprocal space?

Crystallography!

Variation of Bragg peak intensities = where the atoms are



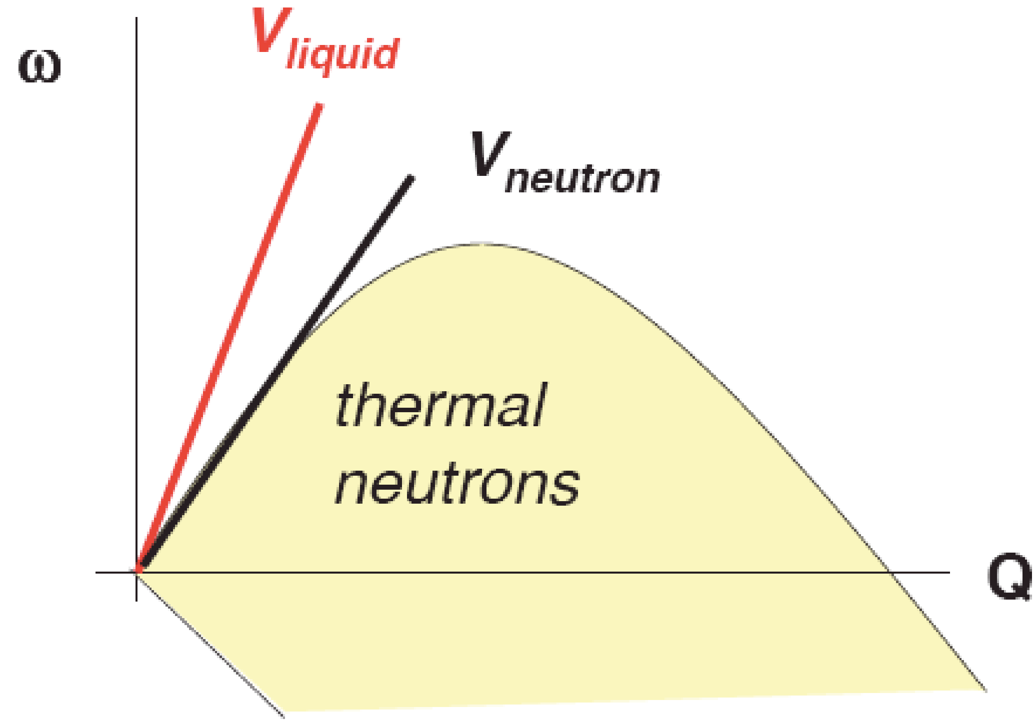
Peakshape gives spatial correlations (if resolution effects can be negated)

Kinematics

- Essentially elastic scattering
- No kinematic limits

$$Q \approx 2k_i \sin\theta$$

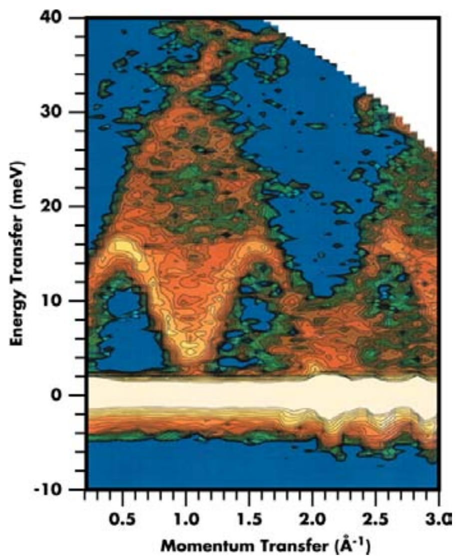
$$\hbar\omega = \hbar c(k_i - k_f)$$

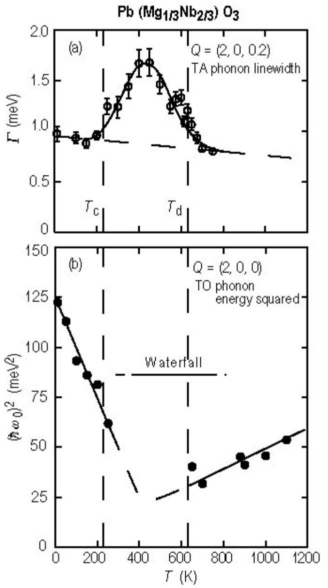


TOF vs. 3-axis

- epithermal (up to 2 eV)
- Total spectra (esp. powder samples)
- Absolute normalization
- Low-dimensional systems
- Hardware inflexible
- Software intensive

- High flux of thermal neutrons
- Focused studies in Q,ω (soft modes, gaps, etc.)
- Three-dimensional systems
- Hardware intensive
- Software inflexible

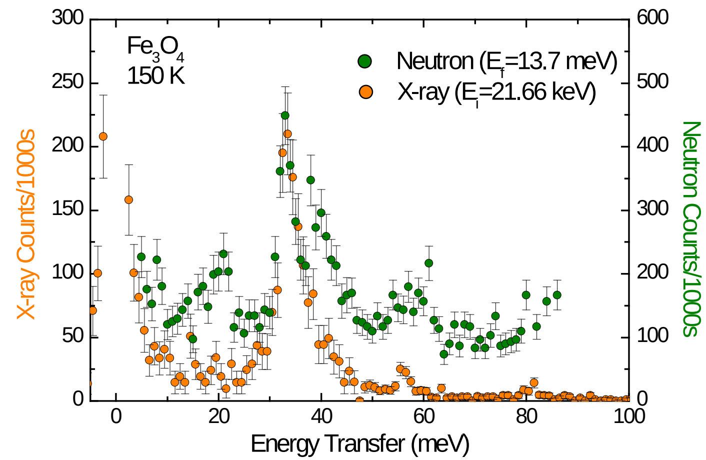


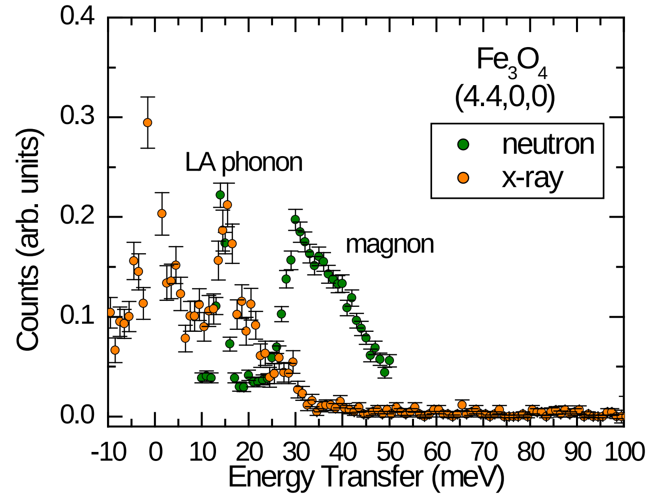


IXS vs. INS

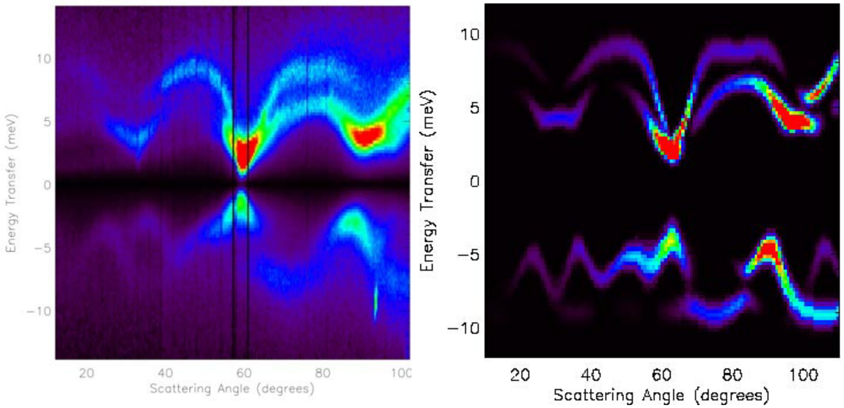
- SAMPLE SIZE

-
  - Simple scattering geometry ($k_i \approx k_f$)
  - Resolution function simpler (most angles fixed, E-scans only)
  - No spurions (high-order refs. keV, no incoherent scat.)
  - *Can only do lattice excitations*

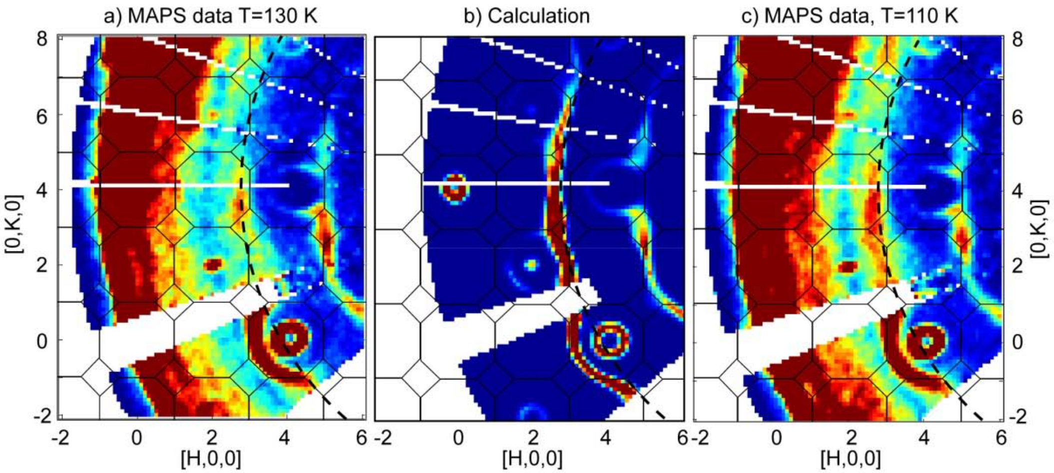




Computation

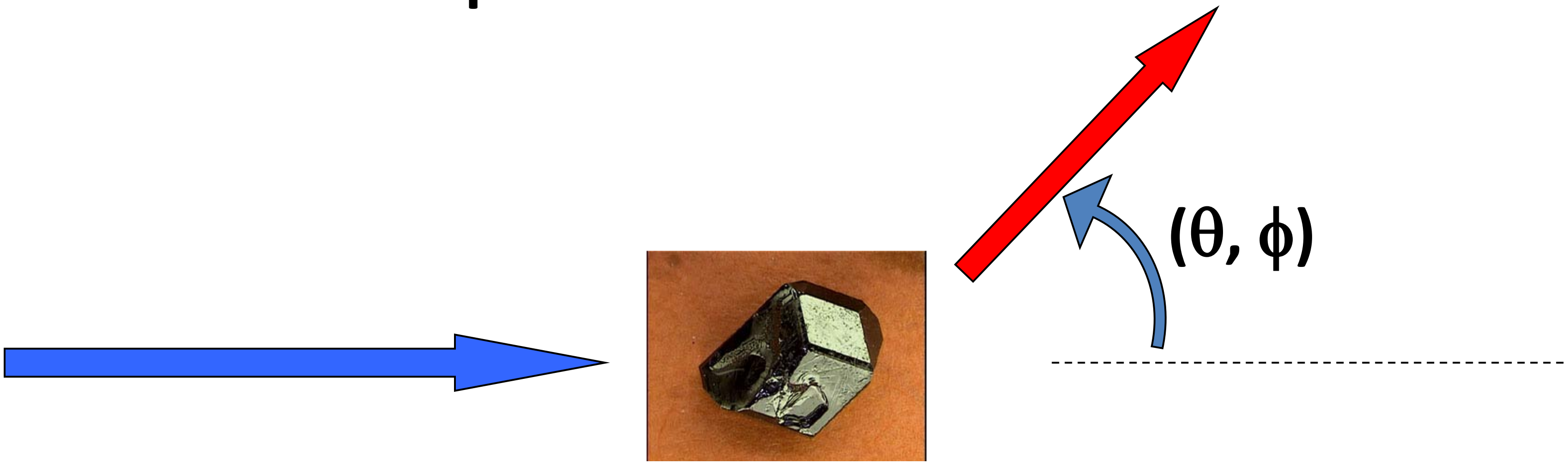


Pb phonons



Fe_3O_4 spin waves

The Basic Experiment:



Incident Beam:

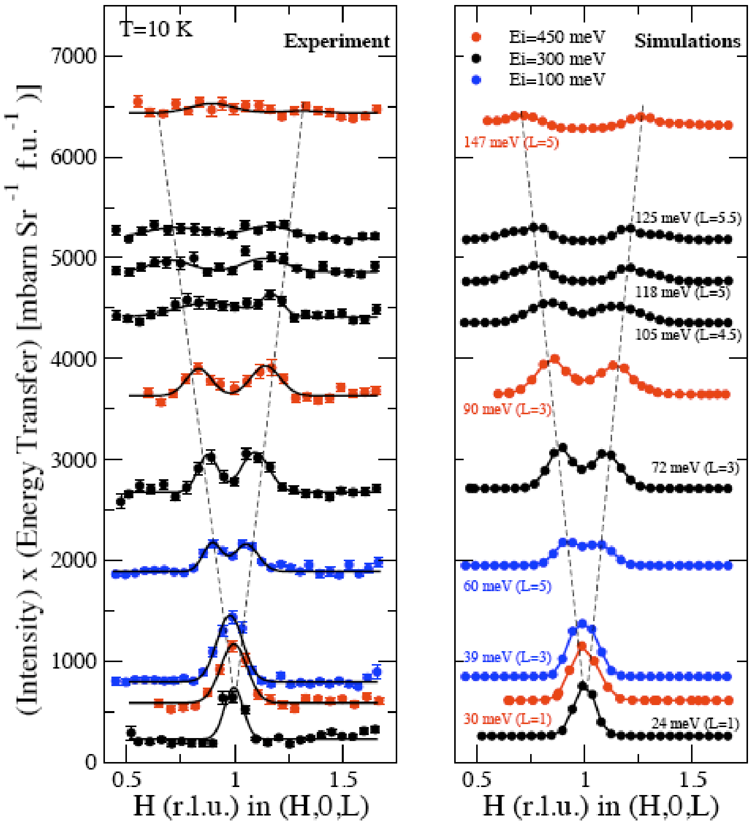
- monochromatic
- “white”
- “pink”

Scattered Beam:

- Resolve its energy
- Don’t resolve its energy
- Filter its energy

Absolute normalization

- **Absolute normalization**
  - Using incoherent scattering from vanadium
  - $\sigma/4\pi$ = 404 mbarns/Sr



Fermi's Golden Rule within the 1st Born Approximation

$$W = 2\pi / h \quad |\langle f \mid V \mid i \rangle|^2 \;\; \rho\,(E_f)$$

$$\delta\sigma = W / \Phi \;=\; (m/2\pi h^2)^2 \;\; k_f / k_i \quad |\langle f \mid V \mid i \rangle|^2 \;\; \delta\Omega$$

$$\delta^2\sigma / \delta\Omega\, \delta E_f = \; k_f/k_i \;\; \sigma_{coh}/4\pi \;\; N \;\; S_{coh}(\mathbf{Q}, \omega)$$

$$+\, k_f/k_i \; \sigma_{incoh}/4\pi \;\; N \;\; S_{incoh}(\mathbf{Q}, \omega)$$

Spin correlation functions

$$\frac{d^2\sigma}{d\Omega dE_f} = \underbrace{\frac{k_f}{k_i}\left[\frac{1}{2}\gamma r_0 g F(Q)\right]^2}_{\text{Scattering cross-section}} \underbrace{\sum_{\alpha\beta}\left(\delta_{\alpha\beta} - \hat{Q}_\alpha \hat{Q}_\beta\right)}_{\text{Dipole interaction}} \sum_{jj'} e^{i\mathbf{Q}\cdot(\mathbf{R}_{j'} - \mathbf{R}_j)} \frac{1}{2\pi\hbar}\int dt e^{-i\omega t} \underbrace{\left\langle S_j^\alpha(0) S_{j'}^\beta(t)\right\rangle}_{\text{Spin-spin correlation function}}$$

$$\left.\frac{d^2\sigma}{d\Omega dE_f}\right|_{inel} = \frac{k_f}{k_i}\left[\frac{1}{2}\gamma r_0 g F(Q)\right]^2 \sum_{\alpha\beta}\left(\delta_{\alpha\beta} - \hat{Q}_\alpha \hat{Q}_\beta\right)\left(1 - e^{\hbar\omega/kT}\right)^{-1} \frac{1}{\pi (g\mu_B)^2} \operatorname{Im}\left\{\chi^{\alpha\beta}(\mathbf{Q},\omega)\right\}$$

The cross-section is proportional to the magnetic susceptibility,
i.e. it is the response of the system to spatially & time varying magnetic field

Paramagnetic scattering

Single ion scattering

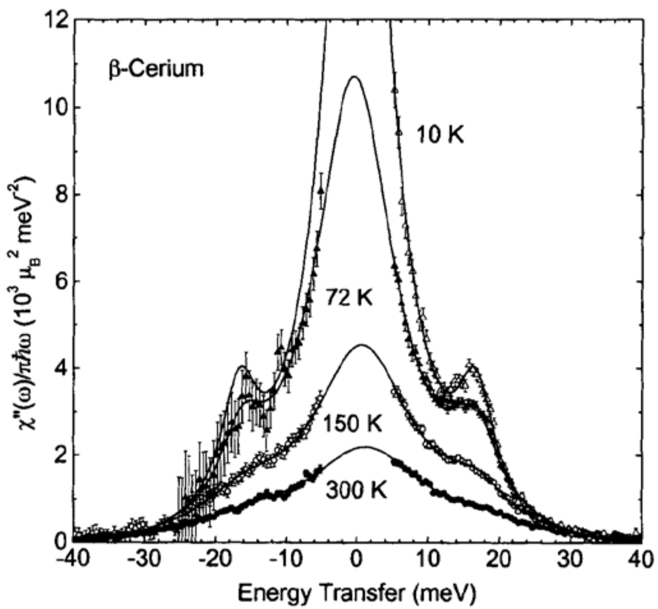
$$\left\langle S_j^{\alpha} S_{j'}^{\beta} \right\rangle = 0 \;(j \neq j')$$

$$\left\langle S_j^z(0) S_j^z(t) \right\rangle = \left\langle \left(S_j^z\right)^2 \right\rangle e^{-\Gamma t} = \frac{1}{3}\left\langle \left(\mathbf{S}_j\right)^2 \right\rangle e^{-\Gamma t} = \frac{1}{3} S(S+1) e^{-\Gamma t}$$

$$\frac{\mathrm{Im}\{\chi^{zz}(0,\omega)\}}{\pi \hbar\omega} = \frac{g^2 S(S+1)\mu_B^2}{3k_B T}\frac{1}{\pi}\frac{\Gamma}{\Gamma^2 + (\hbar\omega)^2}$$

- Inverse width, $1/\Gamma$, gives relaxation time
- Note crystal field excitation

$$\chi_0 = \int_{-\infty}^{\infty} \frac{\mathrm{Im}\{\chi^{zz}(0,\omega)\}}{\pi \hbar\omega} d\omega = \frac{g^2 S(S+1)\mu_B^2}{3k_B T}$$



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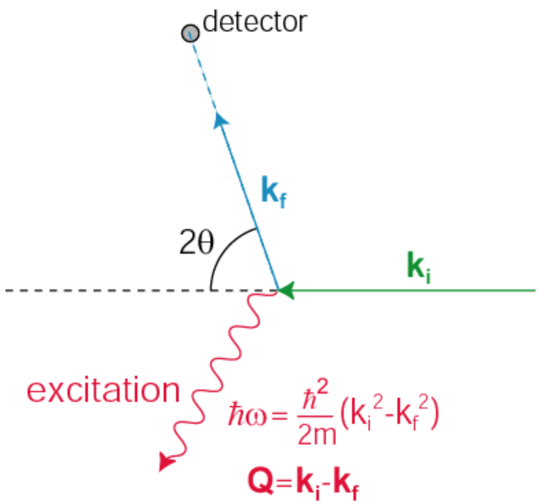
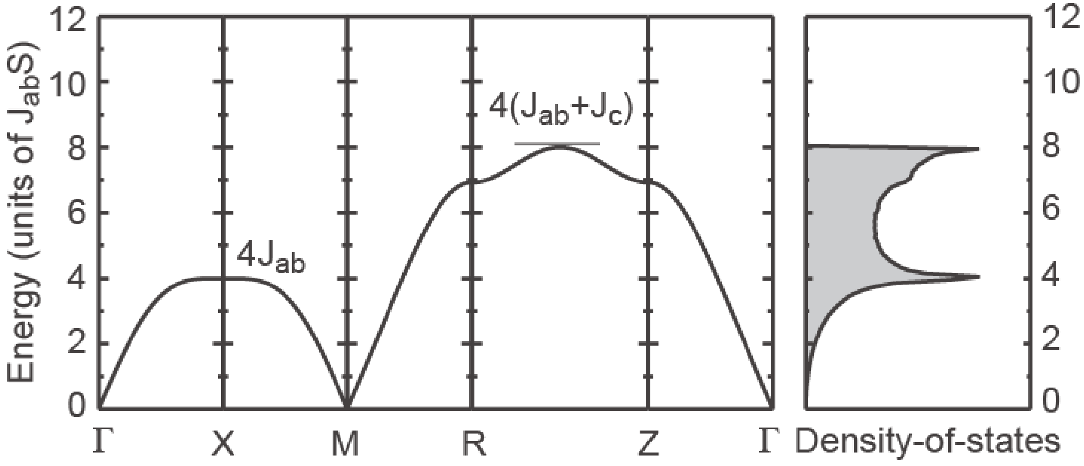
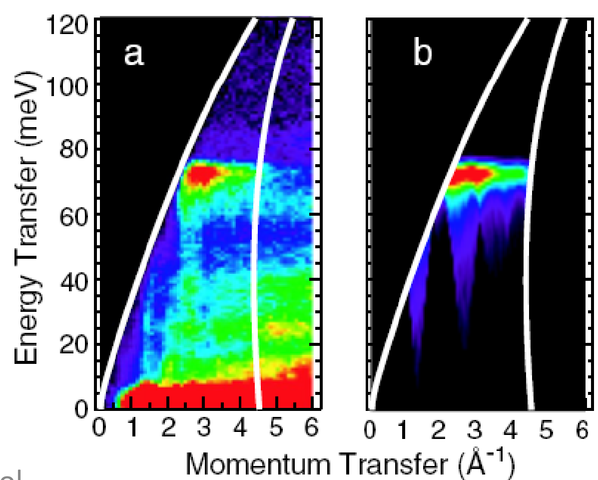
Scattering experiments



Single-crystal



Powder $S(|\mathbf{Q}|,\omega)$

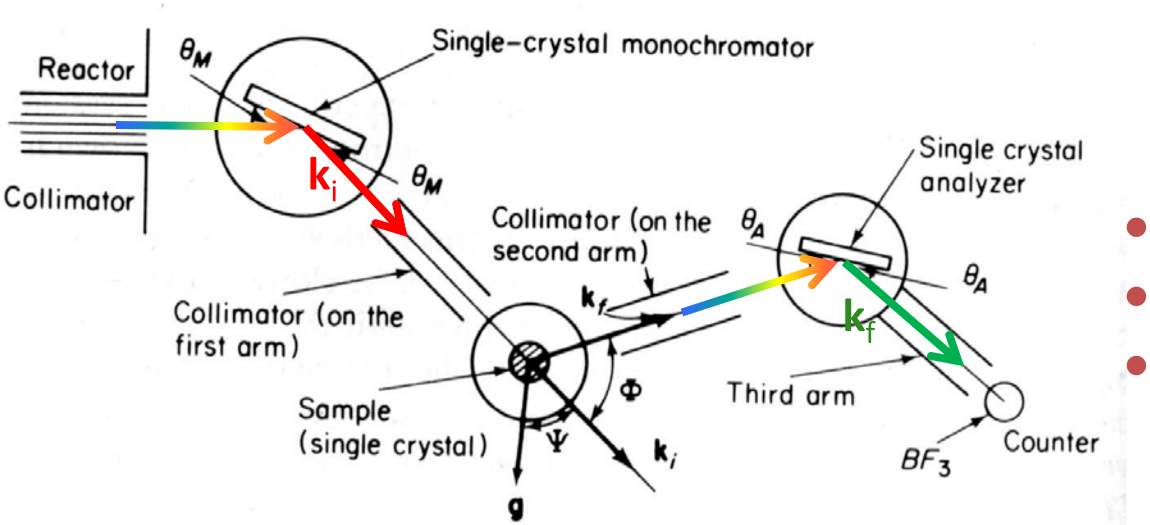


Instrument and sample (powder or single-crystal) determine how ($\mathbf{Q}$,ω) space is sampled

Triple-axis instruments

High flux isotope reactor - ORNL

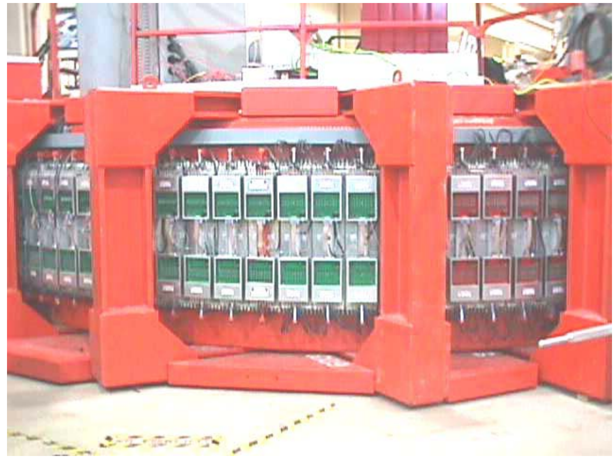
HB-1A 3-axis spectrometer



- Hardware flexibility
- Constant-**Q** (or E) scans
- Ideally suited for single-xtals

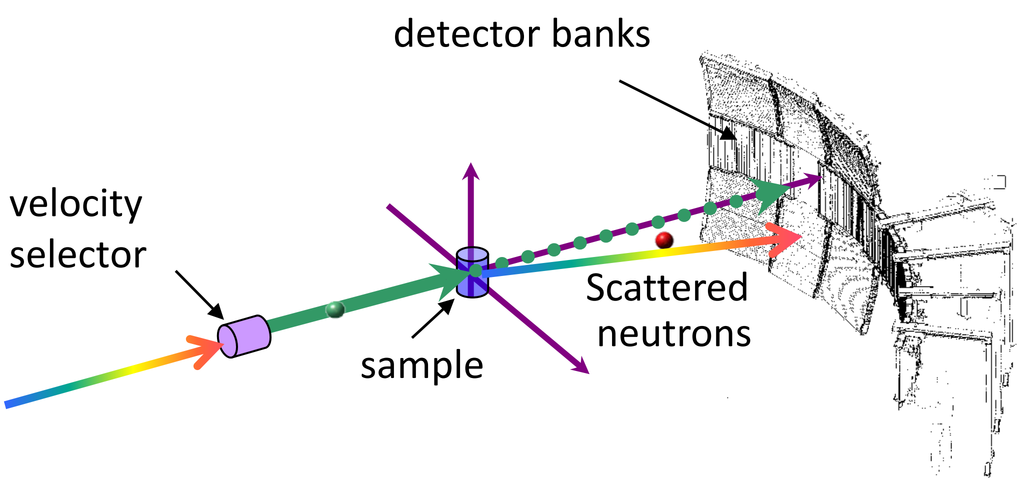
Time-of-flight methods

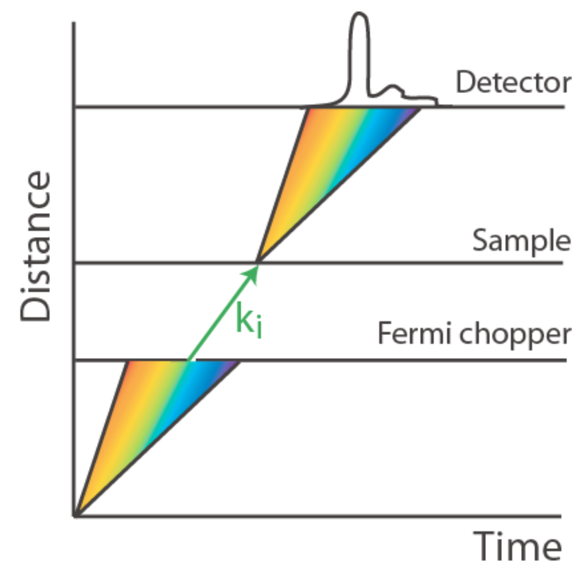
Spallation neutron source



Pharos – Lujan Center

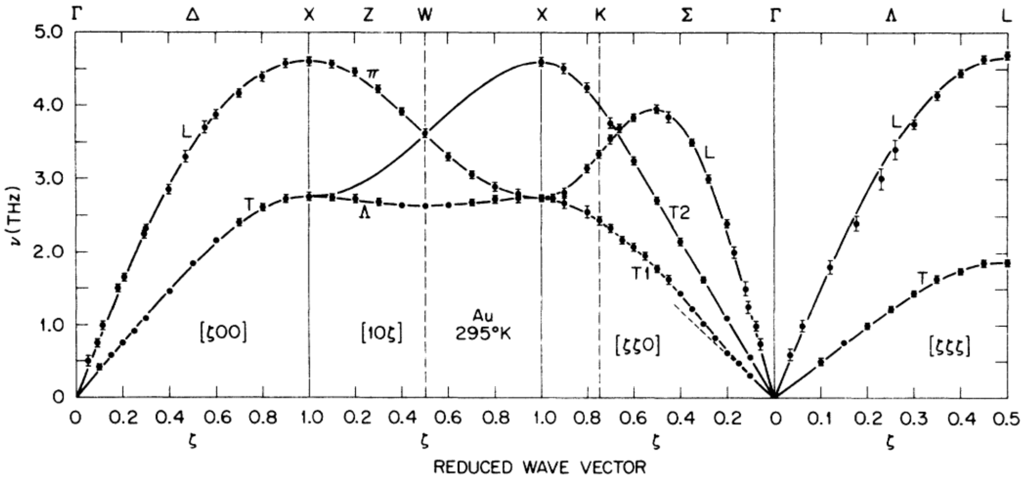
- Hardware inflexible
- Effective for powders
- Complicated **Q**,E-scans a challenge for single-xtals





INS data

- Intensities as a function of **Q** and ω



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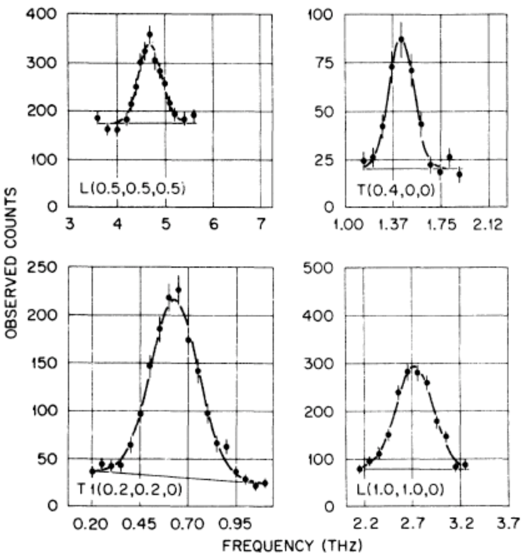
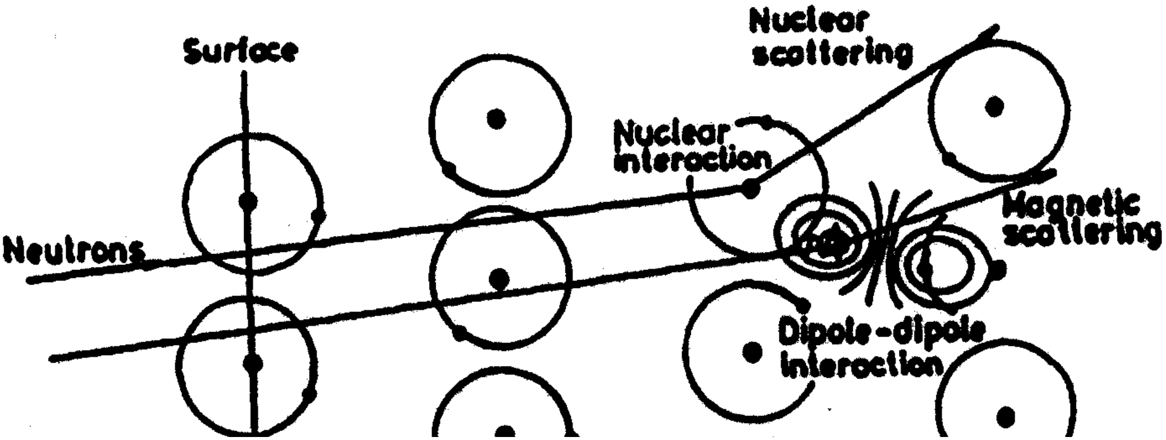
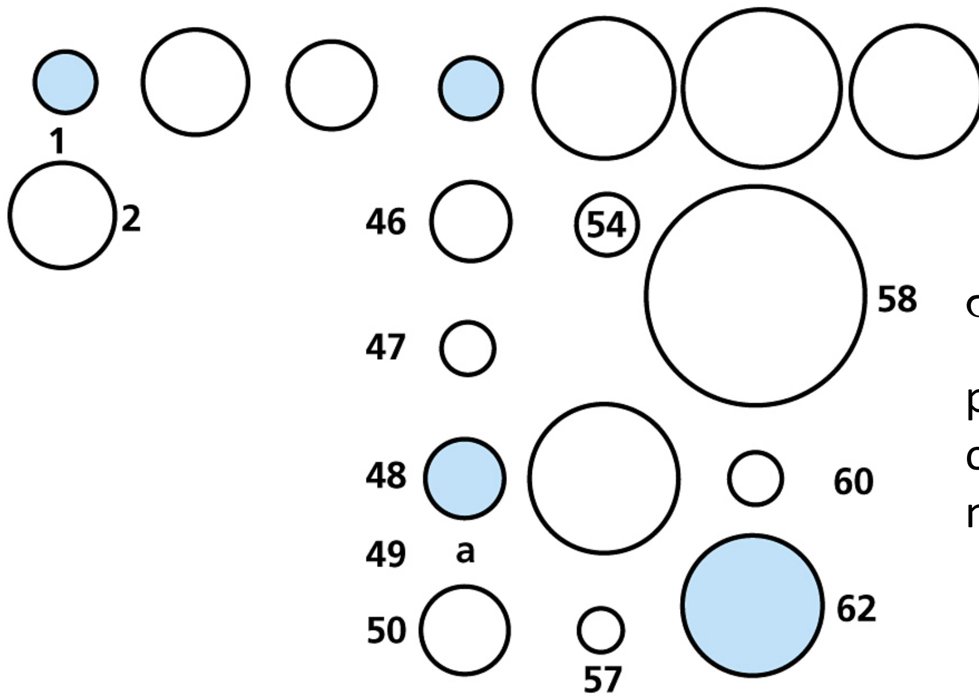




Neutrons

S_{coh} ($\mathbf{Q}$,ω) and S_{incoh}($\mathbf{Q}$,ω) describe the structure and dynamics of the atoms and magnetic moments

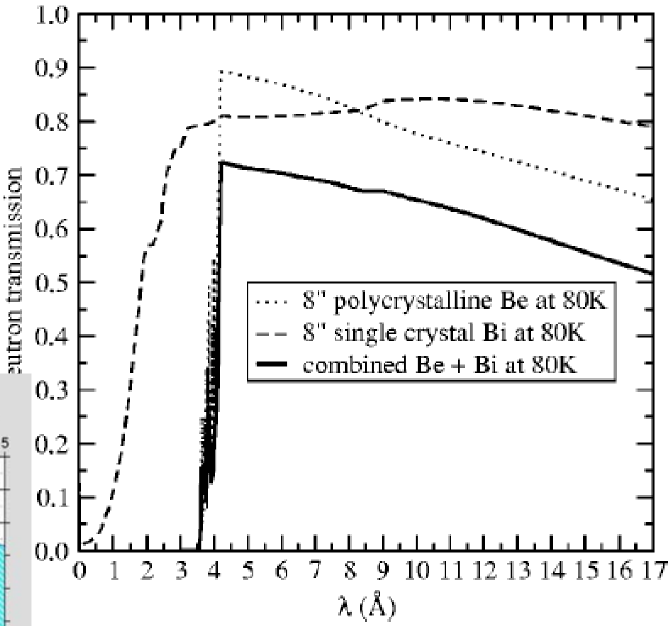


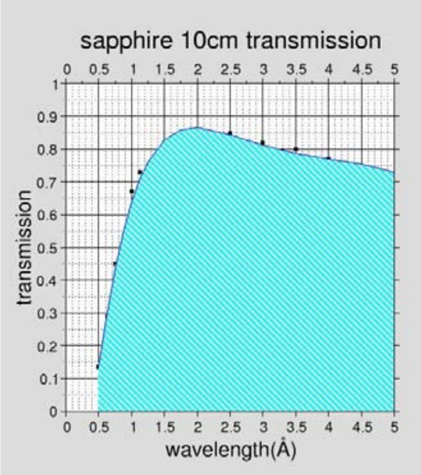
σ_{coh} and σ_{incoh}

parametrize the strength of the scattering from the nuclei or magnetic moments

Other triple-axis stuff

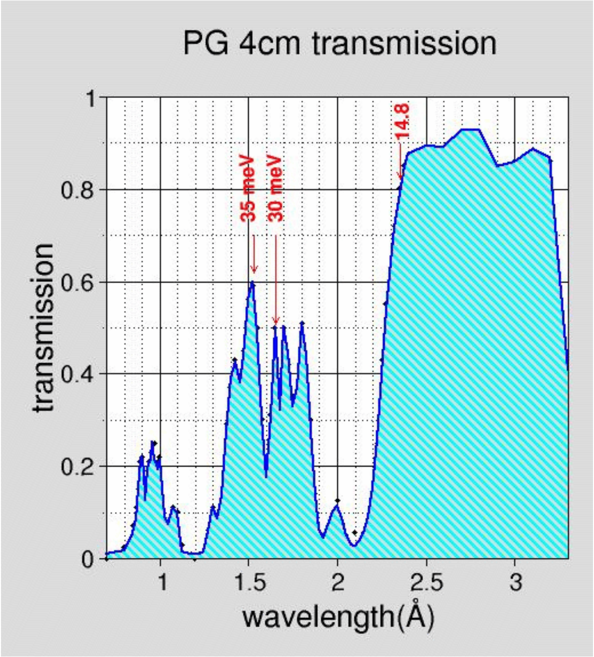
- **Soller Collimators**
  - Define beam divergence
  - Q,ω resolution function
- **Filters**
  - Xtal Sapphire: fast neutron background
  - Poly Be: low-energy (5 meV) band pass
  - PG: higher order contamination
- **Masks**
  - Beam definition
  - Background reduction

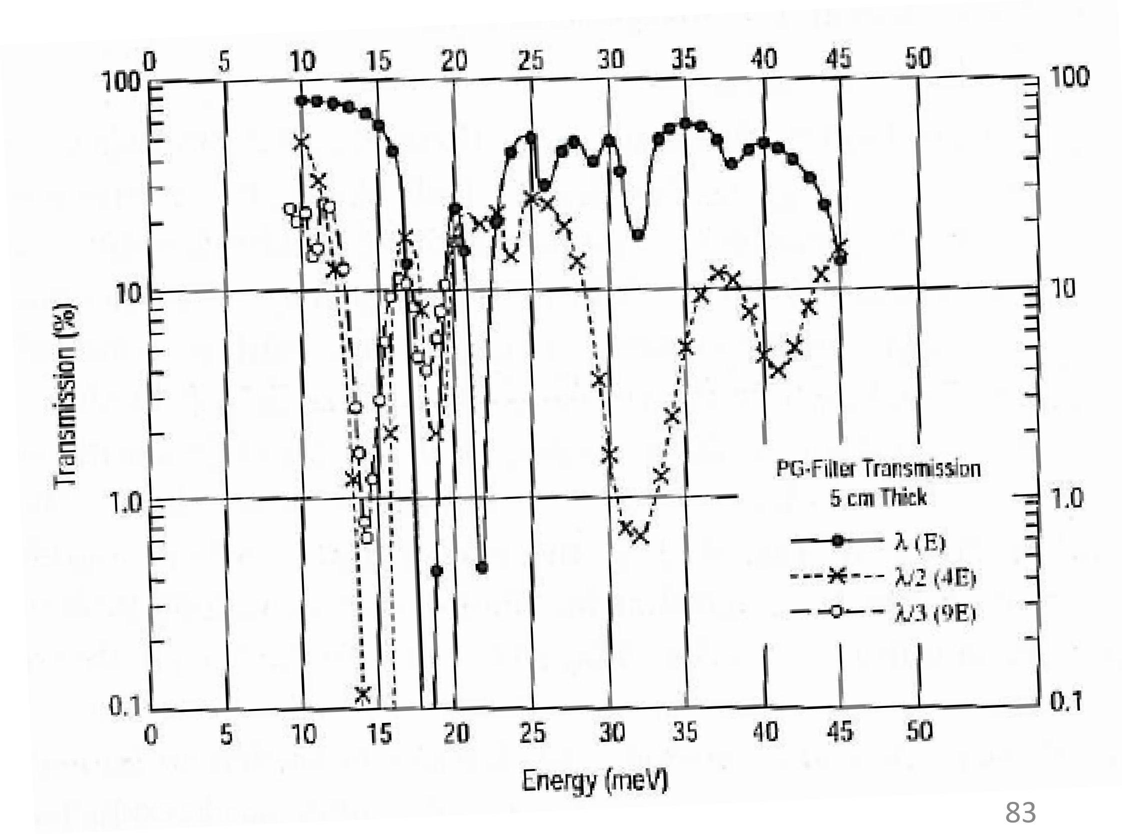




PG filter

- **Magic numbers**
  - Best filter for rejection of $\lambda/2$ contamination
  - E_f = 13.7, 14.7, 30.5, 41 meV





Reciprocal space

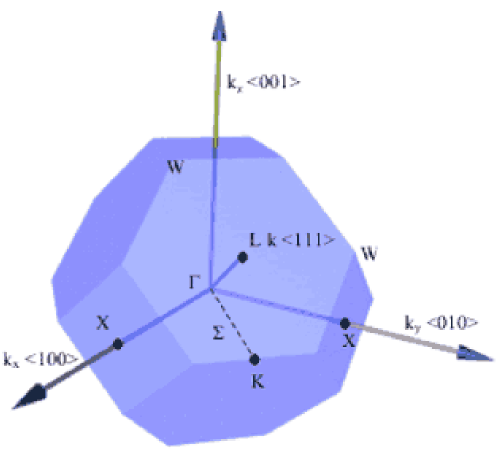
$$\mathbf{Q} = \mathbf{k}_i - \mathbf{k}_f$$

$$\hbar\omega = E_i - E_f$$

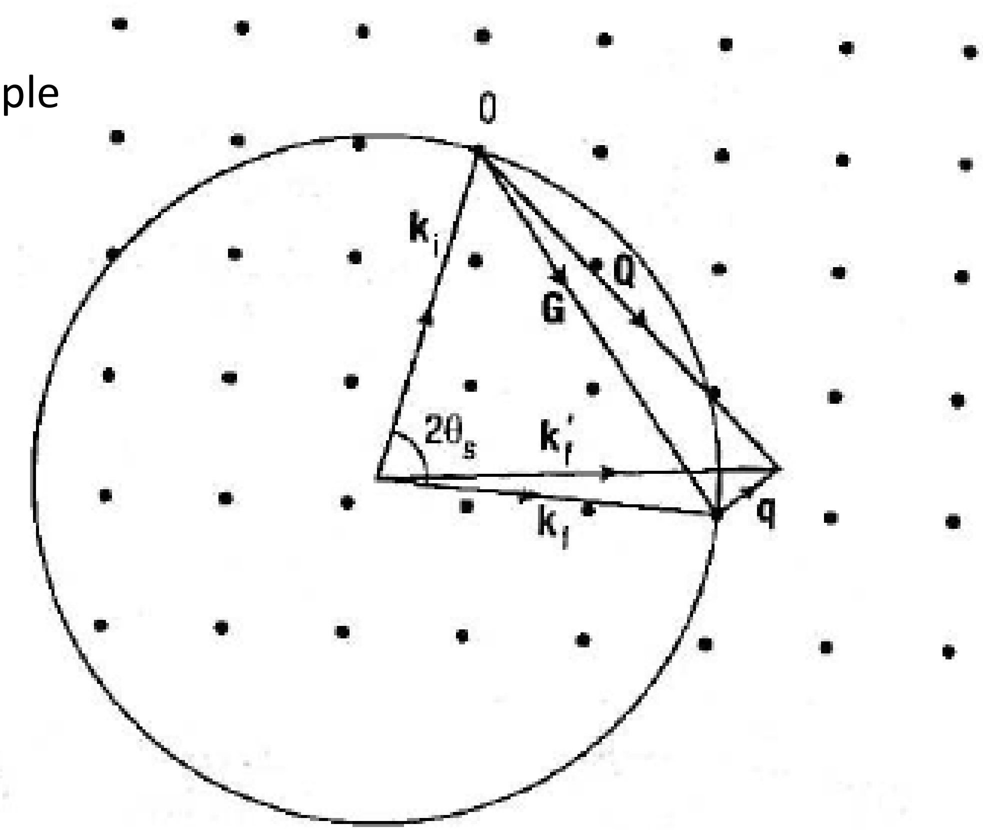
Momentum/energy transferred to sample

$$\mathbf{q} = \mathbf{Q} - \tau$$

Wavevector in 1st Brillouin zone



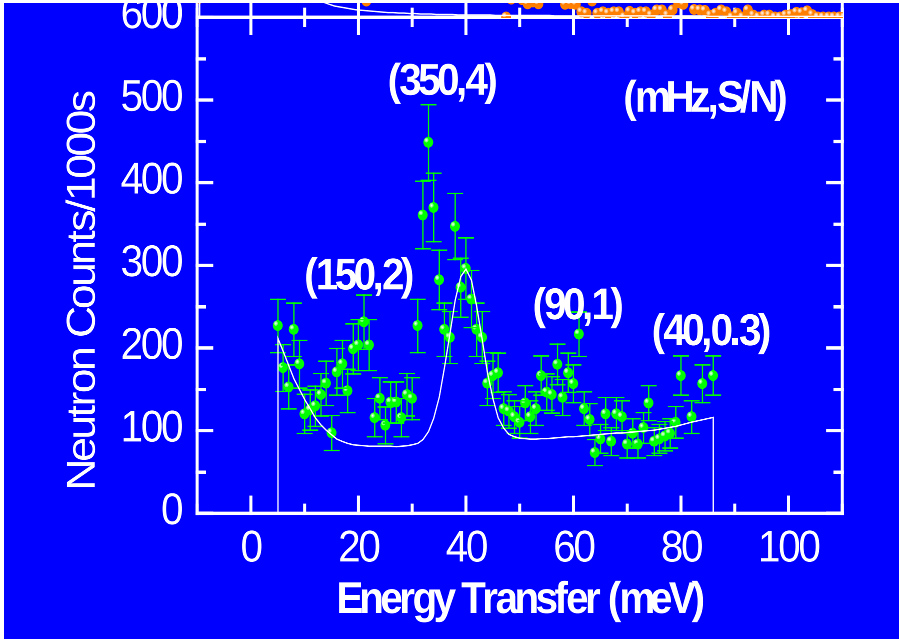
FCC Brillouin zone



Scattering triangle

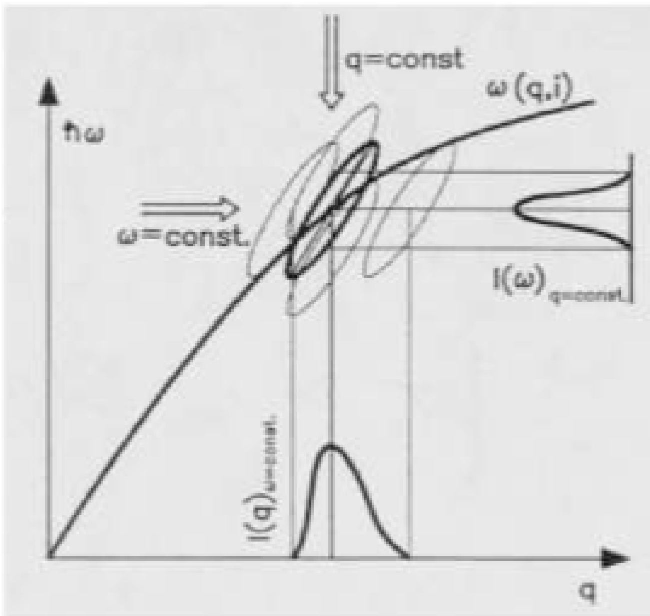
Spurions

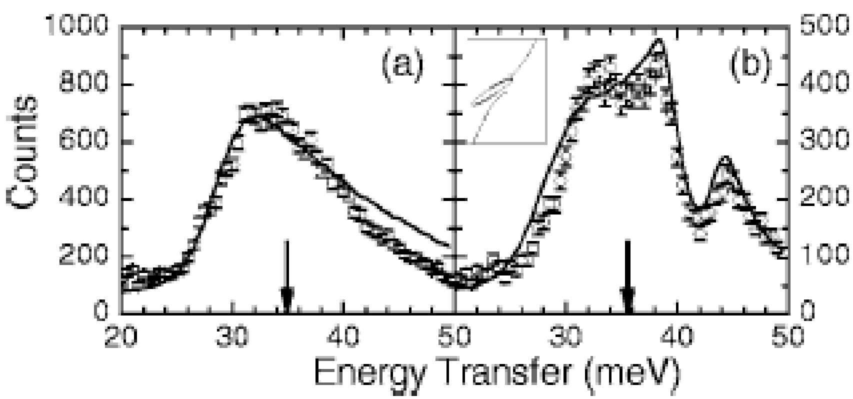
- **Bragg – incoherent – Bragg**
  - Eg. $k_i - 2k_f$
    - $\hbar\omega$ = 41.1 meV
    - E_f = 13.7 meV
      E_i = 54.8 meV
      $4E_f$ = 54.8 meV
    - Incoherent elastic scattering visible from analyzer $\lambda/2$

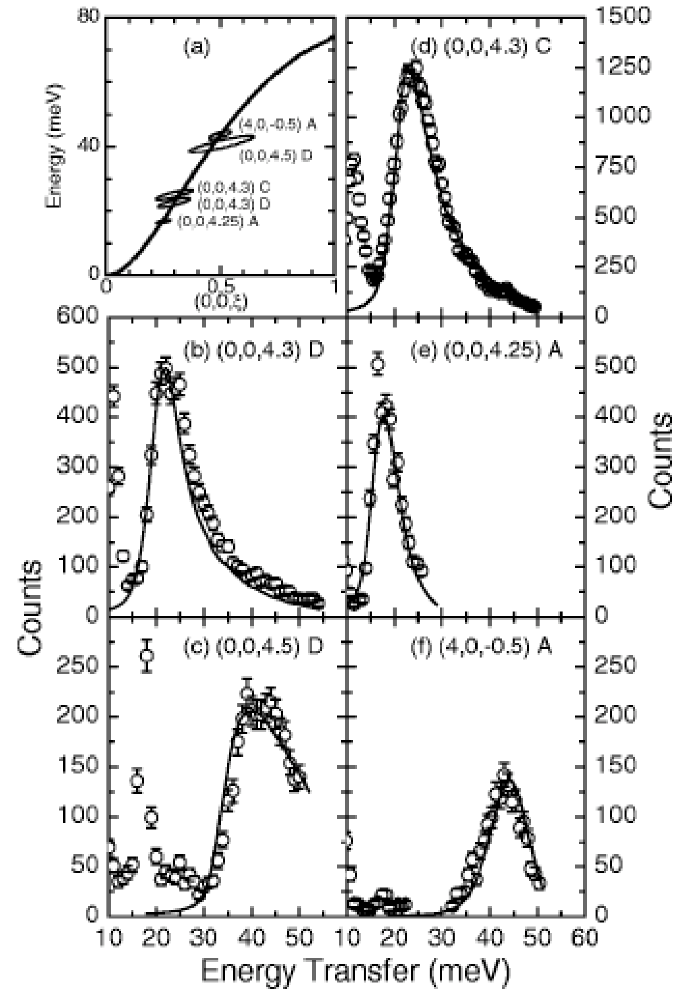


- **incoherent – Bragg – Bragg**
  - Sample 2θ in Bragg condition for k_f-k_f
  - Even for inelastic config, weak incoherent from mono

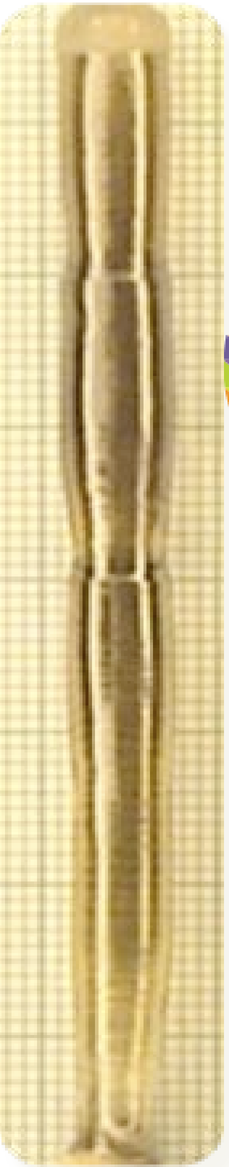
Resolution effects







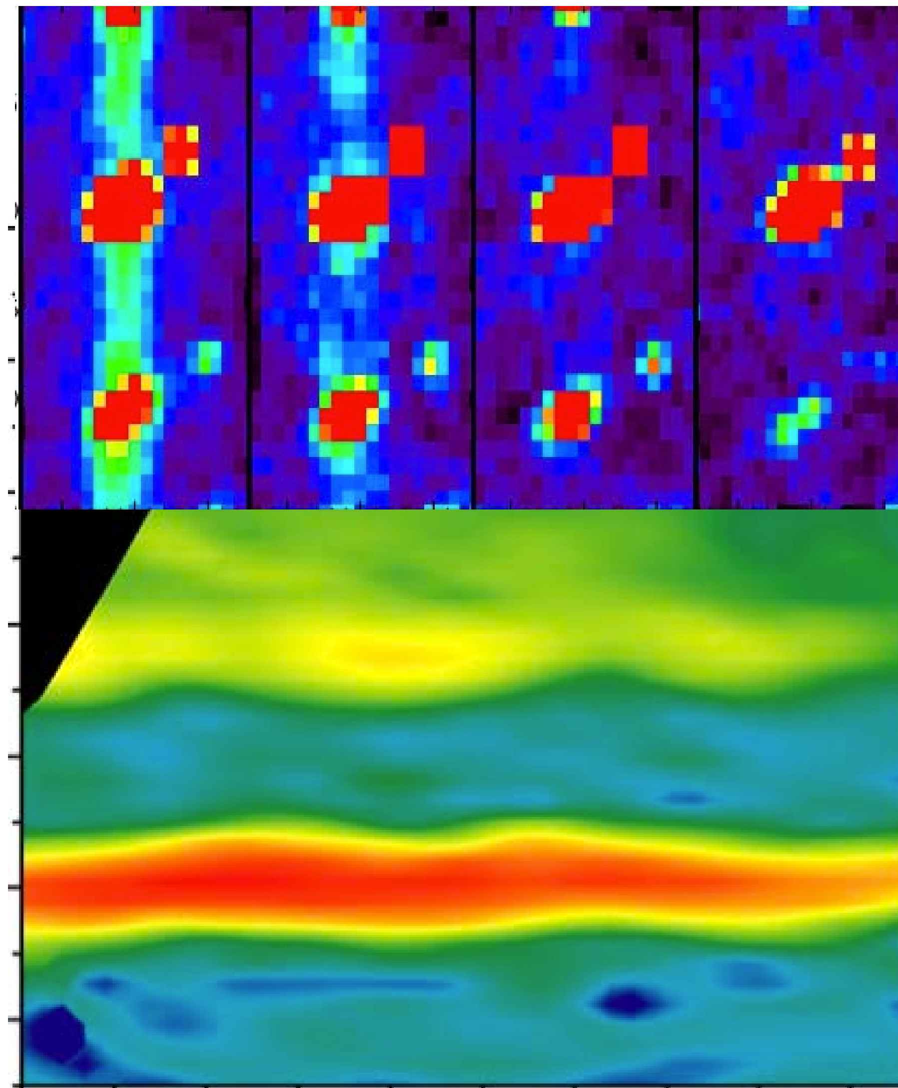
Introduction to Inelastic Neutron Scattering



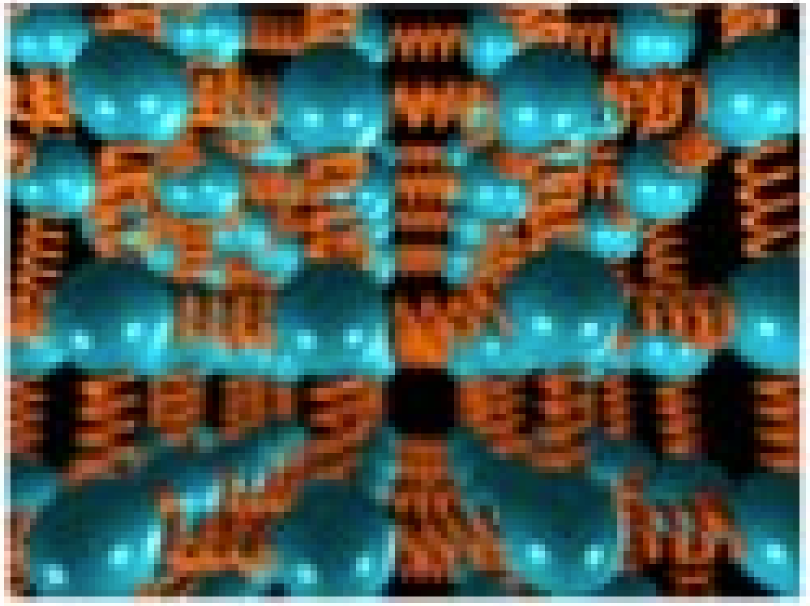
Bruce D Gaulin

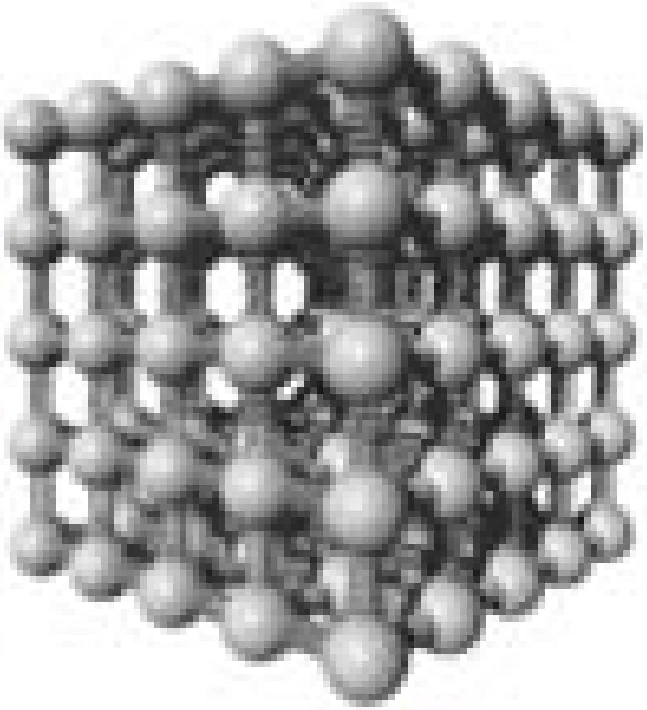
McMaster University

Brockhouse Institute
for Materials Research



Lattice





Cubic lattice