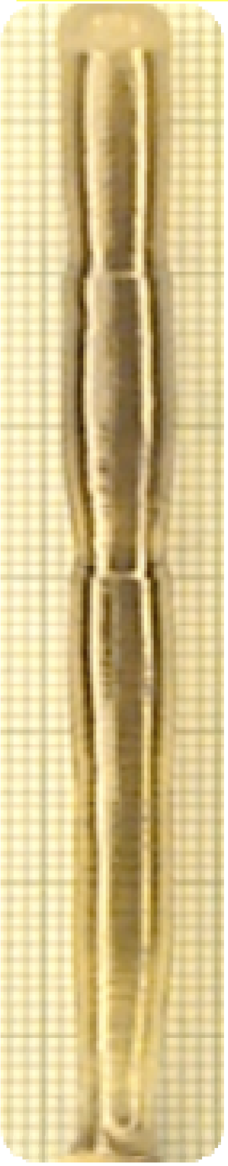
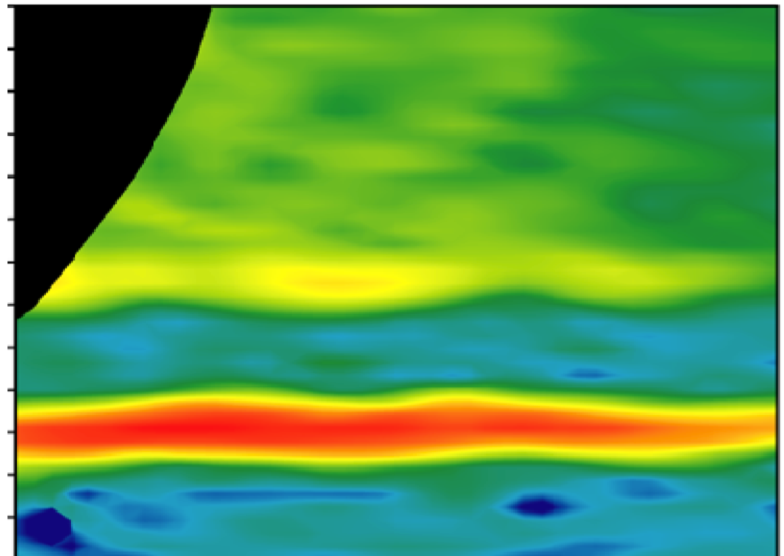
Introduction to Triple Axis Neutron Spectroscopy

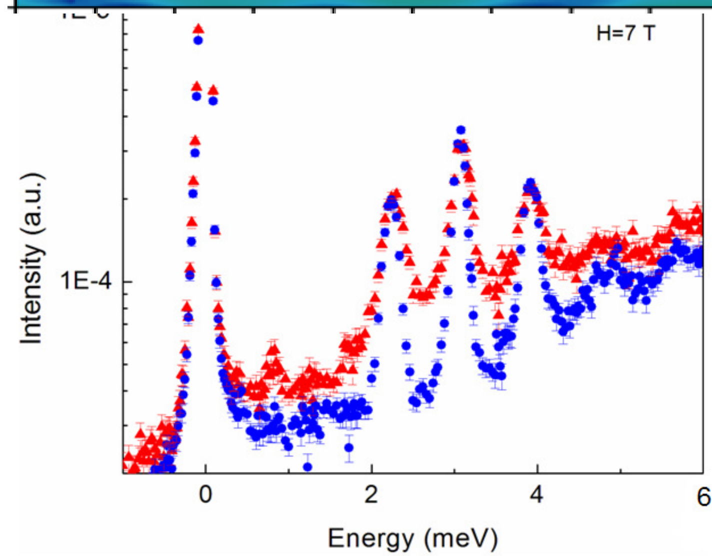


Bruce D Gaulin

McMaster University

Brockhouse Institute for Materials Research



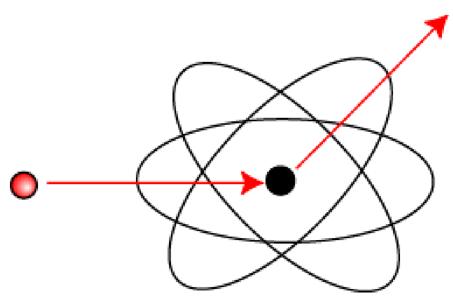


- *The triple axis spectrometer*
- *Constant-Q and constant E*
- *Practical concerns*
- *Resolution and Spurions*

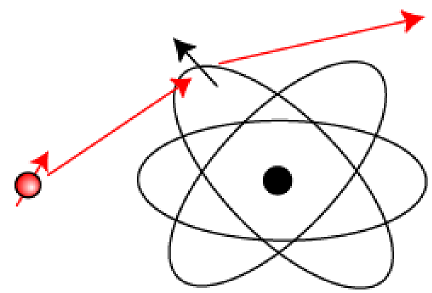
Neutron interactions with matter

- **Properties of the neutron**
  - Mass m_n =1.675 x 10^{-27} kg
  - Charge 0
  - Spin-1/2, magnetic moment $\mu_n = -1.913\ \mu_N$

- **Neutrons interact with…**
  - Nucleus
  - Crystal structure/excitations (eg. Phonons)
  - Unpaired electrons via dipole scattering
  - Magnetic structure and excitations



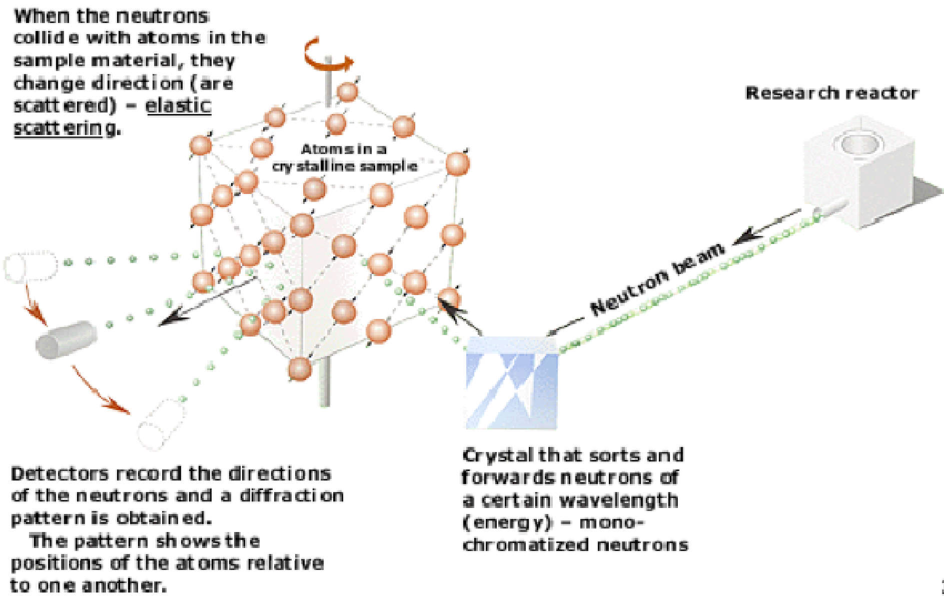
Nuclear scattering

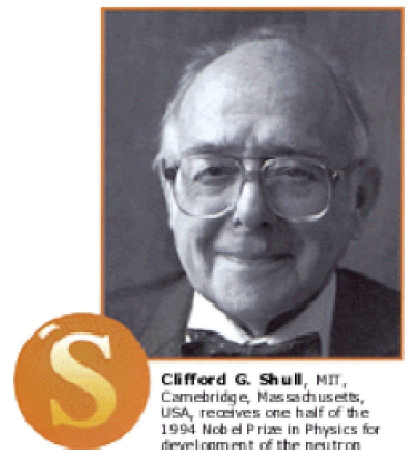


Magnetic dipole scattering

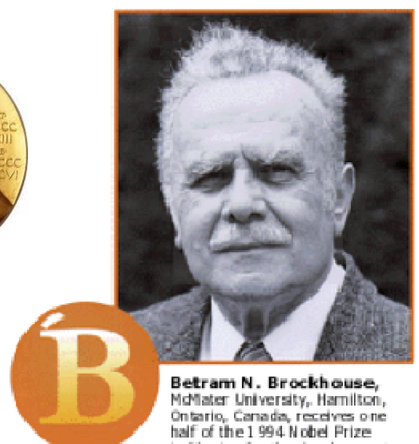
Brockhouse and Shull Share 1994 Nobel Prize in Physics

Most recent Nobel Prize awarded to a scientist working in Canada

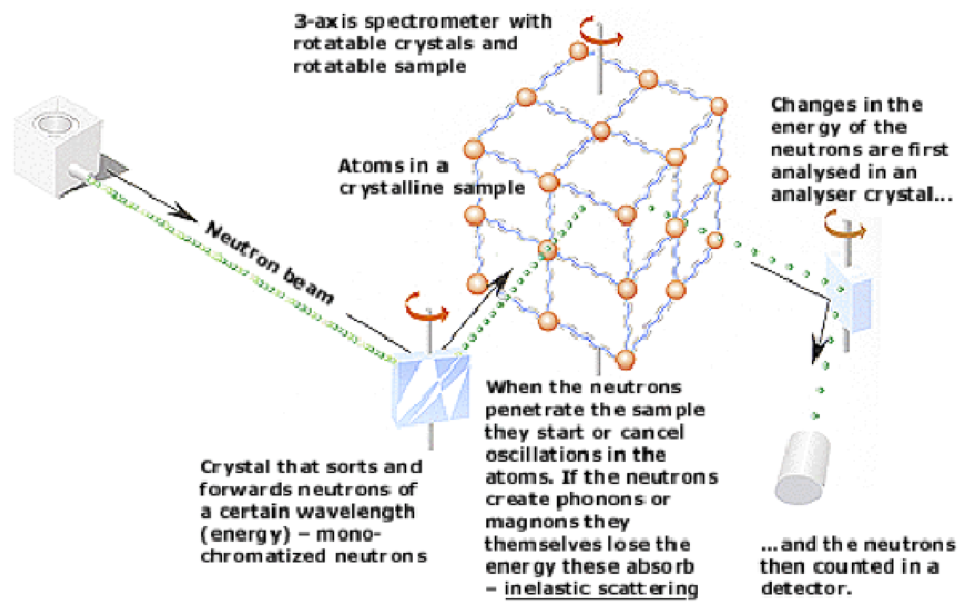




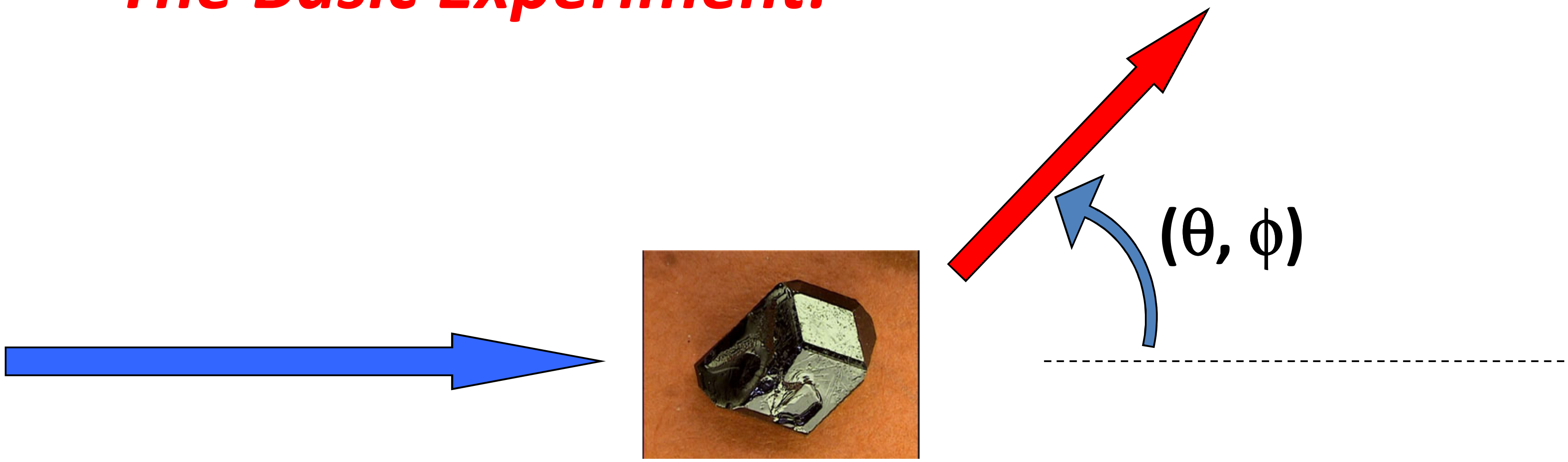
Clifford G. Shull, MIT, Camebridge, Massachusetts, USA, receives one half of the 1994 Nobel Prize in Physics for development of the neutron diffraction technique.



Betram N. Brockhouse, McMaster University, Hamilton, Ontario, Canada, receives one half of the 1994 Nobel Prize in Physics for the development of neutron spectroscopy.



The Basic Experiment:



Incident Beam:

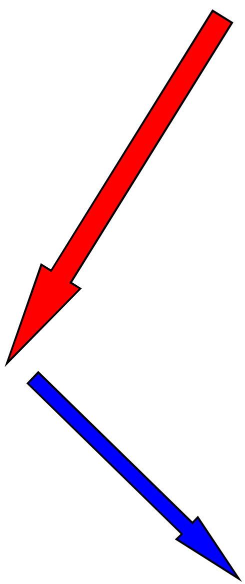
- **monochromatic**
- **“white”**
- **“pink”**

Scattered Beam:

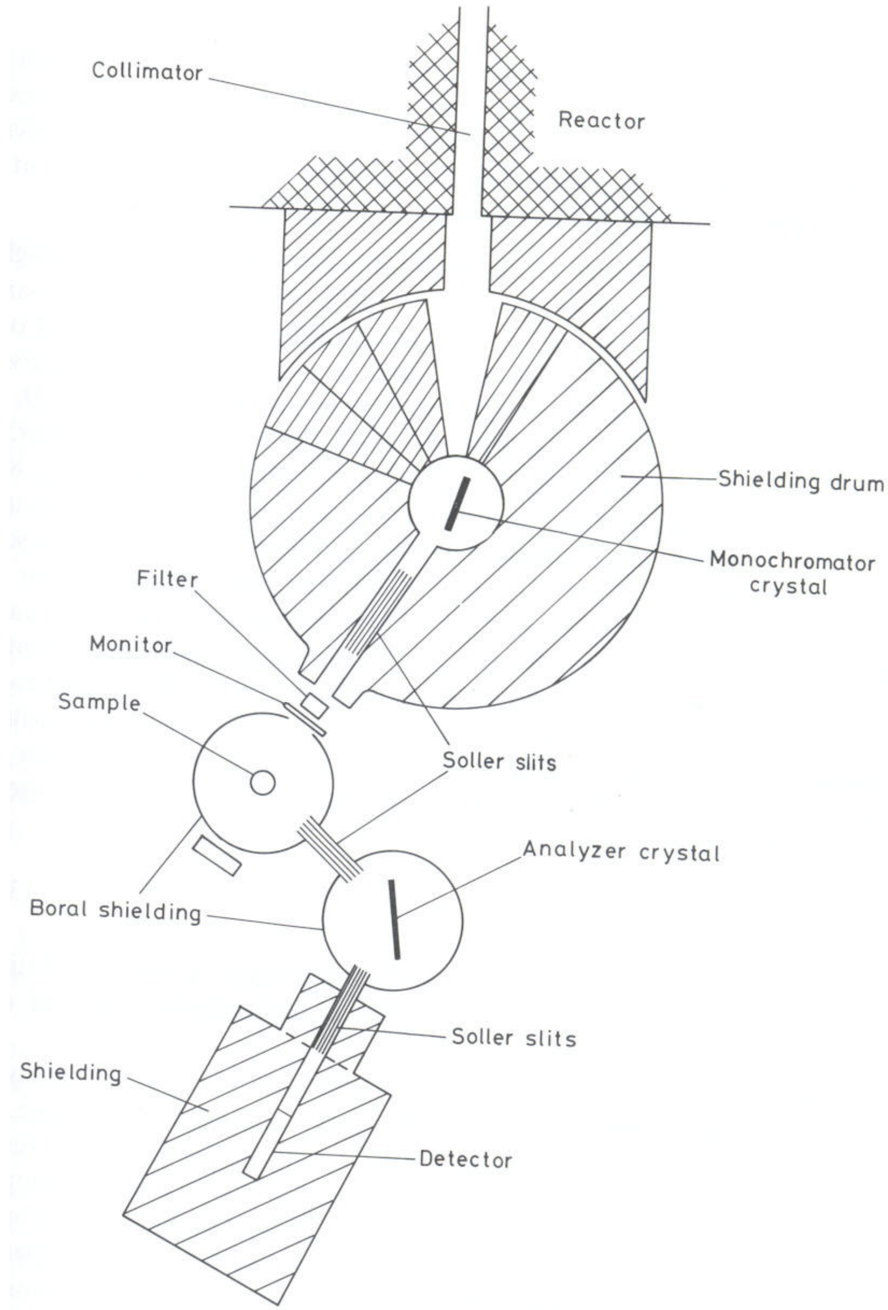
- **Resolve its energy**
- **Don’t resolve its energy**
- **Filter its energy**

Brockhouse's Triple Axis Spectrometer

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

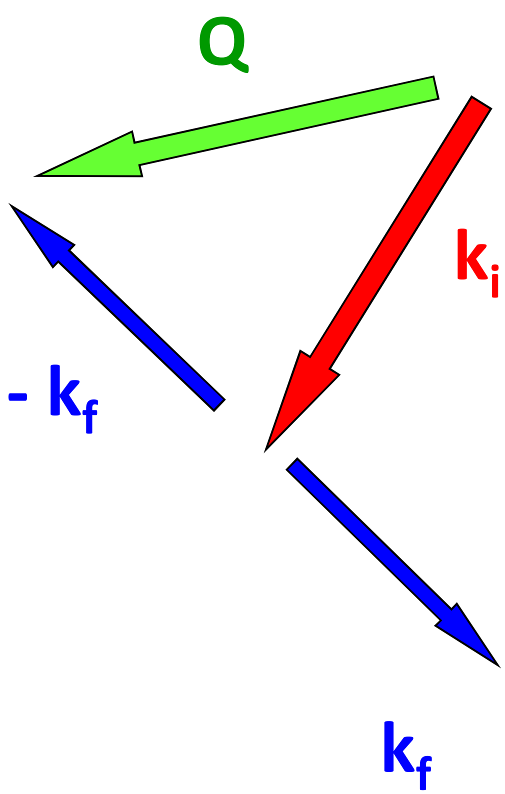


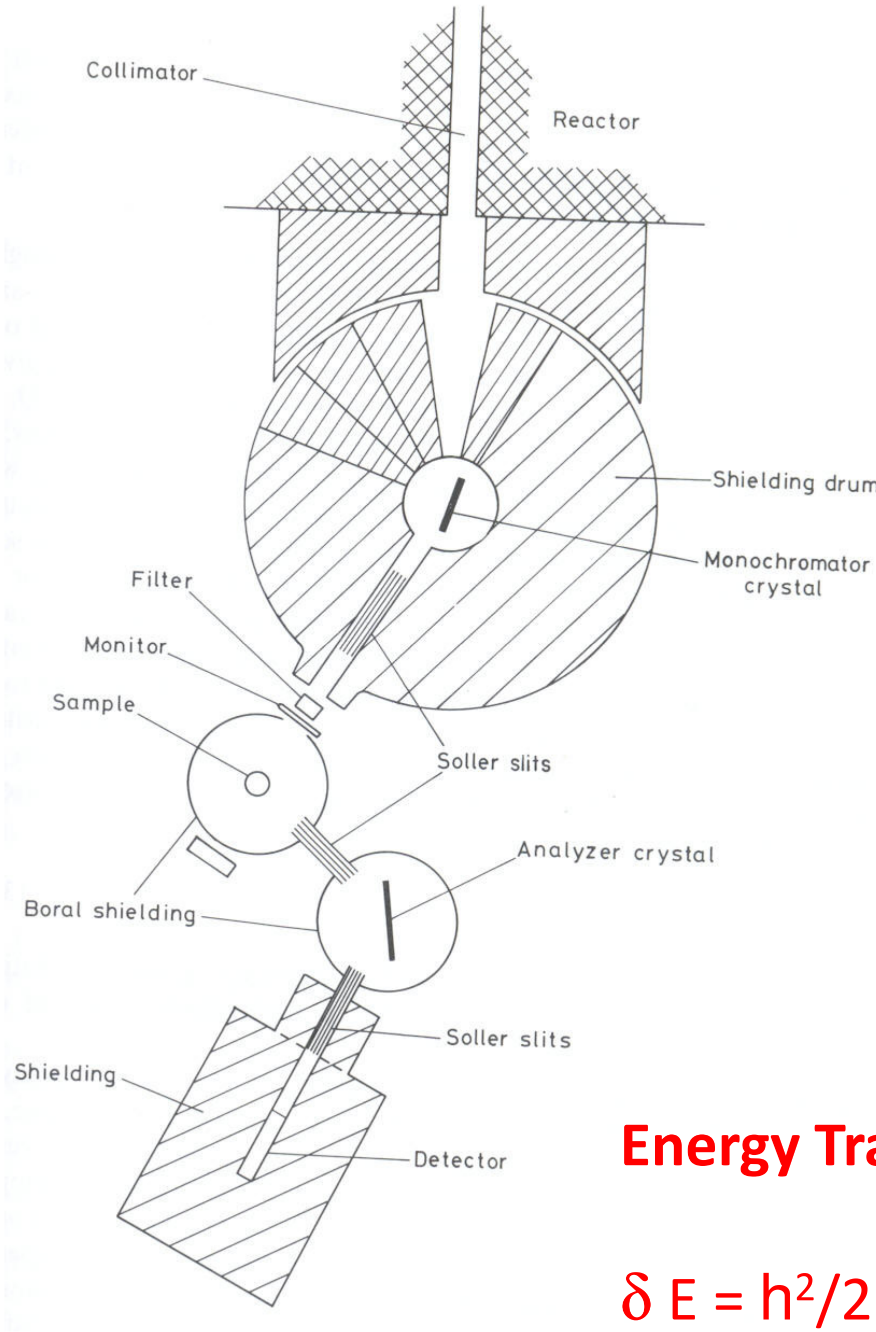
$| \mathbf{k_f} | = 2 \pi / \lambda_f$



Momentum Transfer:

$$Q = k_i - k_f$$





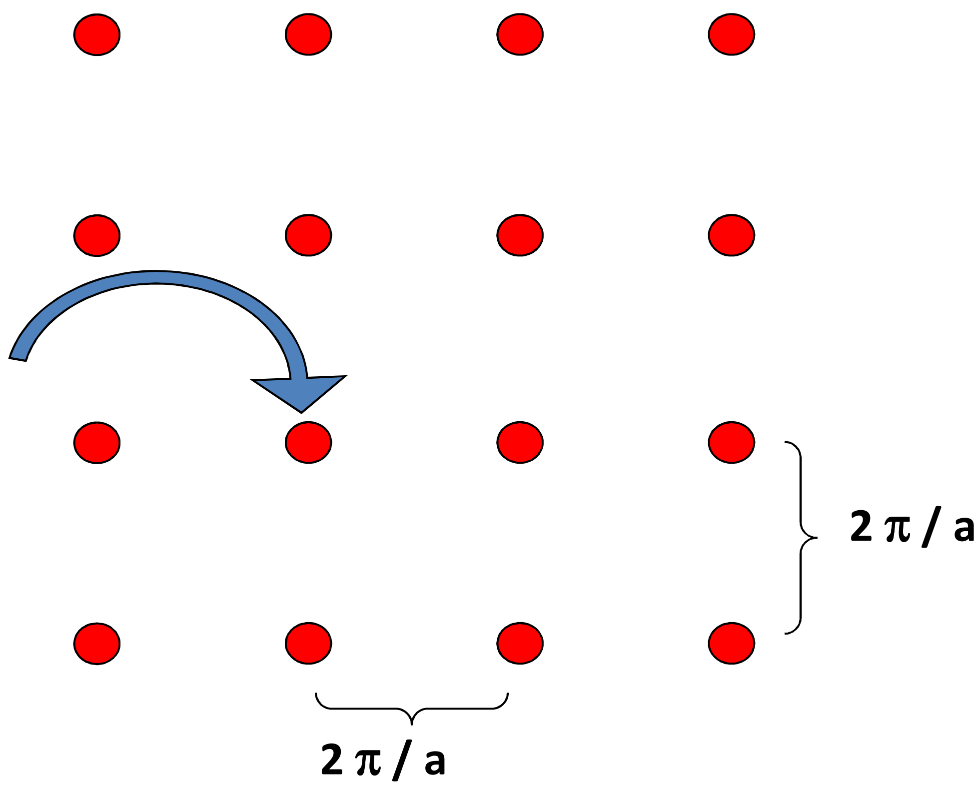
Energy Transfer:

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

Mapping Momentum – Energy (Q-E) space

Origin of reciprocal space;

Remains fixed for any sample rotation

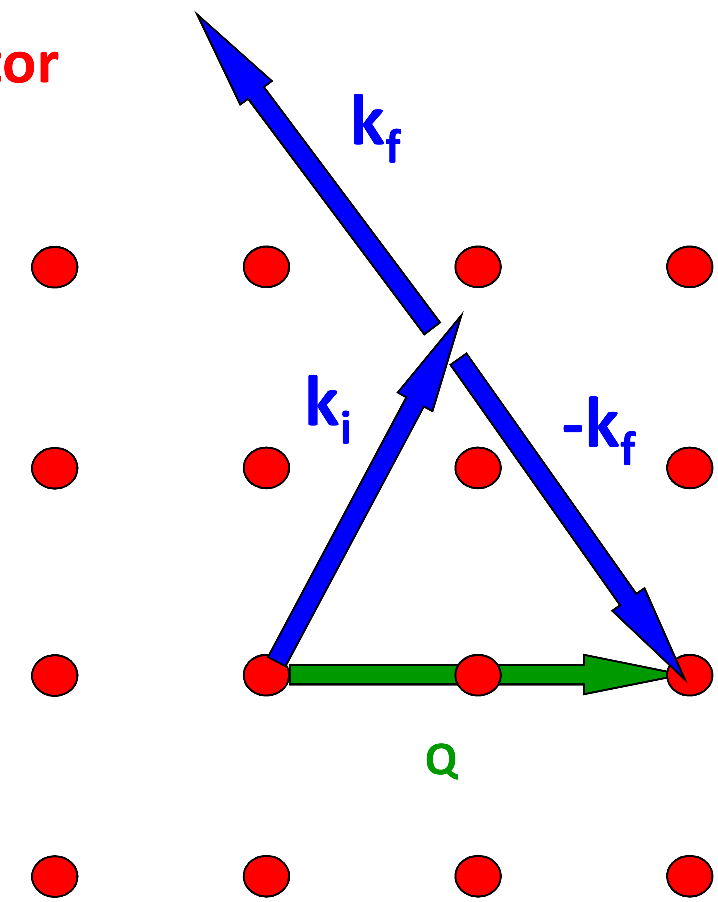


Bragg diffraction:

Elastic scattering : | k_i | = | k_f |

Constructive Interference

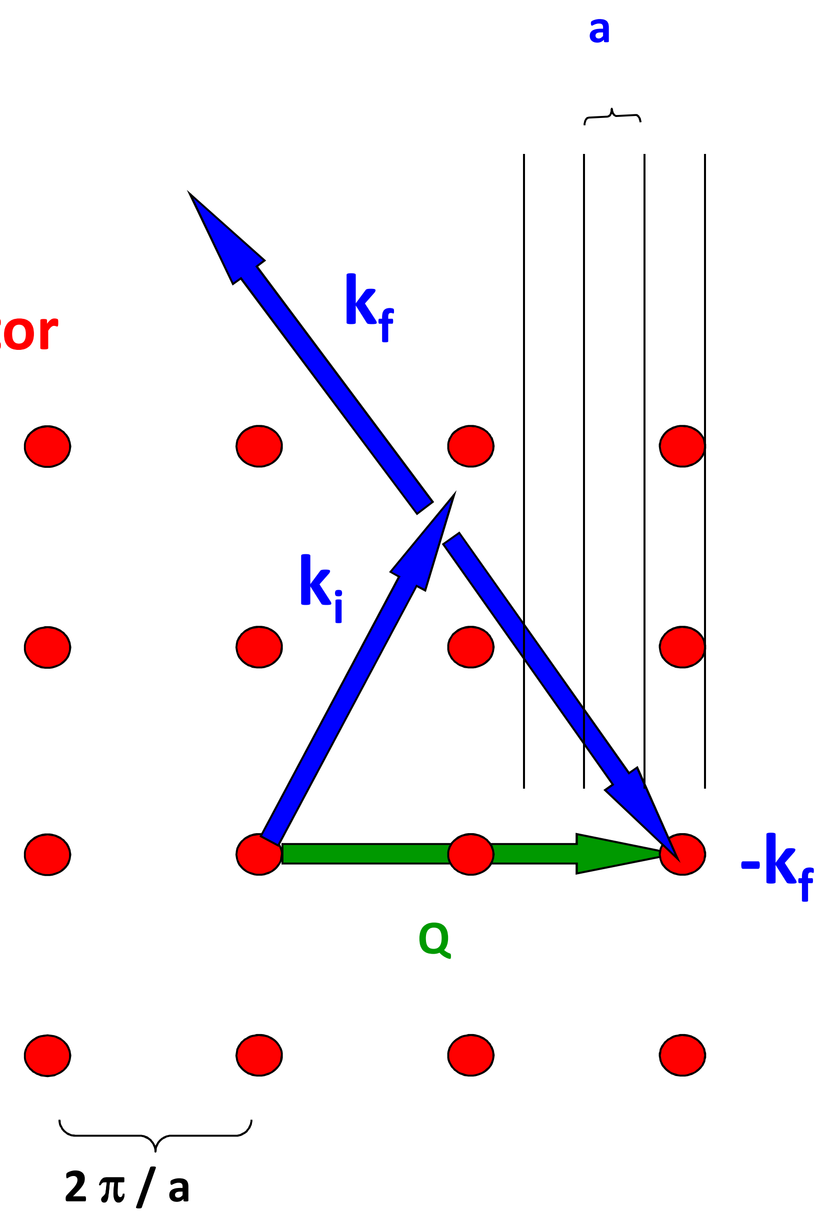
Q = Reciprocal Lattice Vector



Bragg diffraction:

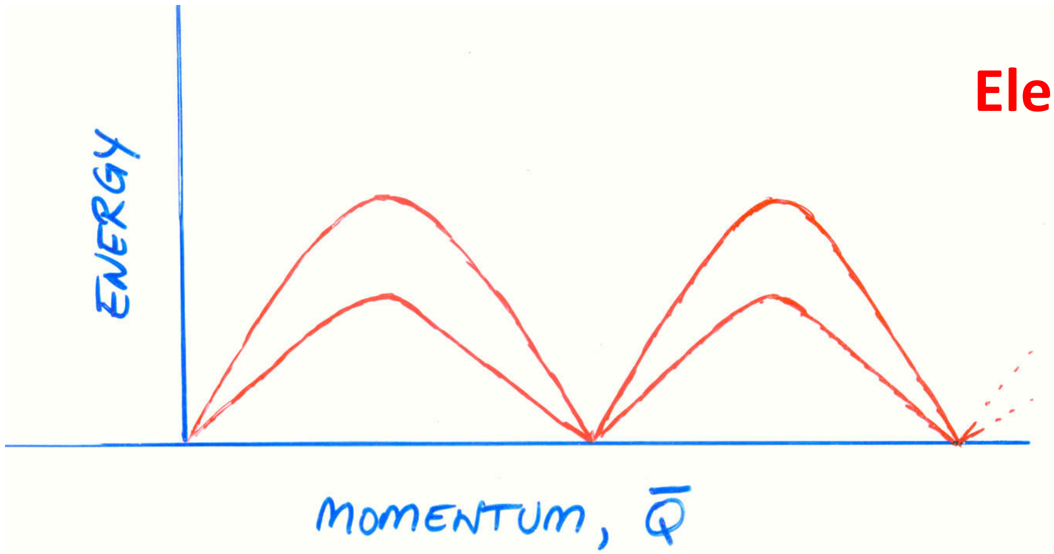
Constructive Interference

Q = Reciprocal Lattice Vector

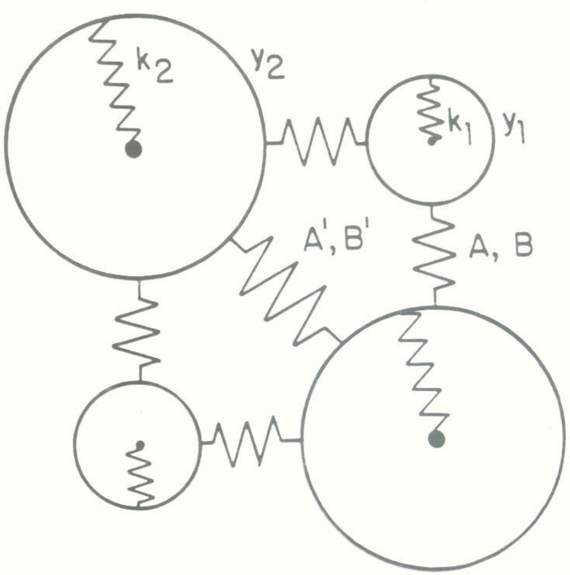


Elastic scattering : | k_i | = | k_f |

Elementary Excitations in Solids

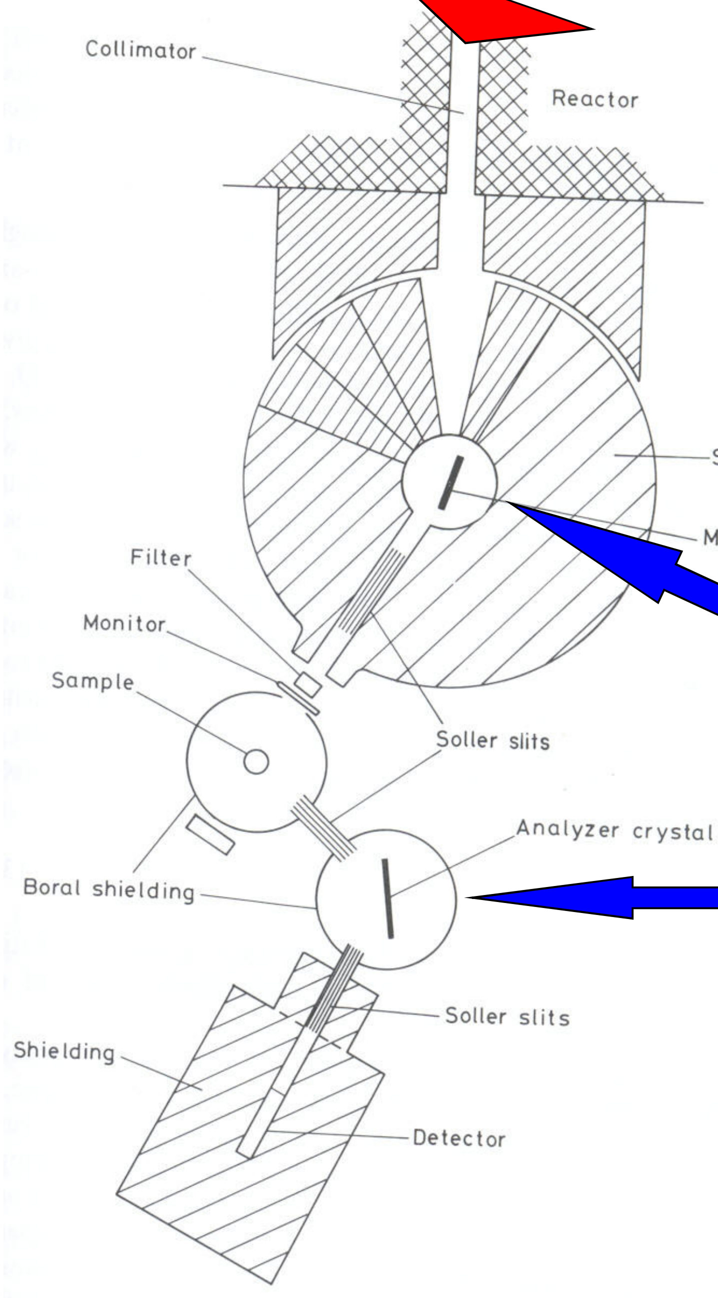


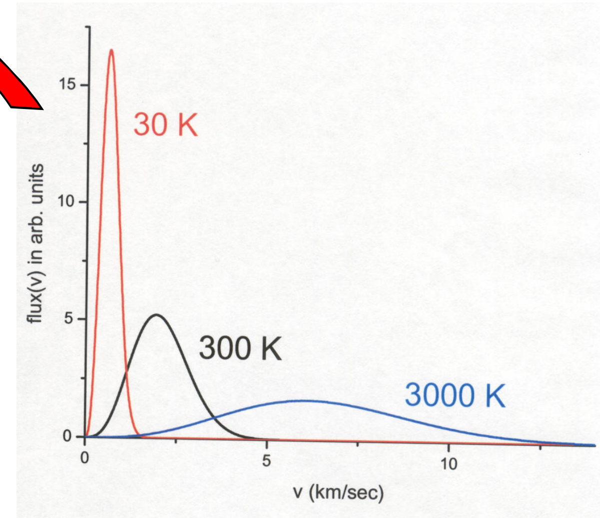
- Lattice Vibrations (Phonons)
- Spin Fluctuations (Magnons)

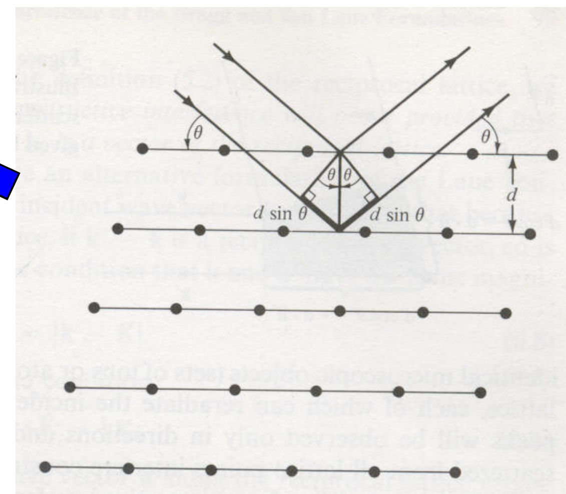


Energy vs Momentum

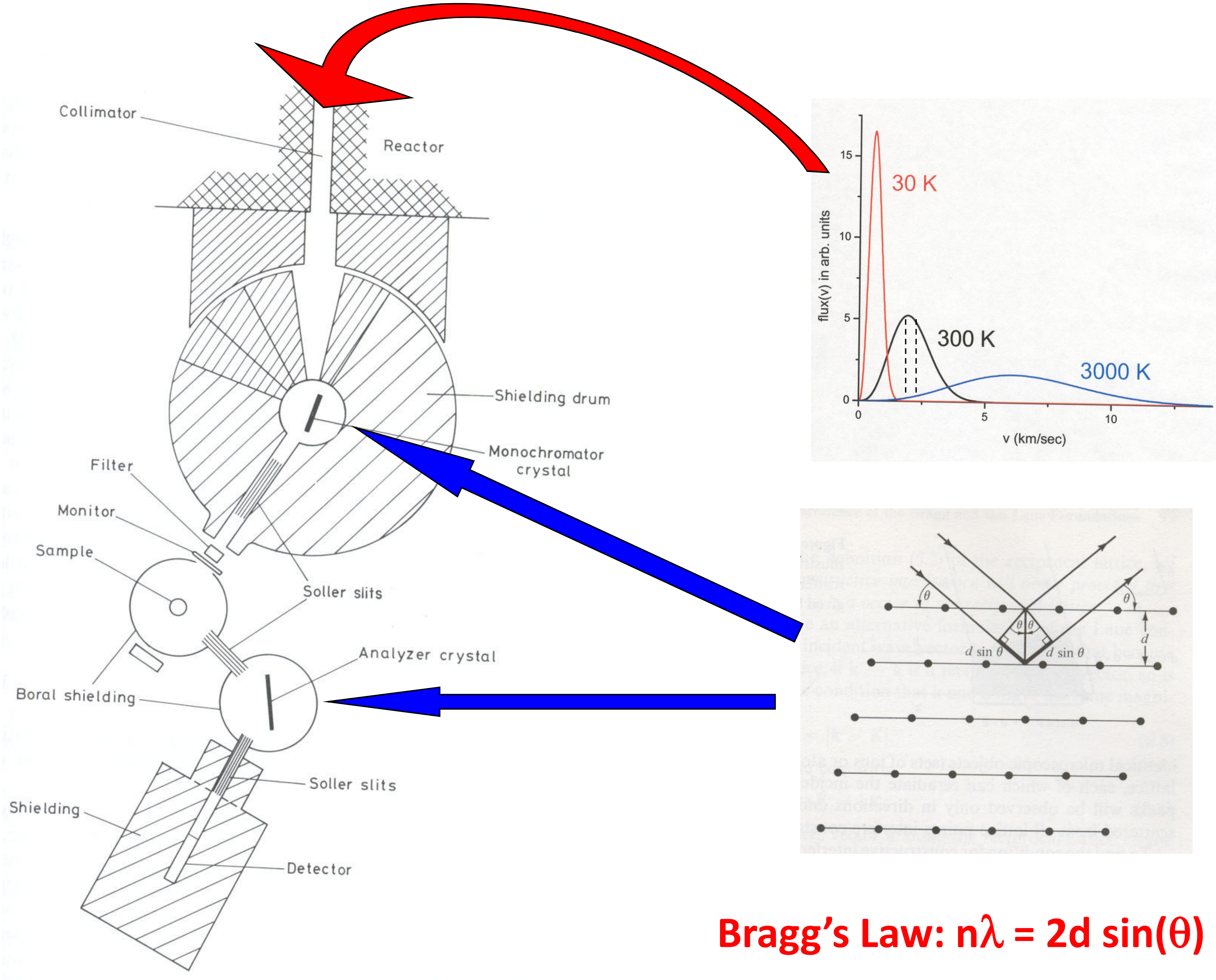
- Forces which bind atoms together in solids







Bragg’s Law: $n\lambda = 2d\sin(\theta)$

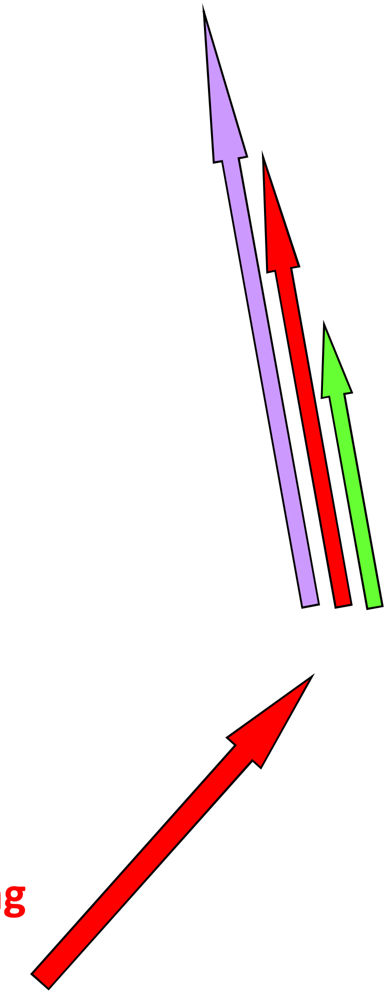


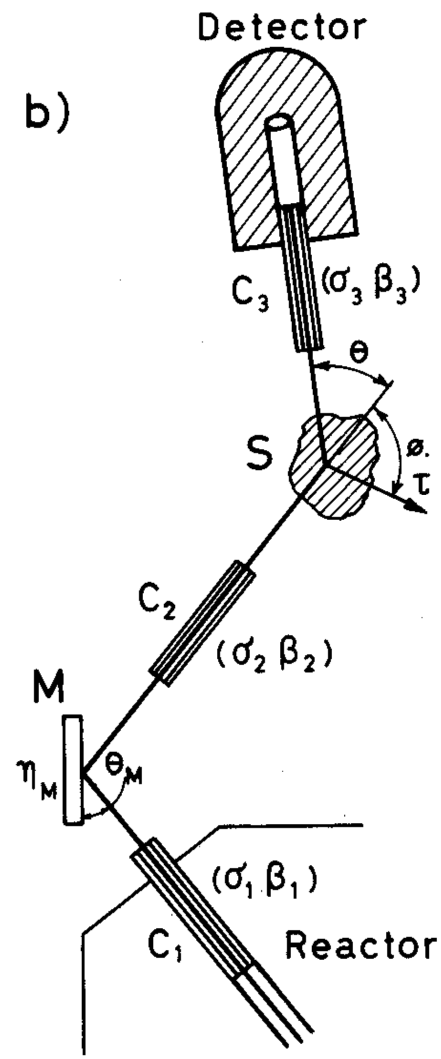
Bragg's Law: $n\lambda = 2d \sin(\theta)$

Two Axis Spectrometer:

- 3-axis with analyser removed

- Powder diffractometer
- Small angle diffractometer
- Reflectometers

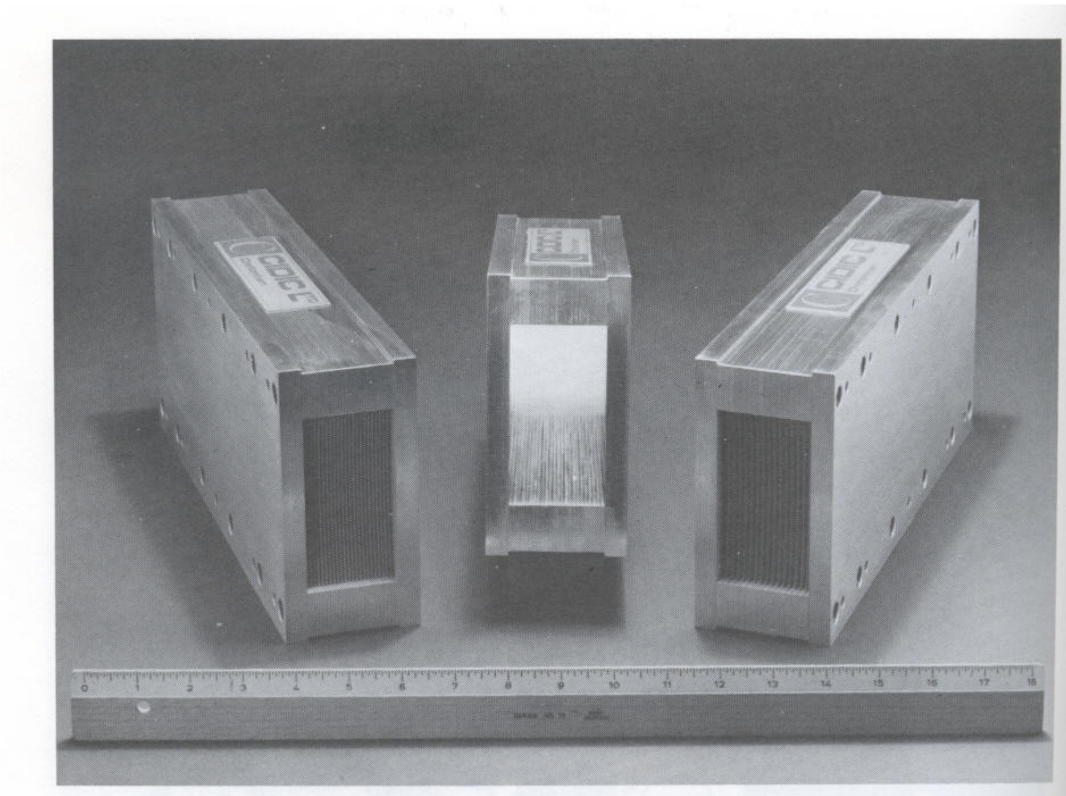


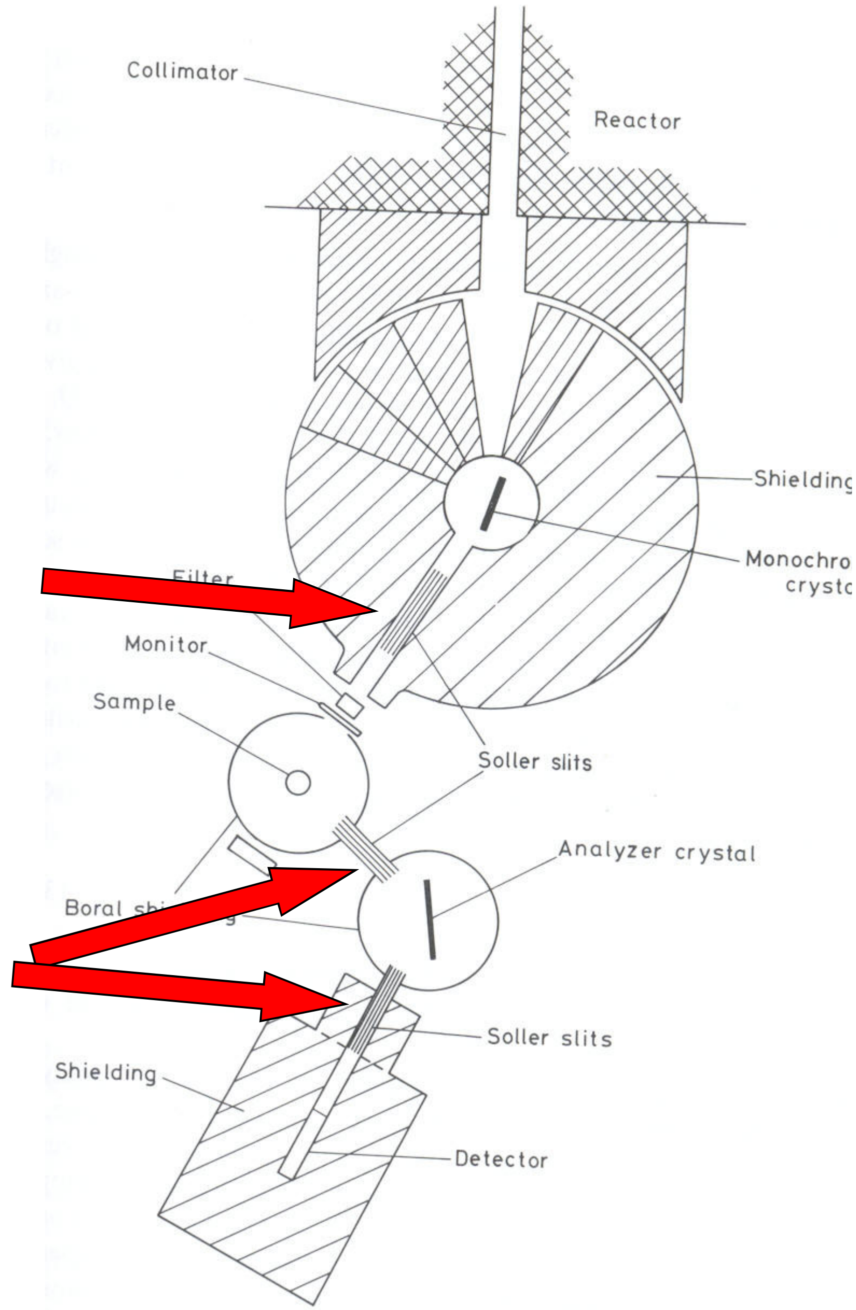


Diffractometers often employ working assumption that all scattering is *elastic.*

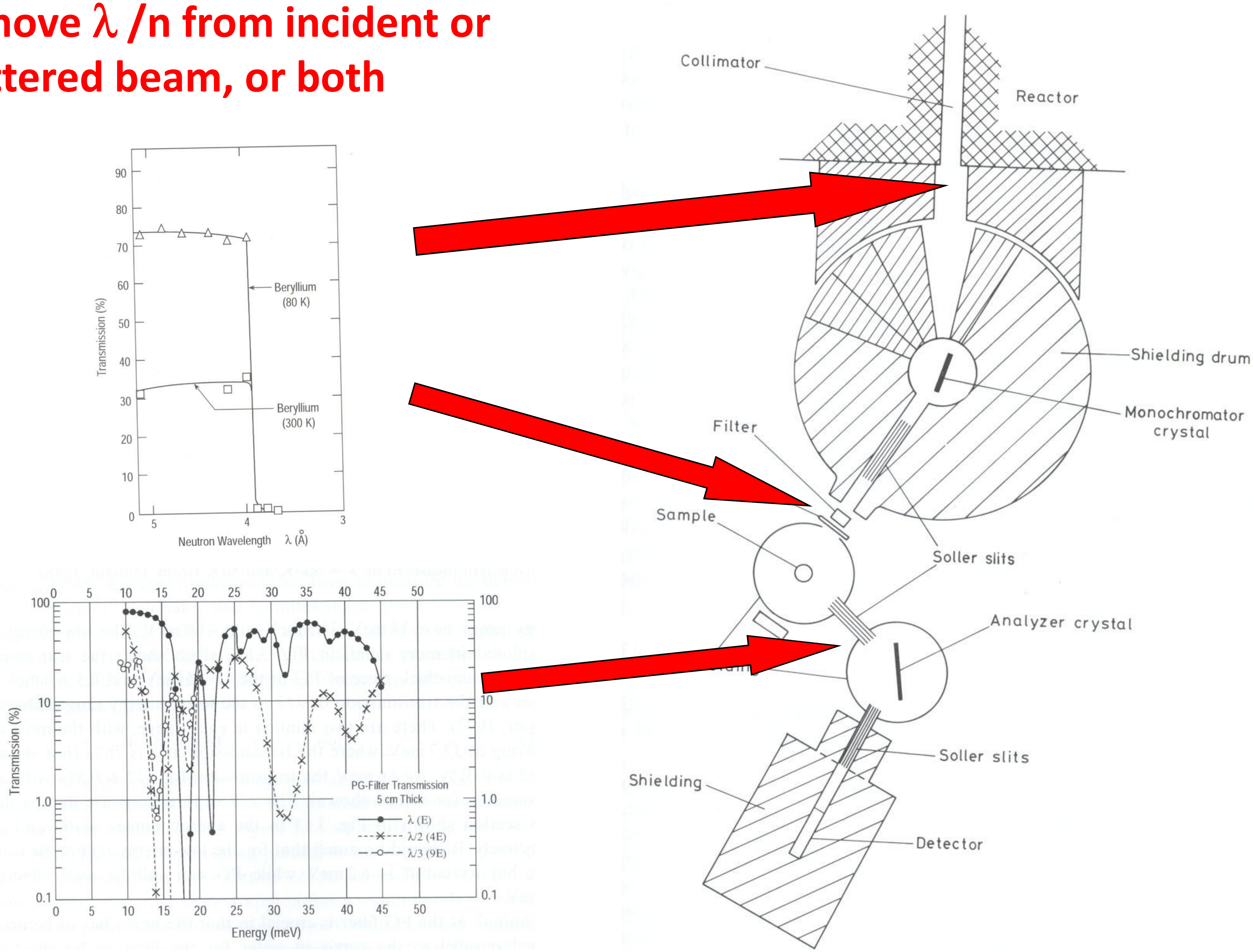
Soller Slits: Collimators

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



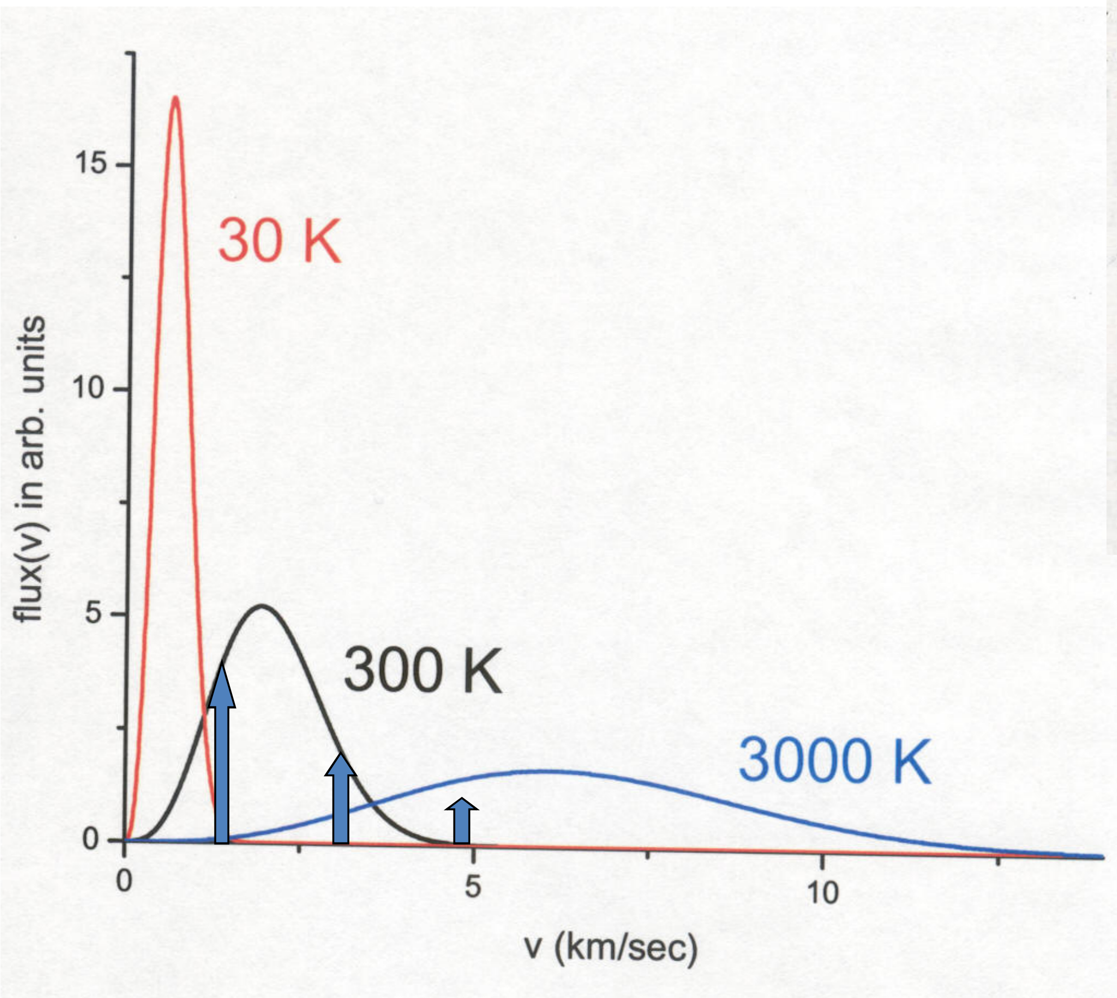


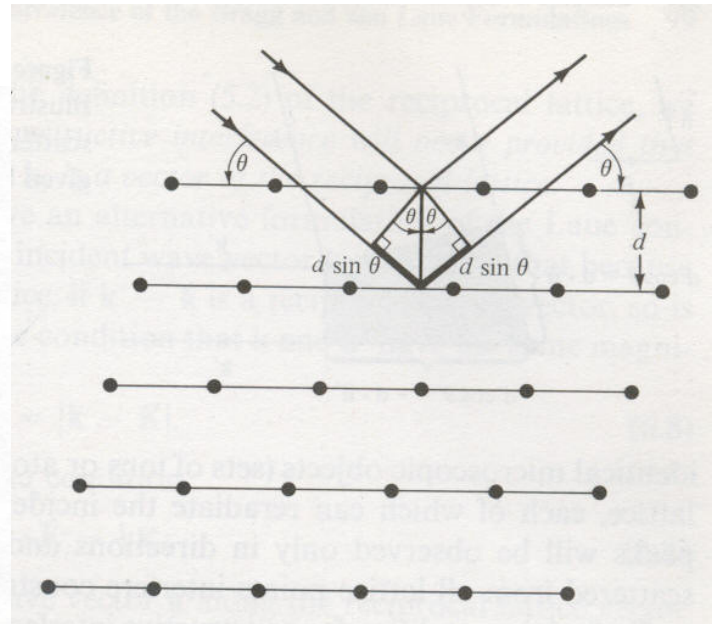
Filters:
Remove λ /n from incident or scattered beam, or both



Single crystal monochromators:

Bragg reflection and harmonic contamination

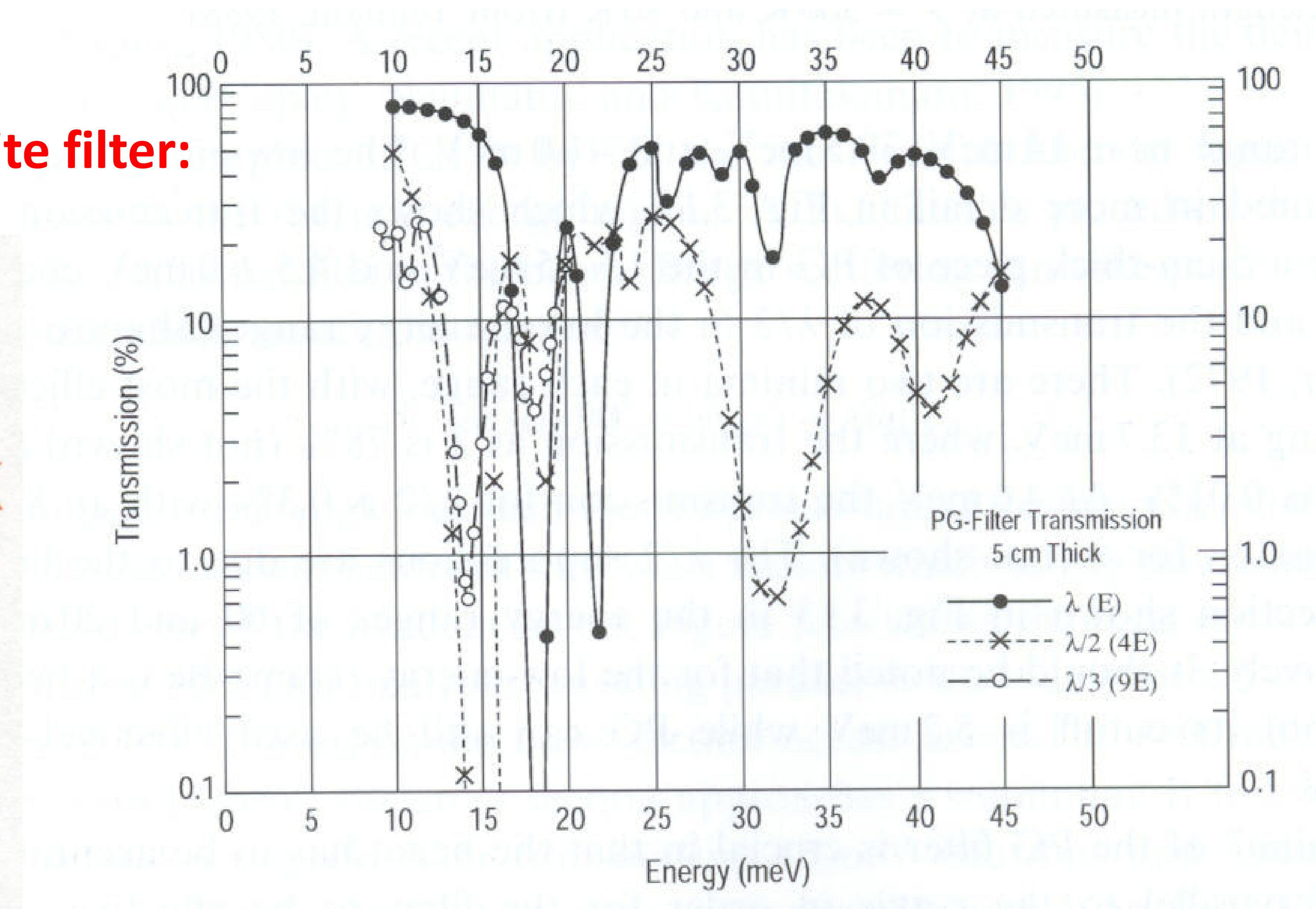


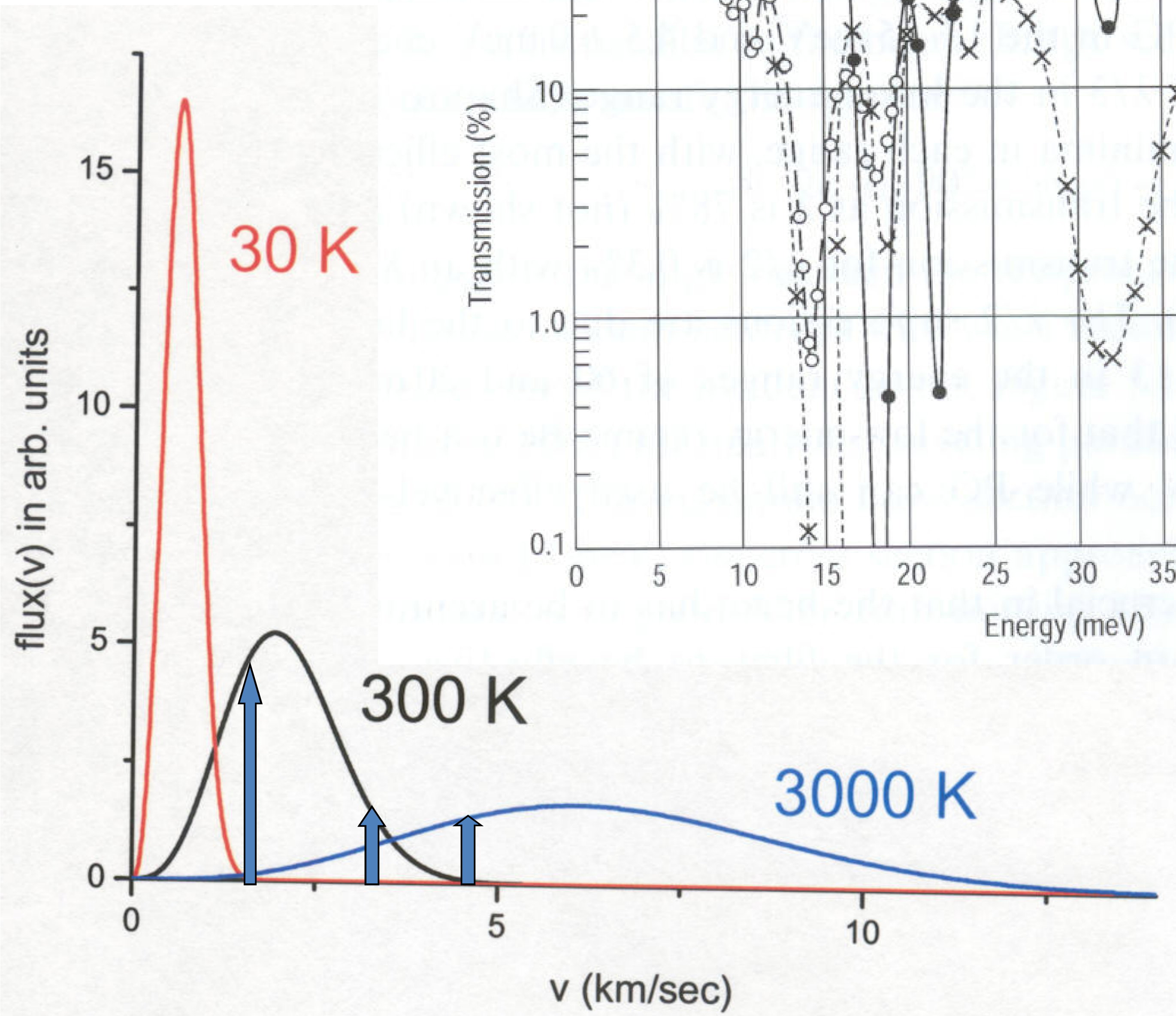


$n\lambda = 2d \sin(\theta)$

Get: λ , $\lambda/2$, $\lambda/3$, etc.

Pyrolitic graphite filter:





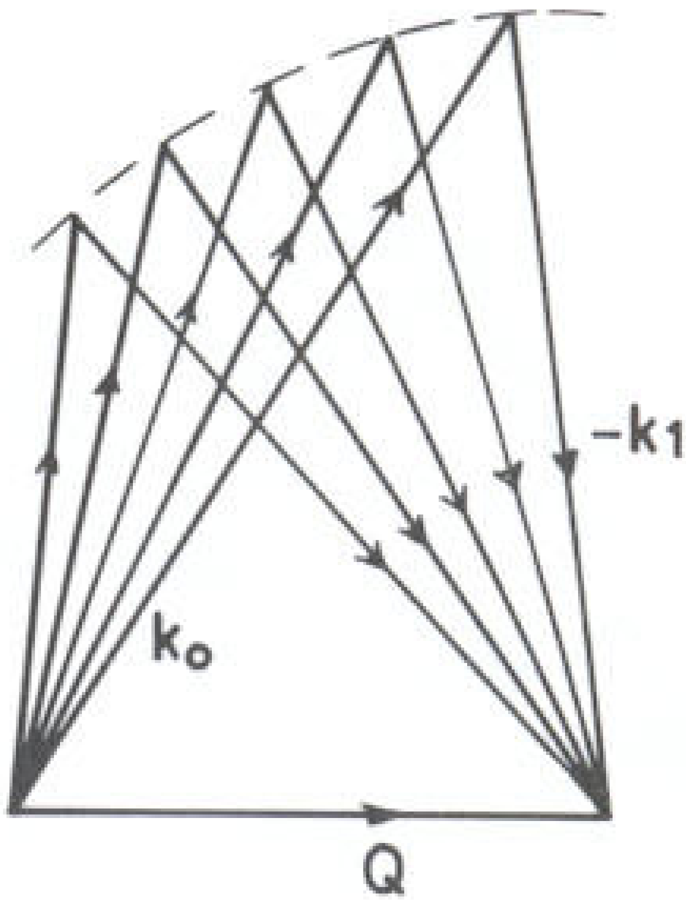
E = 14.7 meV

λ = 2.37 A

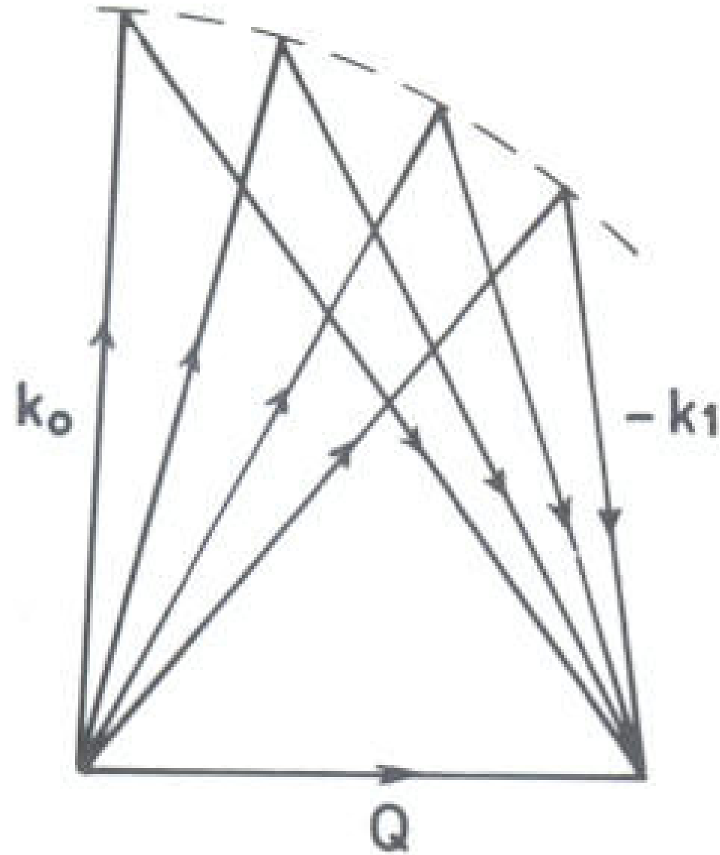
v = 1.6 km/s

2 x v = 3.2 km/s

3 x v = 4.8 km/s



Constant k_f (ii)



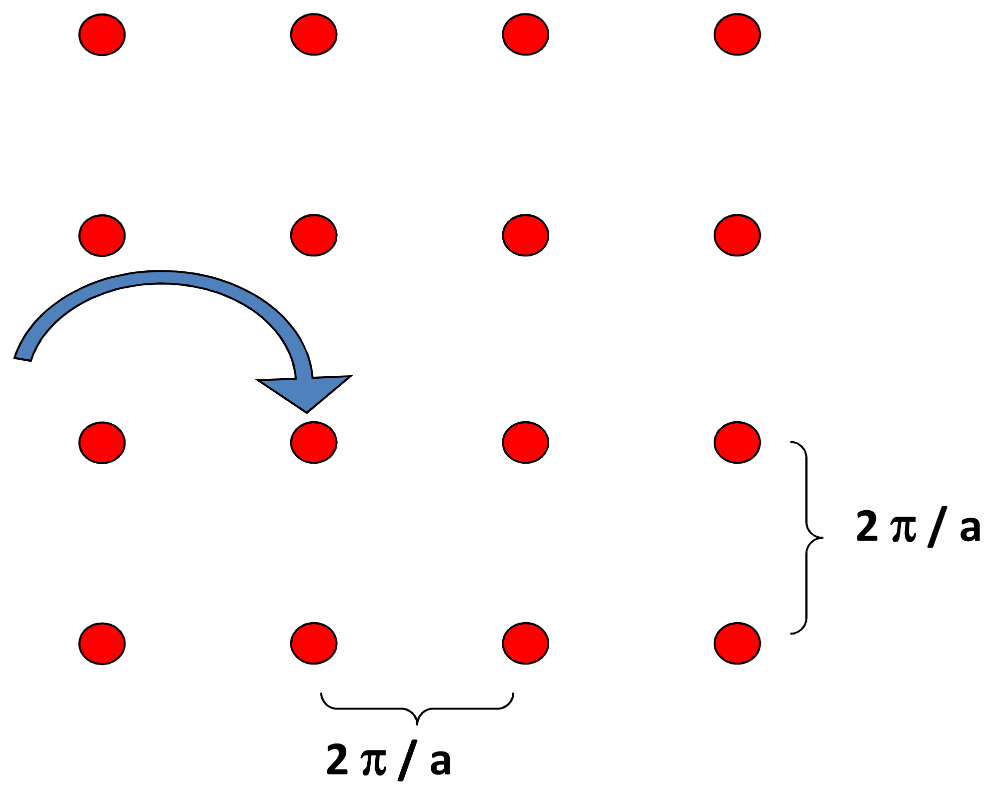
Constant k_i (i)

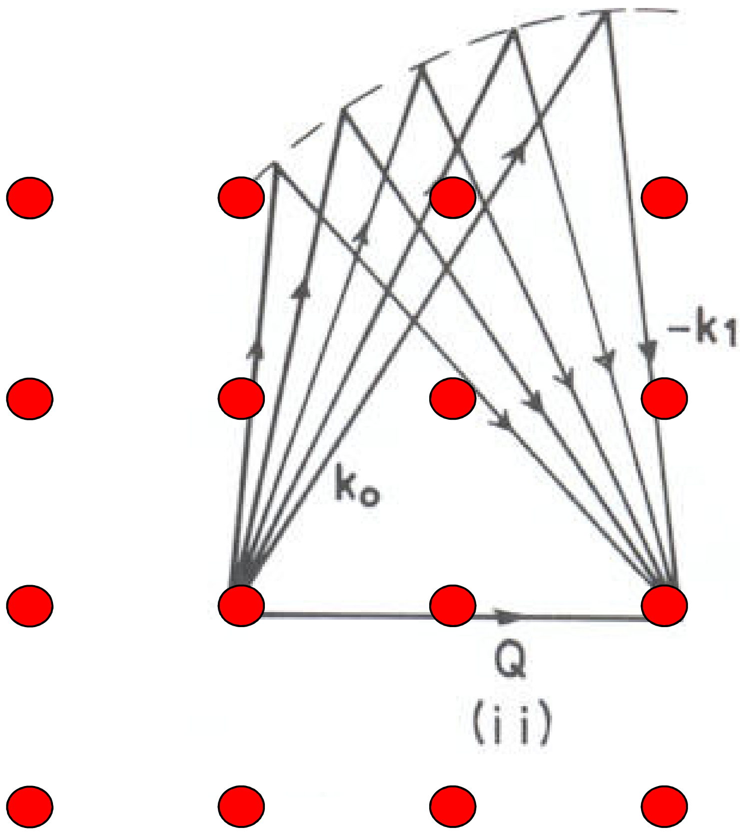
Two different ways of performing constant-Q scans

Mapping Momentum – Energy (Q-E) space

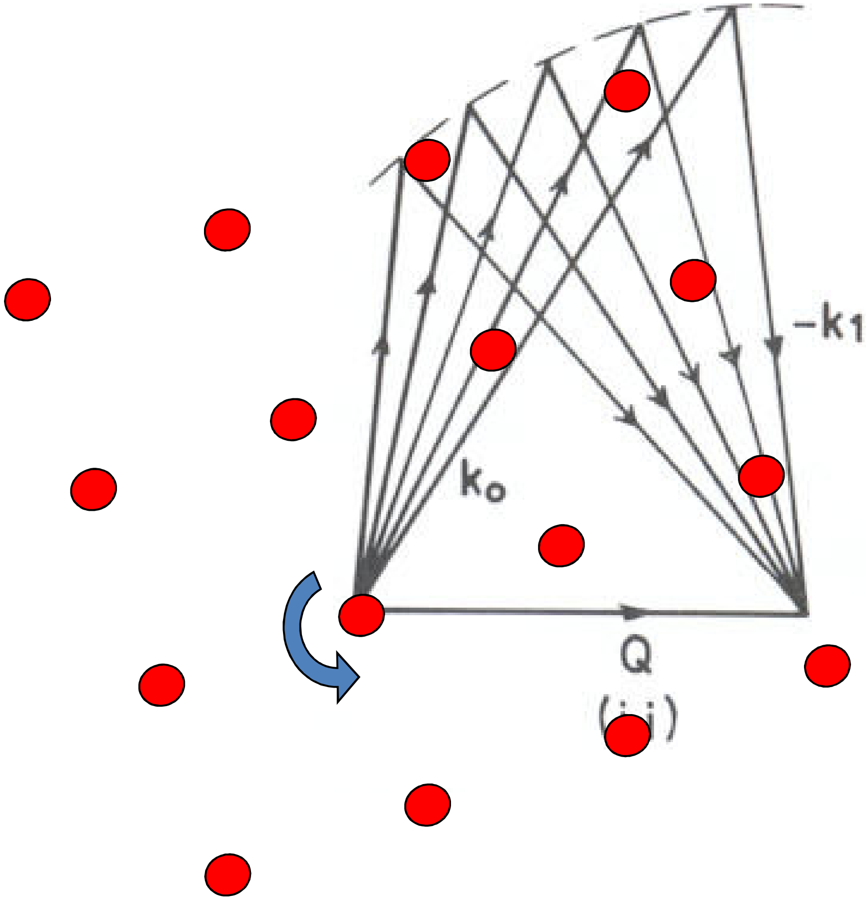
Origin of reciprocal space;

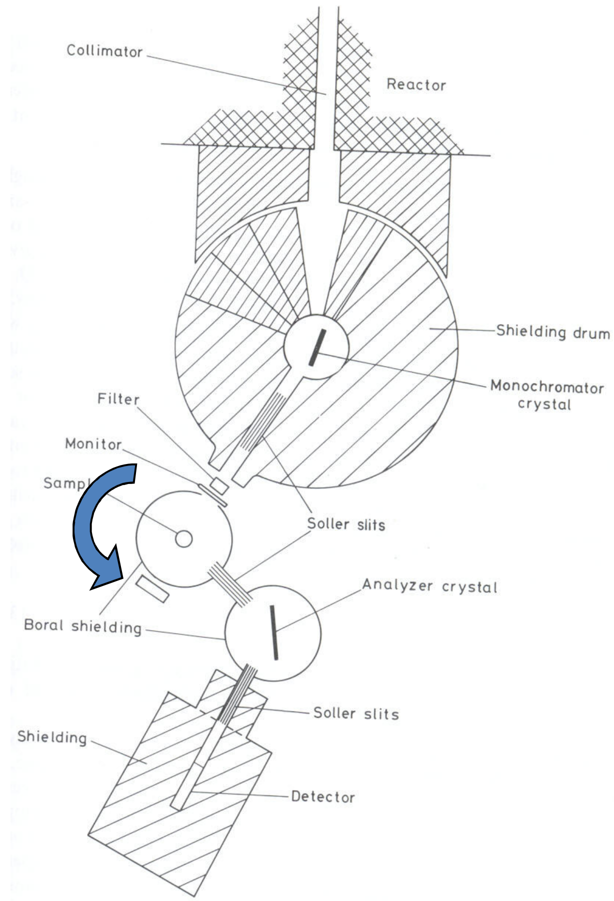
Remains fixed for any sample rotation





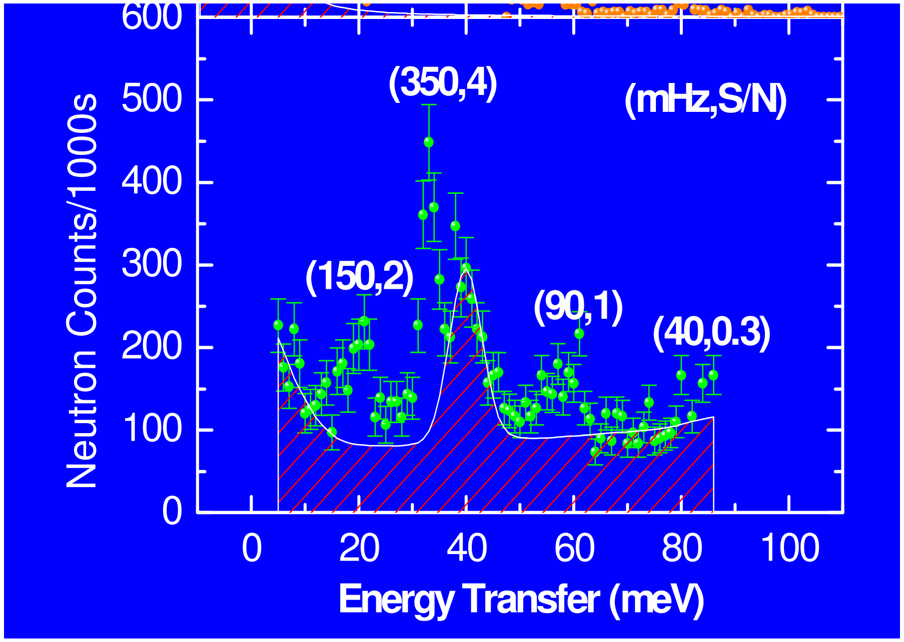
-k1
k0
Q
(ii)


-k1
k0
Q
(i,i)


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

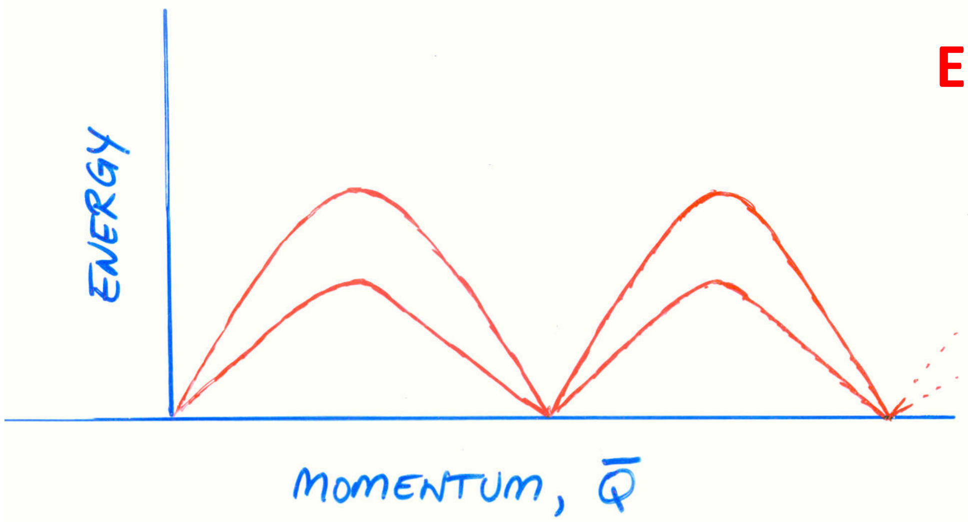
Spurions

- **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 $\lambda/2$

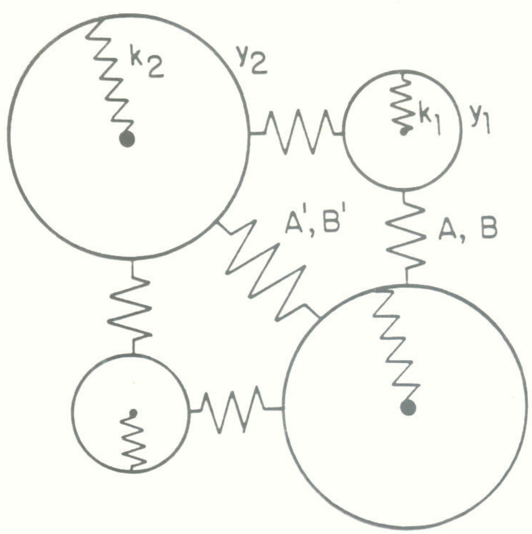


- **incoherent – Bragg – Bragg**
  - Sample 2θ in Bragg condition for k_f-k_f
  - Even for inelastic config, weak incoherent from mono

Elementary Excitations in Solids

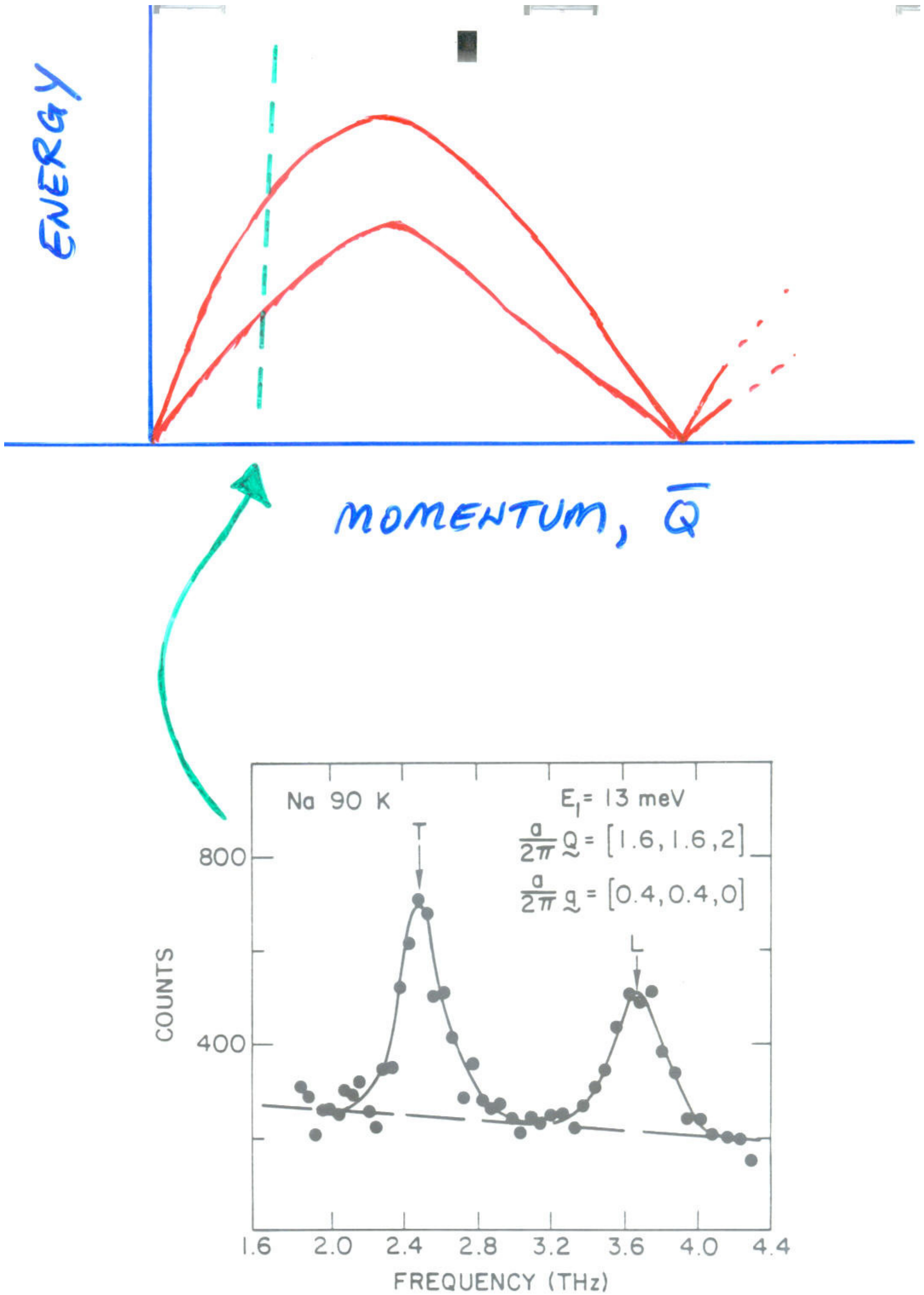


- Lattice Vibrations (Phonons)
- Spin Fluctuations (Magnons)



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

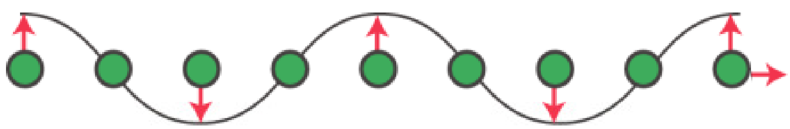
Map out elementary excitations
In Q-energy space (dispersion
Surface)

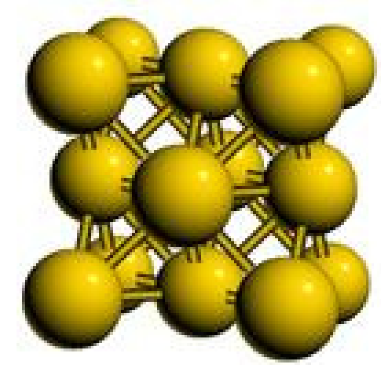
Phonons

- Normal modes in periodic crystal → wavevector

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

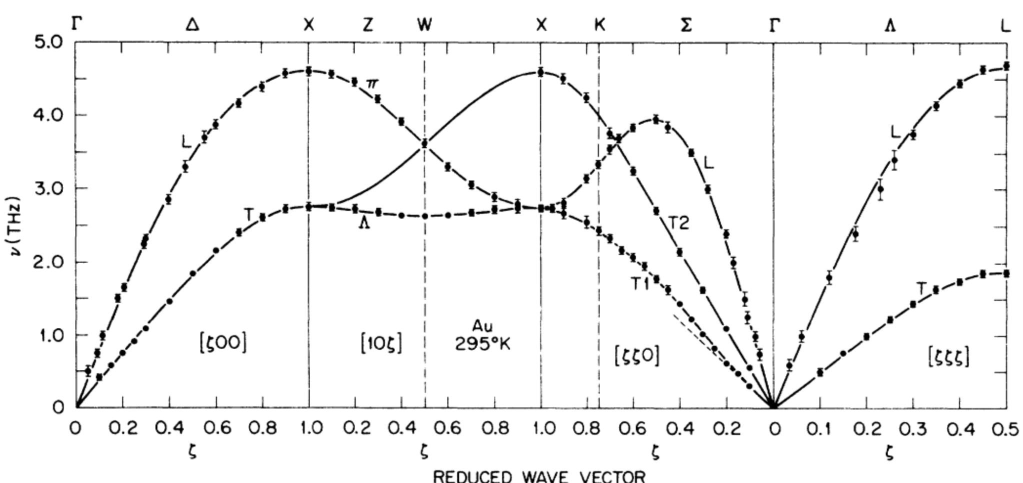
- Energy of phonon depends on **q** and polarization



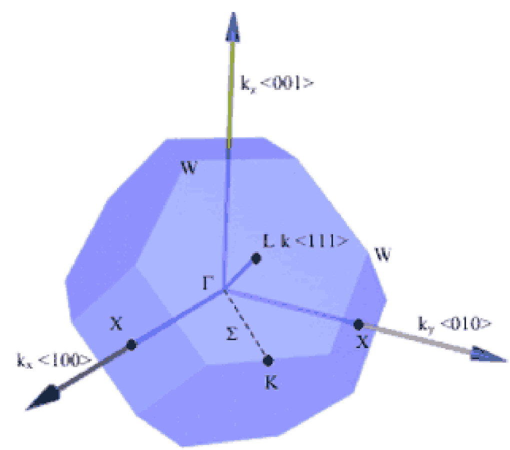


FCC structure

Longitudinal mode / Transverse mode



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

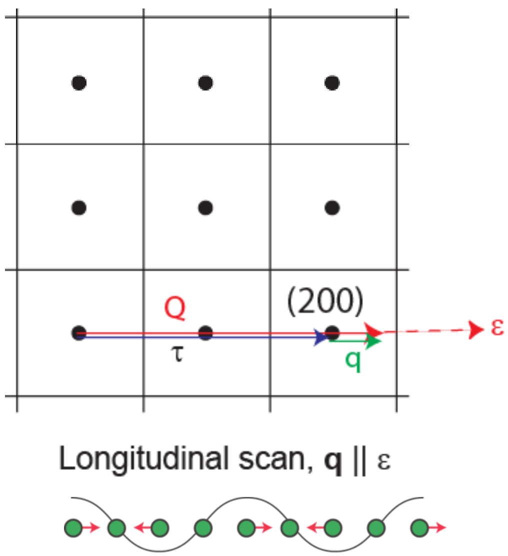


FCC Brillouin zone

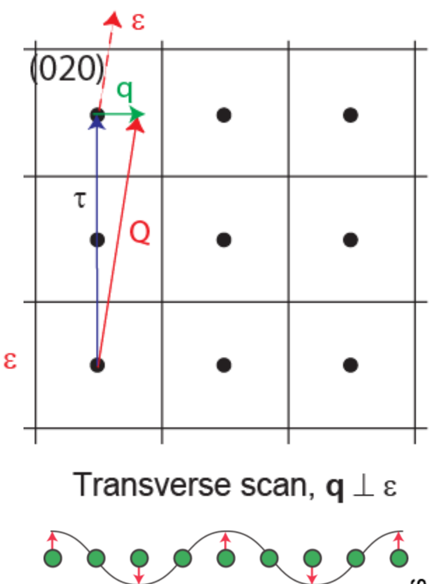
Phonon intensities

Structure (polarization) factor

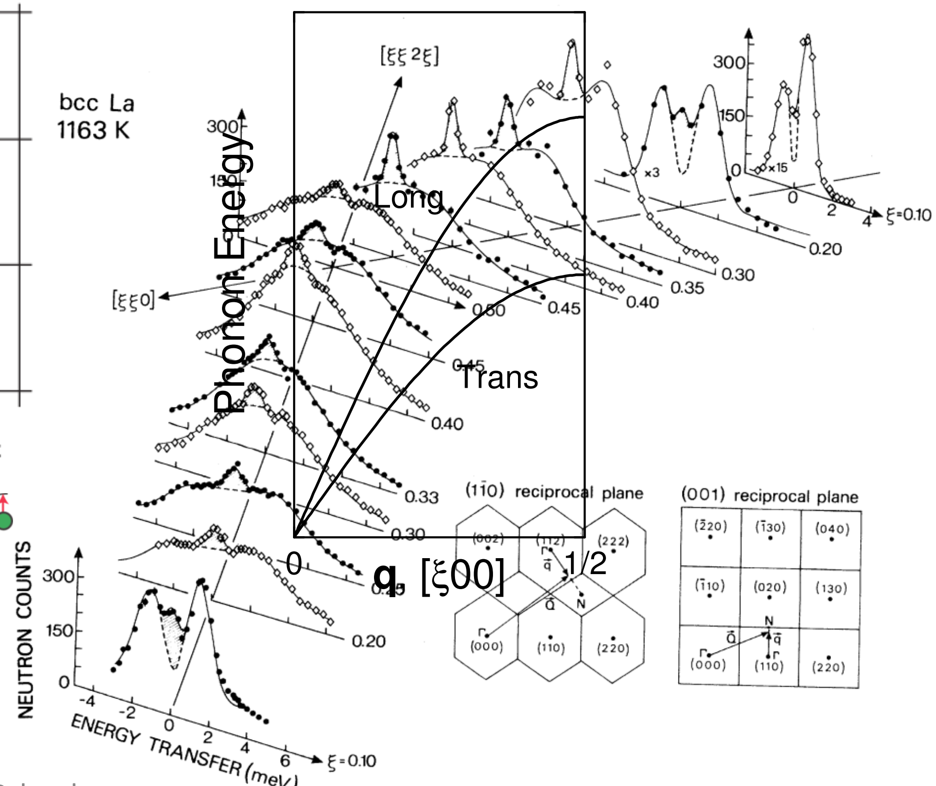
$$S_{1+}(\mathbf{Q},\omega)=\frac{1}{2NM}e^{-Q^2\langle u^2\rangle}\sum_{j\mathbf{q}}\frac{\left|\mathbf{Q}\cdot\boldsymbol{\varepsilon}_j(\mathbf{q})\right|^2}{\omega_j(\mathbf{q})}\left(1+n(\omega)\right)\delta(\mathbf{Q}-\mathbf{q}-\boldsymbol{\tau})\delta\left(\omega-\omega_j(\mathbf{q})\right)$$



Longitudinal scan, **q** || ε

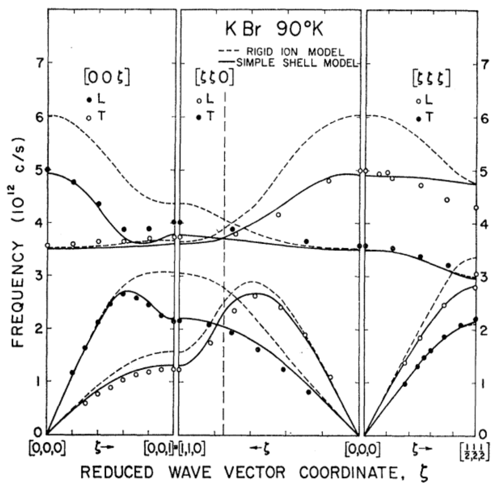


Transverse scan, **q** ⊥ ε

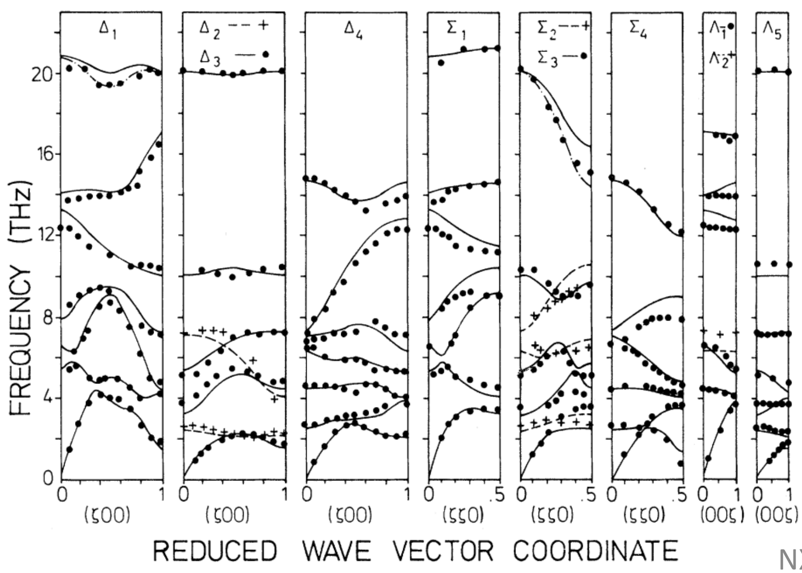


Guthoff *et al., Phys. Rev. B* **47**, 2563 (1993).

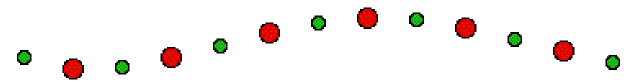
More complicated structures



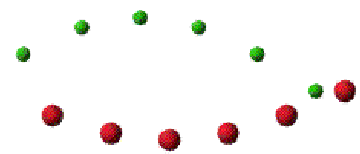
Woods, *et al., Phys. Rev*. **131**, 1025 (1963).



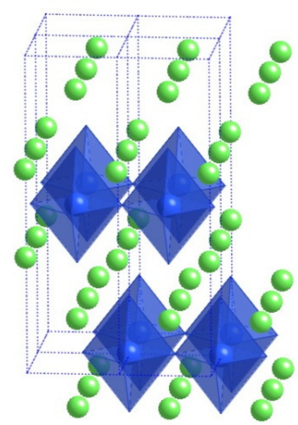
Chaplot, *et al., Phys. Rev*. B **52**, 7230(1995).



Acoustic phonon



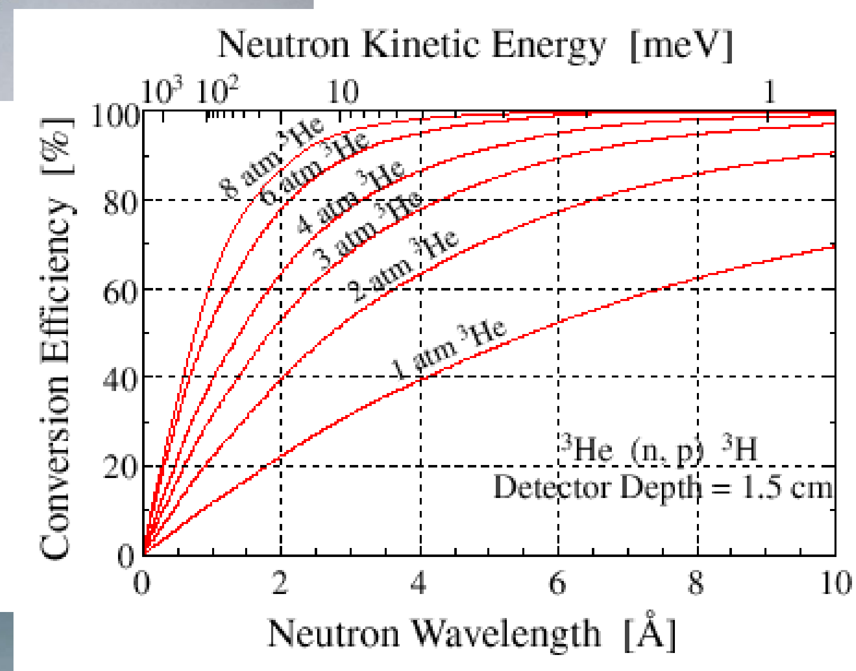
Optical phonon



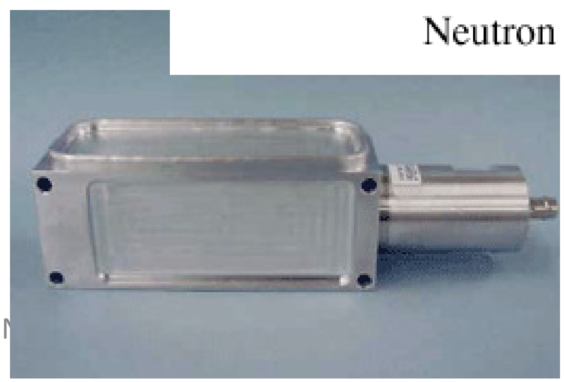
La_2CuO_4

Detectors

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

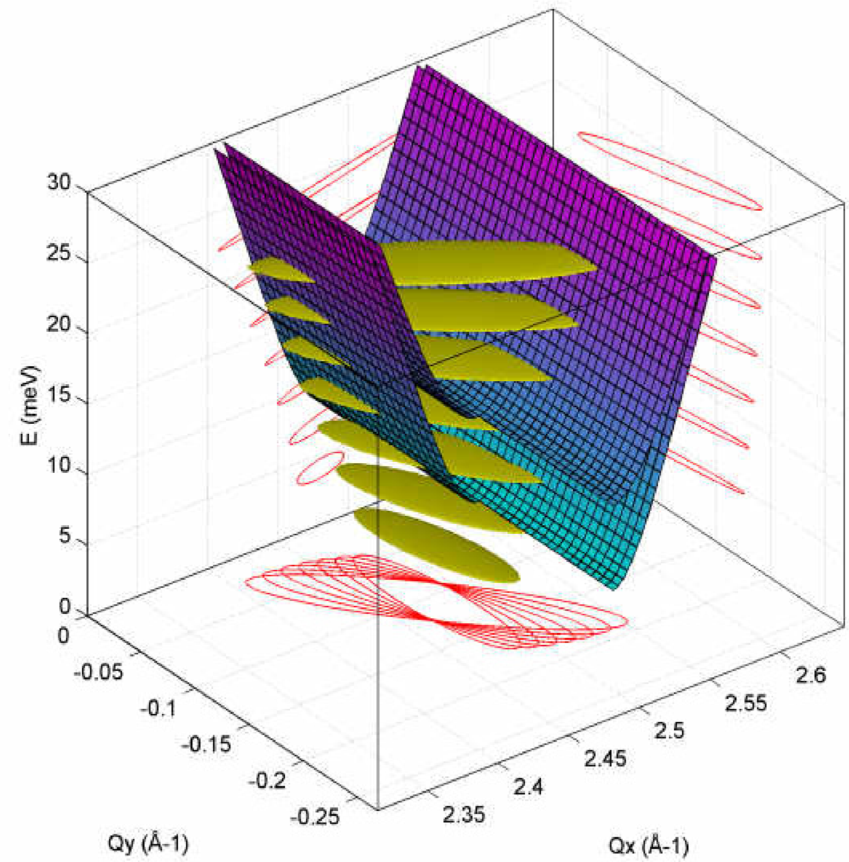


- **Beam monitors**
- Low efficiency detectors for measuring beam flux



Resolution

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

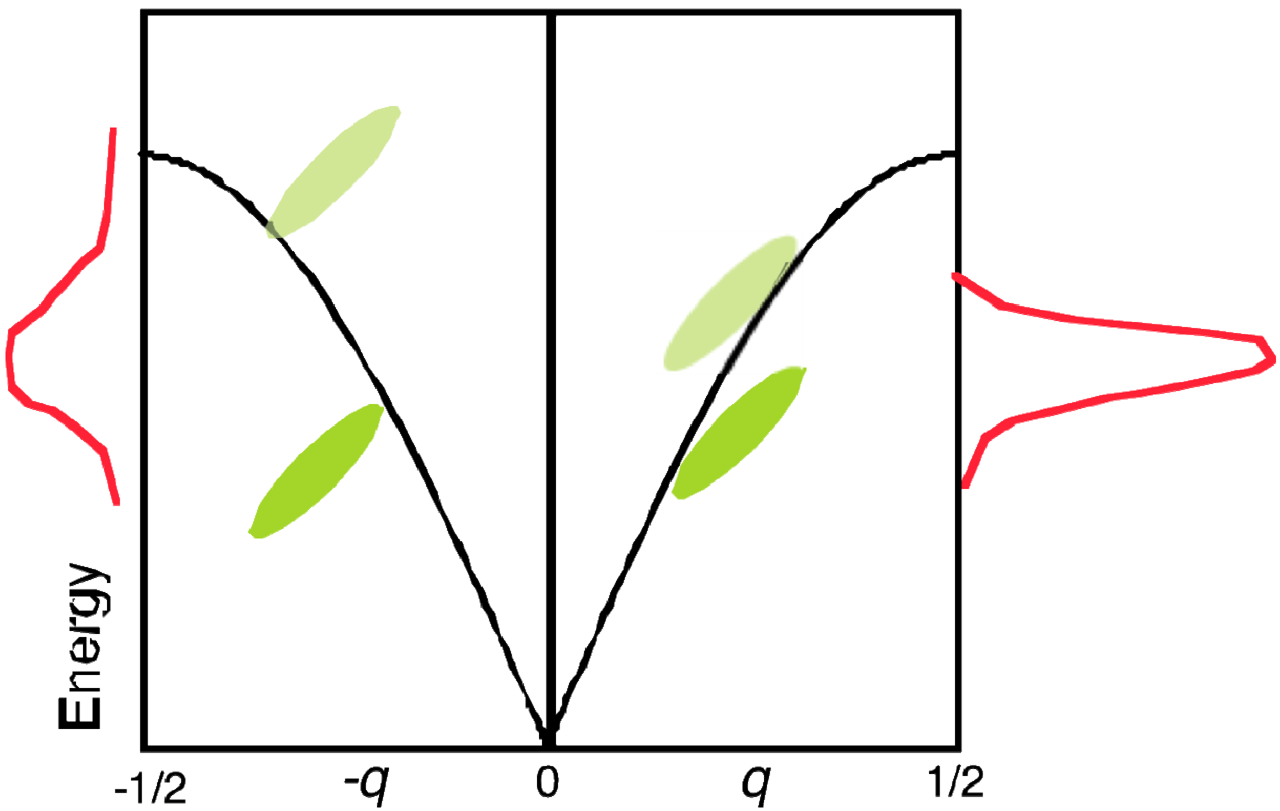


- **Resolution convolutions**

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

Resolution focusing

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



References

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

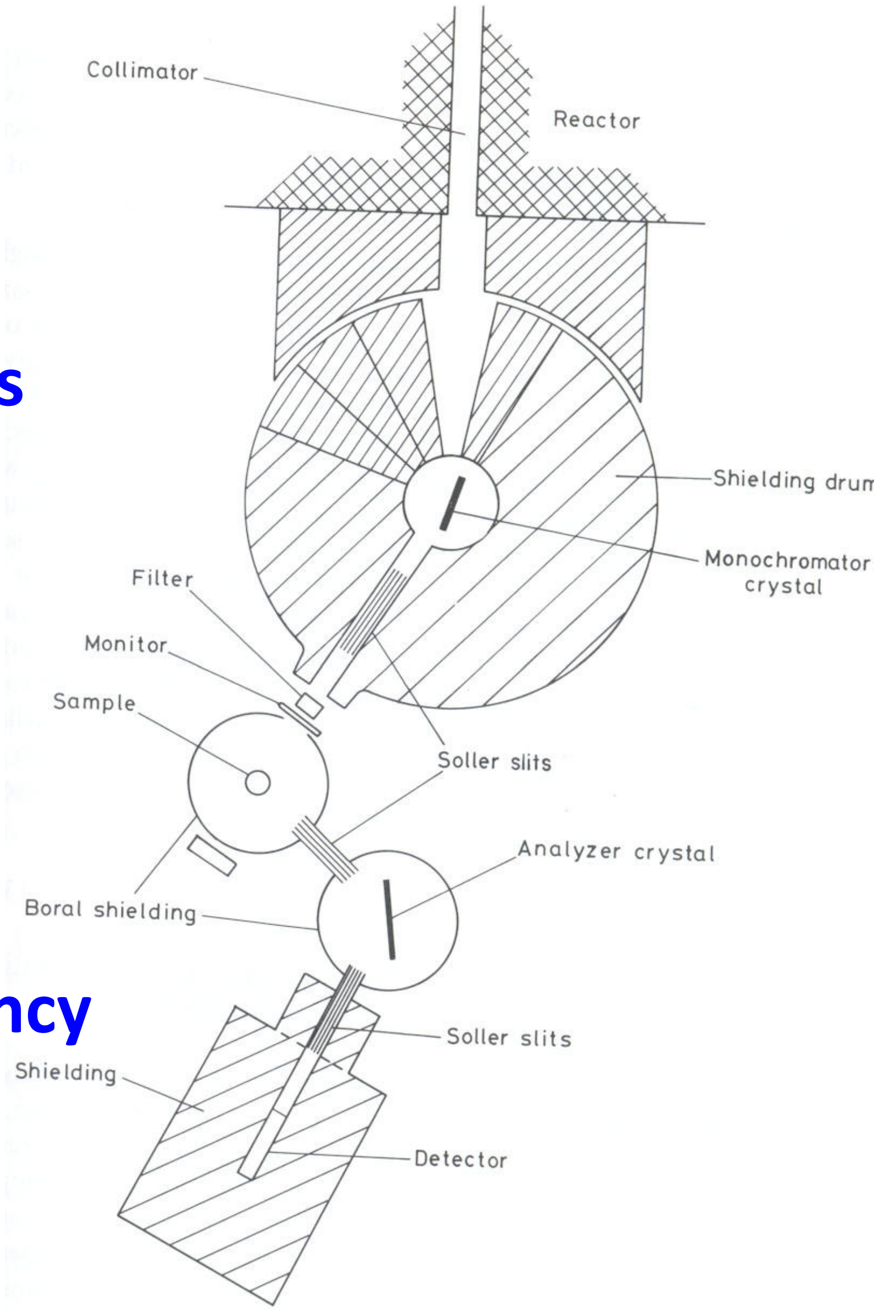
B. Fultz, http://www.cacr.caltech.edu/projects/danse/ARCS_Book_16x.pdf

Constant k_f:

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

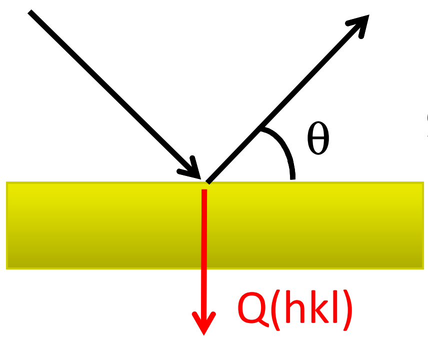
- k_i, θ_M do change, but
monitor detector normalizes to incident neutron flux

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

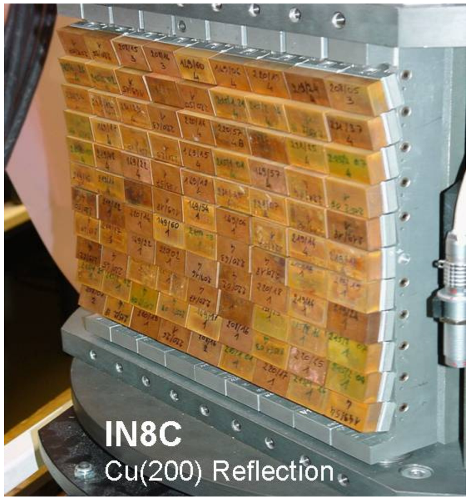


Monochromators

- **Selects the incident wavevector**



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

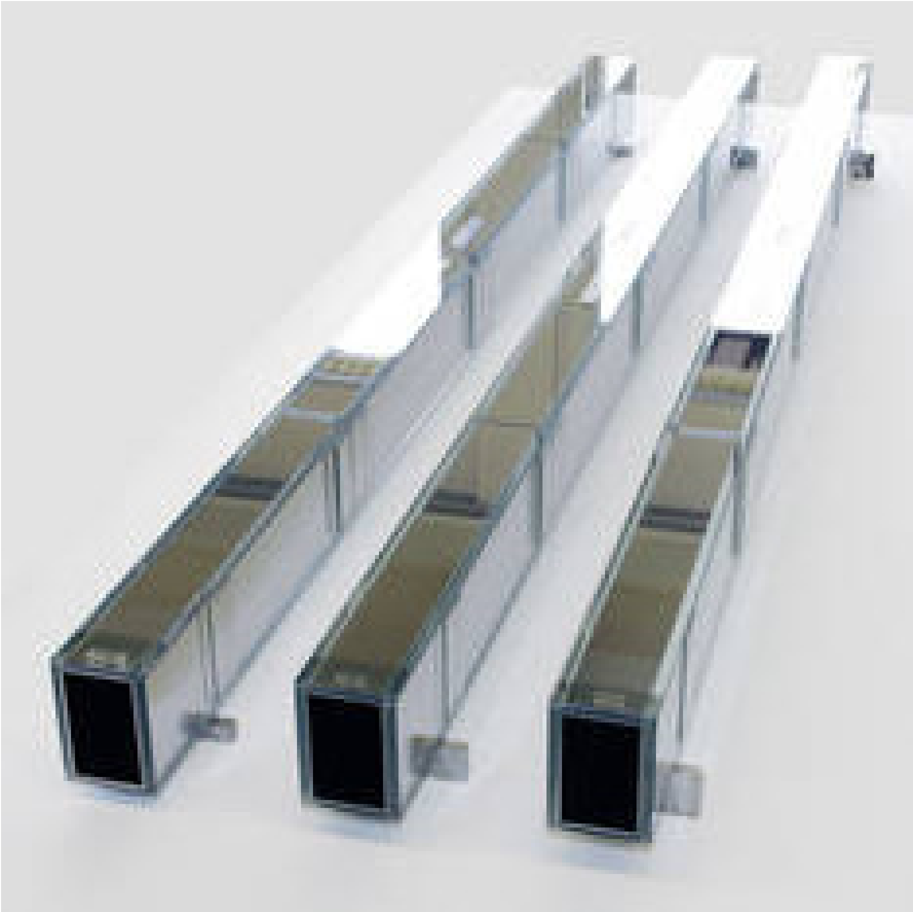


- Reflectivity
- focusing
- high-order contamination
  eg. λ/2 PG(004)

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

Guides

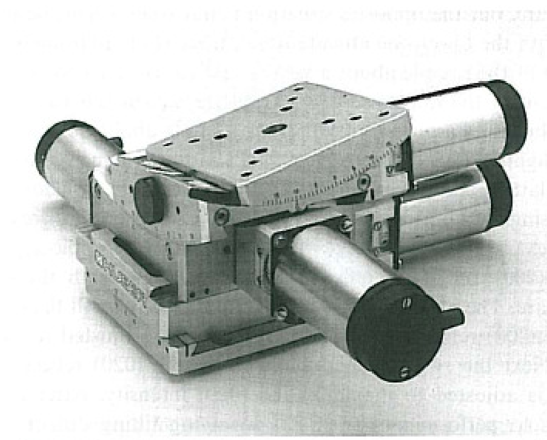
- **Transport beam over long distances**
- **Background reduction**
- **Total external reflection**
  - Ni coated glass
  - Ni/Ti multilayers (supermirror)

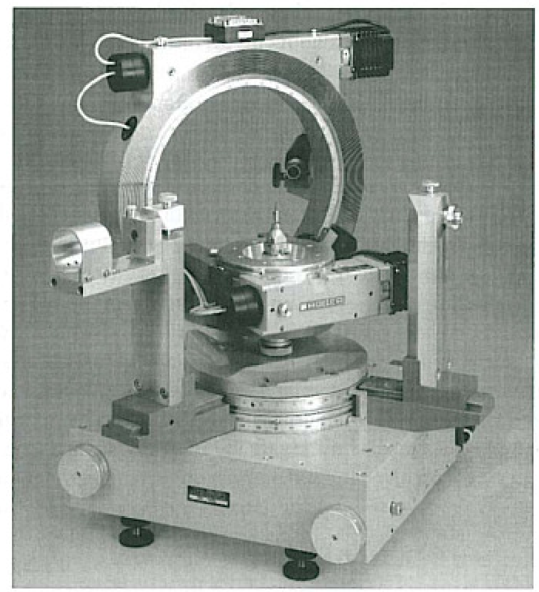


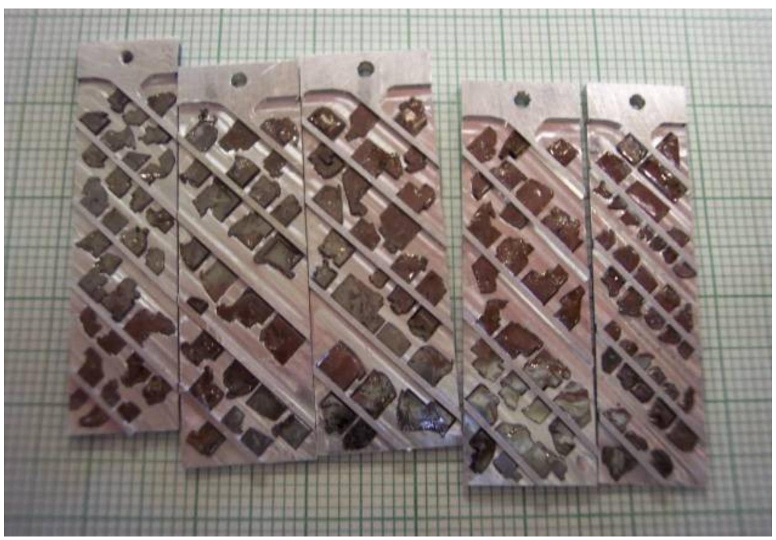
Samples

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

- **Sample rotation**
- **Sample tilt**







Co-aligned $CaFe_2As_2$ crystals