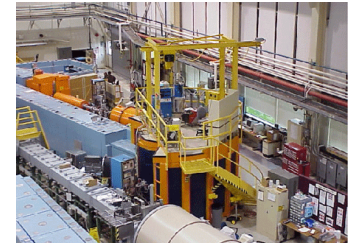
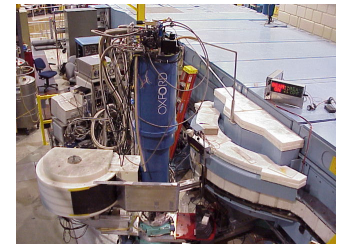
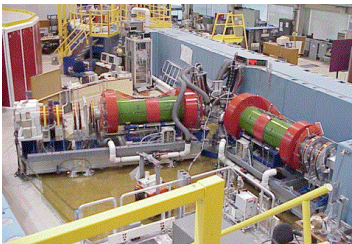


Choosing the Right Neutron Spectrometer



NCNR →

Peter Gehring
NIST Center for Neutron Research



Main Messages of the Week



(1) Neutron scattering experiments measure the flux of neutrons scattered by a sample into a detector as a function of the change in neutron wave vector (\vec{Q}) and energy ($\hbar\omega$).

Momentum

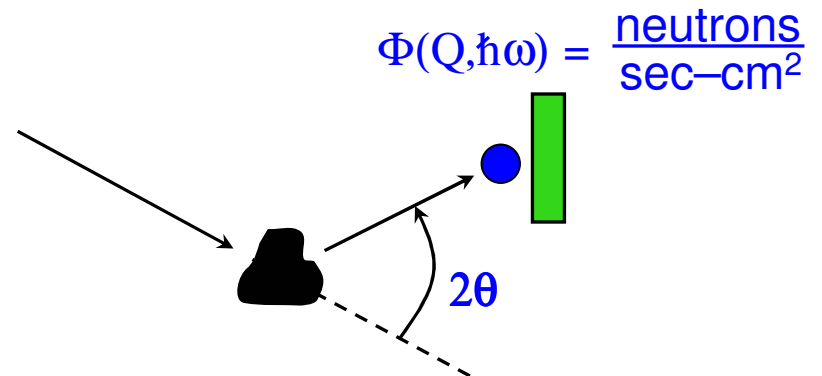
$$\hbar k = \hbar(2\pi/\lambda)$$

$$\hbar Q = \hbar\vec{k}_i - \hbar\vec{k}_f$$

Energy

$$\hbar\omega_n = \hbar^2 k_n^2 / 2m$$

$$\hbar\omega = \hbar\omega_i - \hbar\omega_f$$



(2) The expressions for the scattered neutron flux Φ involve the positions and motions of atomic nuclei or unpaired electron spins.

$$\Phi = f\{\vec{r}_i(t), \vec{r}_j(t), \vec{S}_i(t), \vec{S}_j(t)\}$$



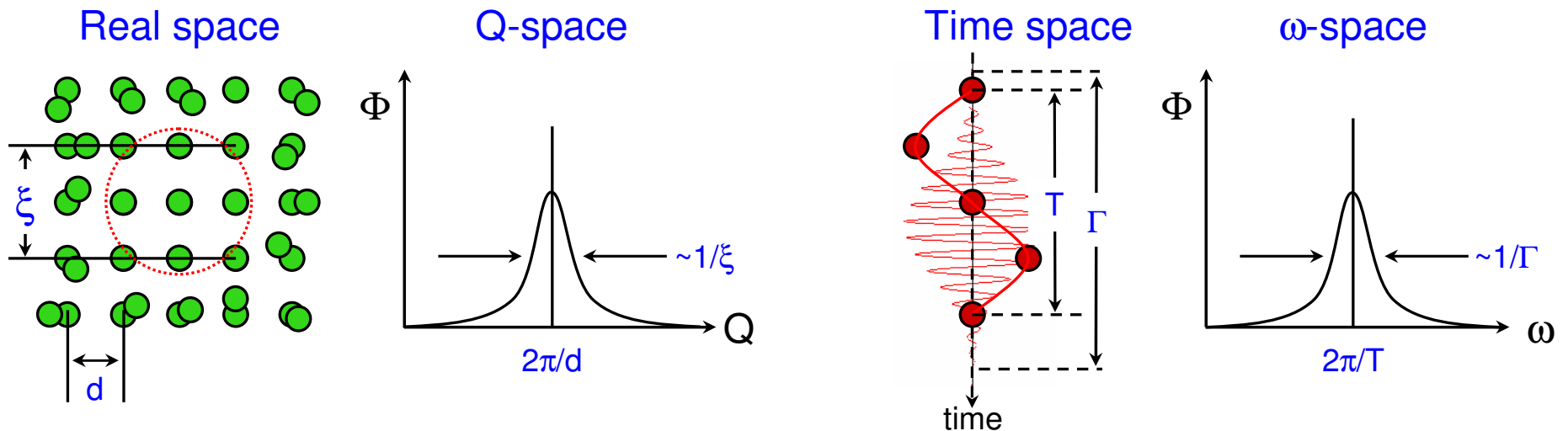
Φ provides information about all of these quantities!

Main Messages of the Week

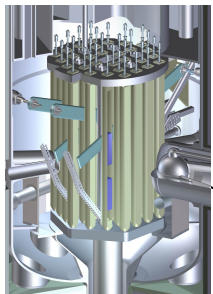


(3) The scattered neutron flux $\Phi(\vec{Q}, \hbar\omega)$ is proportional to the space (\vec{r}) and time (t) Fourier transform of the probability $G(\vec{r}, t)$ of finding one or two atoms separated by a particular distance at a particular time.

$$\Phi \propto \frac{\partial^2 \sigma}{\partial \Omega \partial \omega} \propto \iint e^{i(\vec{Q} \cdot \vec{r} - \omega t)} G(\vec{r}, t) d^3 \vec{r} dt$$



What is required to do an inelastic neutron scattering experiment?



A source

(E_i, \vec{k}_i)

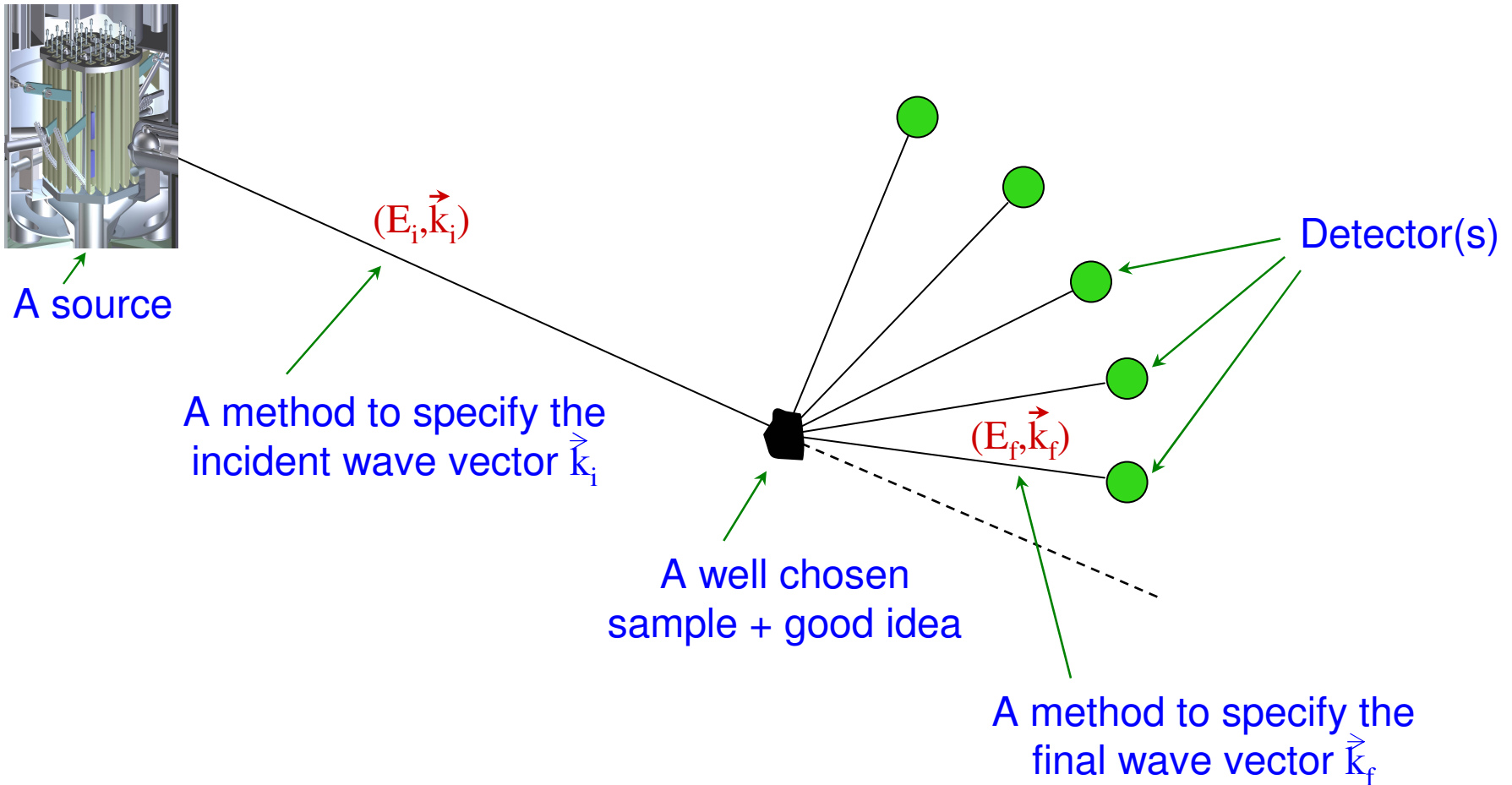
A method to specify the incident wave vector \vec{k}_i

A well chosen sample + good idea

(E_f, \vec{k}_f)

A method to specify the final wave vector \vec{k}_f

Detector(s)

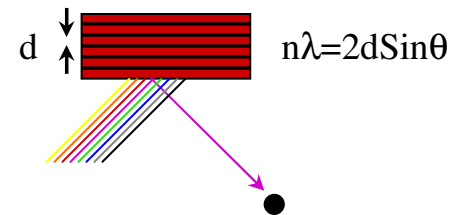


Methods of specifying and measuring \vec{k}_i and \vec{k}_f



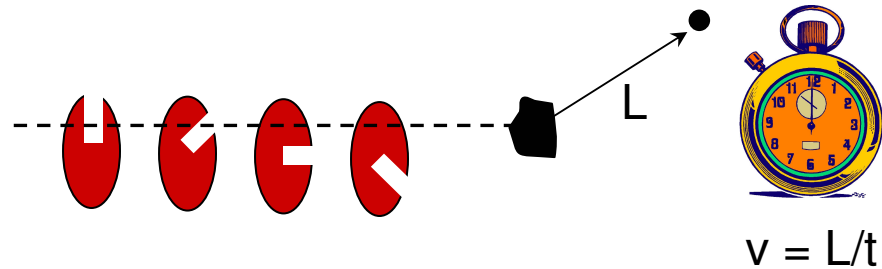
1. Bragg Diffraction

SPINS, FANS, Backscattering



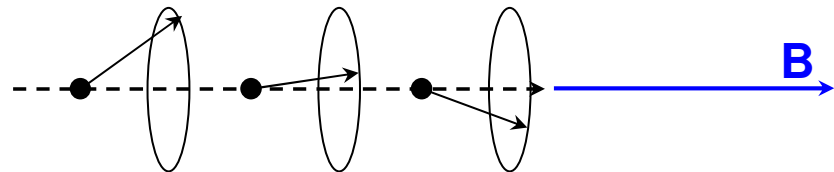
2. Time-of-Flight (TOF)

DCS, Backscattering (?)



3. Larmor Precession

Spin Echo



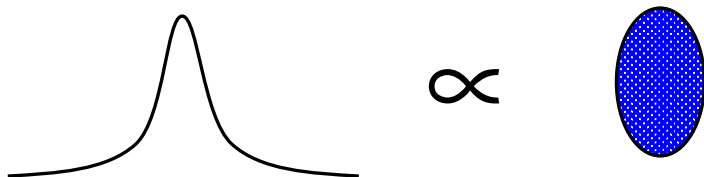
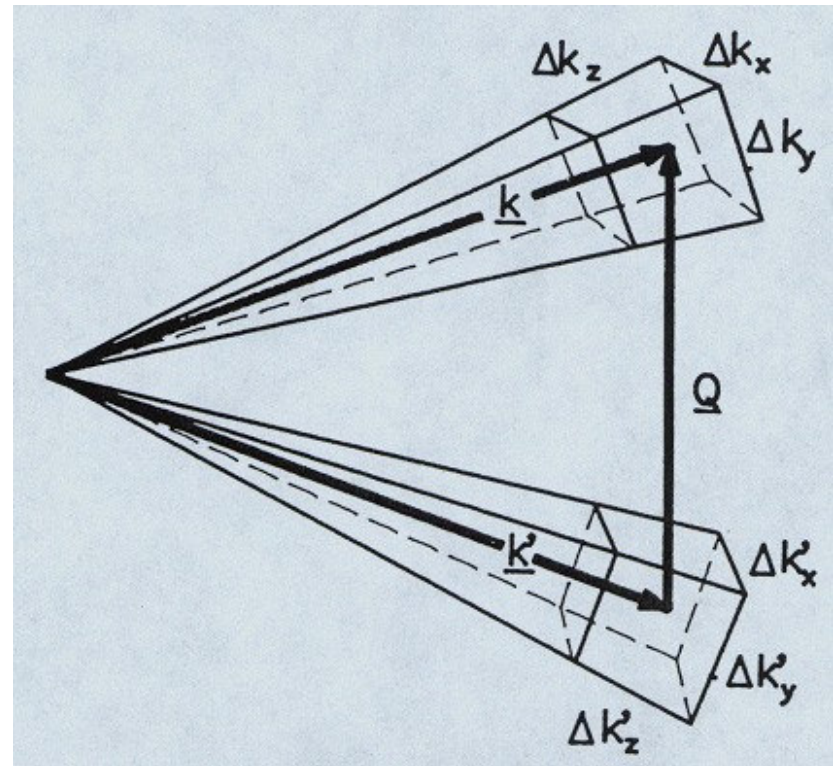
Why are there so many different spectrometers?



Because neutron scattering is an intensity limited technique. Thus detector coverage and resolution **MUST** be tailored to the science.

Uncertainties in the neutron wavelength and direction imply that \mathbf{Q} and $\hbar\omega$ can only be defined with a certain precision.

The total signal in a scattering experiment is proportional to the resolution volume \rightarrow better resolution leads to lower count rates! So choose *carefully* ...



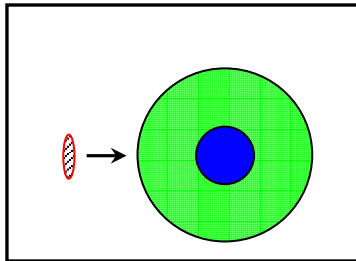
Courtesy of R. Pynn

Q-Resolution Matters!

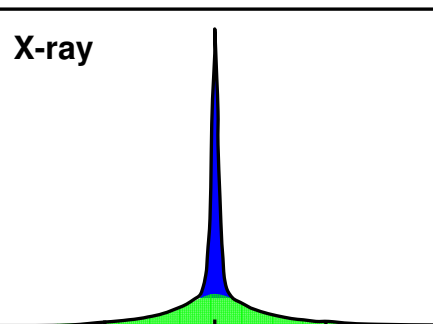
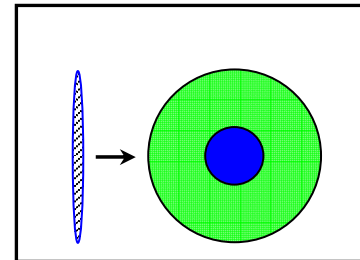


The “right” resolution depends on what you want to study.

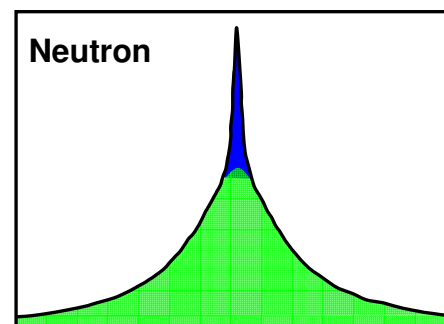
X-ray



Neutron

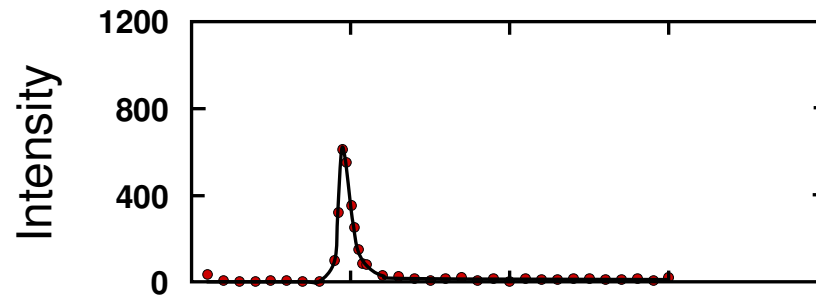
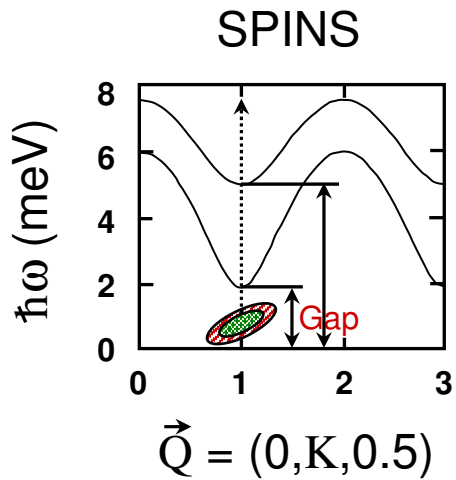


-0.050 -0.025 0.000 0.025 0.050
 q (\AA^{-1})



-0.050 -0.025 0.000 0.025 0.050
 q (\AA^{-1})

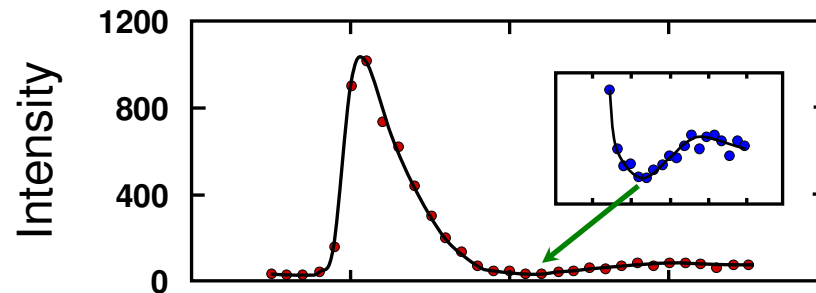
$\hbar\omega$ -Resolution Matters!



Focusing Analyzer



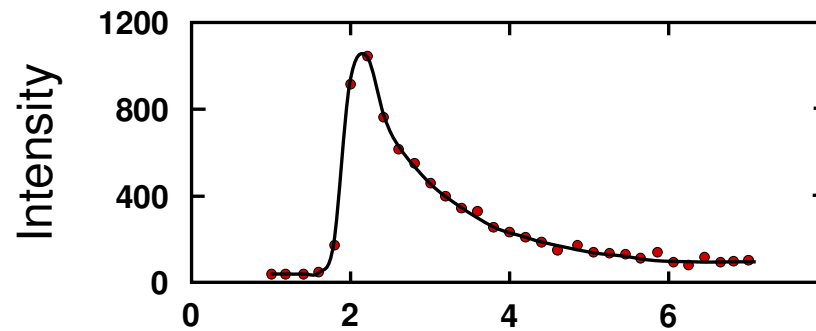
Flat



Focusing Analyzer



5 Blades



Focusing Analyzer



9 Blades

$\hbar\omega$ -Resolution Matters!



Another example ...

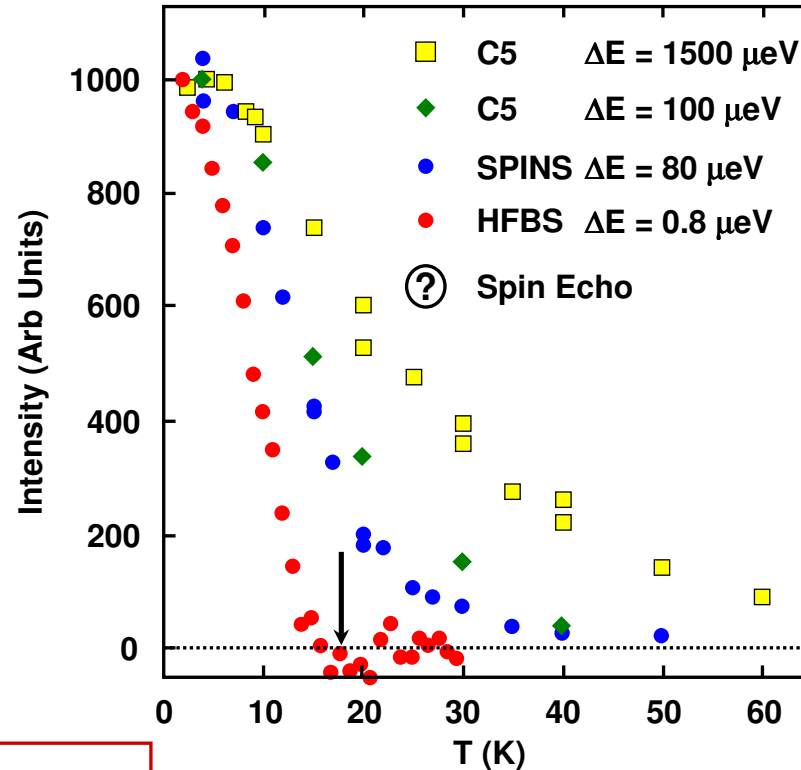
$\text{YBa}_2\text{Cu}_3\text{O}_{6.35}$
 $T_c = 18\text{K}$

Magnetic order occurs
at $Q = (1/2, 1/2, 2)$.

But what is T_N ?

A “fatter” energy resolution integrates
over low-energy fluctuations ...

“Elastic” Bragg Peak Intensity



So, how do I choose the right spectrometer?



Two basic considerations:

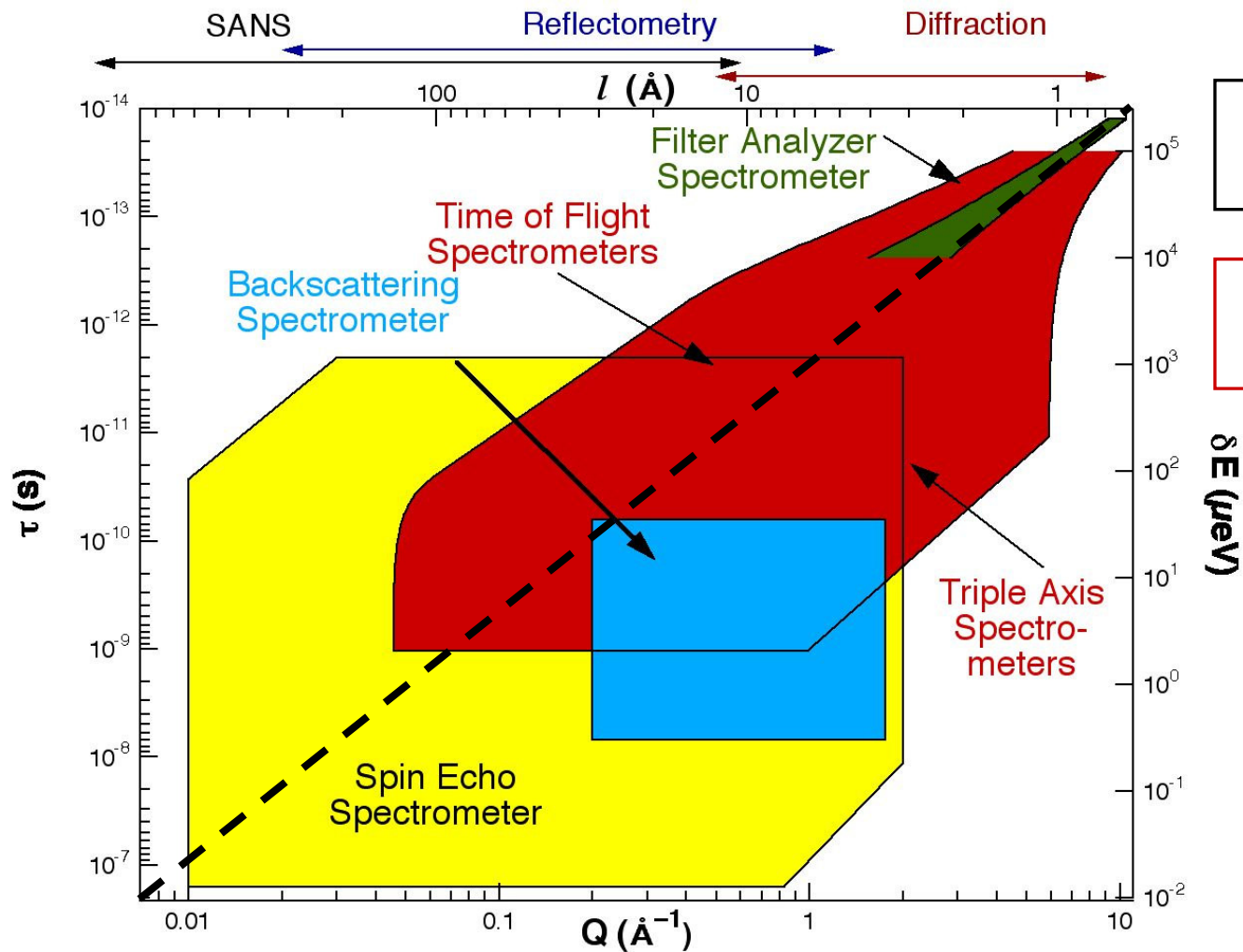
1. What are the **time** scales ($\hbar\omega$) of interest?
2. What are the **length** scales (Q) of interest?

(Some spectrometers overlap \rightarrow the choice may boil down to one of **resolution**)

Two additional considerations:

1. What **energy** resolution ($\Delta\hbar\omega$) is required?
2. What **momentum** resolution (ΔQ) is required?

Different spectrometers cover different regions of phase space



Do you see a pattern here?

Larger "objects" tend to imply slower motions.

Rules of Thumb



1. What are the energies ($\hbar\omega$) / time scales ($\Delta t \sim 1/\omega$) of interest?

$\hbar\omega > 10\text{-}20 \text{ meV}$ - use FANS (or another spectrometer designed for vibrational spectroscopy)

$\hbar\omega < 20\text{-}30 \text{ } \mu\text{eV}$ - use HFBS

In between - use DCS (or another cold neutron TOF spectrometer)

2. Be certain that the length scales of the relevant motions lie within the range of the spectrometer.

As a simple example, consider the HFBS instrument. ($Q \sim 2\pi/L$)

$$Q_{\min} = 0.25 \text{ \AA}^{-1} \rightarrow L_{\max} \sim 25 \text{ \AA}$$

$$Q_{\max} = 1.75 \text{ \AA}^{-1} \rightarrow L_{\min} \sim 3.5 \text{ \AA}$$

REMEMBER - Q_{\min} and Q_{\max} are inversely proportional to the incident neutron wavelength

DCS versus SPINS



DCS – incoherent scattering, surveys

SPINS – limited region of Q - ω

Rules of Thumb: (think carefully before violating)

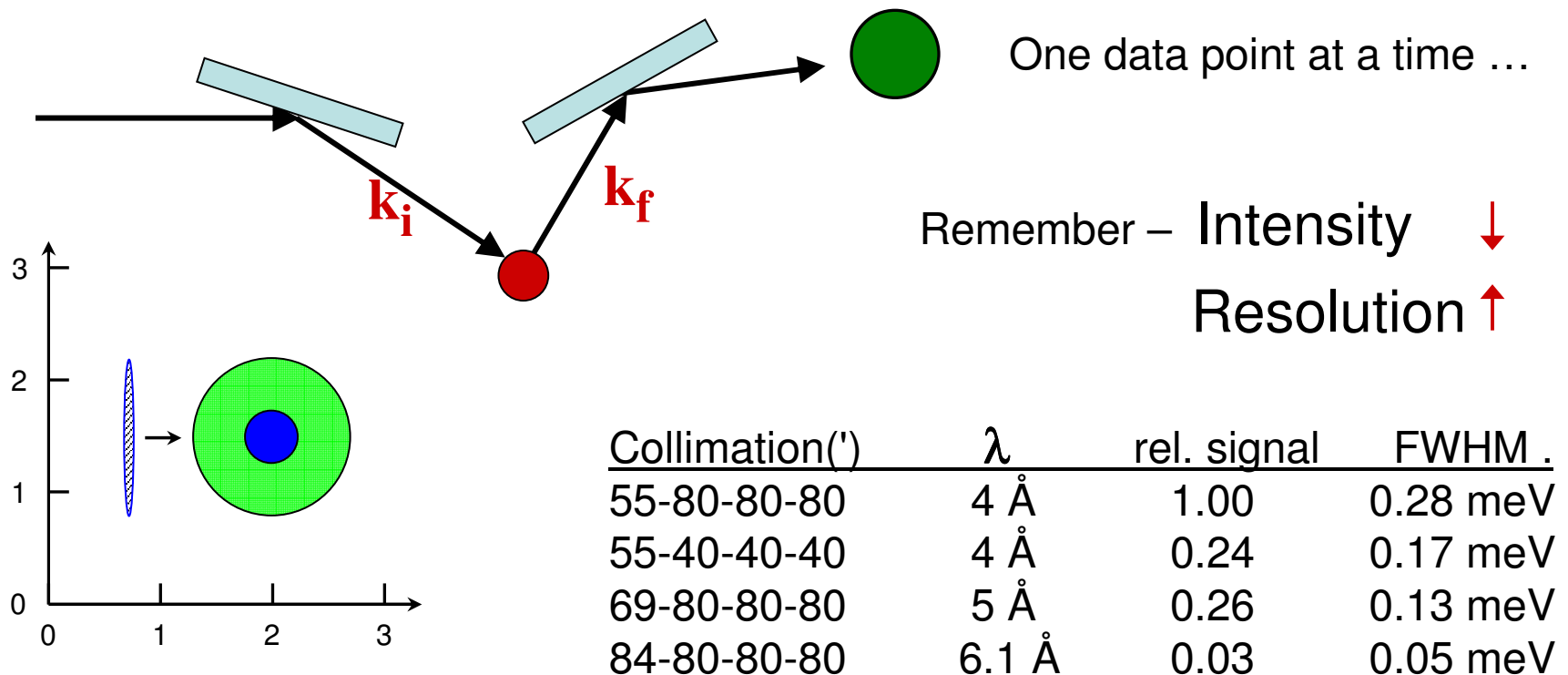
DCS – systems requiring resolution $< 100 \mu\text{eV}$

SPINS – single crystals

Things to consider when choosing SPINS



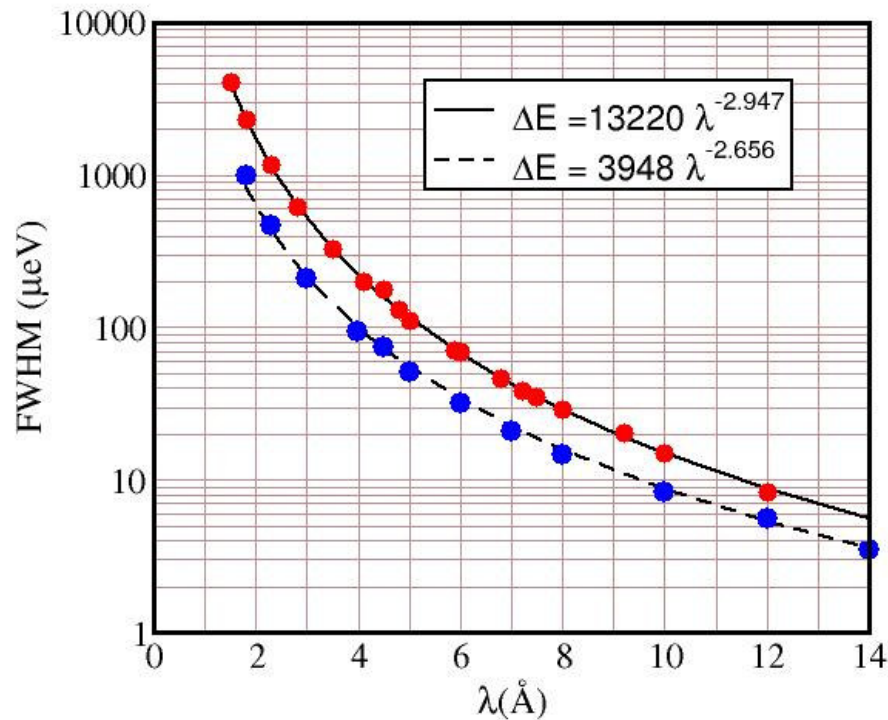
Triple axis spectrometers are typically used when either the direction of \mathbf{Q} is important or the interesting region of \mathbf{Q} - ω space is of limited extent.



Things to consider when choosing DCS



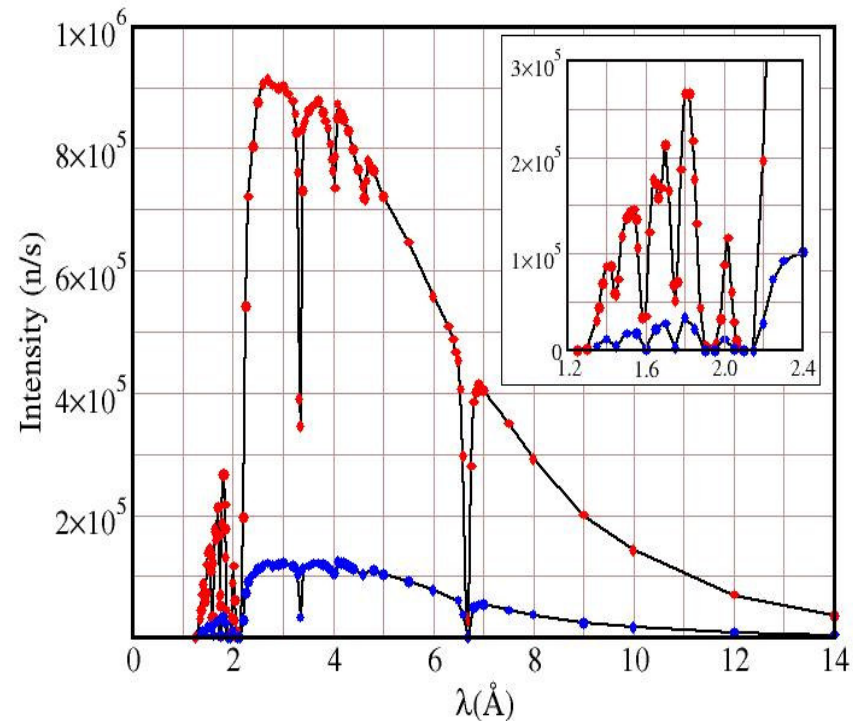
ΔE



Quantities varied

- wavelength λ
- chopper slot widths W

$I(E)$



Remember – Intensity ↓
Resolution ↑

Things to consider when choosing NSE



If the resolution of backscattering is “not good enough” or if you are only interested in a “limited” region of **Q** space (typically small **Q**) ...

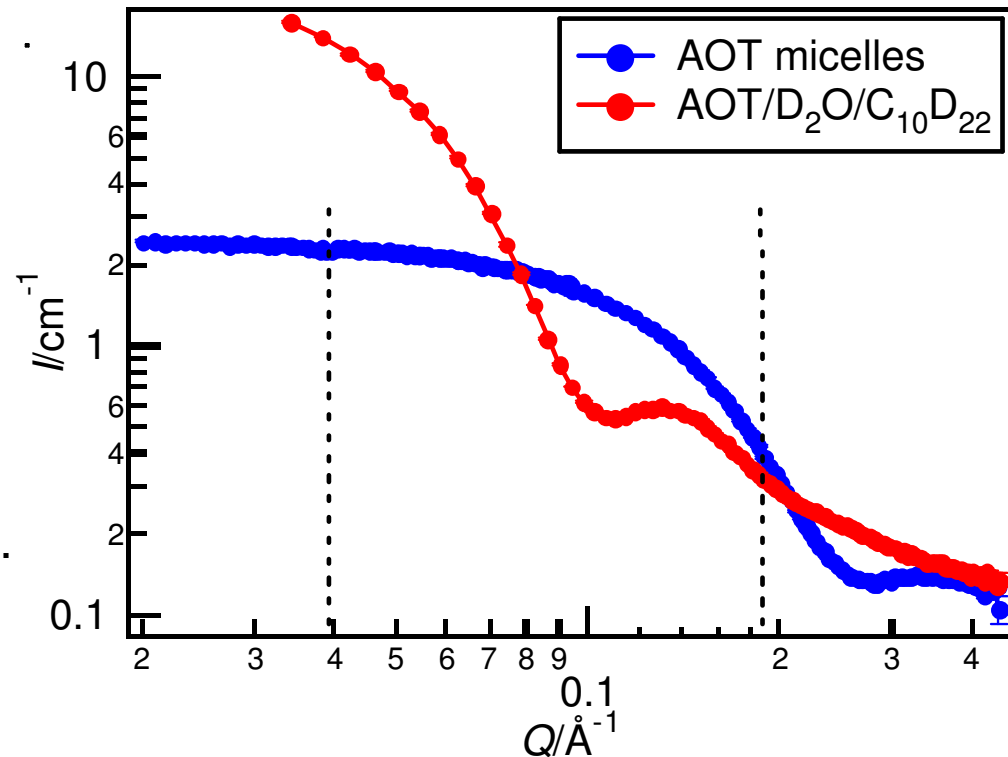
... use NSE (low **Q**, long times)

These cases typically involve coherent scattering, which tends to peak around

$$Q \sim \frac{2\pi}{\text{Relevant length scale of sample}}$$

Remember – slower motions usually imply larger length scales.

Many atoms moving together
=> Coherent scattering



Things to consider about your sample



Is your sample polycrystalline or amorphous?

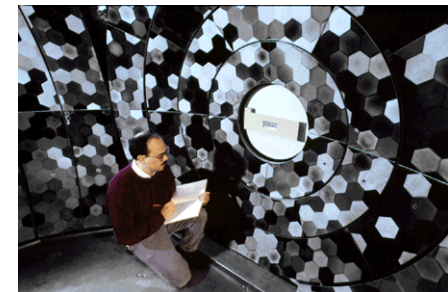
Does **ONLY** the magnitude (not the direction) of **Q** matter?

Is the expected **Q**-dependence of the scattering weak?

This often means that you want to look at a large region of **Q- $\hbar\omega$** space or that you can sum the data over a large region of **Q- $\hbar\omega$** space

If **YES**, consider instruments with large analyzer areas

FANS, DCS, Backscattering



General sample “design”



The most important thing is:

Know as much about your sample as possible
(Beamtime costs ~ \$4000/day!!)

The types of things that you might want to know include:

What's the structure (in a general sense)?

Are there any phase transitions (or a glass transition)?

What isotopes are present?

Supplementary data from other measurements ...

Magnetization vs T

Muon spin relaxation

X-ray data

Specific heat vs T

Raman spectroscopy

General sample “design”



Try to avoid isotopes that are strongly absorbing



For a complete listing go to

<http://www.ncnr.nist.gov/resources/n-lengths>

Sample “design” for triple-axis spectrometers

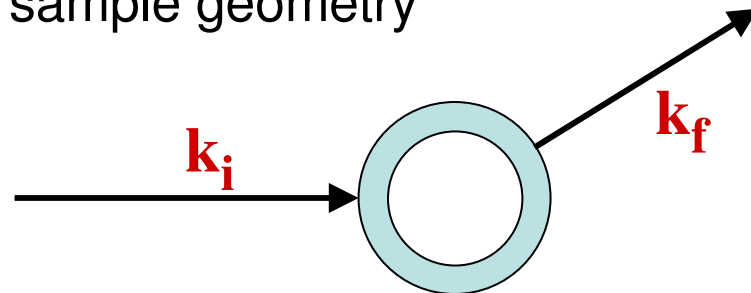


Single Crystals yield the most information

Increase the intensity by increasing the amount of sample

If you have a powder, use a cylindrical container (rather than flat plate)

Annular may be the best sample geometry



Almost all experiments on triple-axis spectrometers involve coherent scattering
→ sample should be deuterated (if it contains H at all)

Sample “design” for DCS and HFBS



Increase the intensity by increasing the amount of sample

→ Fill the beam with sample

maximum beam size is usually given in the instrument description

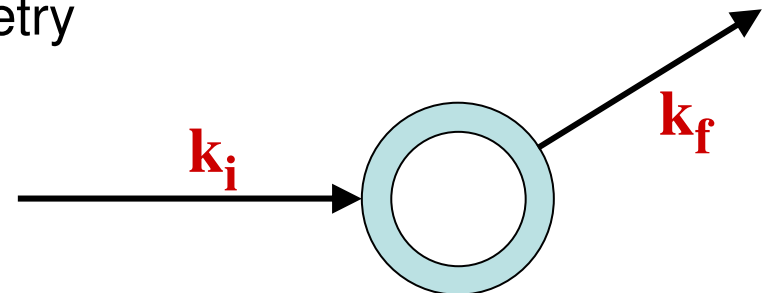
3 cm X 10 cm for DCS (or 1.5 cm X 10cm) 3 cm X 3 cm for Backscattering

If possible, use cylindrical samples (rather than flat plate)

Remember - For incoherent, quasielastic scattering the transmission of the beam should be ~90%

$$I/I_0 = \exp -(n\sigma_T D)$$

Often annular is the best sample geometry



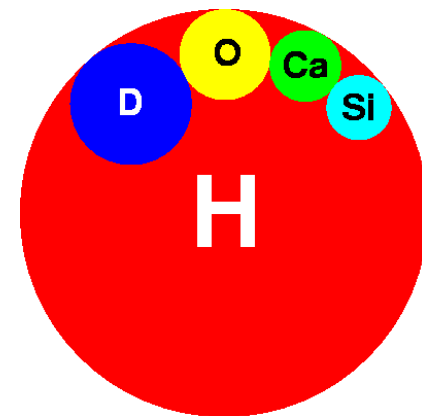
Sample “design” for DCS and HFBS



Does the sample contain H?

Remember: **Neutrons LOVE H!!**

Create a sample where the “interesting” portions of the sample are hydrogenated and the “uninteresting” portions are deuterated.



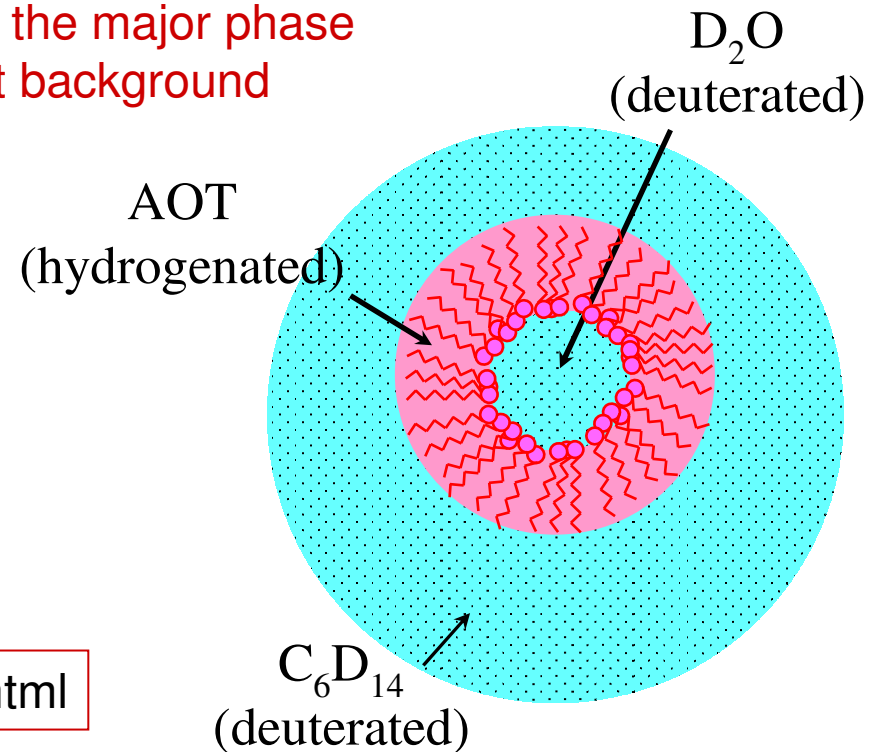
Sample “design” for NSE



Create a sample where the “interesting” portions of the sample have a different SLD than the “uninteresting” portions

Typically this means deuterating the major phase in order to reduce the incoherent background

SLD core	$6.4 \times 10^{-6} \text{ \AA}^{-2}$
SLD shell	$1.0 \times 10^{-6} \text{ \AA}^{-2}$
SLD solvent	$6.5 \times 10^{-6} \text{ \AA}^{-2}$



<http://www.ncnr.nist.gov/resources/sldcalc.html>

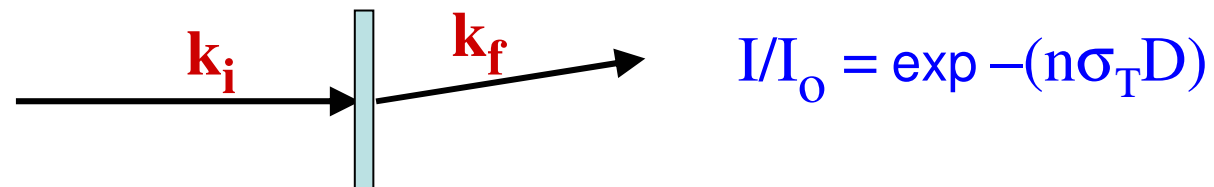
Sample “design” for NSE



Increase the intensity by increasing the amount of sample

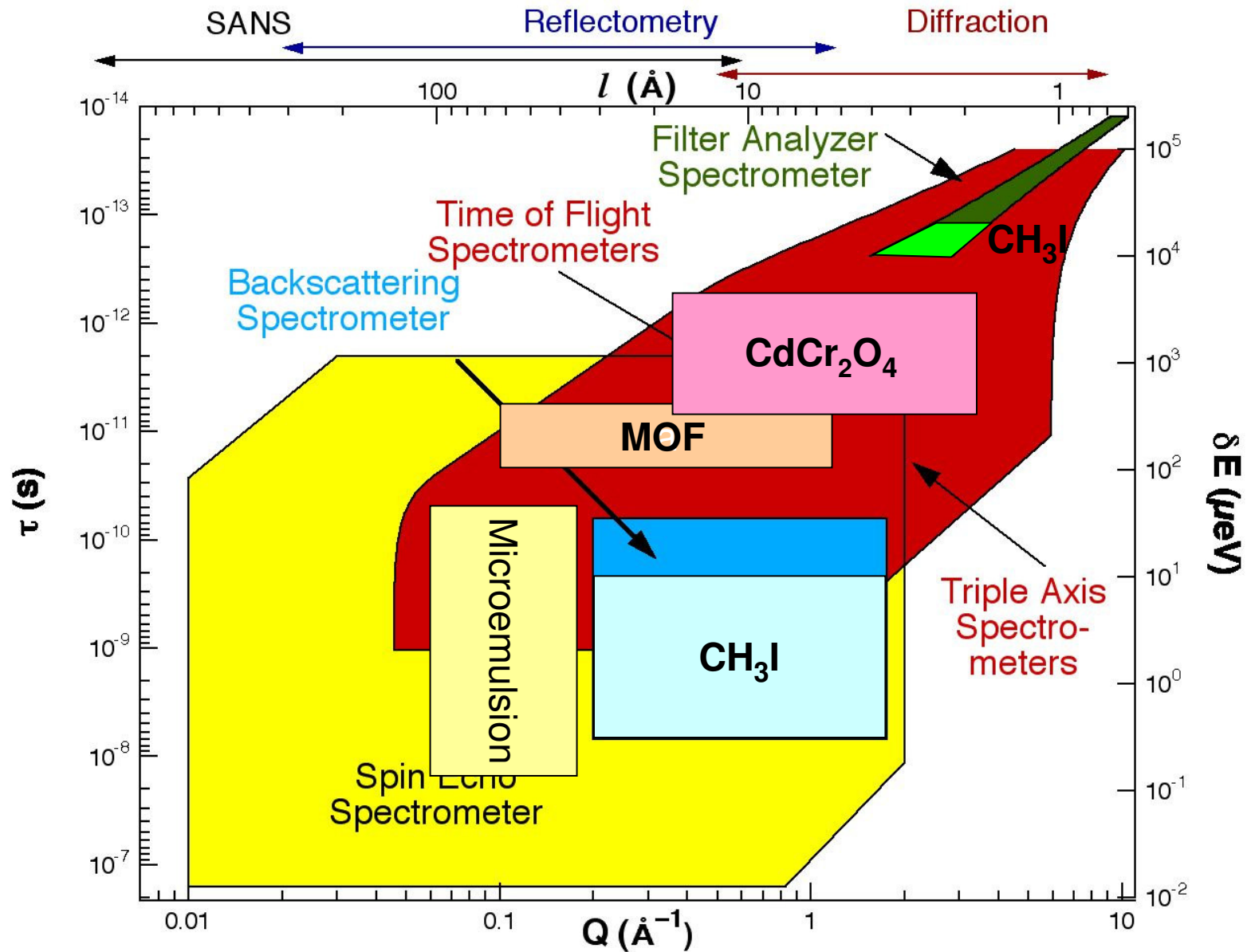
→ Fill the beam with sample

Typically use flat plate samples (at small angles)



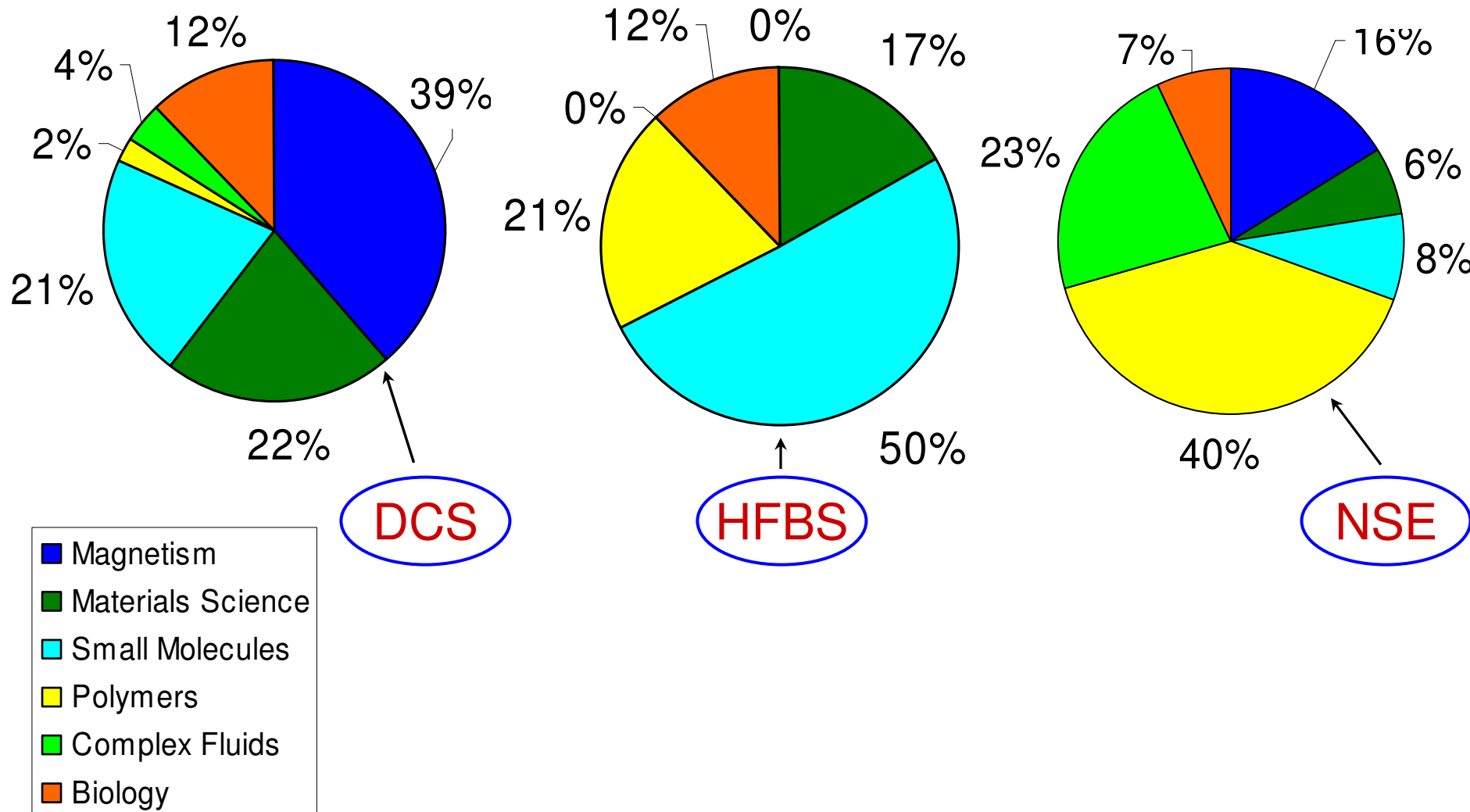
Rule of thumb - the transmission should be ~70%

Samples from this Summer School



Things to consider

NCNR →



Applying for beam time



The use of the neutron scattering instrumentation that you've used over the past week is open to all qualified users based on peer-reviewed proposals. Calls for proposals are issued about twice per year.

The **next deadline** for **new proposals** will be in **Sept. of 2007**.

Further information on submitting proposals can be found at:

http://www.ncnr.nist.gov/programs/CHRNS/CHRNS_prop.html

Summer School Success Stories



2001



Jae-Ho Chung
University Prof.

2003



Vicky Garcia-Sakai
ISIS Staff Scientist

1999



William Ratcliff
NCNR Staff Physicist

1997



Rob Dimeo
NCNR Deputy Director

Ok, so you can't win them all ...

Acknowledgements



Organizers - Antonio Faraone and Yamali Hernandez

Our administrative staff - Julie Keyser

All of the experiment teams

Invited speakers - C.L. Broholm and M.C. Rheinstädter



Thanks for coming!