

## Choosing the Right Neutron Spectrometer



Dan Neumann  
NIST Center for Neutron Research

dan@nist.gov    www.ncnr.nist.gov

## Main Messages of the Week



- Neutron scattering experiments measure the number of neutrons scattered by a sample as a function of the wavevector change ( $\mathbf{Q}$ ) and the energy change ( $\hbar\omega$ ) of the neutron
- Expressions for the scattered neutron intensity involve the positions and motions of atomic nuclei or unpaired electron spins
- The scattered neutron intensity as a function of  $\mathbf{Q}$  and  $\hbar\omega$  is proportional to the space and time Fourier transform of the probability of finding one or two atoms separated by a particular distance at a particular time

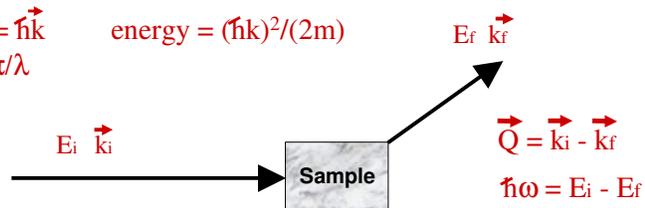
## What is required to do an inelastic neutron scattering experiment



1. A source of neutrons
2. A method to prescribe the wavevector ( $\mathbf{k}_i$ ) of the neutrons incident on the sample
3. A well-chosen sample
4. A method to determine the wavevector ( $\mathbf{k}_f$ ) of the scattered neutrons
5. A detector

$$\text{momentum} = \hbar \vec{k}$$
$$k = 2\pi/\lambda$$

$$\text{energy} = (\hbar k)^2 / (2m)$$



NSE measures  $|\Delta\mathbf{k}|$  directly by attaching a "clock" to each neutron

## Methods of specifying & measuring $\mathbf{k}_i$ and $\mathbf{k}_f$



### 1. Bragg Diffraction

SPINS, FANS, Backscattering

### 2. Time-of-flight

DCS, Backscattering (??)

### 3. Larmor Precession

Spin Echo

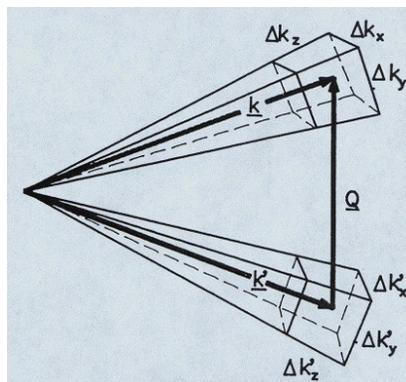
## Why are there so many different spectrometers?



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

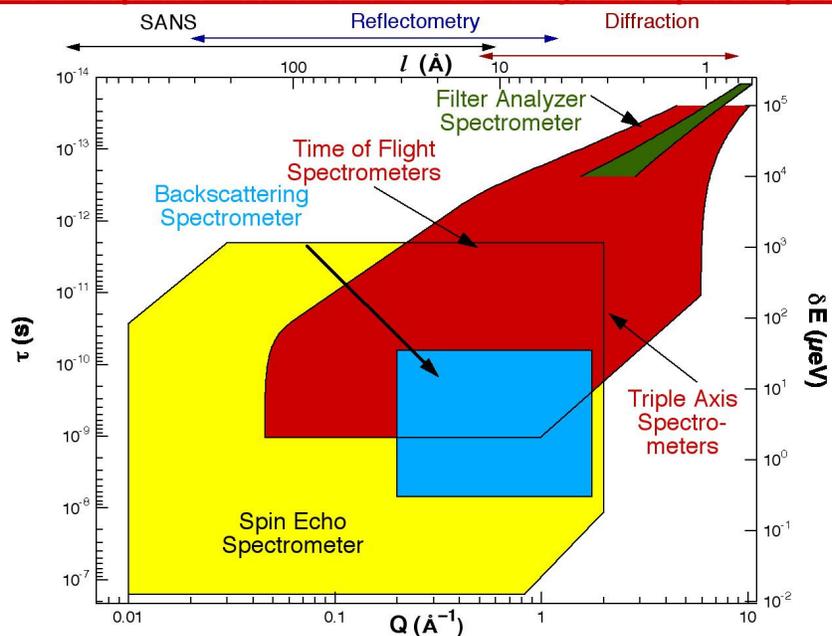
Uncertainties in the neutron wavelength and direction imply that  $Q$  and  $\hbar\omega$  can only be defined with a certain precision.

The total signal in a scattering experiment is proportional to the resolution volume *i.e.* better resolution leads to lower count rates



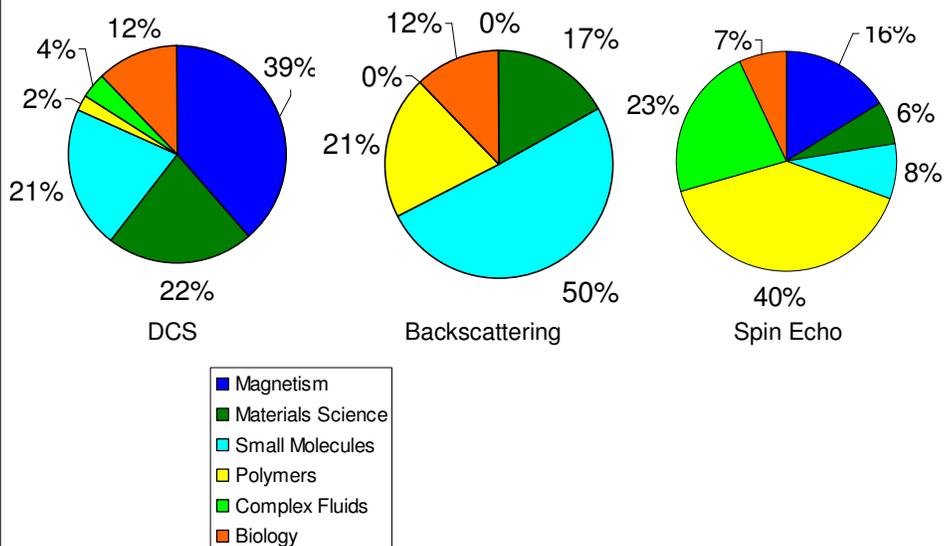
Courtesy of R. Pynn

## Different spectrometers cover different regions of phase space



## Things to consider

**NCNF**



## Things to consider

**NCNF**

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)

## Things to consider



Now consider the energies ( $\hbar\omega$ ) or time scales of interest ( $\delta t \sim 1/\omega$ )

$\hbar\omega > 10\text{-}20$  meV - use FANS (or some other spectrometer  
designed for vibrational spectroscopy)  
 $\hbar\omega < 20\text{-}30$   $\mu\text{eV}$  - use Backscattering

in between - use DCS (or some other cold neutron TOF spectrometer)

BUT – check to make sure that the length scale of the motions that you're interested in is within the range of the instrument. As a simple example of this, consider the Backscattering spectrometer. ( $Q \sim 2\pi/L$ )

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

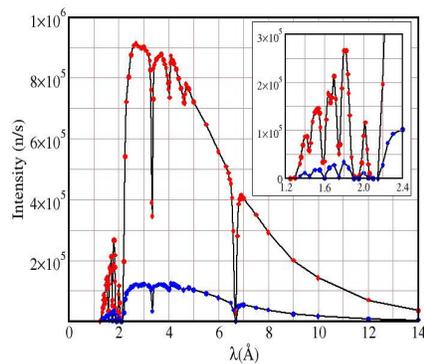
$$Q_{\max} = 1.75 \text{ \AA}^{-1} \Rightarrow L_{\min} \sim 3.5 \text{ \AA}$$

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

## Things to consider after choosing DCS



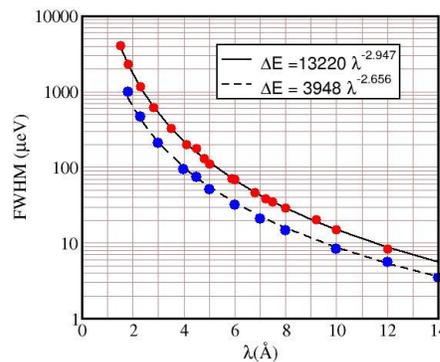
$I(E)$



Quantities varied

- wavelength  $\lambda$
- chopper slot widths  $W$

$\Delta E$



Remember – Intensity  $\downarrow$   
Resolution  $\uparrow$

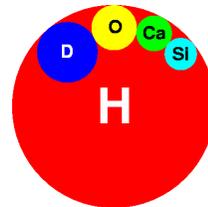
## Sample "Design" for DCS & Backscattering



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 DCS & Backscattering



Increase the intensity by increasing the amount of sample

=> Fill the beam with sample

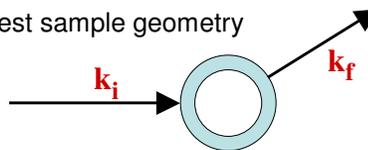
maximum beam size is usually given in the instrument description  
3 cm X 10 cm for DCS (or 1.5 cm X 10cm) 3 cm X 3 cm for Backscattering

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



## Things to consider

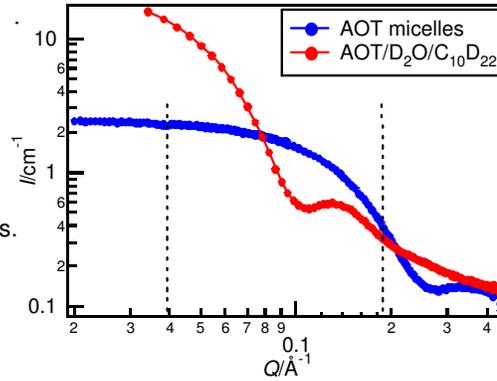


If the resolution of backscattering is “not good enough” or if you are only interested in a “limited” region of  $Q$  space (typically small  $Q$ ), use NSE (low  $Q$ , long times)

These cases typically involve coherent scattering which tends to peak around  $2\pi/(\text{the relevant length scales in your sample})$

Remember – slower motions usually imply larger length scales.

Many atoms moving together  
=> Coherent scattering



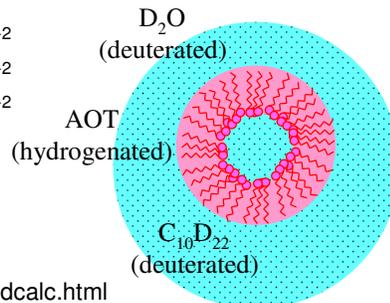
## Sample “Design” for NSE



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	$1.6 \times 10^{-6} \text{ \AA}^{-2}$
SLD solvent	$6.5 \times 10^{-6} \text{ \AA}^{-2}$



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

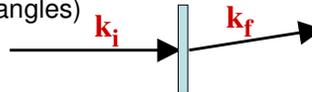
## Sample "Design" for NSE



Increase the intensity by increasing the amount of sample

=> Fill the beam with sample

Typically use flat plate samples (at small angles)



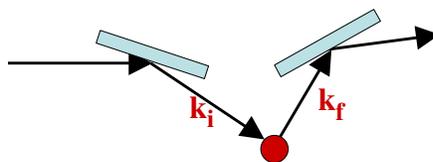
Rule of thumb - the transmission should be ~70%

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

## Triple Axis Spectrometers



Triple axis spectrometers are typically used when either the direction of  $Q$  is important or the interesting region of  $Q-\omega$  space is of limited extent.



Remember – Intensity ↓

Resolution ↑

Collimation(°)	$\lambda$	rel. signal	FWHM
55-80-80-80	4 Å	1.00	0.28 meV
55-40-40-40	4 Å	0.24	0.17 meV
69-80-80-80	5 Å	0.26	0.13 meV
84-80-80-80	6.1 Å	0.03	0.05 meV

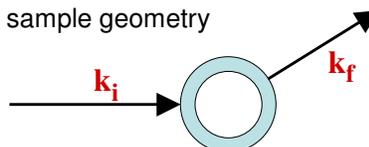
## Sample “Design” for Triple Axis



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)

## General Sample “Design”



Try to avoid isotopes that are strongly absorbing

${}^6\text{Li}$   ${}^{10}\text{B}$   ${}^{113}\text{Cd}$

For a complete listing go to

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

## General Sample "Design"



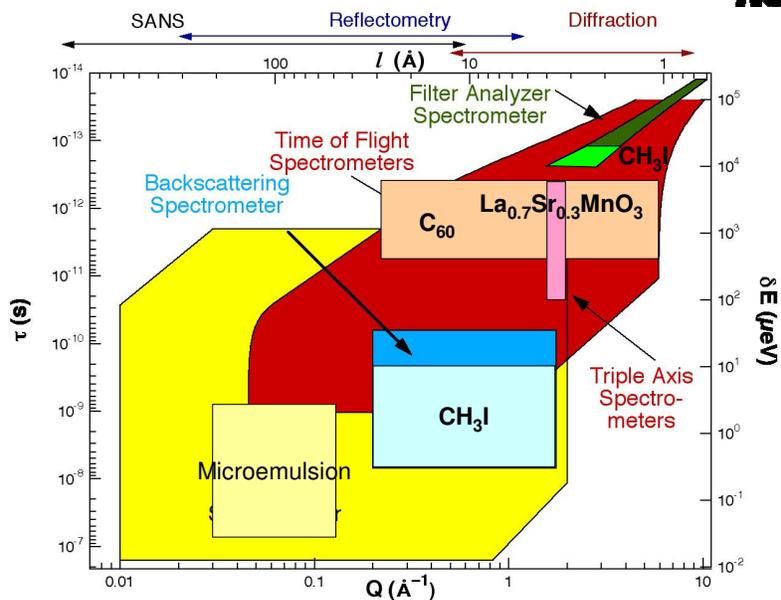
The most important thing is:

**Know as much about your sample as possible**

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?

## Things to consider



## DCS vs. SPINS



DCS – incoherent scattering, surveys  
SPINS – limited region of  $Q$ - $\omega$

Rules of Thumb: (think carefully before violating)

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

SPINS – single crystals

## 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 the Fall of 2005.

Further information on submitting proposals can be found at:

[http://www.ncnr.nist.gov/programs/CHRNS/CHRNS\\_prop.html](http://www.ncnr.nist.gov/programs/CHRNS/CHRNS_prop.html)

## Acknowledgements



John Copley and Peter Gehring  
Our administrative staff (Julie Keyser)  
The experiment teams  
Dobrin Bossev and Seung-hun Lee



**Thanks for coming**