High Flux Back Scattering Spectrometer (HFBS) Experiment Group C 2011 NCNR Summer School



How About Those Neutrons?

- Compared to other spectroscopic probes, neutrons have:
 - Very deep penetration depths
 - No systematic change in scattering cross sections
 - Isotope dependent
 - (Weak) Interactions with all materials
 - Wavelengths on order of molecular bonds
- Disadvantages can be cleverly overcome
 - Low flux, occasional strong adsorption

How neutron travels?



Instrument Resolution

- Smallest exchange of energy that can be seen by instrument
- Backscattering eliminates $\Delta\theta/\tan\theta$ by selecting $\theta = 90^{\circ}$
 - Wavelength spread is then dependent on d (spacing of Bragg planes in crystal)
- Si {111} crystal planes select for wavelength of 6.27Å
 - 1 µev resolution obtained by matching the energy to the silicon d-spacing
 - Doppler motion creates spread in energy

$$\frac{\Delta\lambda}{\lambda} = \frac{\Delta d}{d} + \frac{\lambda}{t}$$

$$As \theta \to 90^{\circ}$$

$$r 2\theta \to 180^{\circ}$$

$$\frac{\Delta E}{E} = 2 \frac{\Delta\lambda}{\lambda}$$

Quasi-elastic and Inelastic Neutron Scattering



- Elastic Neutron Scattering
 - The energy of neutron does not change after the scattering
- Quasi-elastic neutron scattering
 - Energy transfer induced by diffusive or diffusive-like processes
- Inelastic neutron scattering
 - non-zero energy transfer for neutrons, which corresponding to specific energy transfer in materials

Polymer Dynamics as a function of temperature







Analysis

Dynamics of the polymer in quasi-elastic scattering



• α -relaxation :

 $S_{\text{theo}}(Q,\omega) = DWF \times S_{QE}(Q,\omega) + S_{IN}(Q,\omega)$

Analysis

• Continuous diffusion (Simple exponential):

 $S(Q,t) = A(Q,t) \exp(-DQ^2 t)$

Translational Diffusion coefficient

• Non simple diffusion (Stretched exponential):

$$S(Q,t) = A(Q,t) \exp\left[-\left(\frac{t}{\tau_{\alpha}(Q,T)}\right)^{\beta(Q,T)}\right] \rightarrow \text{Stretching Parameter}$$

Characteristic relaxation time

• Pre-factor A(Q,t):

In crystals:

$$A(Q,t) = \exp\left(\frac{-Q^2 < u^2 >}{3}\right)$$

In polymers:

$$\exp\left[-\left(\frac{t}{\tau}\right)^{\beta}\right] \approx \sum A_i \exp\left(-\frac{t}{\tau_i}\right)$$



Diffusion at Different Length Scales



Arrhenius vs. VFT Temp. Dependence



α -Relaxation in PVME

Using BS & dielectric spectroscopy to find the alpha relaxation in PVME, but can't see beta...



Fig.4: A complete relaxation map for one of the famous polymers, polyisoprene by different experimental techniques [8]. a-relaxation at low temperatures is covered by dielectric spectroscopy. Open symbols belong to neutron scattering measurements.

Conclusions

- HFBS is useful for obtaining relaxation times and self diffusion coefficients
 - Only time scales of 100ps 10ns
- Polymers can be readily characterized by HFBS
 - Large length/time scales are limited
 - Observe methyl rotation and α -rotation
- At each temperature, increasing Q results in decreasing β
- At each Q value, increasing temperature -> decreased β