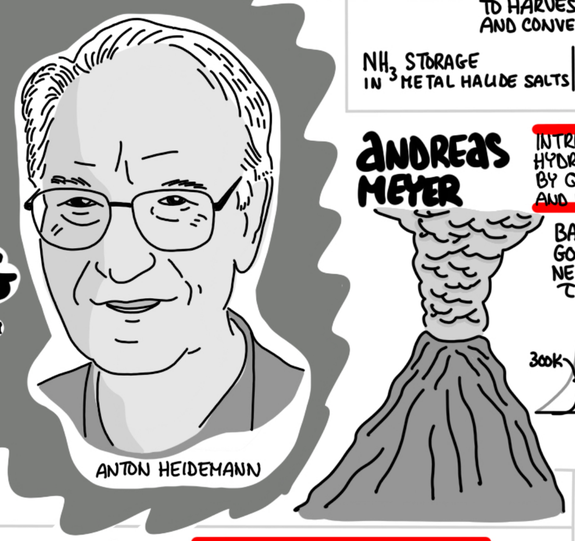
50 Years of Neutron Backscattering

TUM Institute for Advanced Study
September 2–3, 2016

Sketchnotes:



Anton Heidemann

Backscattering spectroscopy: how it all began exactly 50 years ago

Alefeld is the father of backscattering spectroscopy.

Manfred and myself... consider ourselves lucky guys who participated in opening a new field. This does not happen very frequently to thesis students.

"The development of a new method, whenever its precision, sensitivity or resolution is much better than everything that existed in this field before, creates new physics."
-Heinz Maier-Leibnitz

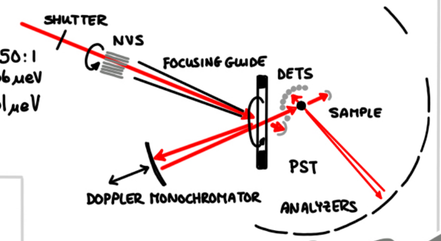
Joachim Wuttke

Spheres: the Spectrometer for High Energy Resolution at FRM II

In memory of Michael Prager (1945-2008)

Catastrophic failure of PST when spinning up to 300 m/s | Now PST spins at x-tal speed of 225 m/s

SNR = 1750:1
δE = 0.66 μeV
ΔE = ±31 μeV

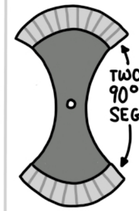


Bernhard Frick

A performance boost for reactor backscattering — IN16B at ILL

Old IN16 – 336 pubs / 18 years
1999 – Began lobbying for PST
2007 – Green light for PST

IN16B = 16× IN16



PST – the heart of IN16B

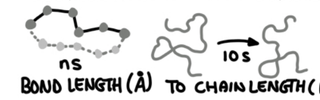
Gain ~ 2.1–2.5
Φ_{sample} ~ 3.8×10^5 n/cm²/s
SNR ~ 40000:1
Analyzer x-tals (Si 111) coated on backside w/ Gd_2O_3

Q_{max}(Si 311) ~ 3.7 Å⁻¹
δE (Si 311) ~ 1.9 μeV
δE (Si 111) ~ 0.7 μeV

Valeria Arrighi

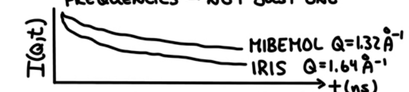
Using backscattering to study dynamics of soft matter and complex systems

Polymer motions → many decades in time



Early QENS | Extracted linewidths depended on resolution and dynamic range
Leads to inappropriate modeling

➡ Use distribution of rotational frequencies — not just one



KWW or Gaussian distribution
Heterogeneity matters!

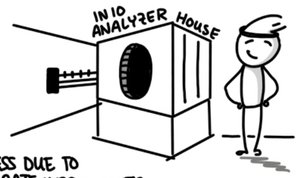
Andreas Magerl

The pathway of neutron backscattering: from Garching to Grenoble

Joined ILL BSS group

Learned rotational tunneling from NIST's Norm Berk

Progress due to count rate improvements



Whoever had to crawl into the manhole had to be "sporty"

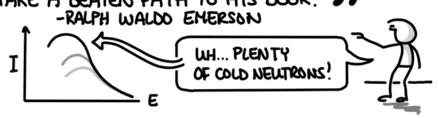
Colin Carlile

Backscattering on pulsed sources: a personal account

... but there are no cold neutrons on pulsed sources!

"If a man can write a better book, preach a better sermon, or make a better mousetrap than his neighbor, though he builds his house in the woods, the world will make a beaten path to his door."
-Ralph Waldo Emerson

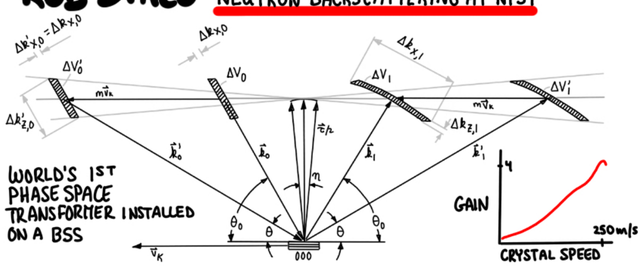
IRIS @ ISIS "INIO ON END OF A LONG GUIDE"



"Backscatter Kindness"

Rob Dimeo

Neutron backscattering at NIST



World's 1st phase space transformer installed on a BSS

Ken Herwig

The design and construction of the SNS near-backscattering spectrometer BASIS

Kaoru Shibata

A time-of-flight type near-backscattering spectrometer DNA in J-PARC

Near backscattering TOF w/ Si analyzer
Spring 2012 – available

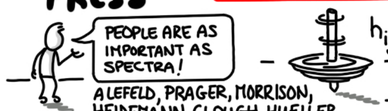
Analyzer
16 Si 111 units + 11 Si 311 units → Installed 2014

Si 111	Si 311
ΔE (μeV) 1.6, 2.4, 3.5	ΔE (μeV) 12
$0.08 < Q(Å^{-1}) < 1.92$	$1.4 < Q(Å^{-1}) < 3.79$

SNR > 10^5

Werner Press

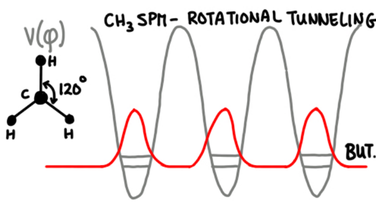
History < 50 y: rotational tunneling with high resolution neutron scattering



Alefeld, Prager, Morrison, Heidemann, Clough, Hueller, Yamamoto, ...

$h_{ij} = \langle \Phi_i | \hat{H} | \Phi_j \rangle$ Pocket states

Methane CH_4 on MgO (Larese)



CH_3 spin – rotational tunneling

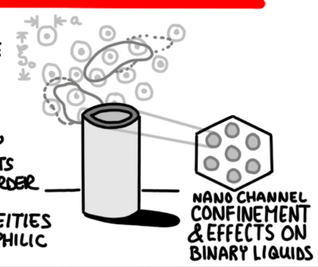
But... tunneling is largely a curiosity-driven endeavor – few groups

Denis Morineau

On the confinement of liquids in mesoporous hosts: recent and less recent achievements from neutron studies

Confinement can dramatically change dynamics w.r.t. bulk behavior

Why?
- Pore size
- Dimensionality
- Surface effects
- Quenched disorder



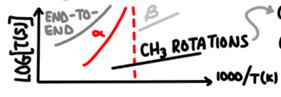
Surface heterogeneities & hyrophobic/hydrophilic

Arantxa Arbe

Polymer dynamics: highlights from neutron backscattering

Rich dynamics depend on the length scale of observation

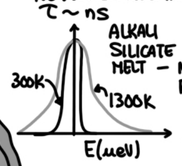
Monomers → side grp motions
Intermolecular → 2nd-ary relaxations
Chain → α relaxation
Chain dynamics

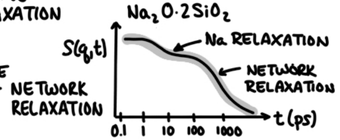


Andreas Meyer

Intrinsic proton dynamics in hydrous silicate melts as seen by QENS at elevated temperature and pressure

Backscattering good for probing network relaxation τ ~ ns





Want to understand lava flows & melts on a molecular level using neutron scattering ➡ QENS

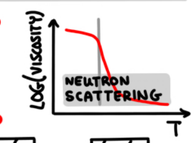
Lava flow vs. Explosive volcanism

How is water dissolved in system? → In molecular H_2O & OH groups

Recommendation: Build BSS instruments with smaller beams → extreme environments

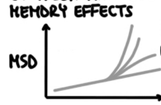
Christiane Alba-Simionesco

How neutrons perceive the formation of a glass, or, how to become a neutron scattering user thanks to backscattering!



Supercooled liquids, polymers, proteins, metals, spin glasses

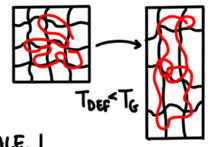
Characterized by
- Disordered structure
- Very slow relaxation
- Complex rheology
- Memory effects



Fixed window scans | Useful observable MSD

Polymers & plasticity

PMMA stretched at $T < T_G$



On monomer scale, plastic deformation remains

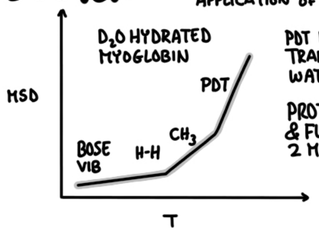
BSS validates models & theories
BSS probes props of new matls at nanoscale

Wolfgang Doster

The protein dynamical transition from backscattering displacements

Protein dynamical transition | PDT

Application of BSS to molecular biology



PDT is a water (solvent) transition – must change water amt to see it

Protein dynamics & function
2 major components

1. Internal rot transitions of side chains, CH_3 indep of protein env. & viscosity
2. Solvent viscosity dependent displacements coupled to trans diffusion of hydration water