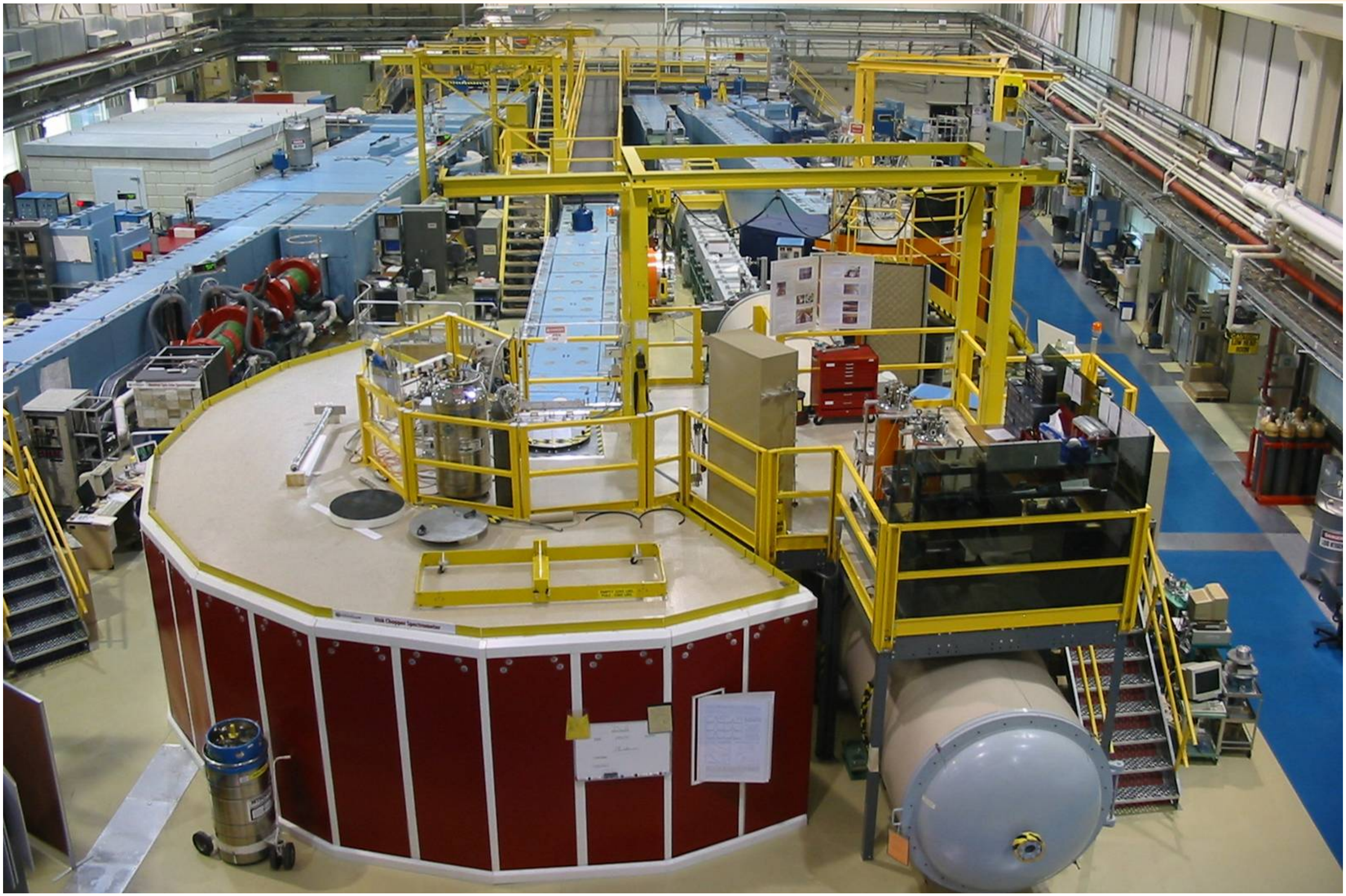
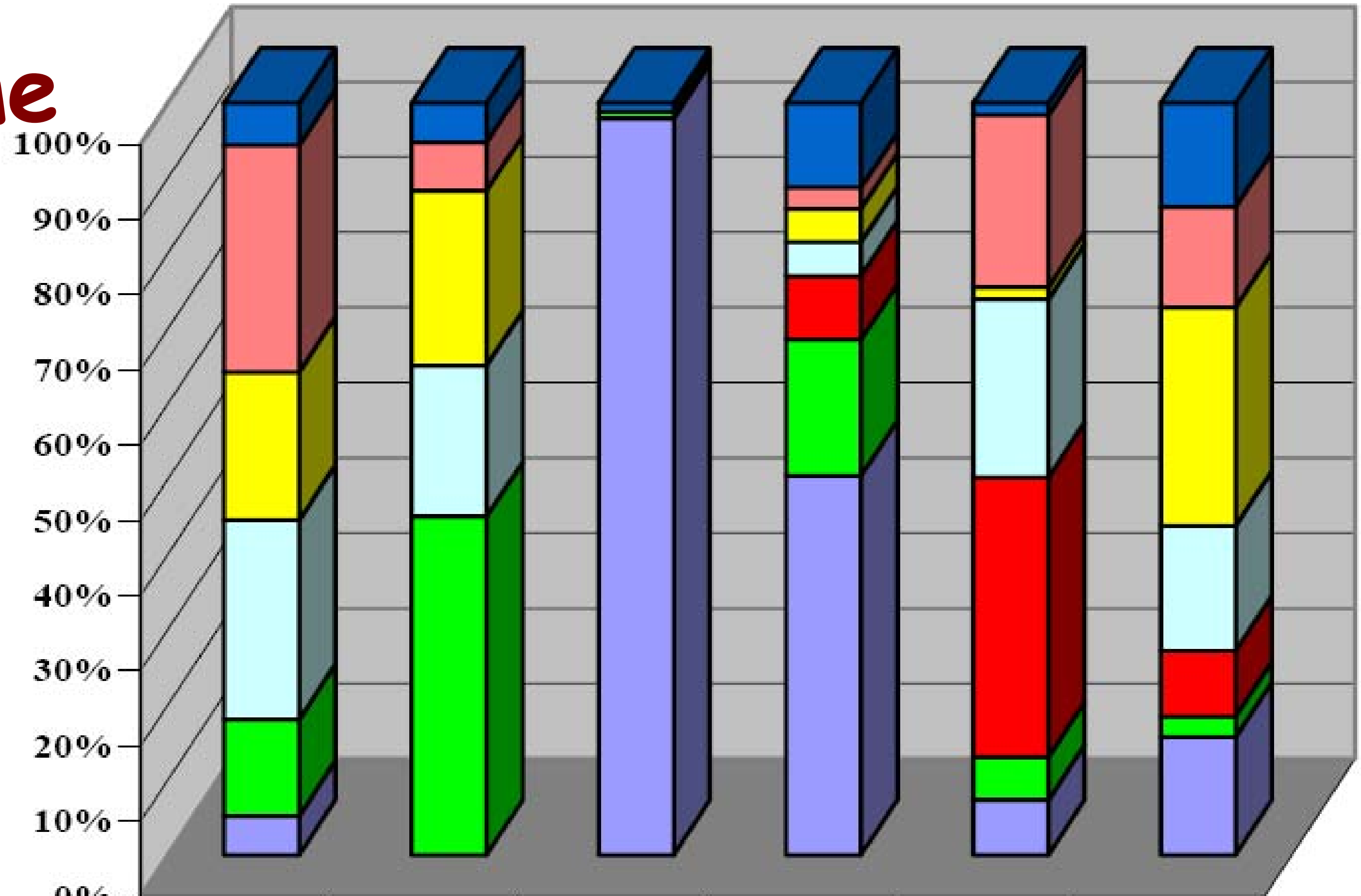
Disk Chopper Spectrometer

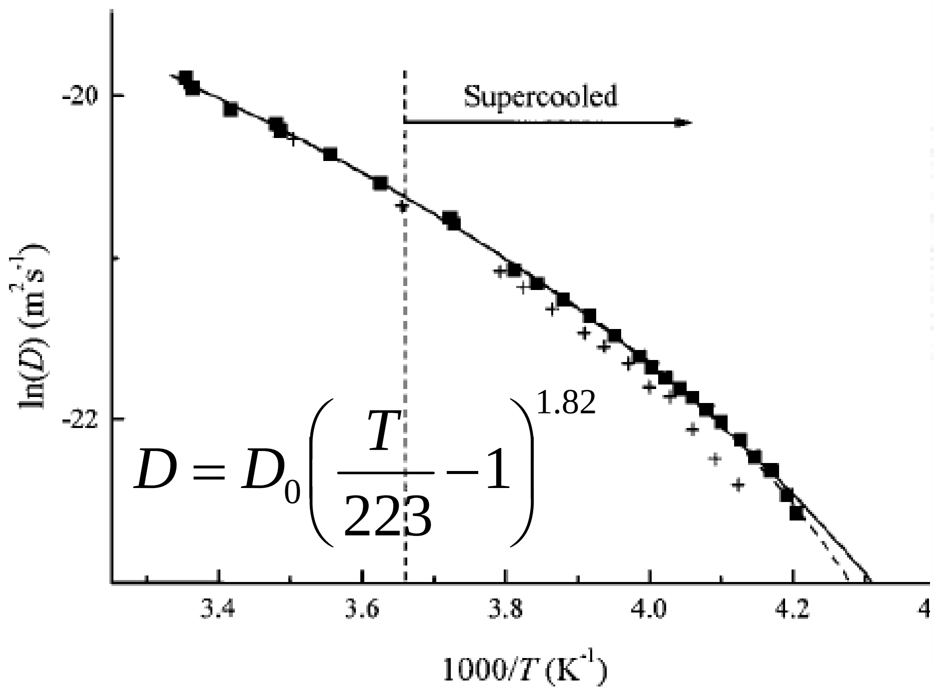


Beam Time

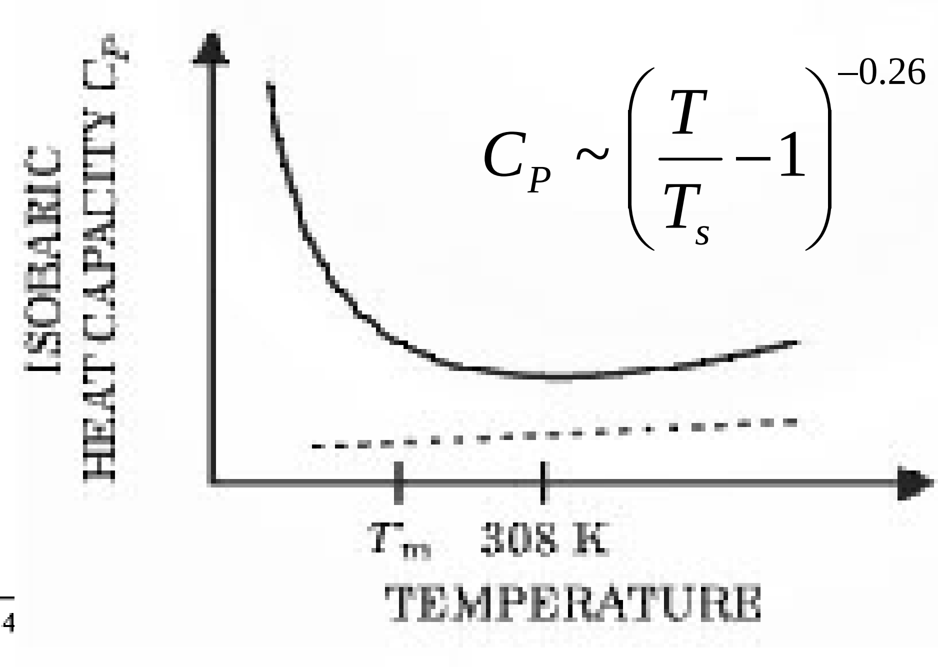


	SANS	USANS	SPINS	DCS	HFBS	NSE
Instrument development	6%	5%	1%	11%	2%	14%
Biology	30%	6%	0%	3%	23%	13%
Complex fluids	20%	23%	0%	4%	2%	29%
Polymers	27%	20%	0%	4%	24%	17%
Small molecules	0%	0%	0%	8%	37%	9%
Materials science	13%	45%	1%	18%	6%	3%
Magnetism	5%	0%	98%	50%	7%	16%

Water in Confinement (MCM-41S)



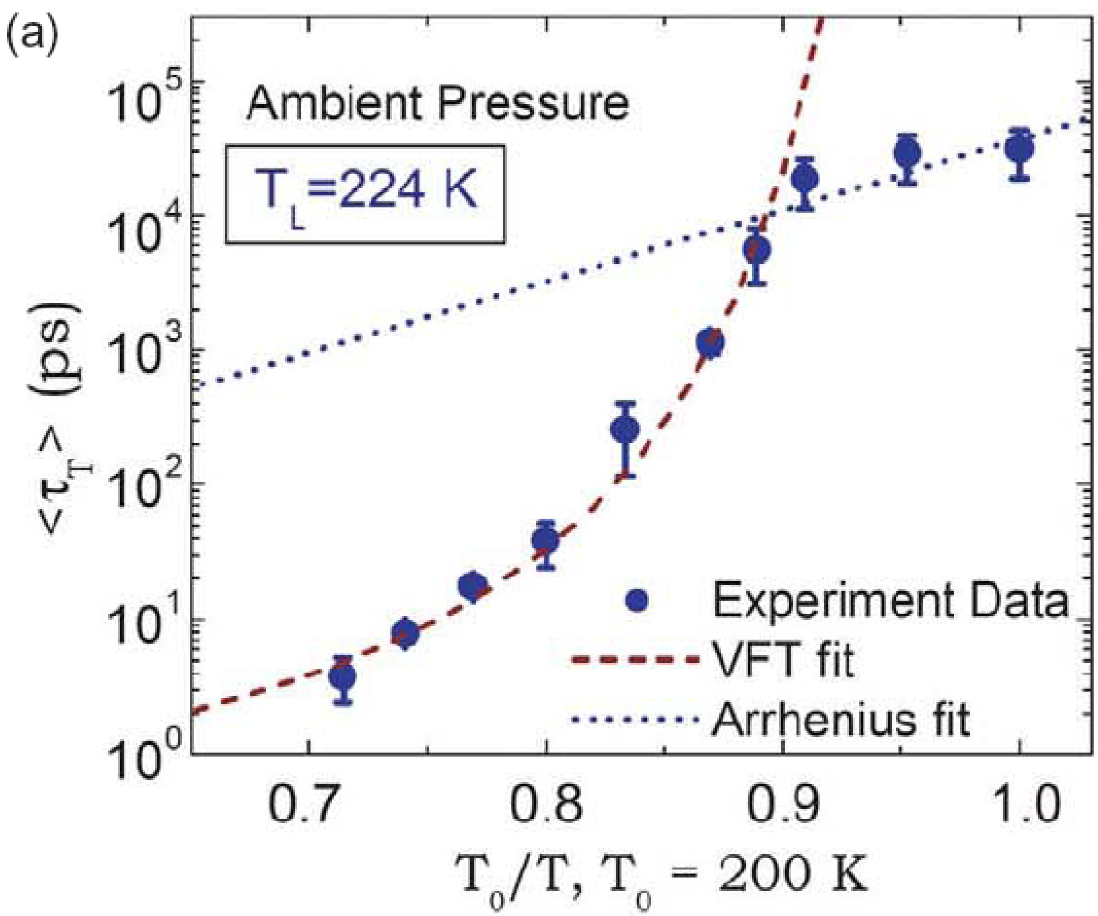
W.S. Price, H. Ide, Y. Arata, J. Chem. Phys. A **103**, 448 (1999).



C. A. Angell, J. Shuppert, and J. C. Tucker, J. Phys. Chem., **77**, 3092 (1977).

Thermodynamic and transport measurements suggest that supercooled water should undergo a fragile-to-strong transition between two liquid phases at around 228 K. However, supercooled bulk water reaches its homogeneous nucleation point and crystallizes into ice at 235 K.

Water in Confinement (MCM-41S)



Fragile to strong transition in the translational relaxation time observed at 224K.

Transition from a high-density to a low density liquid?

Vogel-Fulcher-Tammann law

$$\tau = \tau_o \exp[DT_o/(T - T_o)],$$

A. Faraone, L. Liu, C.-Y. Mou, C.-W. Yen, and S.-H. Chen, J. Chem. Phys., **121**, 10843 (2004).

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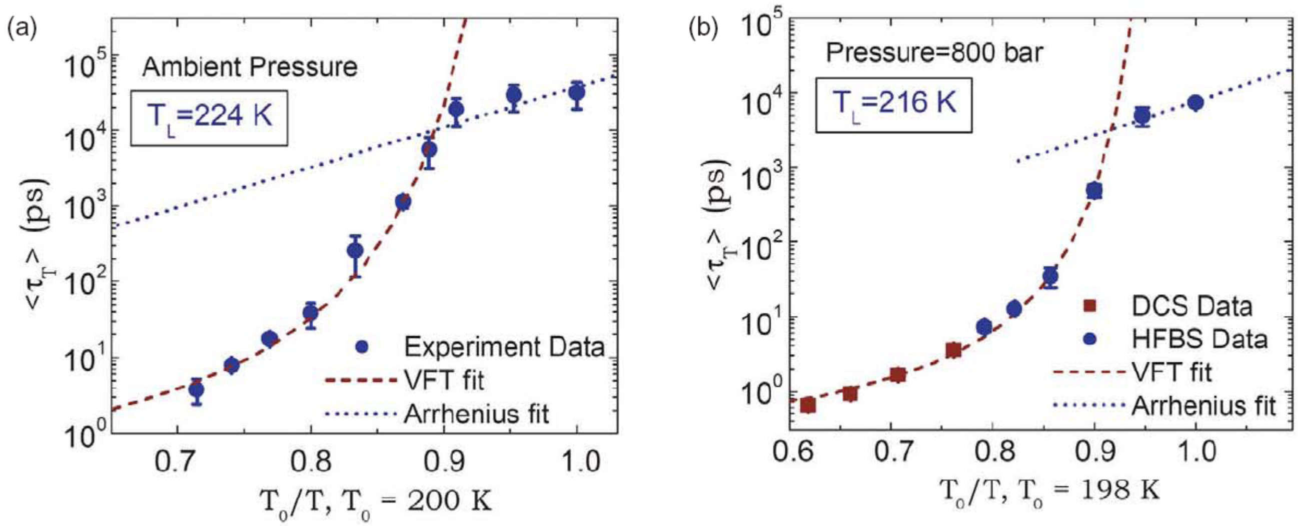
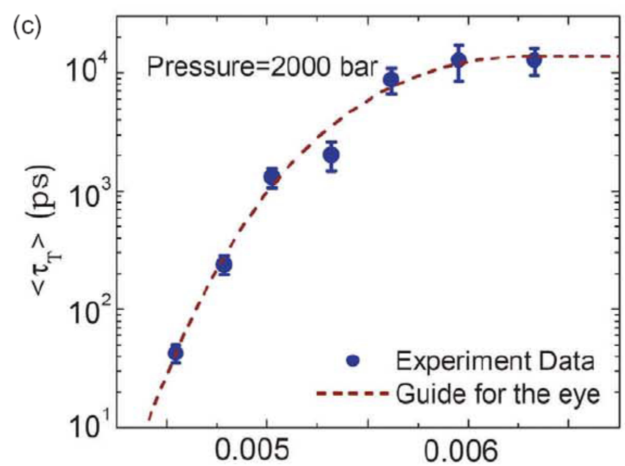
Water in Confinement (MCM-41S)





The anomalies in the thermodynamic quantities also indicate the possible existence of a low-temperature critical point near this transition temperature, but at somewhat elevated pressure.

L. Liu, S.-H. Chen, A. Faraone,
C.-W. Yen, and S.-Y. Mou,
Phys. Rev. Lett., **95**, 117802 (2005).

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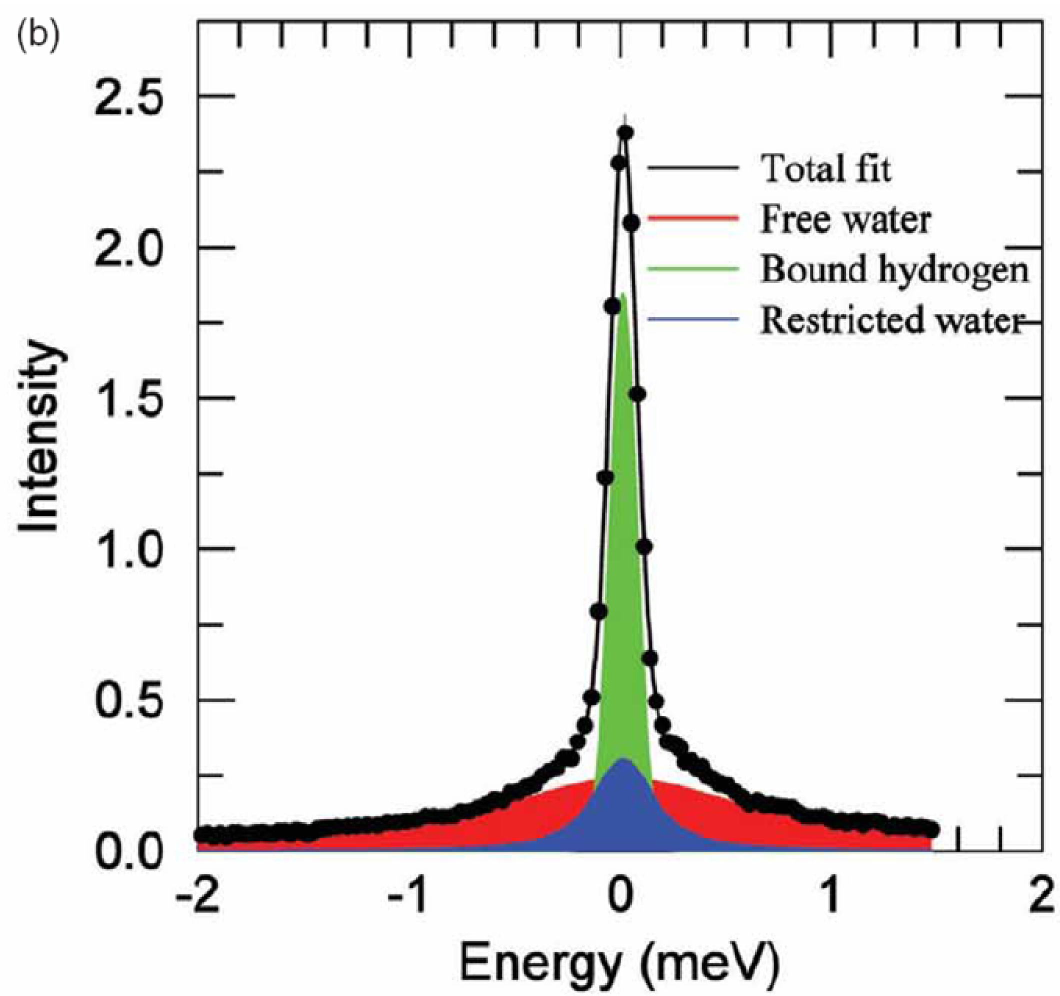
Quasielastic Scattering from Cement



More than 800 million metric tons of Portland cement are produced each year.

Tricalcium silicate (Ca_3SiO_5) is the most important and abundant component of Portland cement.

Dicalcium silicate (Ca_2SiO_4) is the second most abundant component.

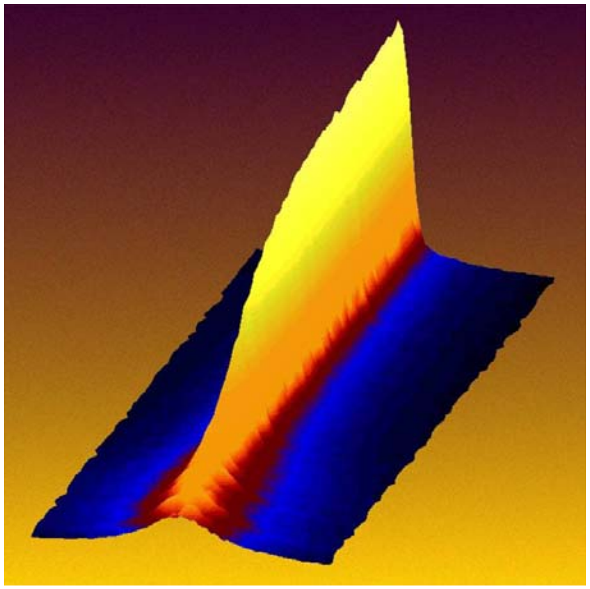
These two components typically account for approximately 80 wt.% of Portland cement.

$$BWI = \frac{Green + Blue}{Green + Blue + Red}$$

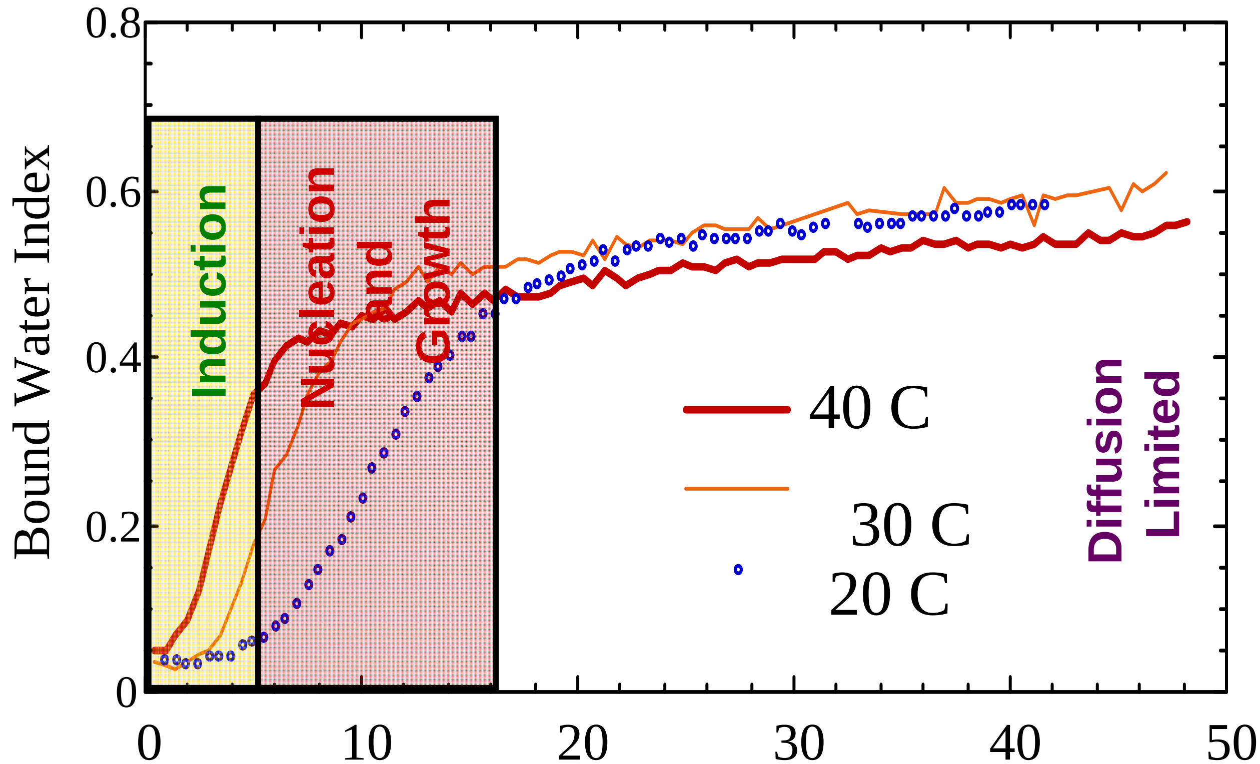
J.J. Thomas, D.A. Neumann, S.A. FitzGerald, and R.A. Livingston, J. Am. Ceram. Soc. **84**, 1811 (2001).

NIST

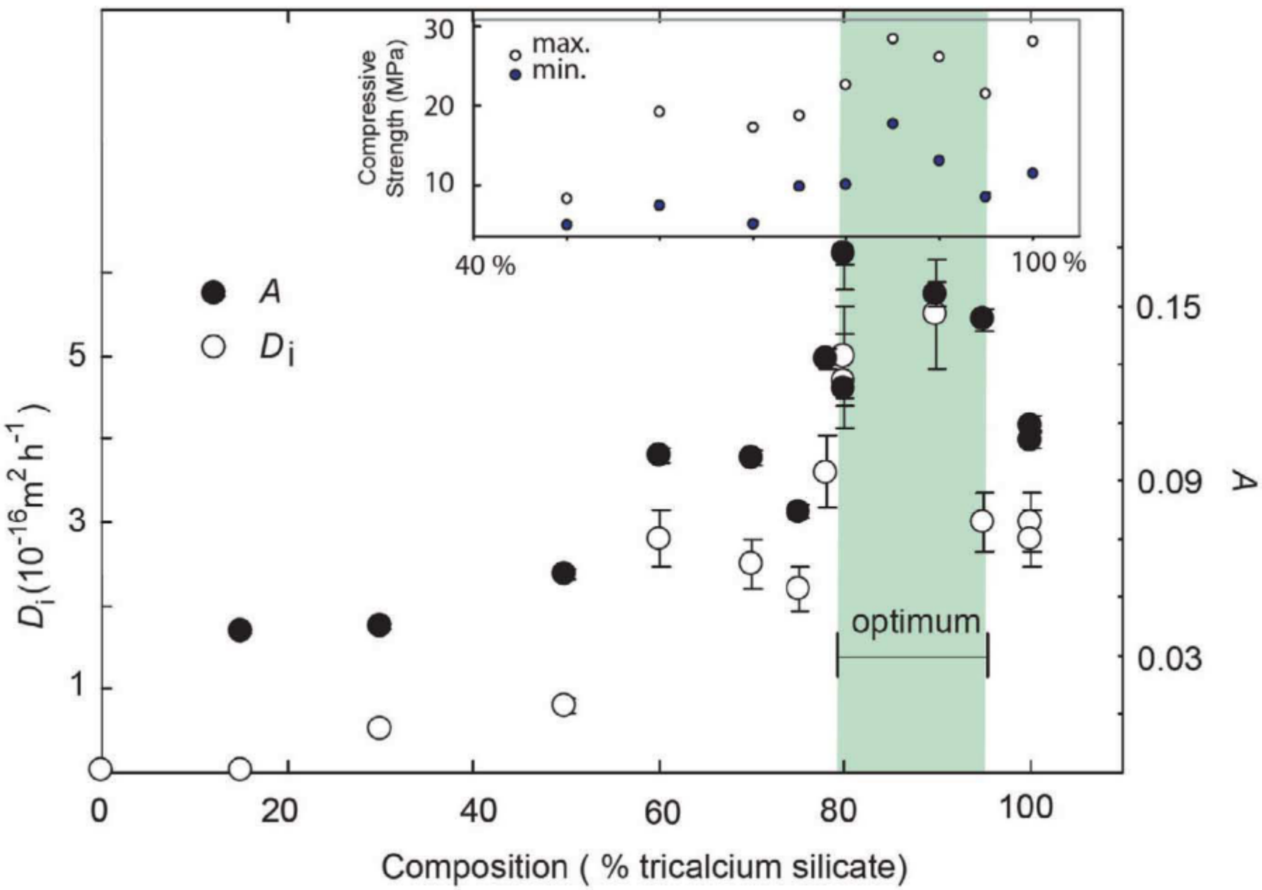
Kinetics of the hydration of cement



The main hydration reaction occurs over 24-48 hours. There are 3 periods.



Quasielastic Scattering from C3S-C2S Mixtures



Data is fit to kinetic models.

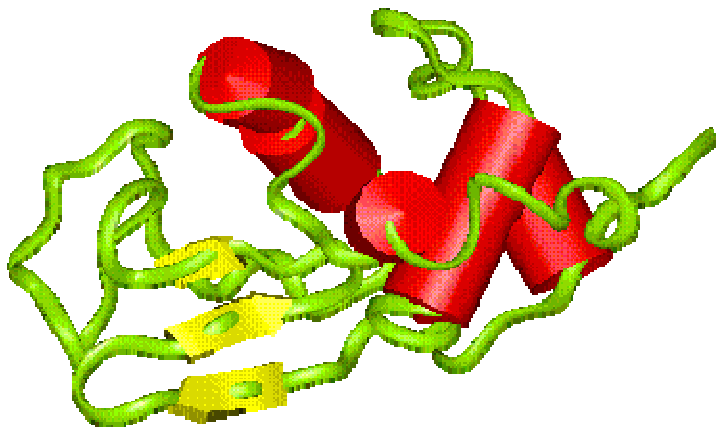
A is the amount of product that would have been formed if the "nucleation and growth" regime had continued to ∞ time.

D_i is the effective diffusion constant that controls the reaction in the "diffusion limited" regime.

V.K. Peterson, D.A. Neumann, and R.A. Livingston, J. Phys. Chem. B **109**, 14449 (2005); Physica B **385-386**, 481 (2006).

NIST

Dynamics of α-lactalbumin

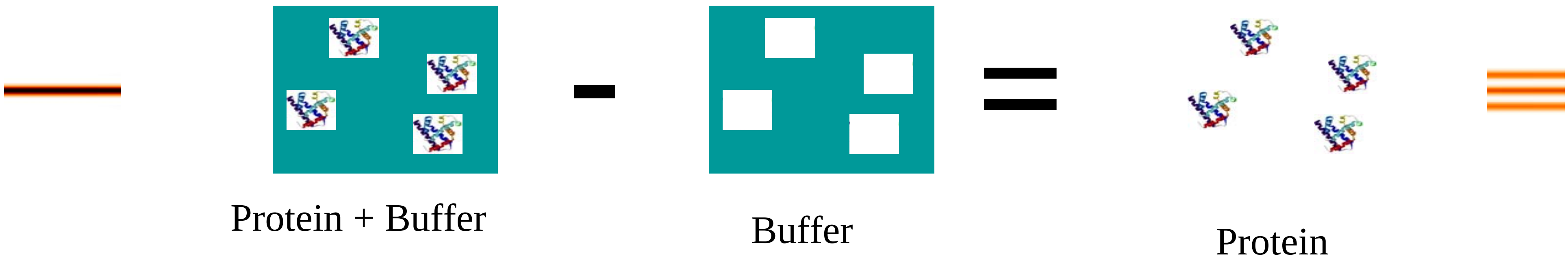


Combining MD simulations and inelastic neutron scattering can lead to new insights into protein dynamics.

1) Dynamics results demonstrate the accuracy of the force-field in a substantially more rigorous way than does structure alone
2) MD results allow a more complete interpretation of the neutron spectroscopic results and can guide future experiments

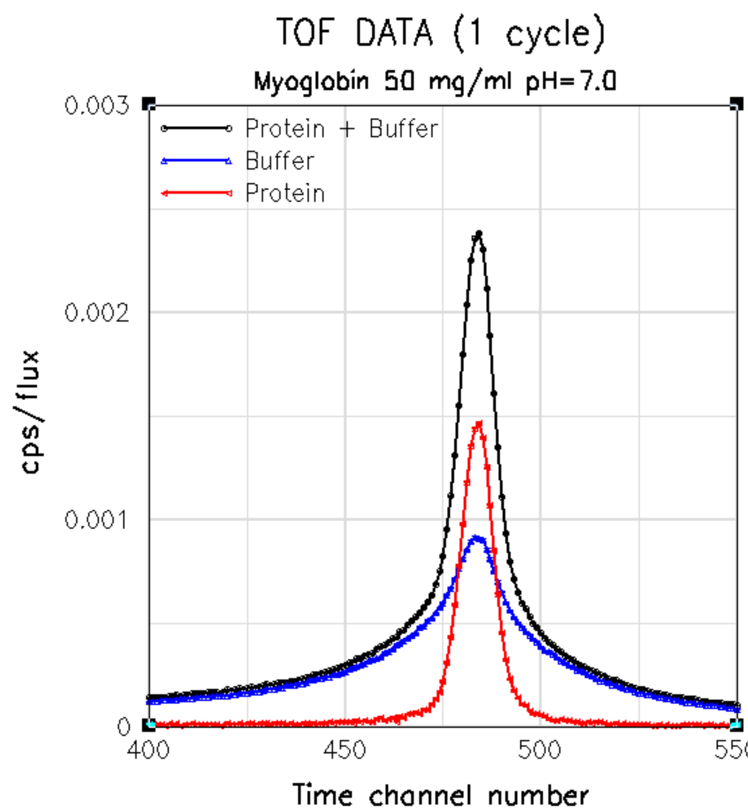
M. Tarek, DA. Neumann, D.J. Tobias, Chem. Phys. **292**, 435 (2003).

NIST



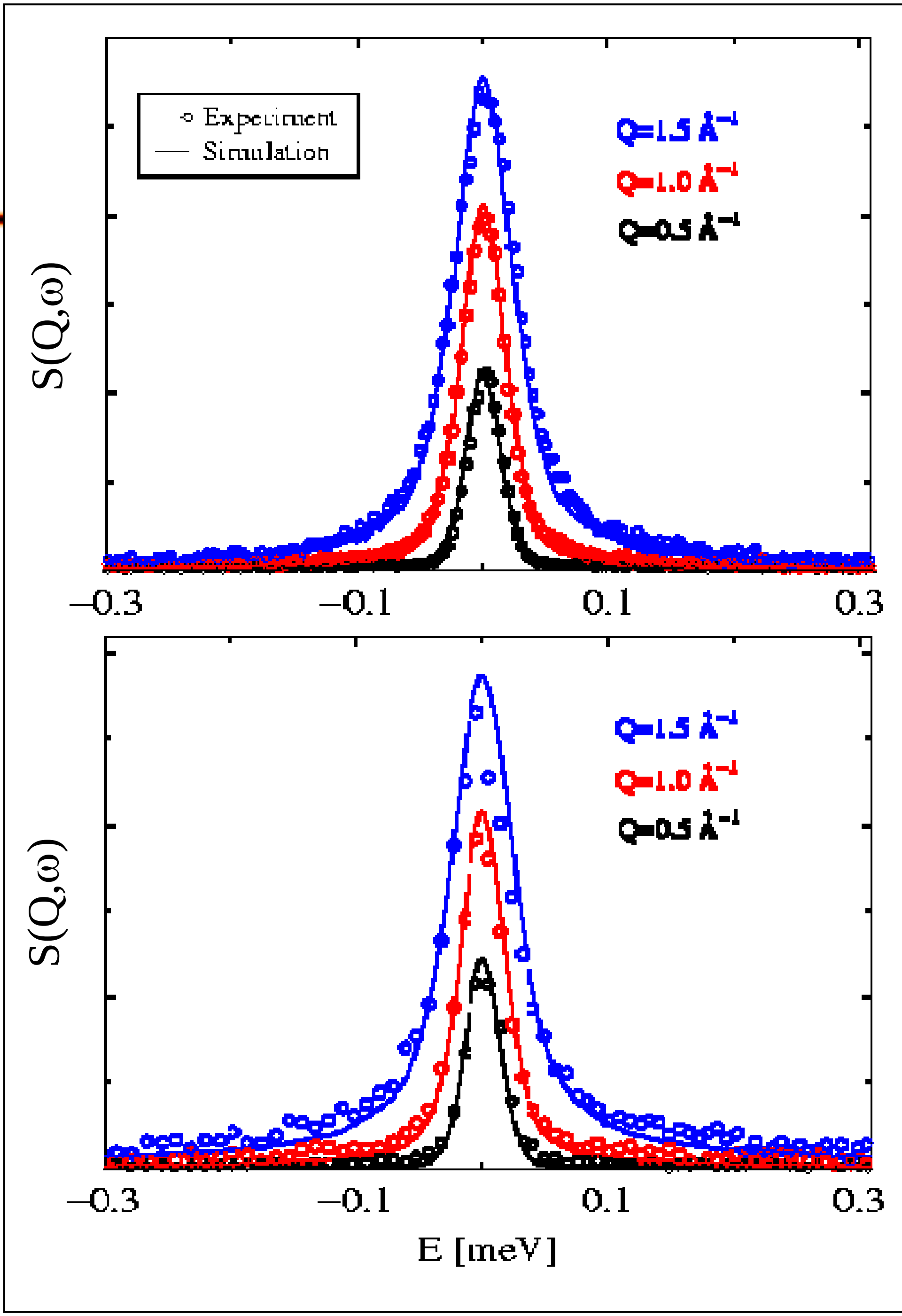
1. All exchangeable protons on the protein are exchanged with deuterium ($H_{ex} \Rightarrow D$) since hydrogen has a much higher scattering cross-section than deuterium

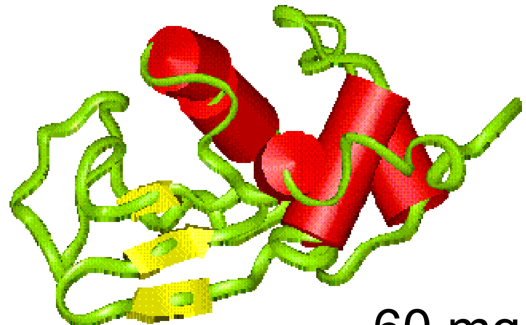
   => NS probes the <u>motions</u> of H atoms and since H atoms are distributed throughout proteins
2. Measure the QENS of a solution containing **non-aggregating** biomolecules in D_2O with fully deuterated buffer (~2% concentration)
3. Measure the QENS of only the D_2O with fully deuterated buffer
4. Solvent subtraction yields QENS from the protein!



Data courtesy of A. Pivovar

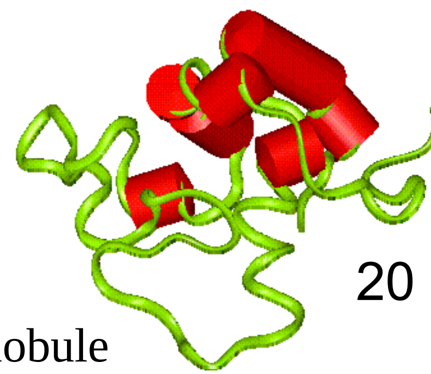
α-lactalbumin





native state

60 mg/ml

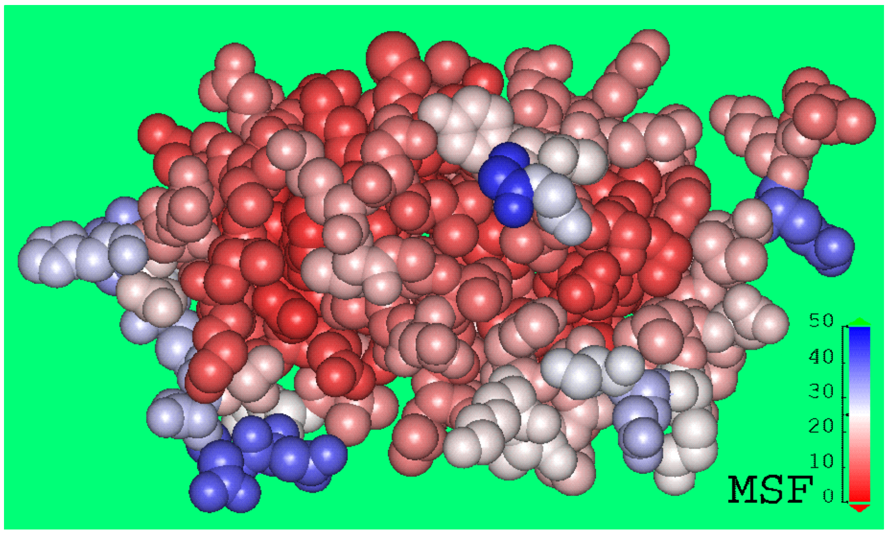


20 mg/ml

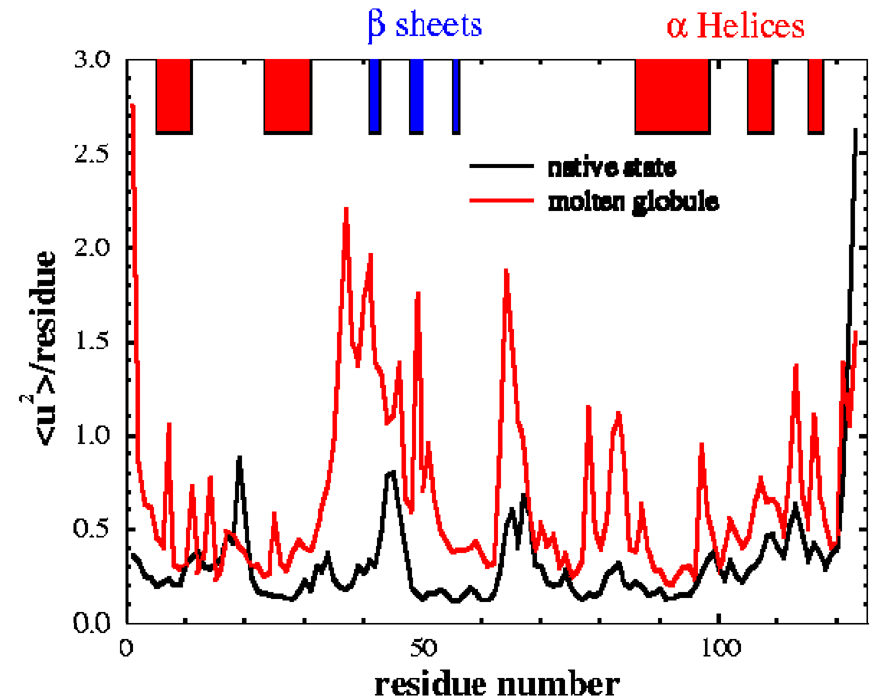
molten globule

INS : additional broadening of the spectra
=> more motion for the MG state
MD: good agreement with INS

Dynamics of α-lactalbumin



Mean squared fluctuations per amino-acid from MD



The observed enhancements in the dynamics of the molten globule state of α-lactalbumin compared to the native state arise from changes in the secondary structure

M. Tarek, DA. Neumann, D.J. Tobias, Chem. Phys. **292**, 435 (2003).

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VDOS of Hyperquenched Glasses

The “Boson peak” is a ubiquitous feature in the VDOS of glasses

Angell and his co-workers have used DCS to investigate how the “Boson peak” changes as a glass is annealed

The complex mineral glass-former called Rockwool is commercially produced by cascade spinning (cooling rate of 10^6 K/s)

Measurements were performed on the material in

1) the hyperquenched glassy state
2) the “standard” glassy state produced by a series of annealings
3) crystallized samples

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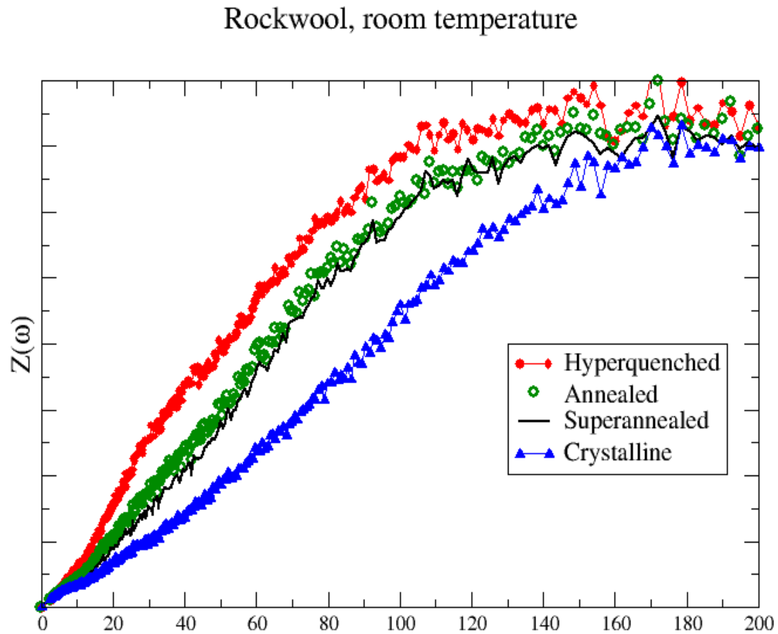
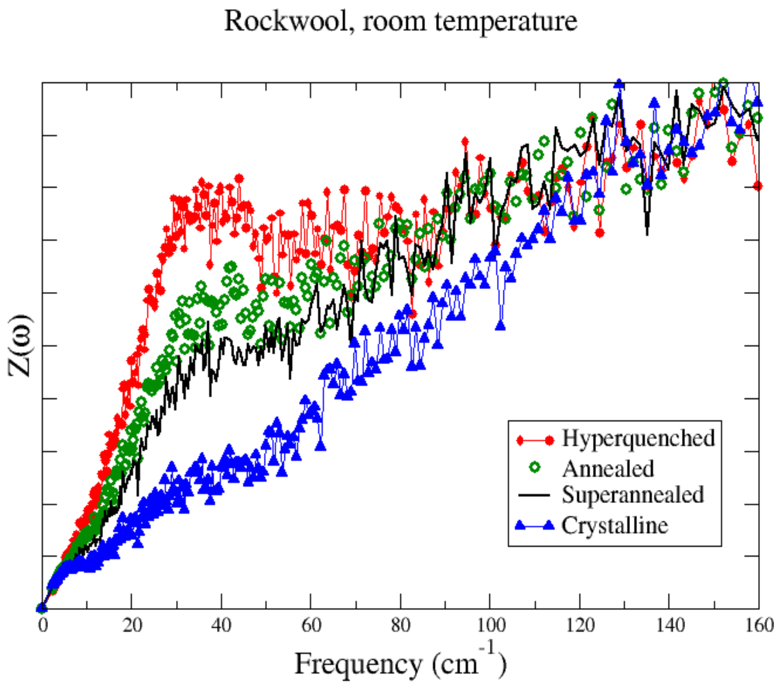




Hyperquenched Glasses

"Vibrational Density of States" averaged over the Q-range of the measurement

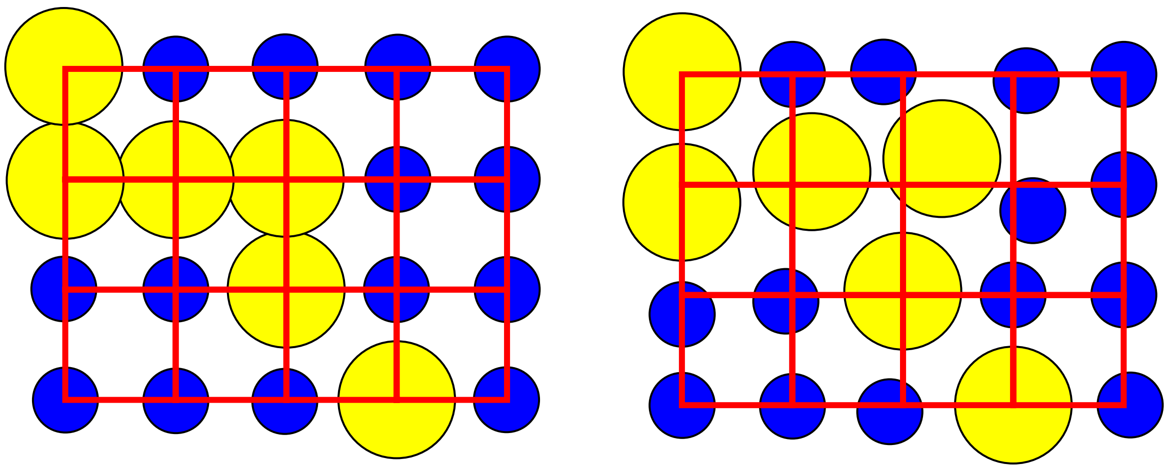
"Vibrational Density of States" averaged over the Q-range 0.4 to 0.7 A^{-1}

The "Boson peak" is enhanced on a length scale of about 1 nm

C.A. Angell, et al.,
J. Phys.: Cond. Matter **15**, S1051 (2003).

Elastic diffuse scattering from binary alloys

$$I_{Total}(Q) = I_{Bragg}(Q) + I_{SRO}(Q) + I_{SE}(Q) + I_{Huang}(Q) + I_{TDS}(Q)$$



Null matrix alloy $^{62}Ni_{0.52}Pt_{0.48}$

Pt $b_{Pt} = 9.6$ fm

^{62}Ni $b_{Ni} = -8.7$ fm

Quantities that depend on $b_{Pt} + b_{Ni}$ are nearly zero

Courtesy of J.L. Roberston

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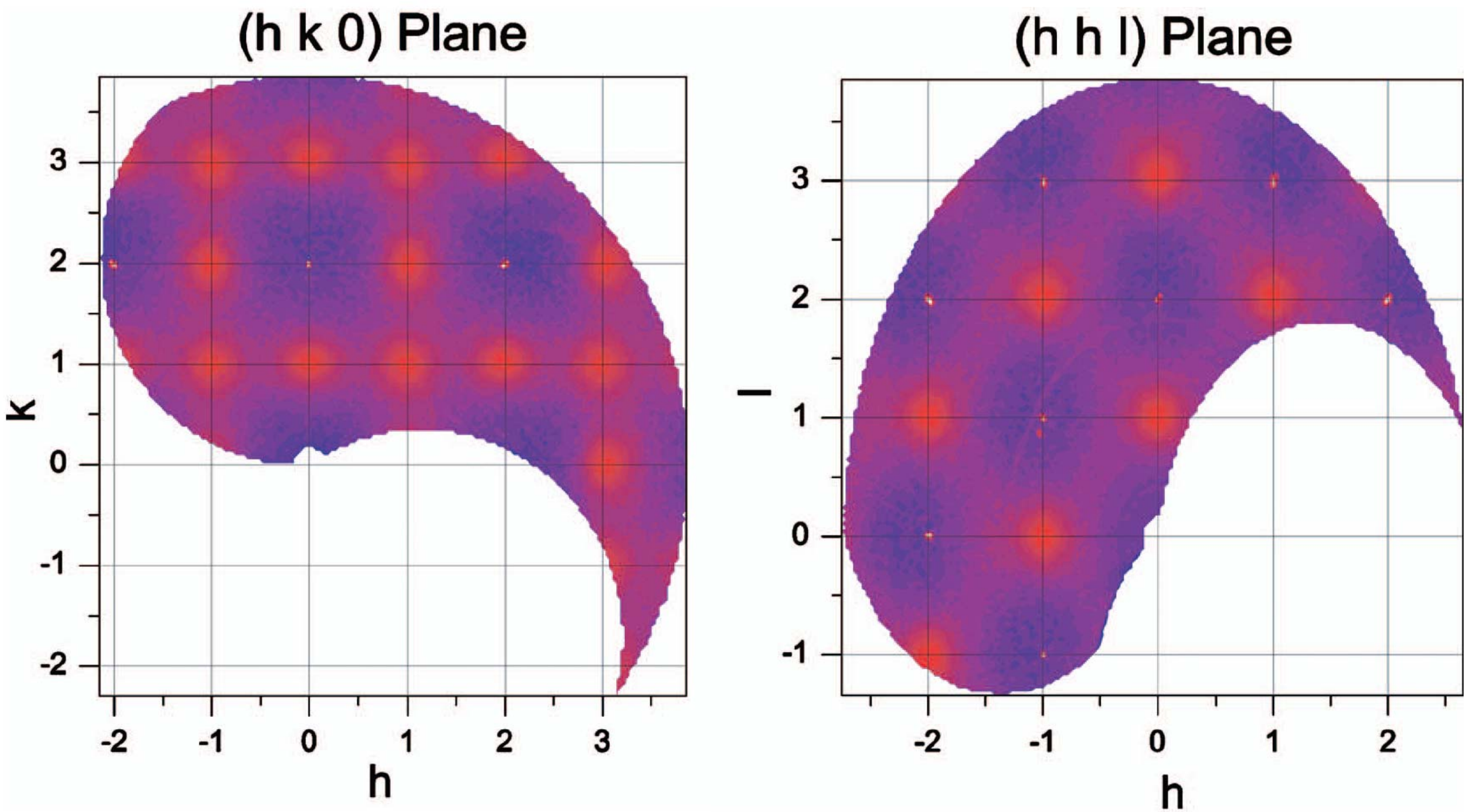
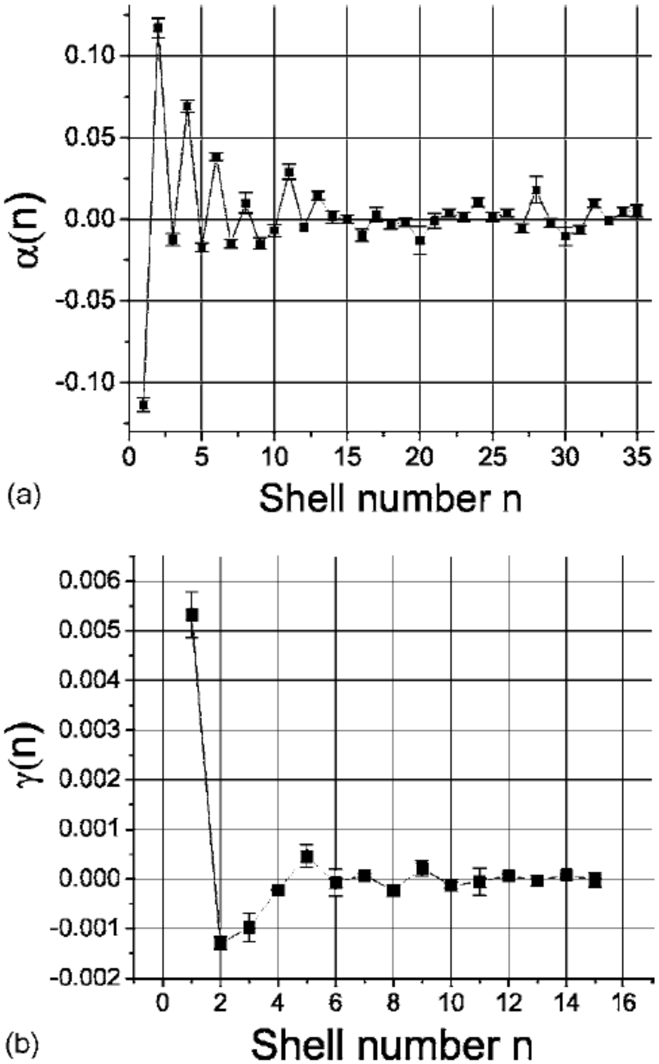
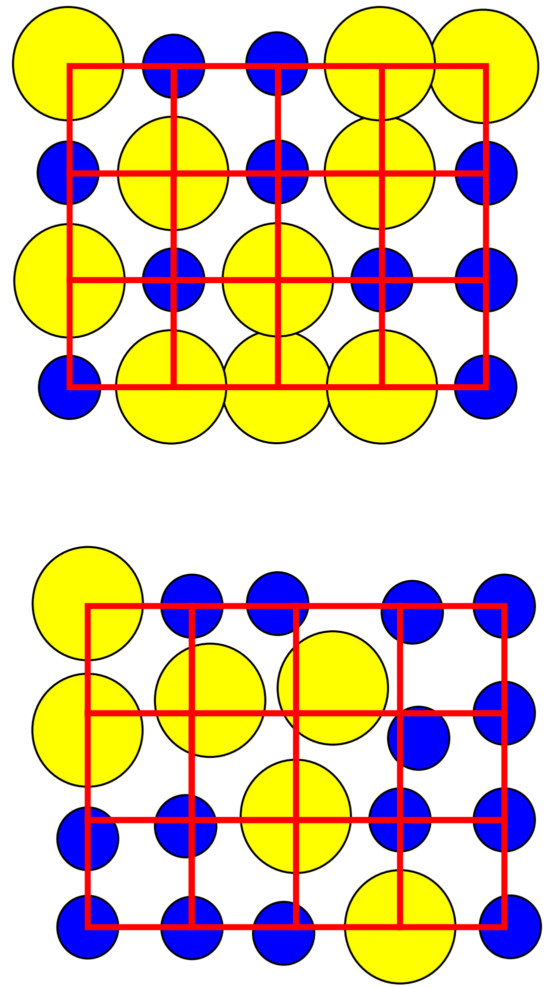
Short-Range Order and Atomic Displacements in a Null-Matrix $^{62}Ni_{0.52}Pt_{0.48}$ Crystal



J.A. Rodriguez, S.C. Moss, *et al.*, PRB **74,** 104115 (2006).

Short-Range Order and Atomic Displacements in a Null-Matrix $^{62}Ni_{0.52}Pt_{0.48}$ Crystal





J.A. Rodriguez, S.C. Moss, et al., PRB **74**, 104115 (2006).

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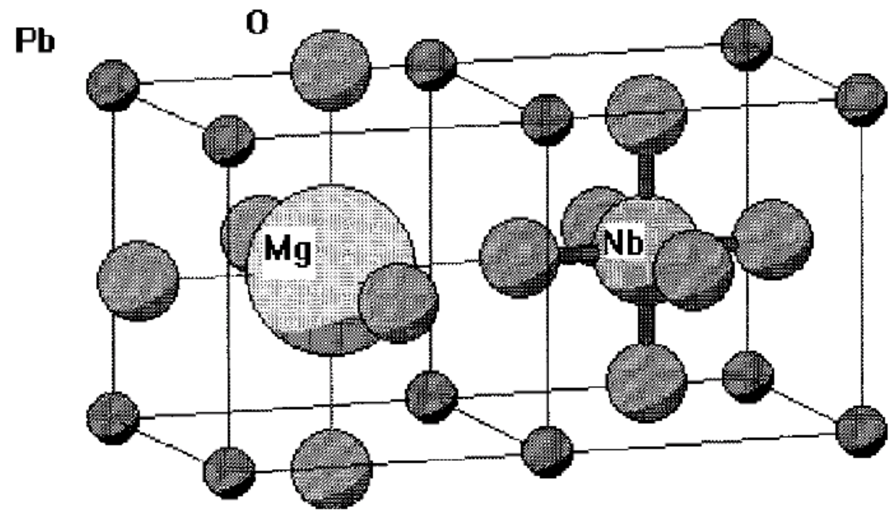
Lead-based Relaxors

Prototypical relaxor is $Pb(Mg_{1/3}Nb_{2/3})O_3$ (or PMN).

Perovskite structure (ABO_3): A or B-site randomly occupied with different cations → quenched chemical disorder.

The addition of Ti^{4+} on the B-site greatly enhances the piezoelectric properties of PMN.

In the case of PMN, B-site has a mixed valence character from Mg^{2+} and Nb^{5+}.



D. M. Fanning *et al.*,
J. Appl. Phys. **87**, 840 (2000)

Random field effects are expected

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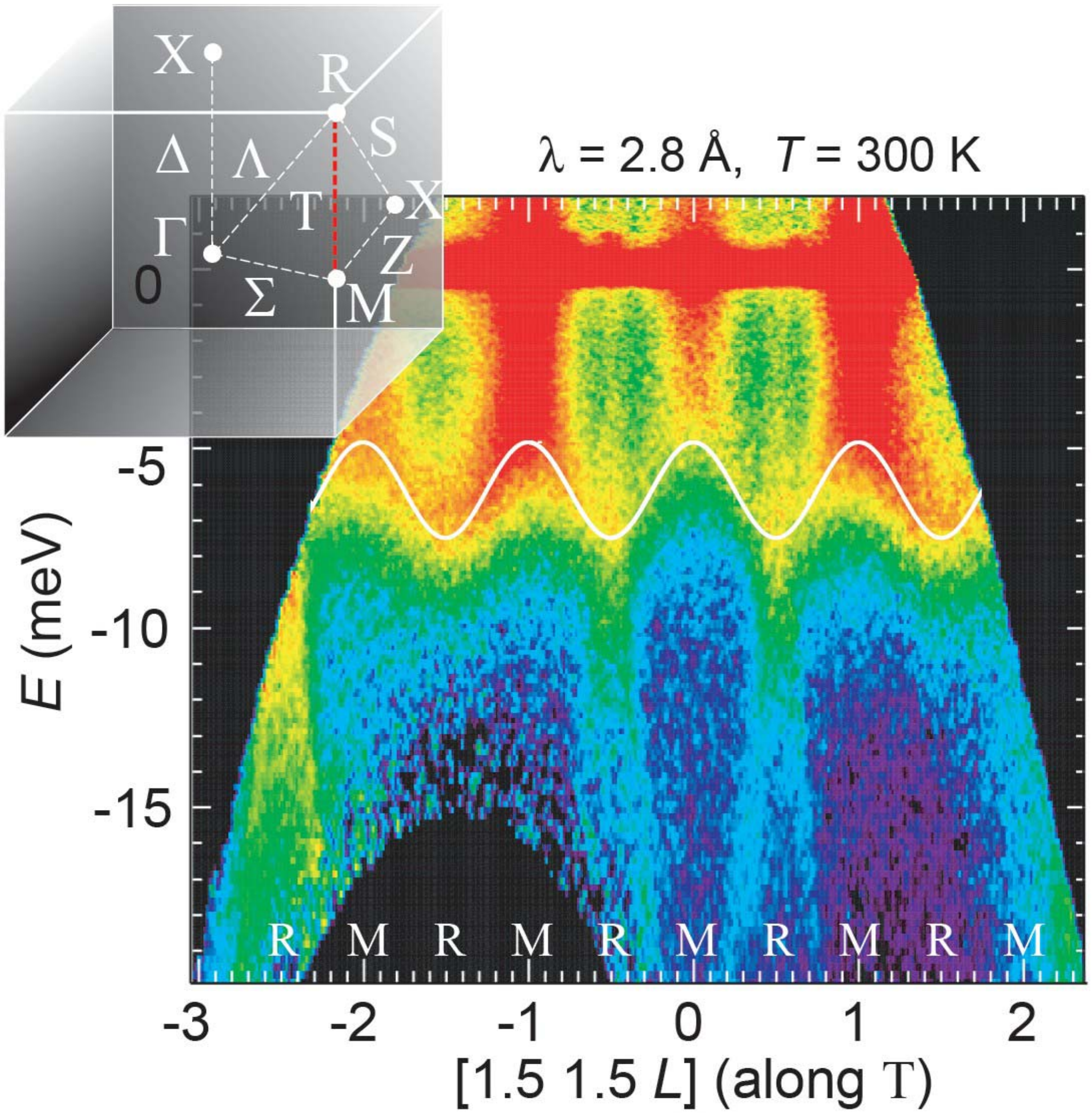
"Columns" of Inelastic Scattering



"Columns" of inelastic scattering soften and extend towards the elastic channel upon cooling from high temperature at both the M and R points.

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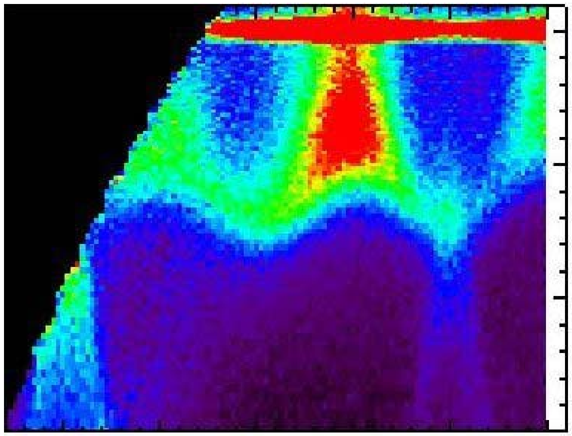
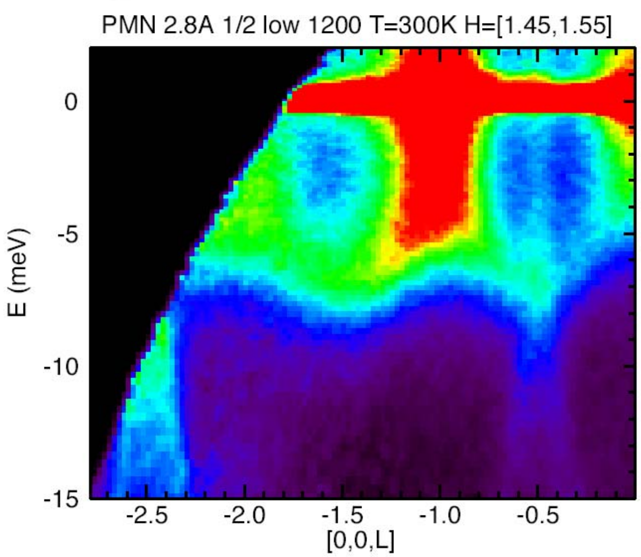
Zone Boundary Soft Modes



600 K



300 K

The structure factors will help determine what these soft zone boundary modes are.

Do not believe that they are the tilt modes (*e.g.* ½(hh0) do not involve oxygen rotations).

Believe that they are due primarily to Pb and Nb displacements.

The presence of the soft ZB modes suggests a competition between FE and AFE short range ordered nano scale regions.

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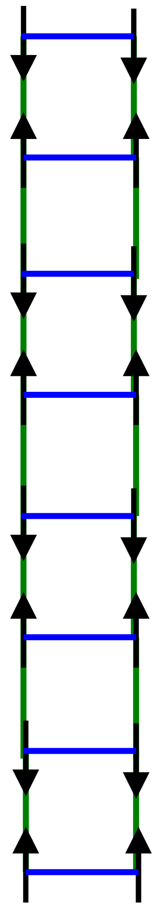
Quantum Phase Transitions in Coupled Spin Ladders

s=½



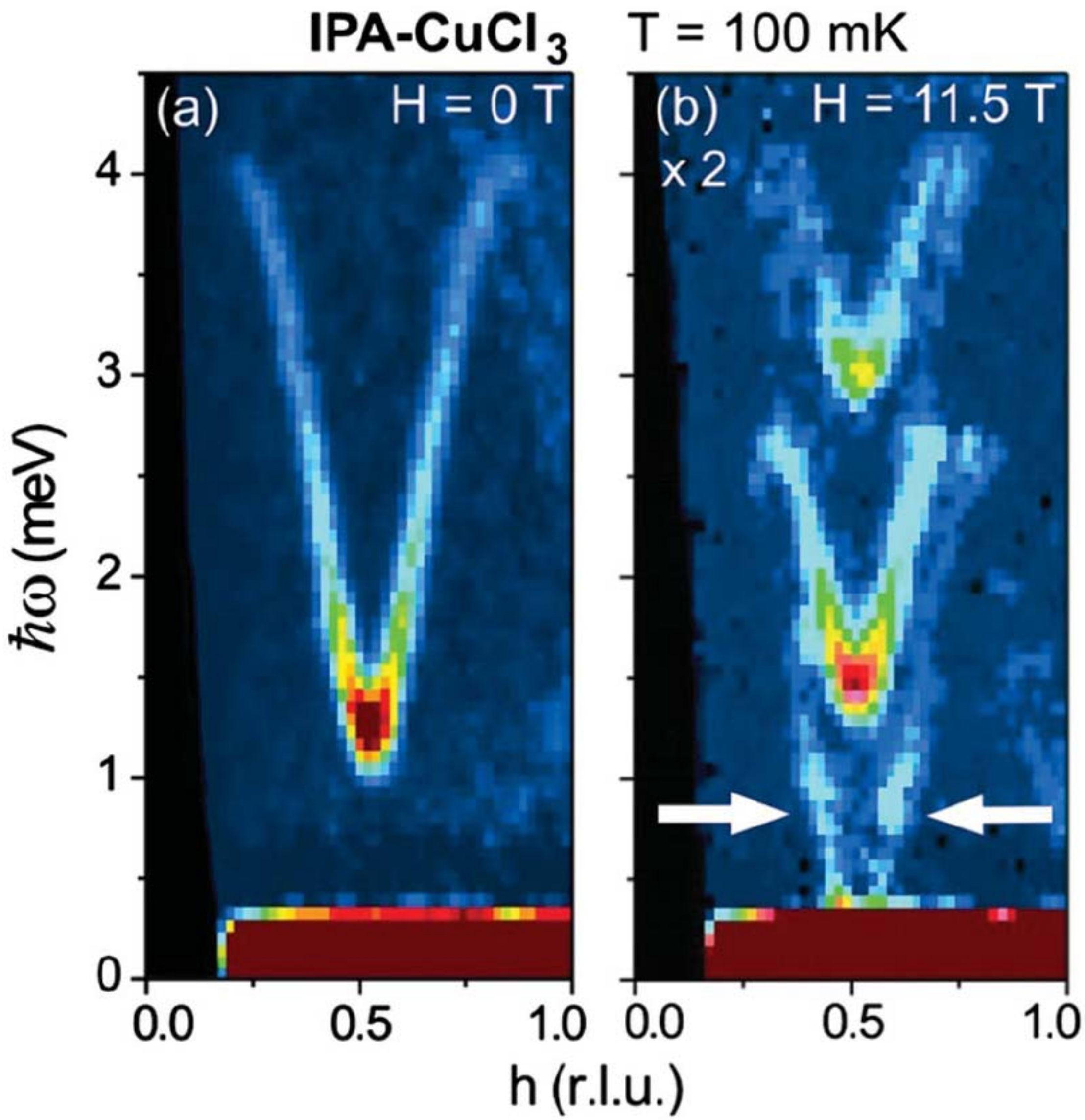
Quantum phase transitions

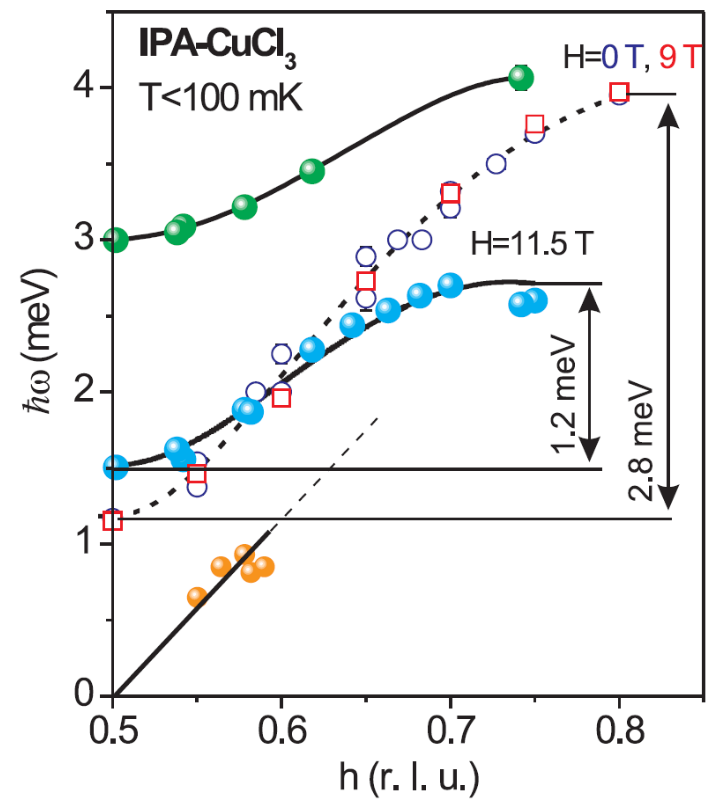
The elementary excitations in a 1-d, spin 1 antiferromagnet are a triplet of magnons

An external magnetic field modifies the magnon energies via the Zeeman effect

At H=Hc the gap of one of the magnon branches approaches 0.
=> equivalent to conventional BEC

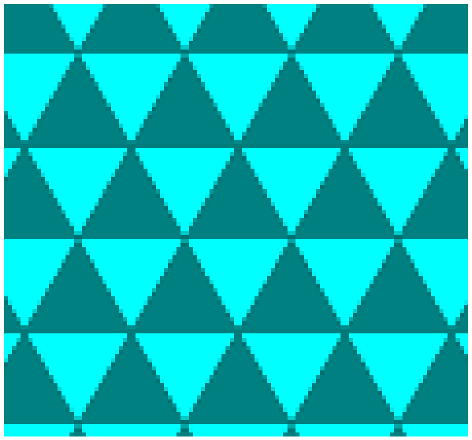
Bose-Einstein Condensate of Magnons in isopropylammonium-$CuCl_3$





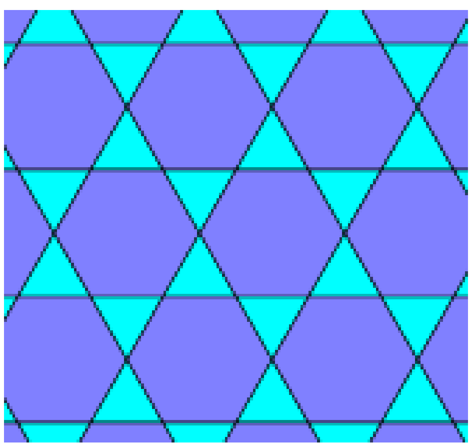
Garlea, Zheludev *et al.*,
PRL **98**, 167202 (2007).

Geometrically Frustrated Magnets



triangular lattice

Kagome lattice



Geometrical frustration occurs when there is an ordered lattice structure where the spin interactions cannot be simultaneously satisfied

The most common systems are quasi 2 dimensional (triangles)

In 3 dimensions, the corresponding structure is a tetrahedron

It turn out that cubic pyrochlore structure with four magnetic atoms/ions residing on the four corners are often excellent model systems

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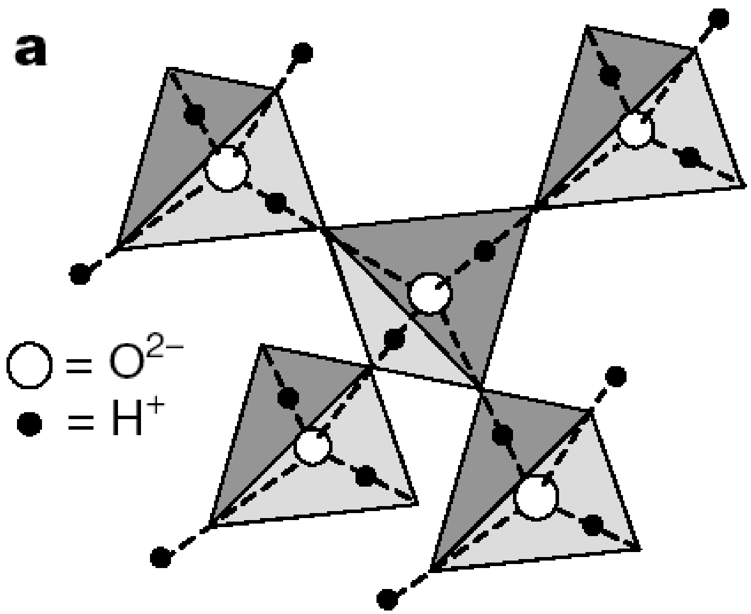
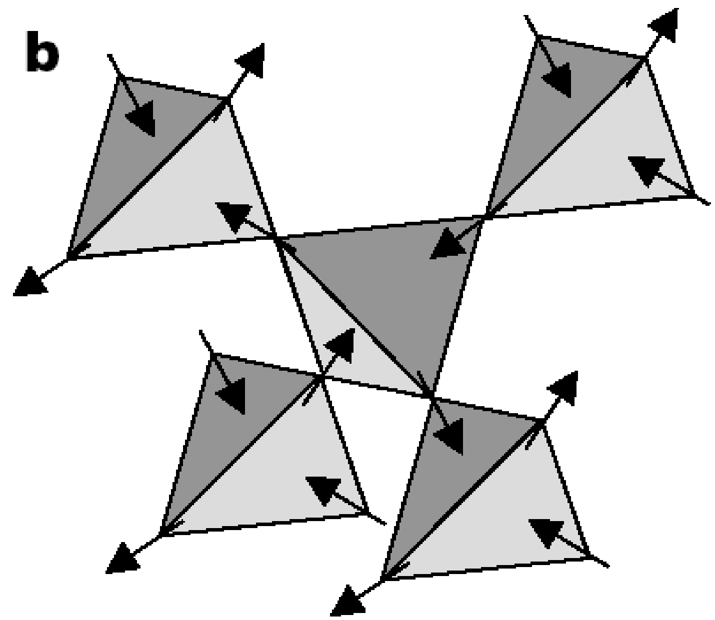
Analogy to Water Ice



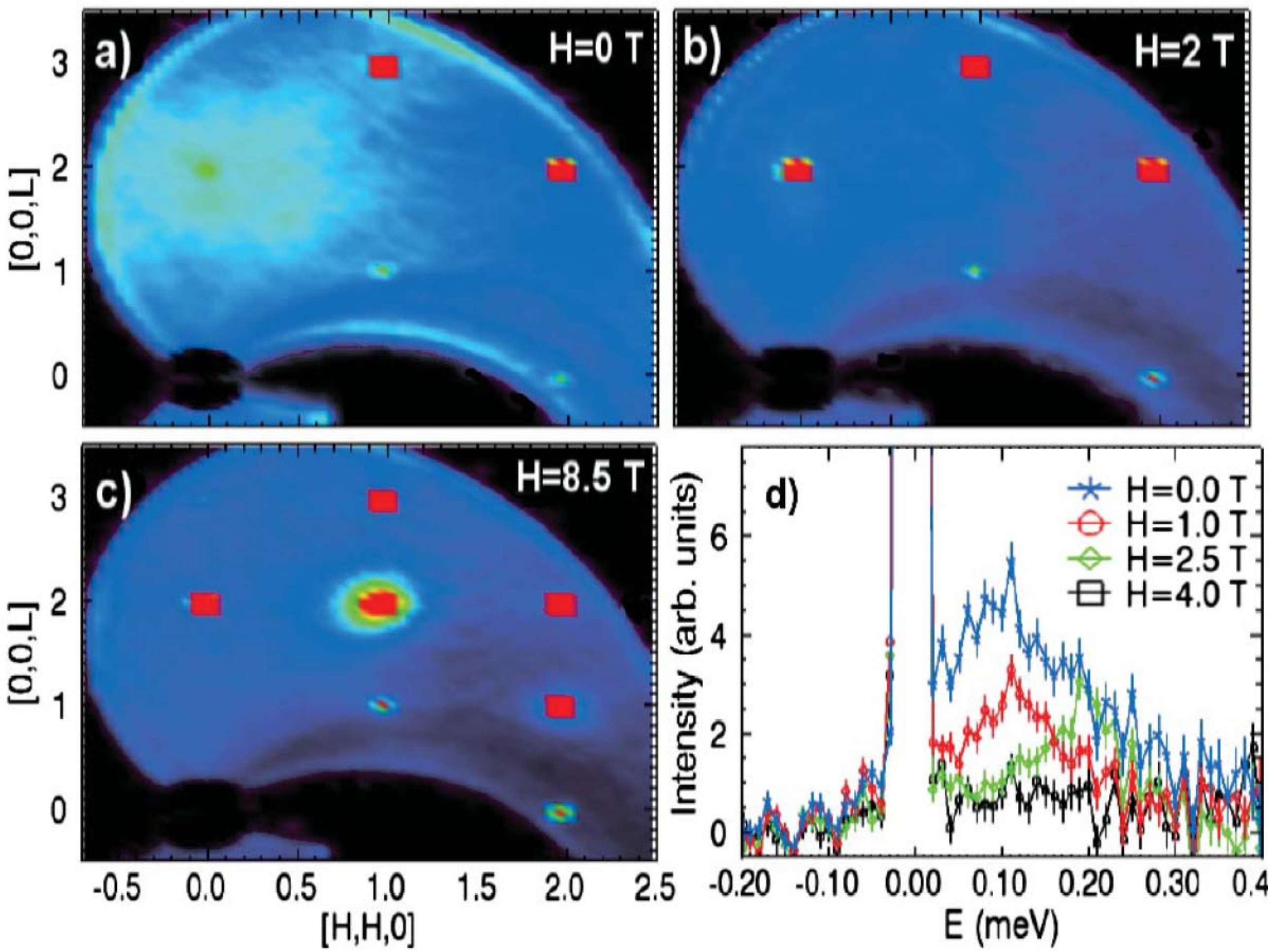
Water ice



Spin ice

CEF constrains spins to local <111> axes

Field-Induced Order in $Tb_2Ti_2O_7$



In zero field $Tb_2Ti_2O_7$ is a highly correlated cooperative paramagnet with disordered spins

At 2 T there is a polarized paramagnet phase where the magnetic peaks arise from single-ion polarization of much of the paramagnetic moment along the field direction.

At higher fields, there is a long-range ordered magnetic phase

T = 1K magnetic field applied along a 110 direction

K.C. Rule, B.D. Gaulin, et al., PRL **96**, 177201 (2006).

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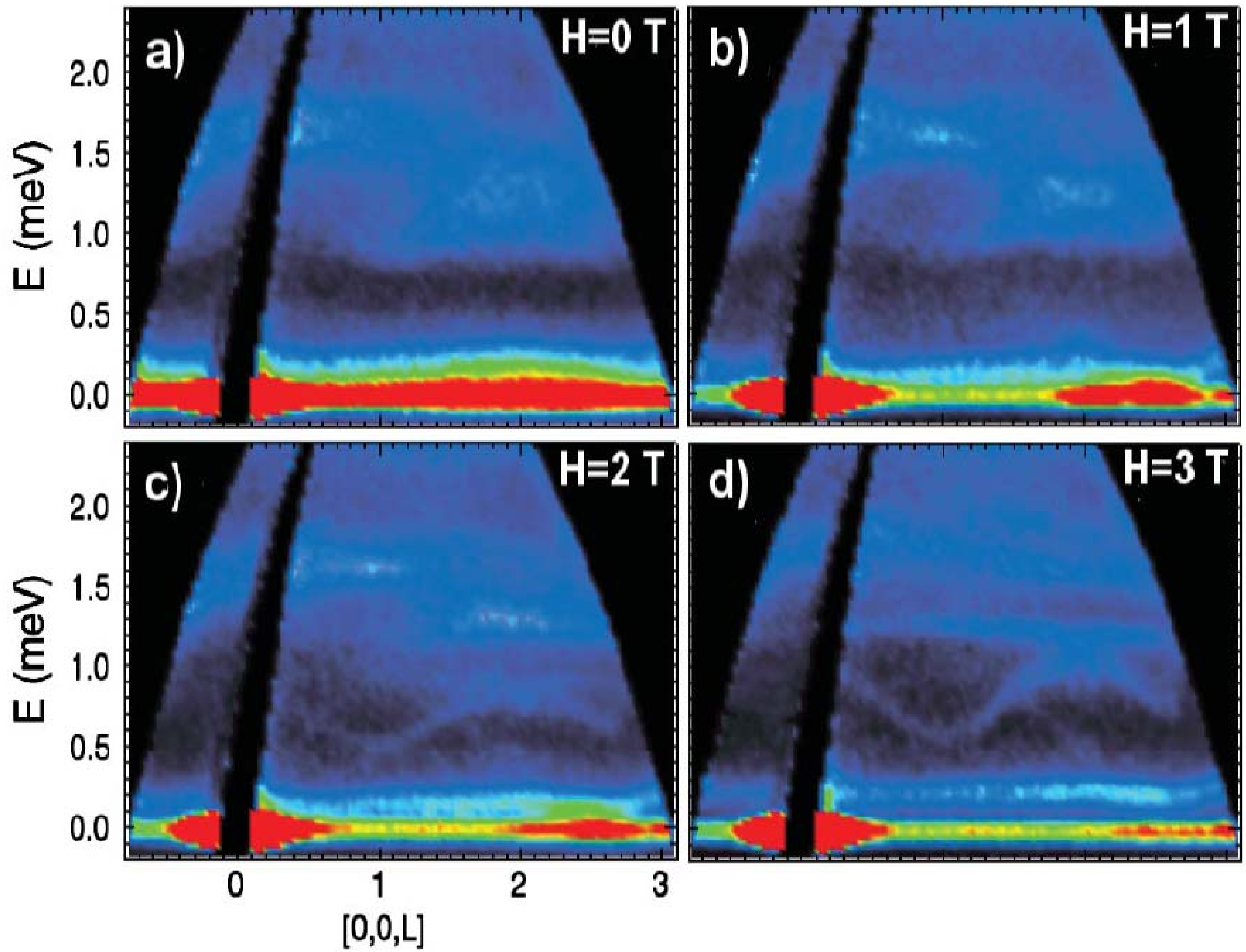
Spin Waves in $Tb_2Ti_2O_7$



K.C. Rule, B.D. Gaulin, et al., PRL **96**, 177201 (2006).

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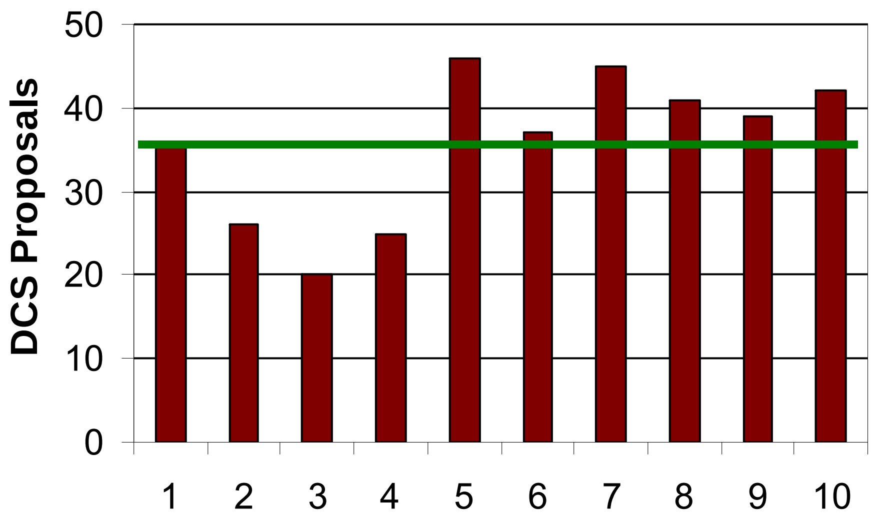
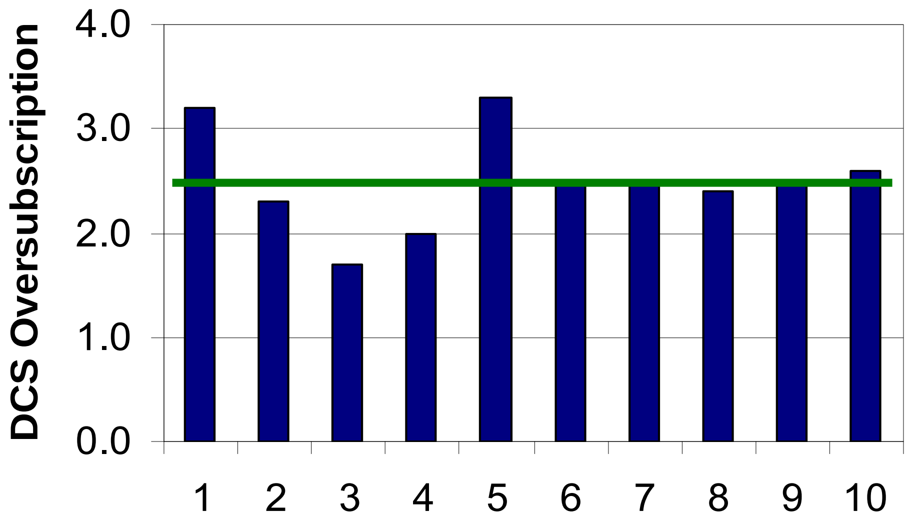
Disk Chopper Spectrometer





Our last 10 "Calls for Proposals"

Ave. Proposals : **36**

Ave. Oversubscription : **2.5**

76 Publications since 2004

13 PRL

4 Nature, Science, PNAS

Acknowledgements

John Copley, Craig Brown, and Yiming Qiu

Yamali Hernandez

Thanks for your interest in the NCNR