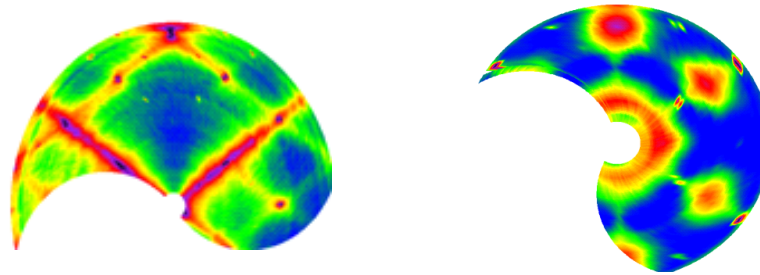


Higgs transition from a magnetic Coulomb liquid to a ferromagnet in $\text{Yb}_2\text{Ti}_2\text{O}_7$



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14th June 2013
EQPCM 2013,
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Japan Atomic Energy Agency

JAEA: K. Kakurai

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Contents

- Geometrically frustrated Pyrochlores

- Quantum spin ice $\text{Yb}_2\text{Ti}_2\text{O}_7$ & Higgs transition
 - *Introduction*

 - *Polarized neutron scattering experiments*

- Summary & future works

- Sample dependent

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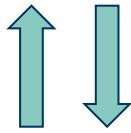
- Geometrically frustrated Pyrochlores

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 - *Introduction*

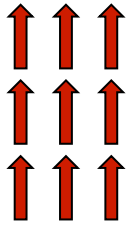
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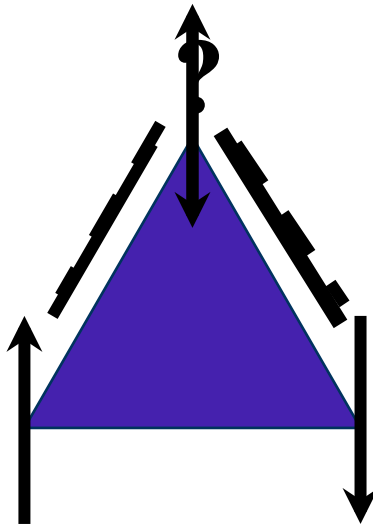


Classical Ising spins, $s_i = +/- 1$



Exchange interaction, $H = J s_i s_j$
 $J < 0$, ferromagnetic;
 $J > 0$, antiferromagnetic

Geometrical Frustration: what happened?



Not all the terms in H can be minimized

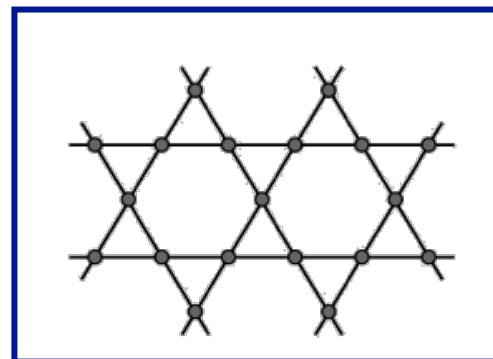
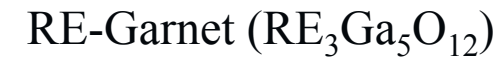
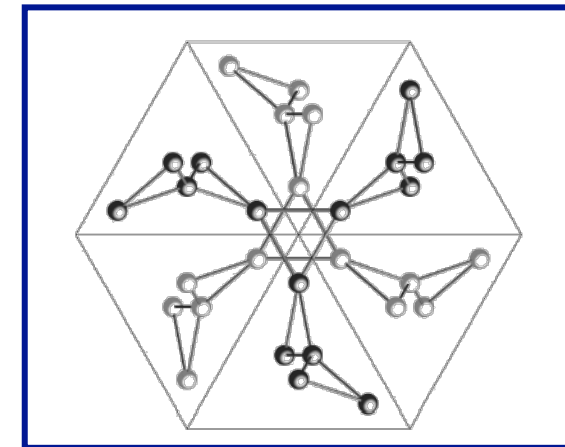
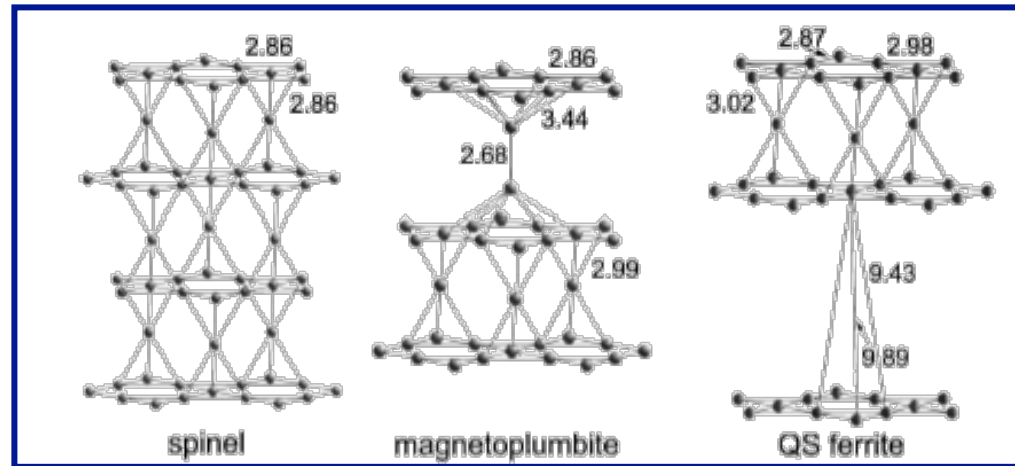
$$\text{But } H = J / 2 \left(\sum_{i=1}^n s_i \right)^2 + C$$

Can be minimized

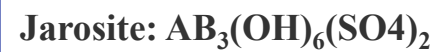


ground state degeneracy

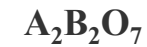
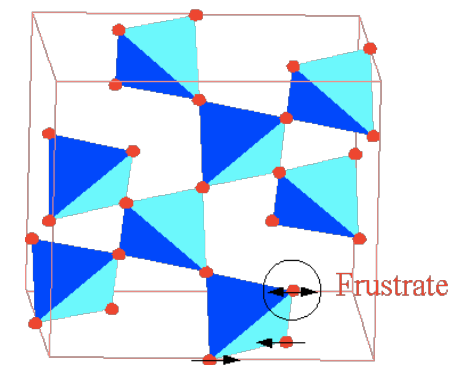
Famous Frustrated lattices



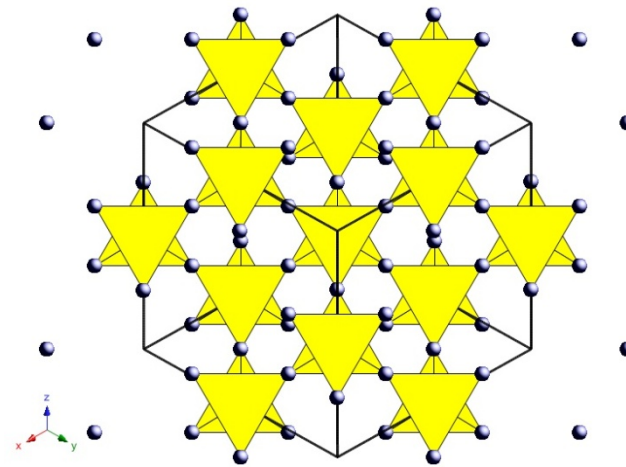
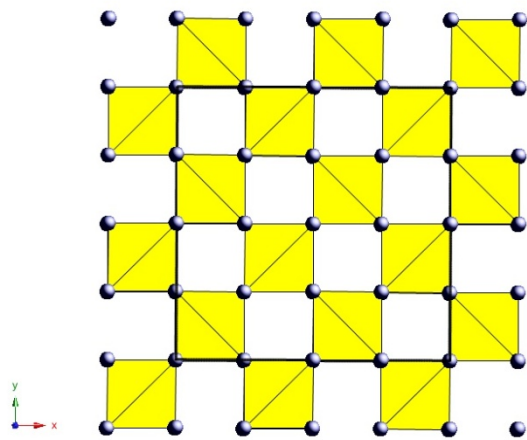
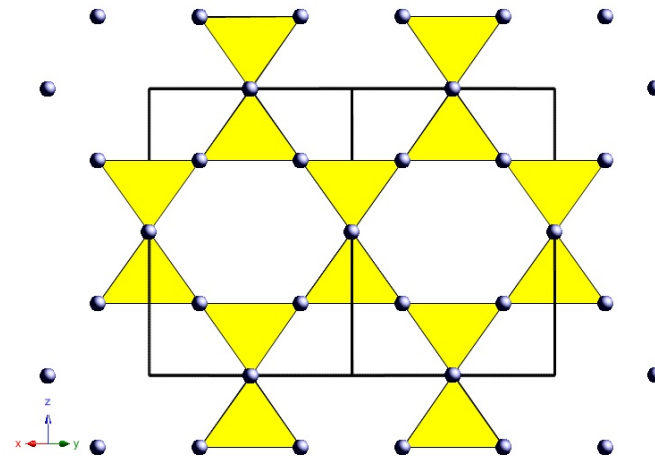
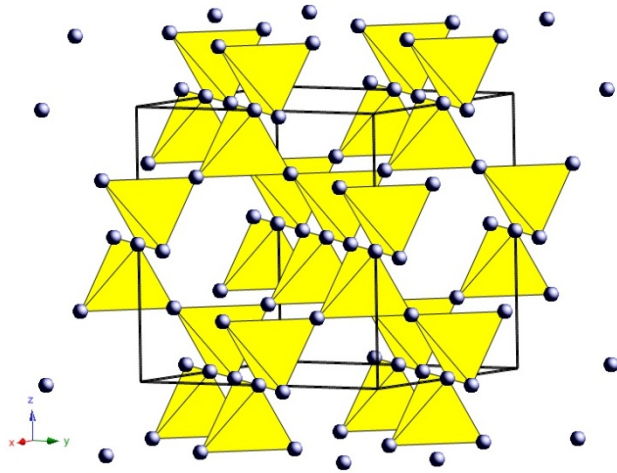
Kagomé
Lattice



Pyrochlore
Lattice

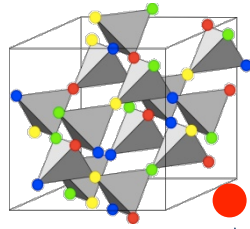


Pyrochlore lattice

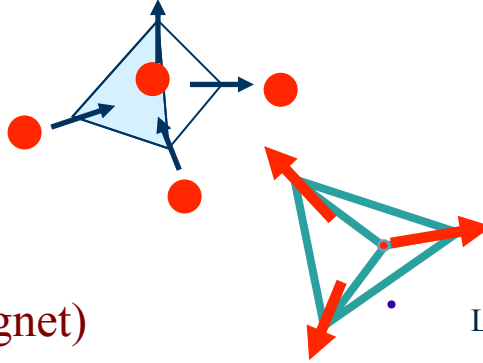


Famous examples for 3D

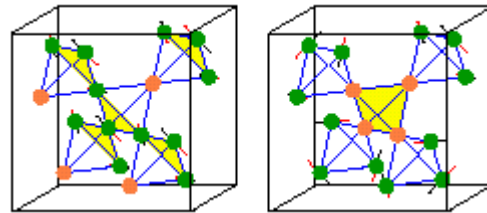
- **Spin glass**
randomly frozen
 $Y_2Mo_2O_7$



- **Spin ice**
frozen local order
 $Ho_2Ti_2O_7, Dy_2Ti_2O_7$



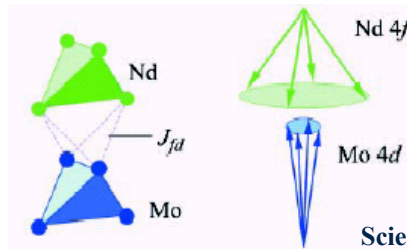
- **Spin liquid**
(Cooperative paramagnet)
very dynamic
 $Tb_2Ti_2O_7$



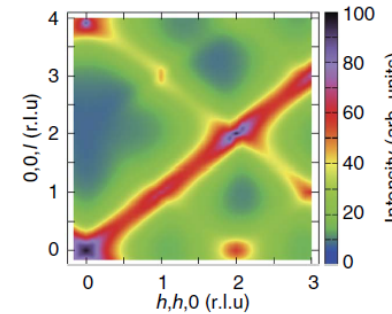
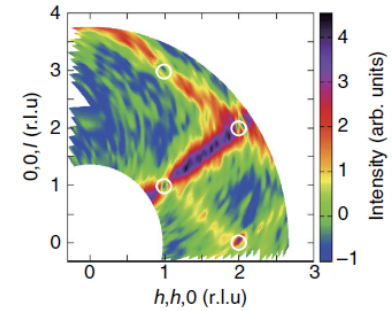
- **Spin slush**
partially ordered
 $Gd_2Ti_2O_7$

J. Phys. Cond. Matter. 16, L321 (2004)

- **Spin Chirality**
transition metal sites
 $Nd_2Mo_2O_7$

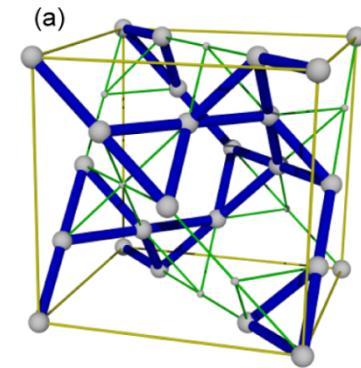


- **XY pyrochlore**
2-D
 $Yb_2Ti_2O_7$



L. J. Chang/ S. Onoda *et al.*, Nat. Commun. 3, 992 (2012)

- **HyperKagome**
 $Na_4Ir_3O_7$



PRL. 105, 237202 (2010)

Science. 291, 2573 (2001)

Contents

- Geometrically frustrated Pyrochlores

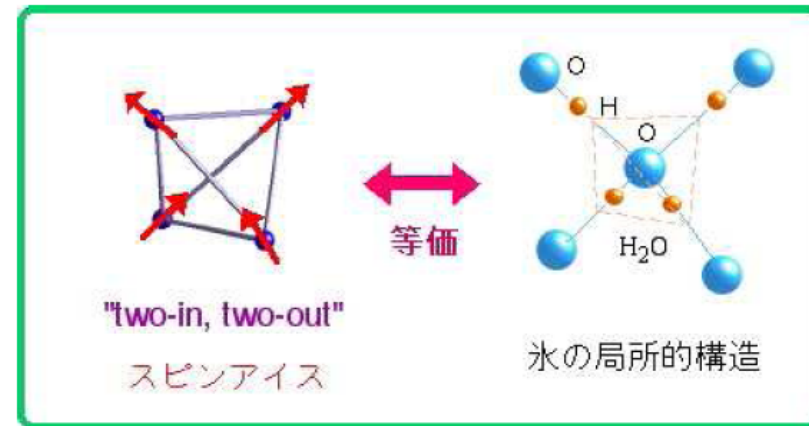
- **Quantum spin ice $\text{Yb}_2\text{Ti}_2\text{O}_7$ & Higgs transition**
 - *Introduction (spin ice)*

 - *Polarized neutron scattering experiments*

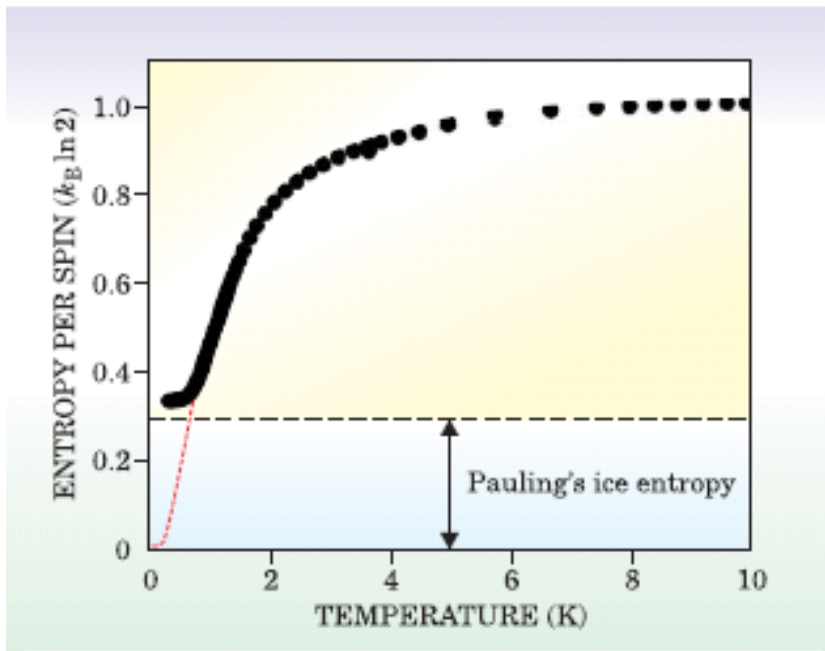
- Summary & future works

- Sample dependent

Spin Ice



150.69.54.33/takagi/matuhirasan/SpinIce.jpg



Zero point entropy:

$$S/k_B N = \ln 2 - (1/2) \ln(3/2)$$

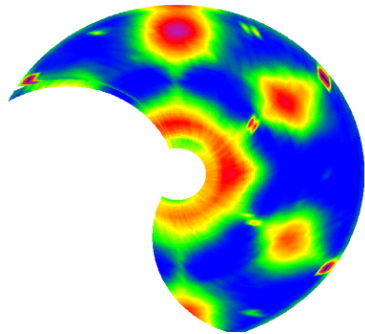
Microstates: N spins, $N/2$ tetrahedra;

Constraints: two-in, two-out;

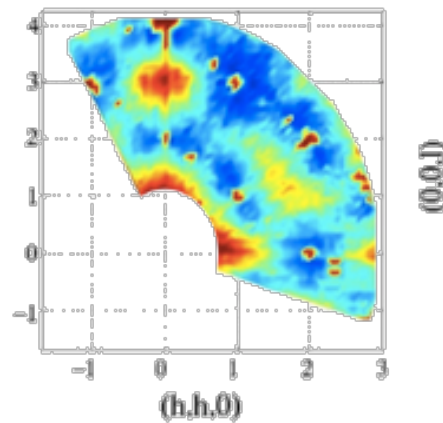
No. of ground state: $2^N (6/16)^{N/2}$

Entropy: $1/2 \ln(3/2)$

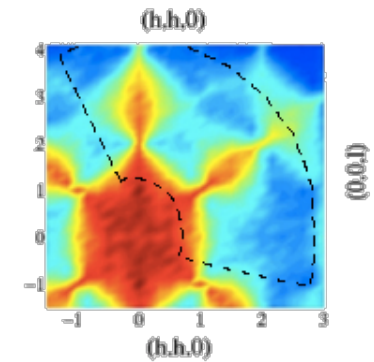
Diffuse neutron scattering for spin ice



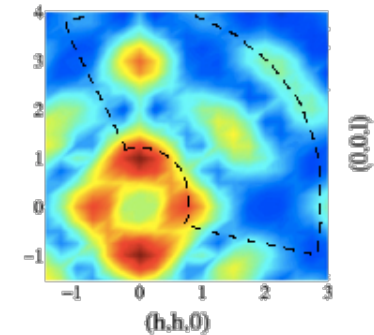
L. J. Chang et al., PRB, **82**, 172403 (2010).



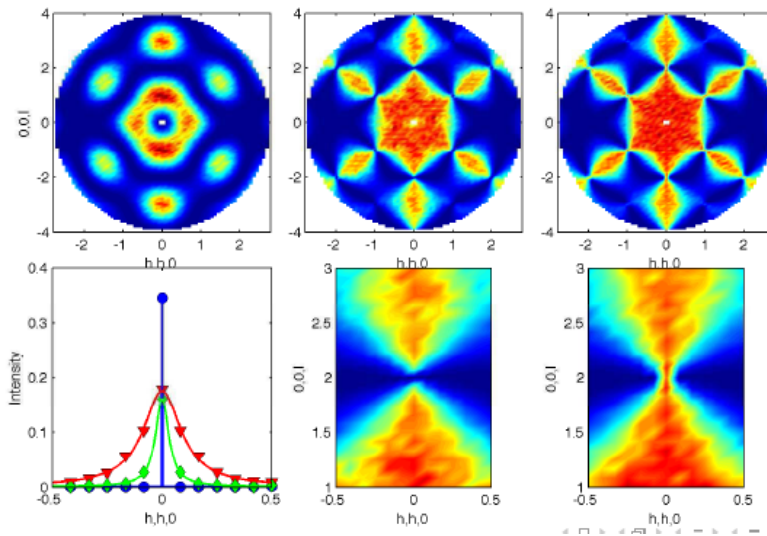
nn Spin Ice



Dipolar Spin Ice



Strings as ferromagnetic fluctuations



T. Fennell et al. Science **326**, 415 (2009)

S.T. Bramwell et al., PRL, **87**, 047205 (2001).

$$H = -J \sum_{\langle ij \rangle} S_i^{z_i} \cdot S_j^{z_j} + D r_{nn}^3 \sum_{i>j} \frac{S_i^{z_i} \cdot S_j^{z_j}}{|\mathbf{r}_{ij}|^3} - \frac{3(S_i^{z_i} \cdot \mathbf{r}_{ij})(S_j^{z_j} \cdot \mathbf{r}_{ij})}{|\mathbf{r}_{ij}|^5}$$

Yb₂Ti₂O₇

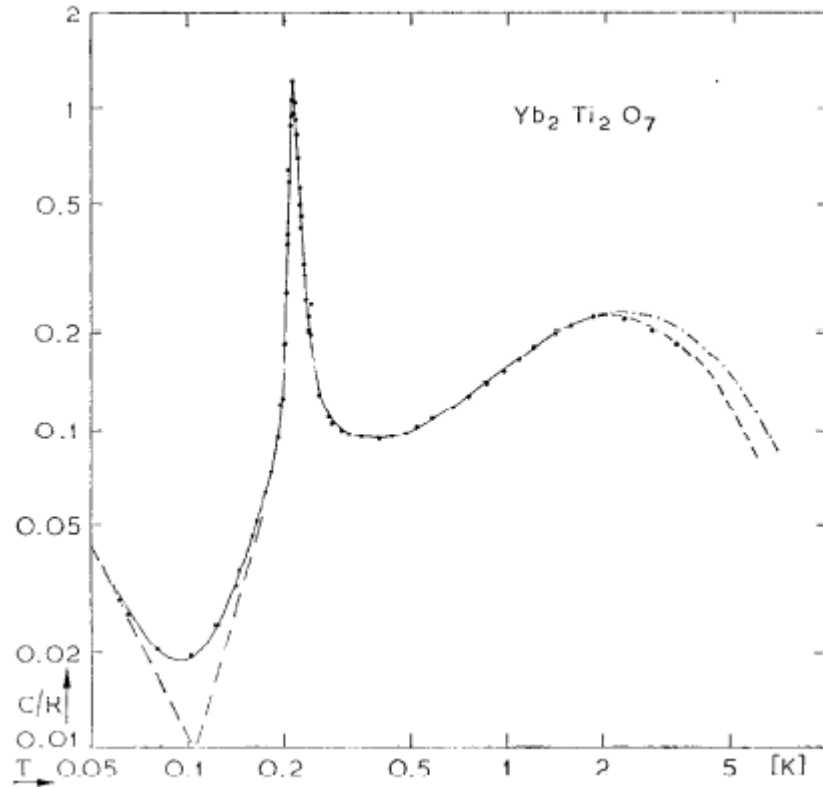


Fig. 12. Heat capacity of Yb₂Ti₂O₇.

H. W. J. Bloete *et al.*, *Physica* **43**, 549–568 (1969).

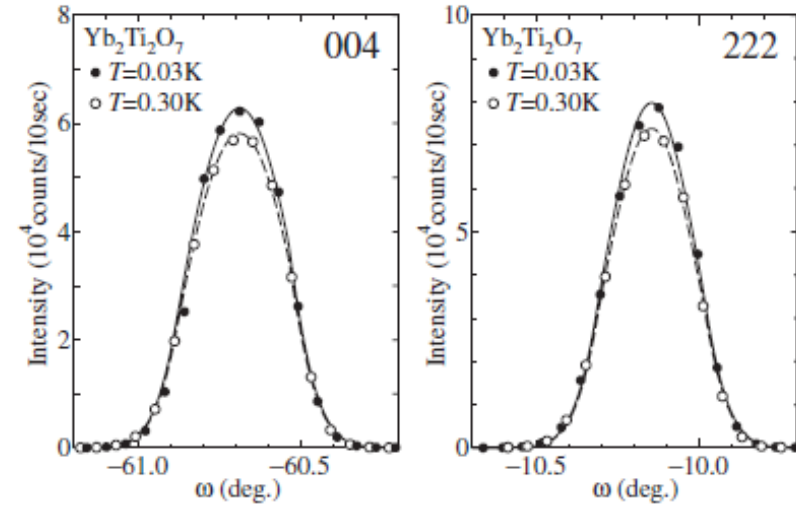


Fig. 3. Profiles of the ω -scans for 004 and 222 reflections taken at 0.03 K and 0.30 K. Solid and Broken lines are guides for the eye.

Y. Yasui *et al.*, *JPSJ* **72** 3014 (2003)

ferromagnetic

CW temperature ~ 0.6 K
 1st order transition ~ 210 mK
 LRO?

Quantum spin ice approach

The Yb^{3+} 4f magnetic moment at a site r is described with the pseudospin-1/2 operator $\hat{\mathbf{S}}_r = (\hat{S}_r^x, \hat{S}_r^y, \hat{S}_r^z)$

$$\mathbf{m}_r = \mu_B \left(g_{\perp} (\hat{S}_r^x \mathbf{x}_r + \hat{S}_r^y \mathbf{y}_r) + g_{\parallel} \hat{S}_r^z \mathbf{z}_r \right)$$

the g -tensor components $g^{\perp} = 4.18$ and $g^{\parallel} = 1.77$

where the z direction is taken along the $\langle 111 \rangle$ direction

$$H_D = \frac{\mu_0}{4\pi} \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} \left[\frac{\mathbf{m}_r \cdot \mathbf{m}_{r'}}{(\Delta r)} - 3 \frac{(\mathbf{m}_r \cdot \Delta \mathbf{r})(\Delta \mathbf{r} \cdot \mathbf{m}_{r'})}{(\Delta r)^5} \right],$$

Spin ice

+

Quantum fluctuations

=

Quantum spin Ice

$$H_{se} = J \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle}^{n.n.} \left[\hat{S}_r^z \hat{S}_{r'}^z + \frac{\delta}{2} (\hat{S}_r^+ \hat{S}_{r'}^- + h.c.) + \frac{q}{2} (e^{2i\phi_{r,r'}} \hat{S}_r^+ \hat{S}_{r'}^+ + h.c.) + \frac{K}{2} (e^{i\phi_{r,r'}} (\hat{S}_r^z \hat{S}_{r'}^+ + \hat{S}_{r'}^+ \hat{S}_r^z) + h.c.) \right].$$

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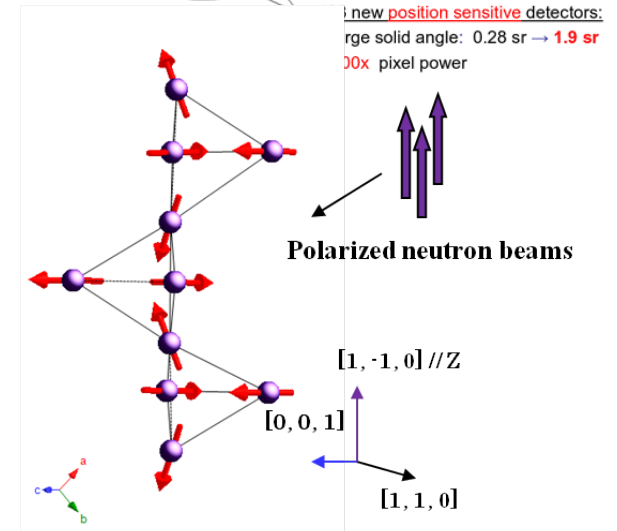
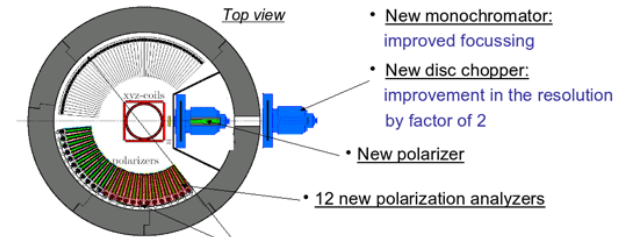
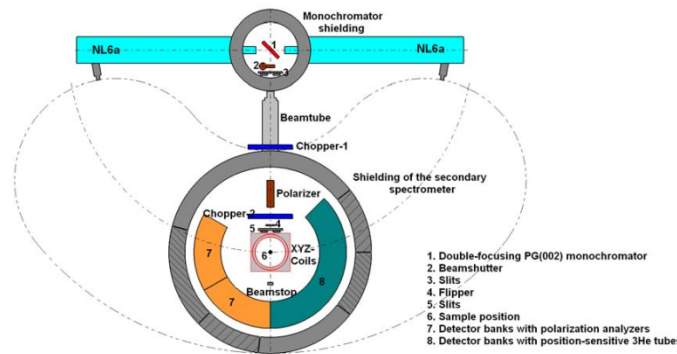
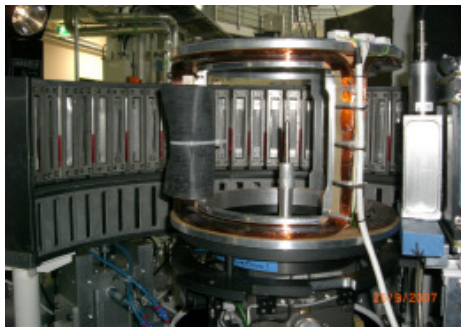
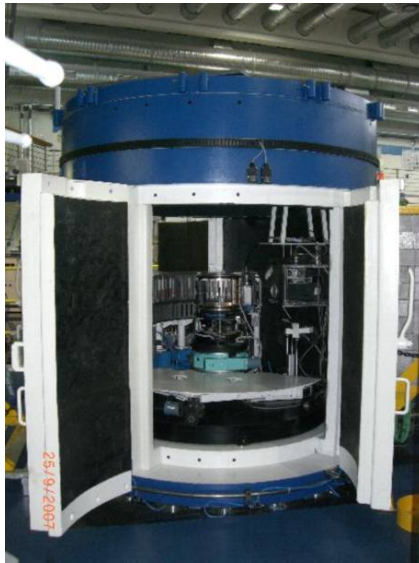


**Single crystals were grown from
IR furnace (Y. Yasui, Nagoya
U.)**



•DNS@FRM-II, Germany

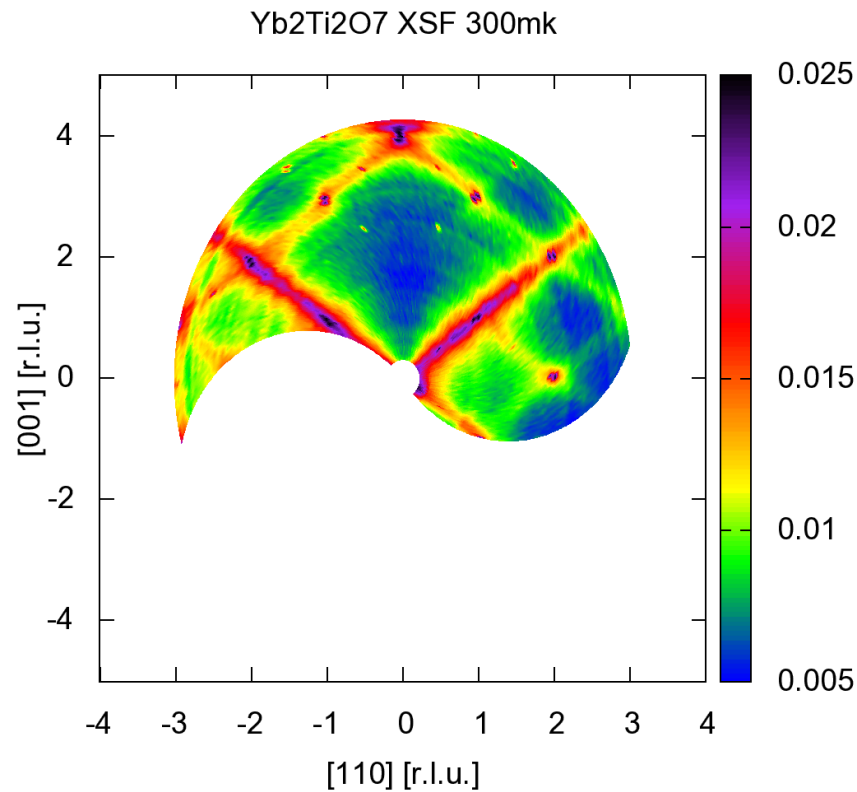
Diffuse Neutron Scattering



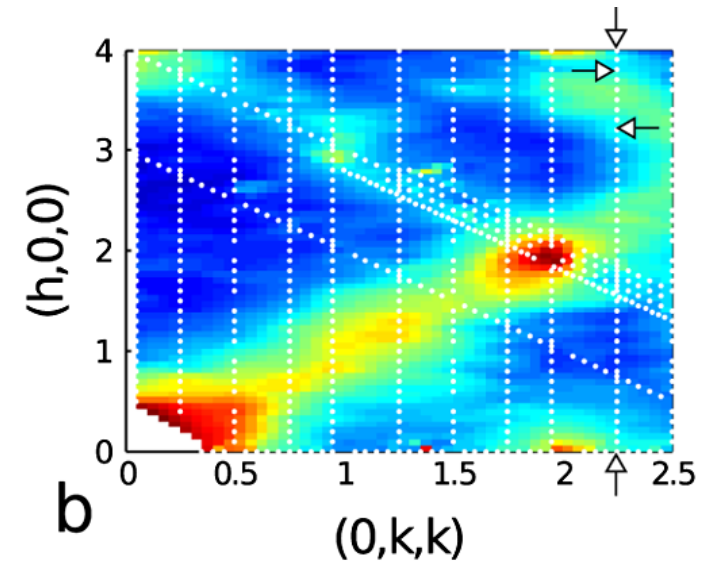
Spin-flip channel

Non-Spin-flip channel

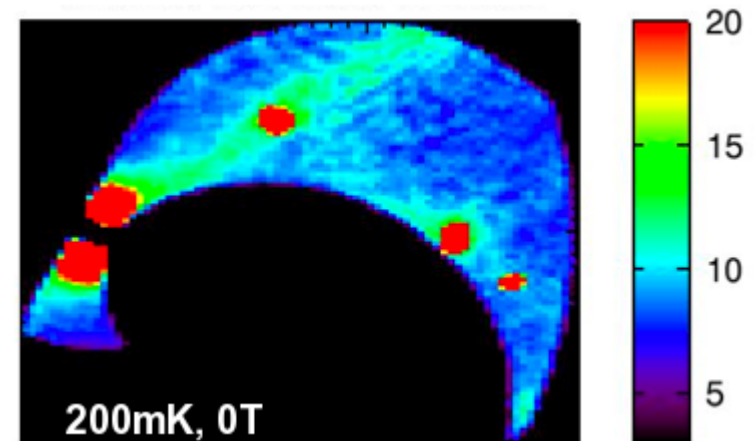
Rod structure along [111]: 2 D correlations on kagome plane above transition temperature



L. J. Chang *et al.*



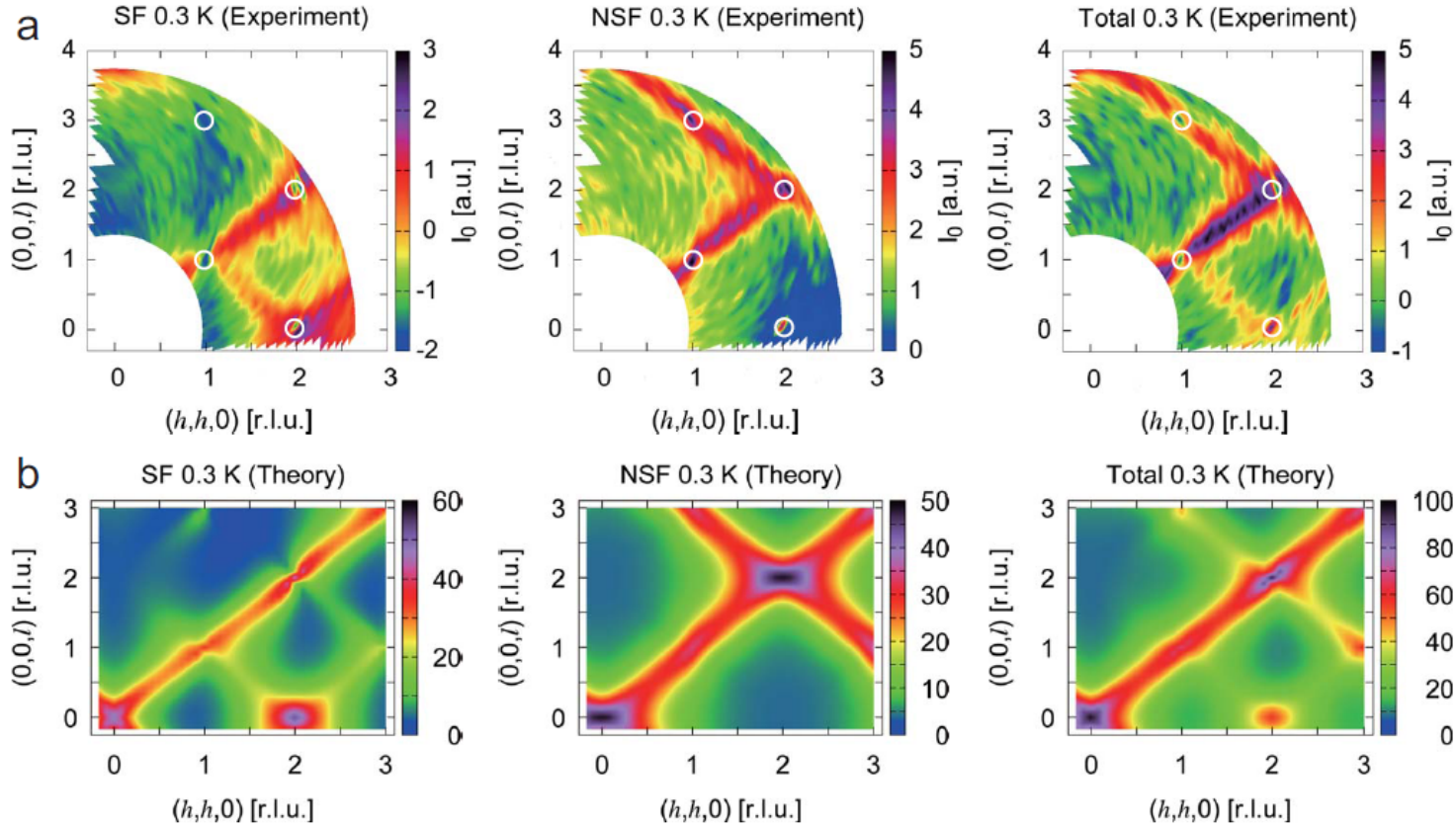
J. D. Thompson *et al.*, PRL. **106**, 187202 (2011)



K. A. Ross *et al.*, PRL **103** 227202 (2010)

Diffuse neutron scattering with polarization analysis

Calculated by RPA
$$I(Q) = \sum_n \sum_{i,j=1}^4 f_{Q,i,j}^{\mu\nu} \frac{\phi_{-Q,n,i}^\mu \phi_{Q,n,j}^\nu}{3 + \epsilon_{Q,n}/T}.$$



$$f_{Q,i,j}^{\mu\nu} = \frac{1}{4|Q|^4} [\mathbf{Z} \cdot (\mathbf{Q} \times (g_\mu \mathbf{e}_i^\mu \times \mathbf{Q}))] [\mathbf{Z} \cdot (\mathbf{Q} \times (g_\nu \mathbf{e}_j^\nu \times \mathbf{Q}))],$$

with $\mathbf{Z} = (1, -1, 0)/\sqrt{2}$ for the NSF channel and $f_{Q,i,j}^{\mu\nu} = \frac{1}{4|Q|^4} [\mathbf{Q} \times (g_\mu \mathbf{e}_i^\mu \times \mathbf{Q})] \cdot [\mathbf{Q} \times (g_\nu \mathbf{e}_j^\nu \times \mathbf{Q})]$

for the total. The SF channel is obtained as the difference between the above two.

Coupling constants we obtained: $(J, \delta, q, K) = (0.68 \text{ K}, -0.8, 0.2, -1.0)$

Similar to the results from neutron inelastic scattering in fields

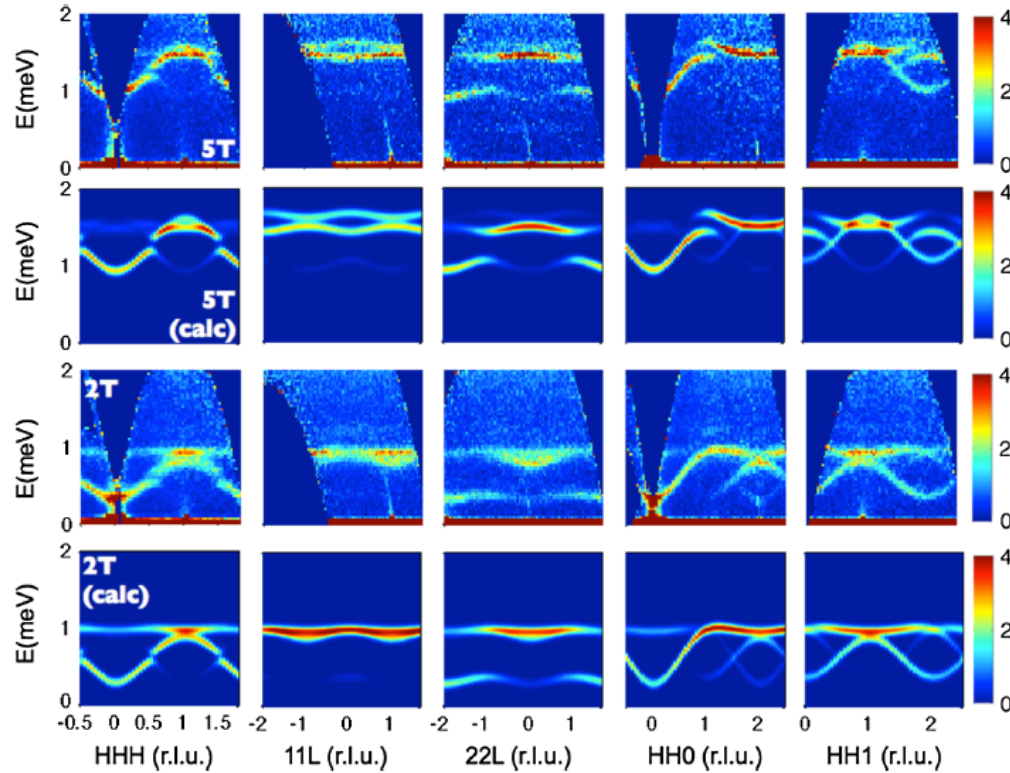
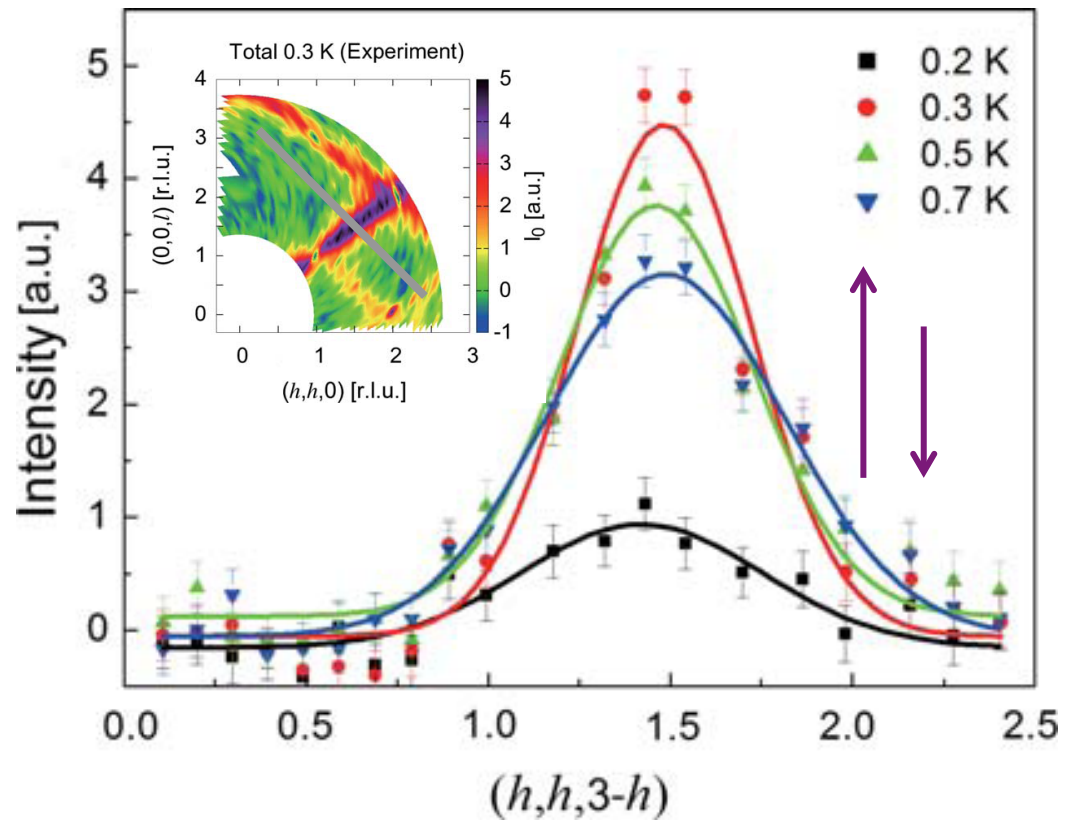
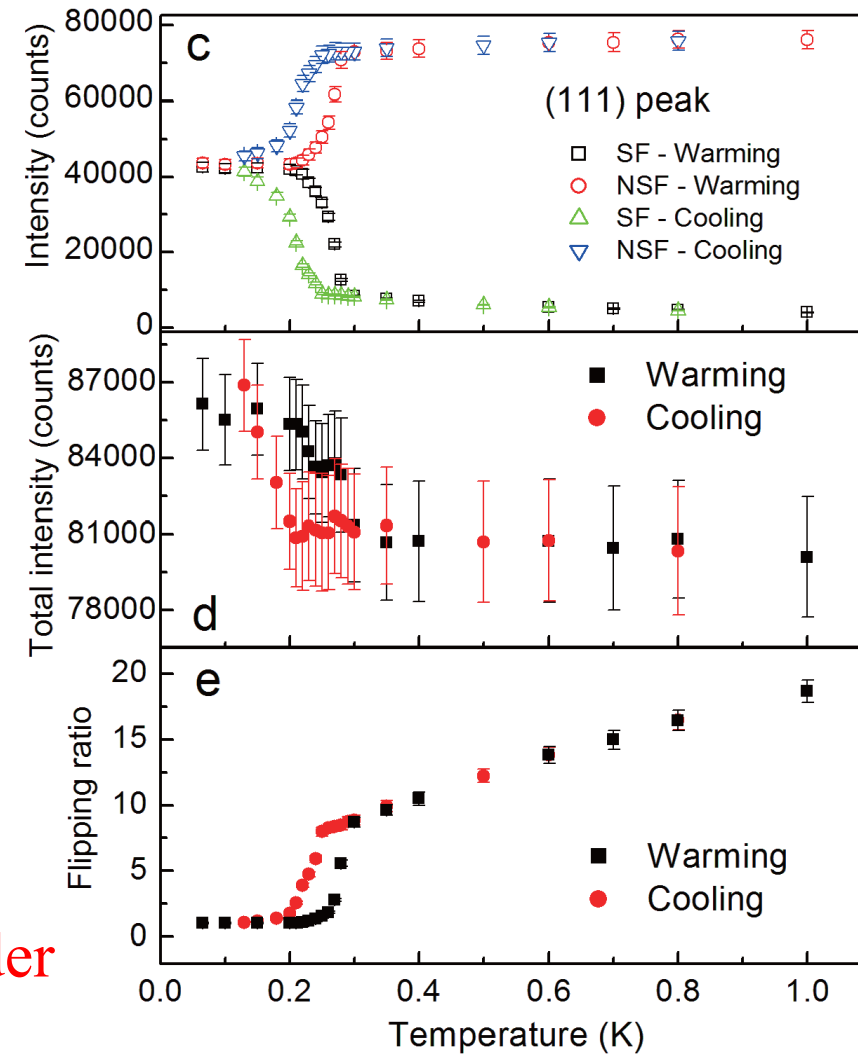
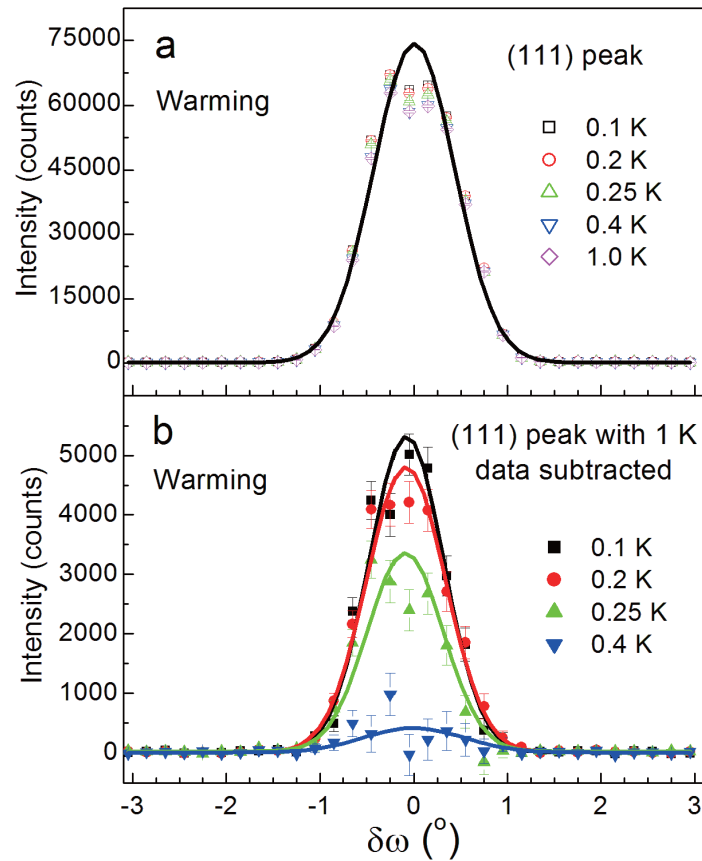


FIG. 1. The measured $S(\mathbf{Q}, \omega)$ at $T = 30 \text{ mK}$, sliced along various directions in the HHL plane, for both $H = 5 \text{ T}$ (first row) and $H = 2 \text{ T}$ (third row). The second and fourth rows show the calculated spectrum for these two field strengths, based on an anisotropic exchange model with five free parameters (see text) that were extracted by fitting to the 5 T data set. For a realistic comparison to the data, the calculated $S(\mathbf{Q}, \omega)$ is convoluted with a Gaussian of full-width 0.09 meV . Both the 2 T and 5 T data sets, composed of spin wave dispersions along five different directions, are described extremely well by the same parameters. (Note that r.l.u. stands for reciprocal lattice units.)

Z-TOTAL cross-section cut on rod

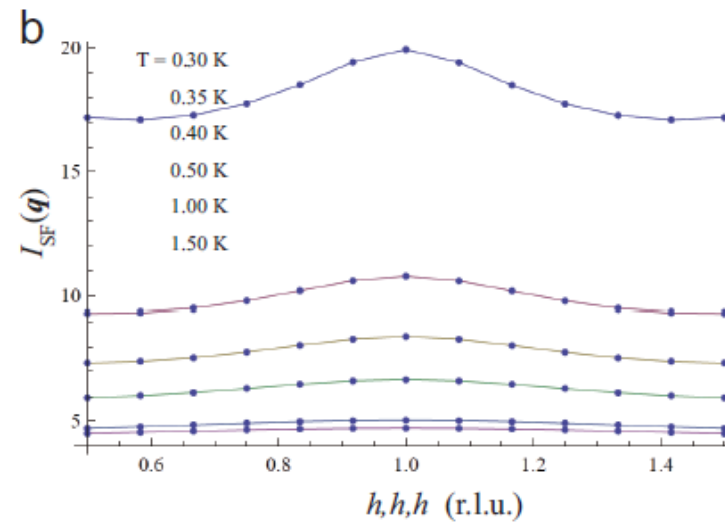
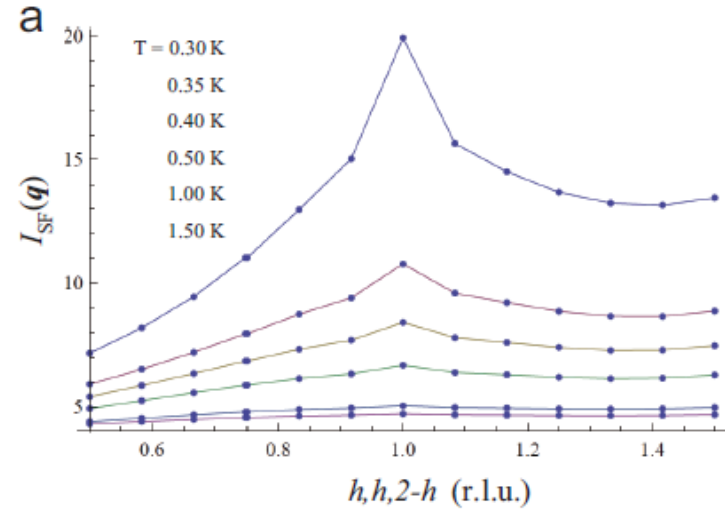
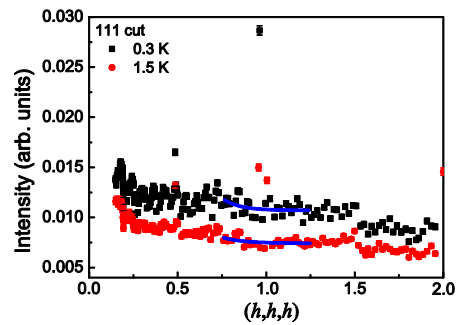
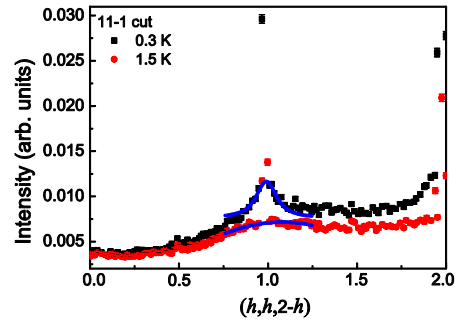


Peak (111) intensities



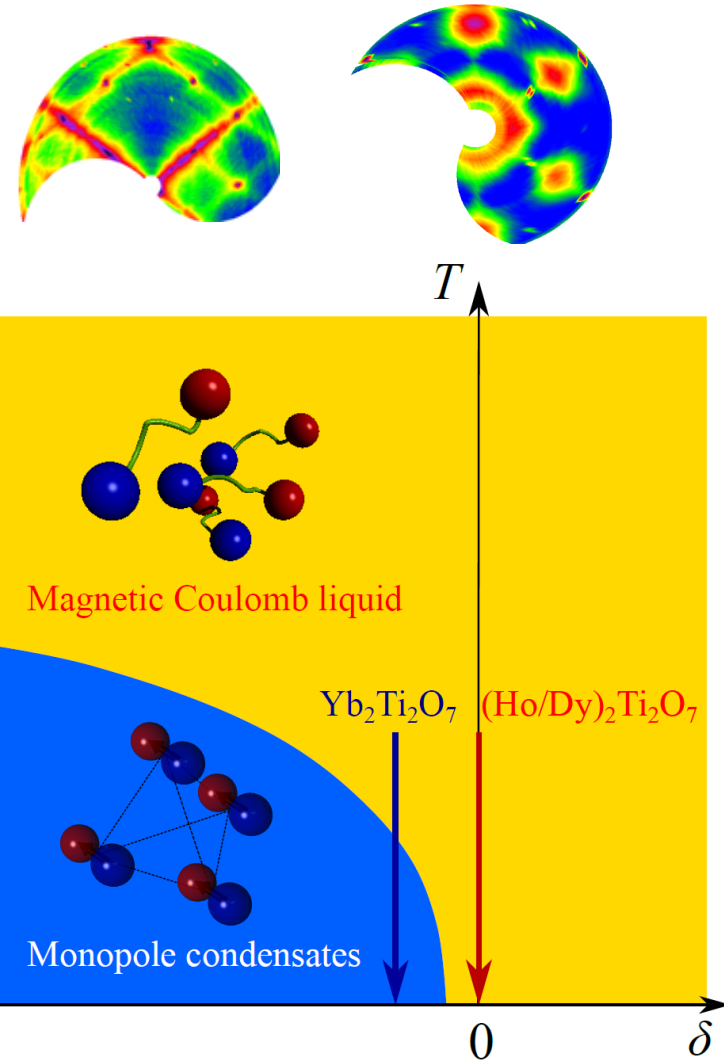
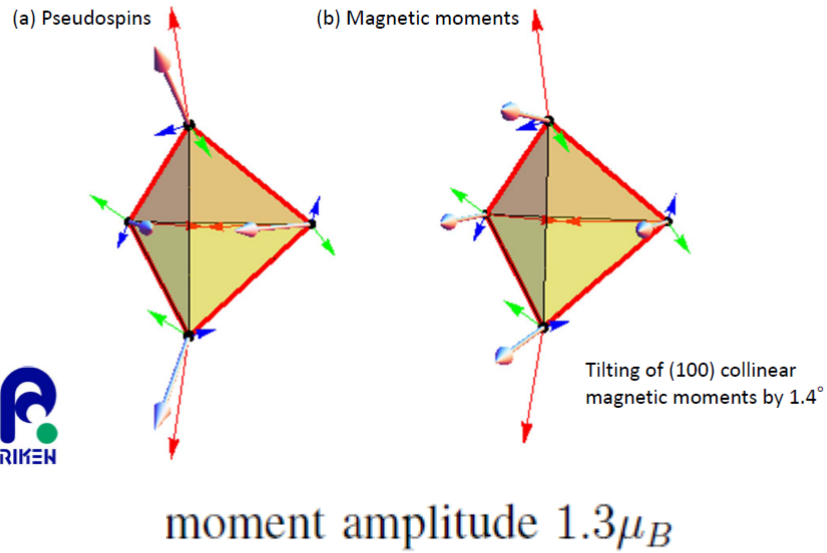
Depolarization: ferromagnetic order
First-order transition
The widths of 111 peaks are identical

Pinch point cut

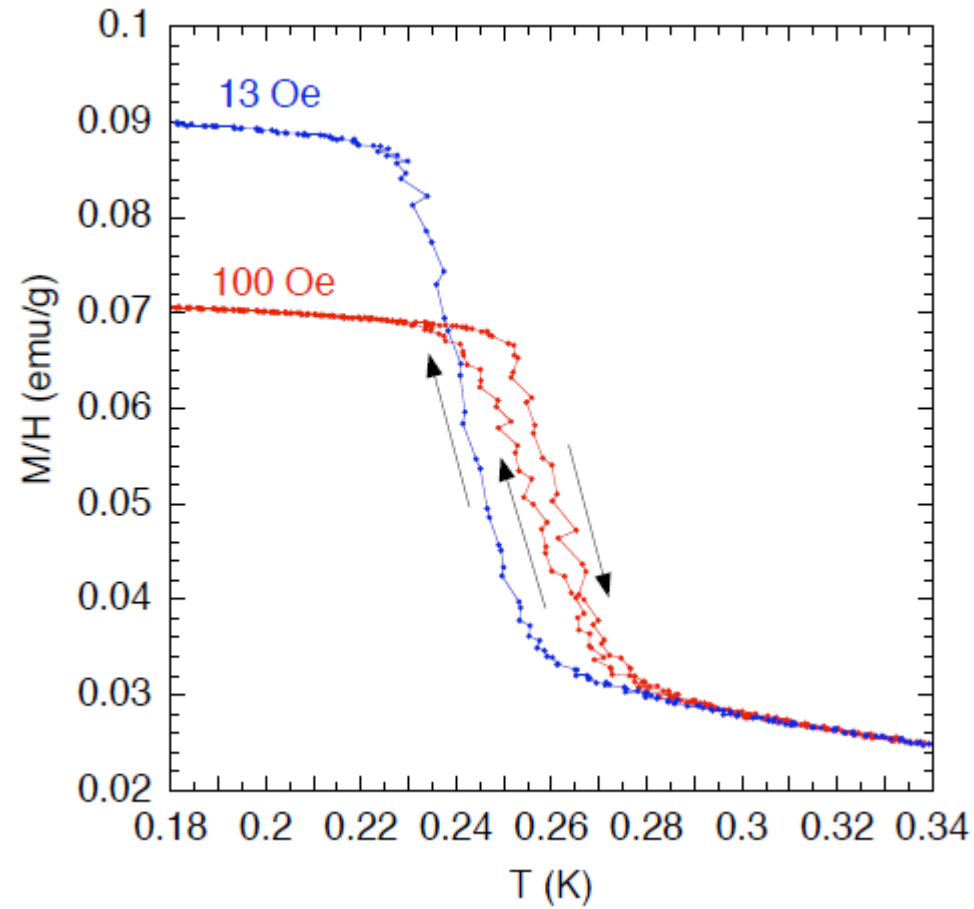


Phase diagram

Ground-state pseudospins and magnetic moments



Low Temperature Magnetization of $\text{Yb}_2\text{Ti}_2\text{O}_7$ powder



L.J. Chang *et al.*, unpublished

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- **Sample dependent**

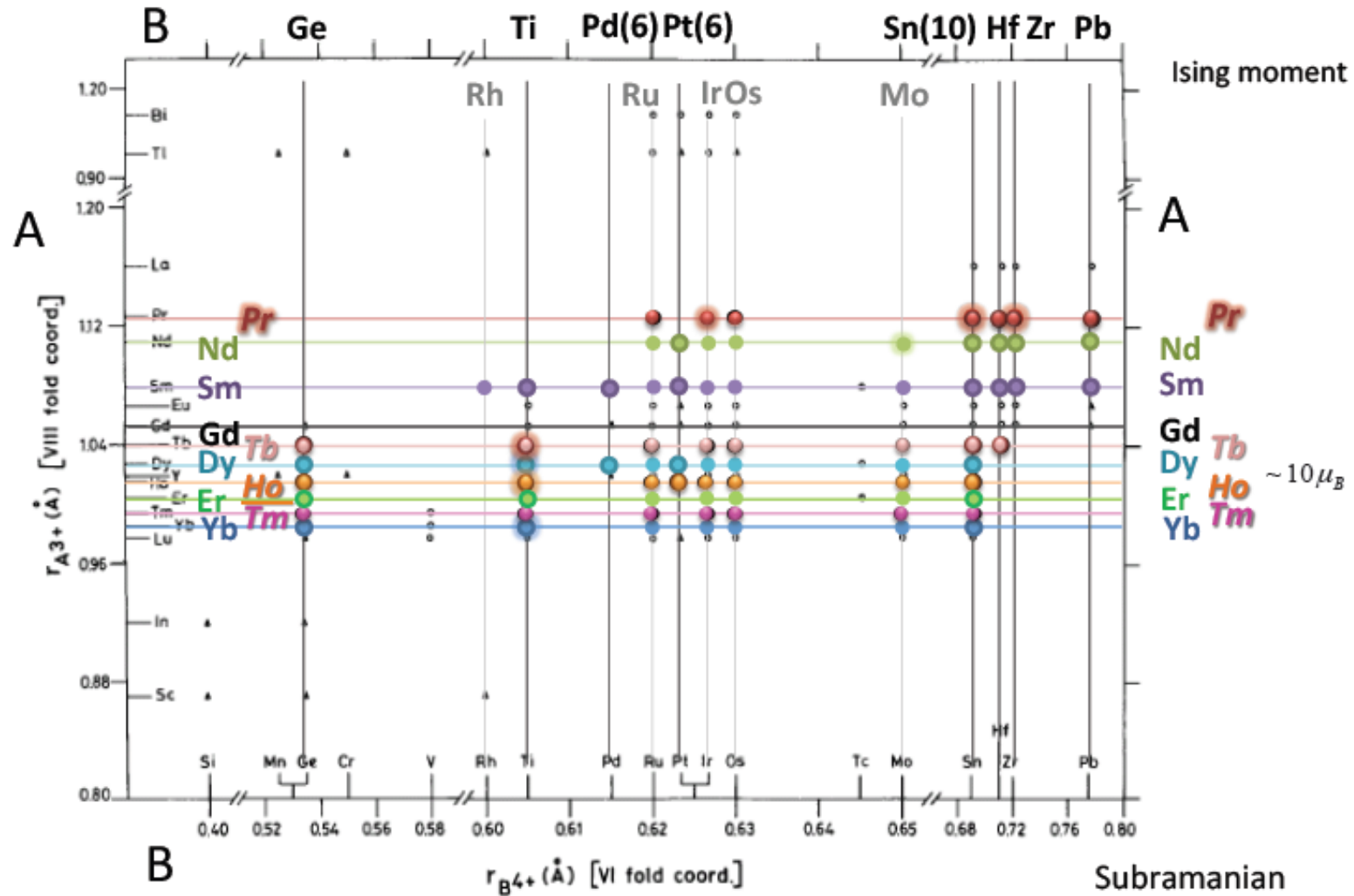
Summary

- $\text{Yb}_2\text{Ti}_2\text{O}_7$, a quantum spin ice, first CEF ~ 620 K
- Pinch points
- Ferromagnetic order at ~ 0.21 K for crystal: neutron depolarization, hysteresis.
- Quantum critical points: magnetic Coulomb phase to Higgs phase, or quantum spin liquid phase etc.???

Future plans:

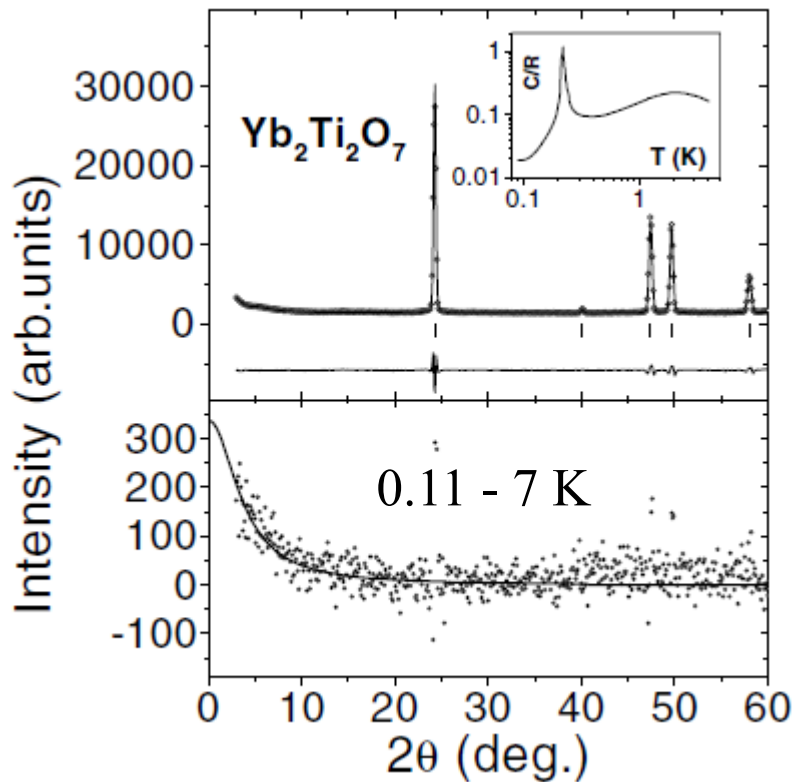
- Quantum excitations: 3D spinon excitations, Higgs-boson
- Search for quantum phase transitions: by mean of pressure or substitutions
- Other pyrochlores

Magnetic pyrochlore oxides $A_2B_2O_7$



Modified by: S. Onoda

Sample dependent



J. A. Hodges *et al.*, PRL **88** 077204 (2002)

No magnetic peaks

CW temperature ~ 0.6 K

1st order transition ~ 210 mK

LRO?

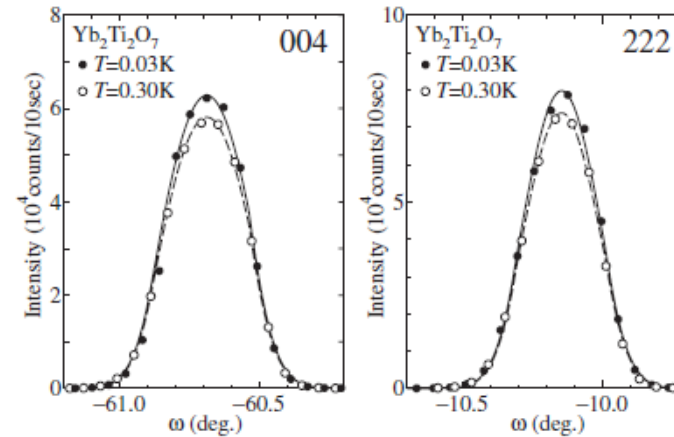


Fig. 3. Profiles of the ω -scans for 004 and 222 reflections taken at 0.03 K and 0.30 K. Solid and Broken lines are guides for the eye.

Y. Yasui *et al.*, JPSJ **72** 3014 (2003)

ferromagnetic

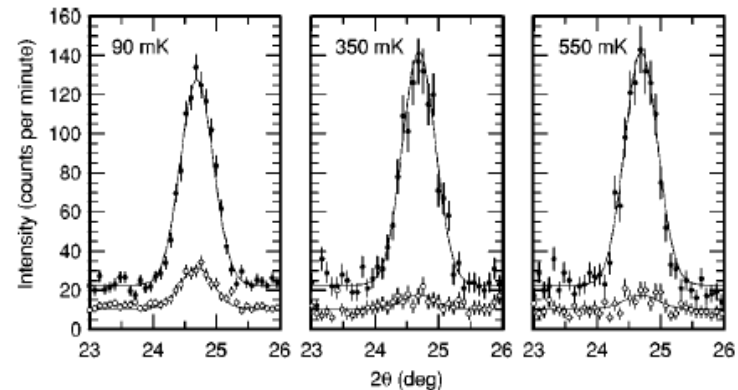
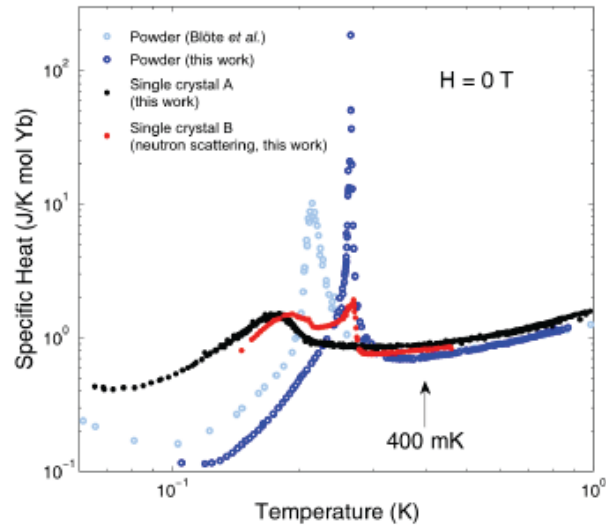


FIG. 3. Spin-flip (open circles) and non-spin-flip (closed circles) scattering at the (111) Bragg position. Above 240 mK there is only a small amount feed through due to incomplete polarization. At 90 mK, a peak is clearly seen in the spin-flip data.

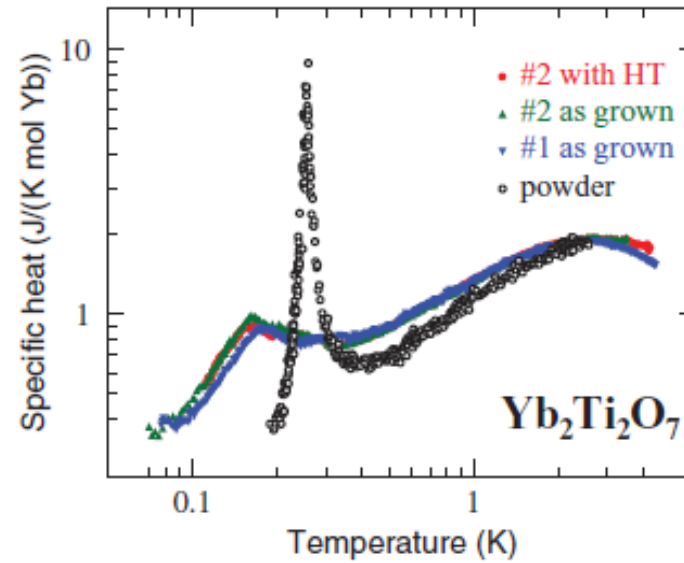
J. S. Gardner *et al.*, PRB **70** 180404(R) (2004)

No neutron depolarization

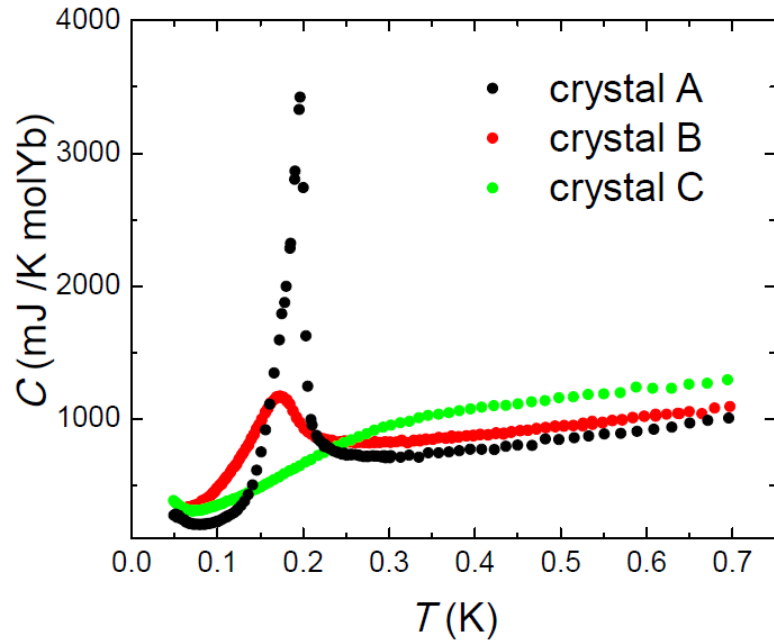
Sample dependent



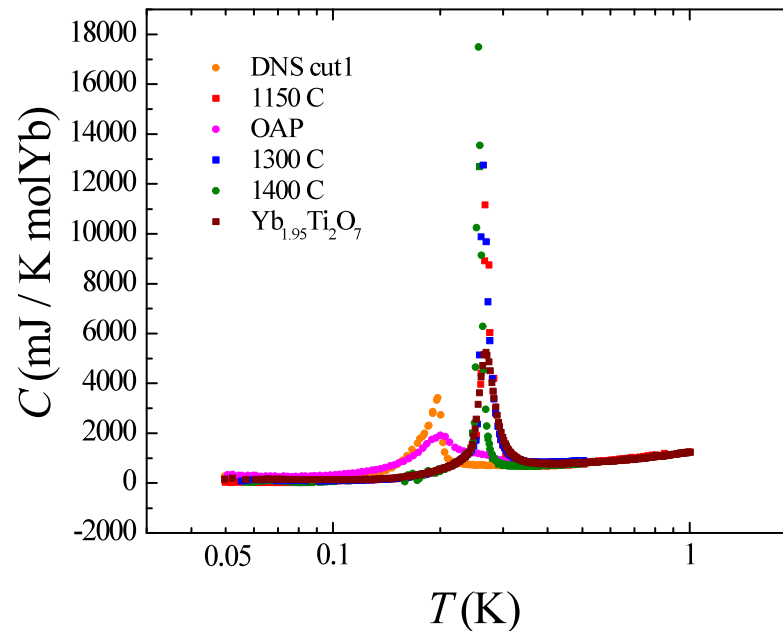
K. A. Ross *et al.*, PRB **84**, 174442 (2011)



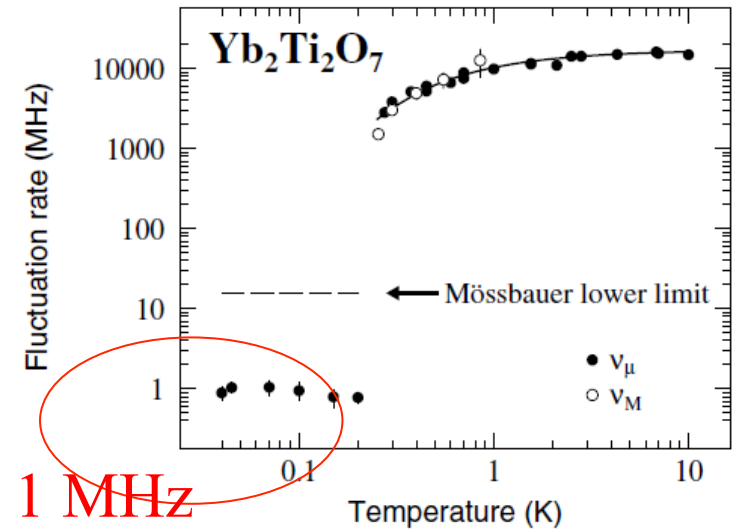
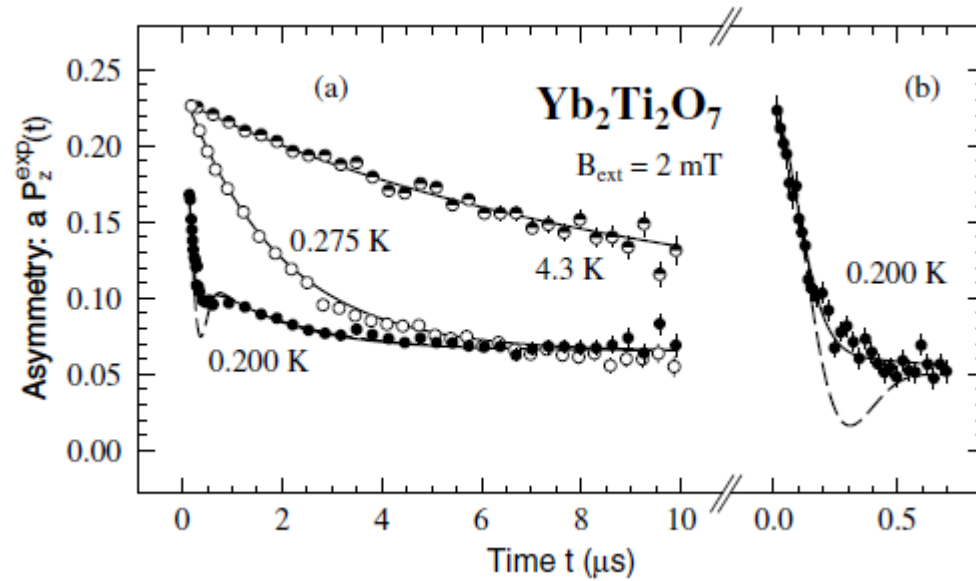
A. Yaouanc *et al.*, PRB **84**, 172408 (2011)



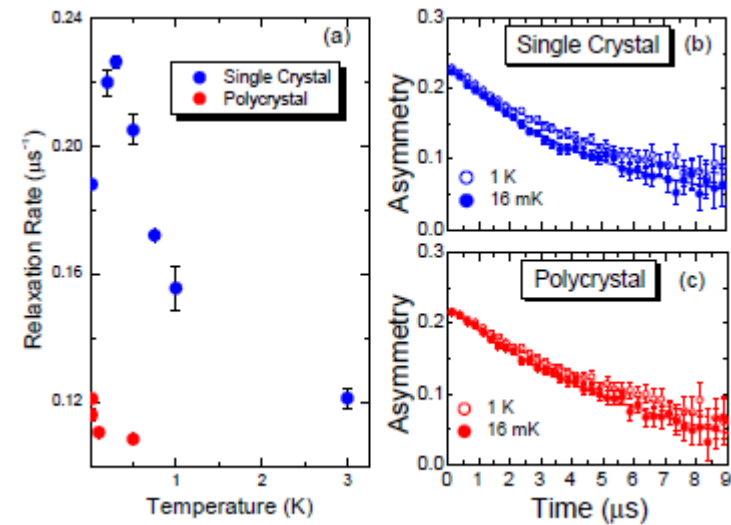
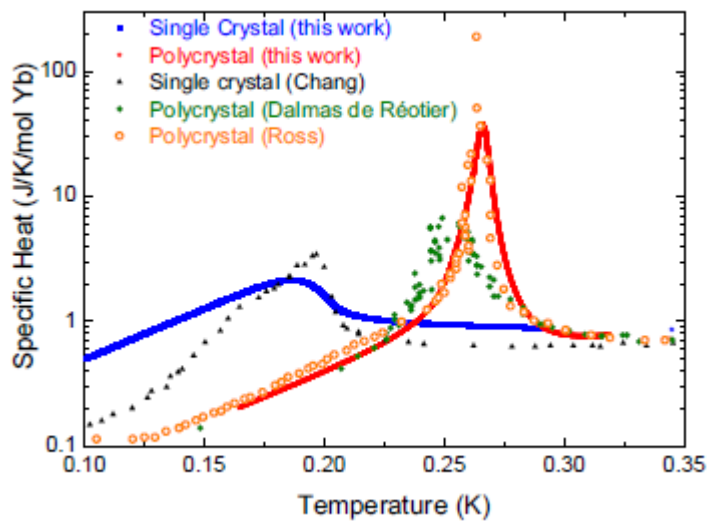
L. J. Chang/ S. Onoda *et al.*, Nat. Commun. **3**, 992 (2012)



M. R. Lees/ L.J. Chang *et al.*, unpublished



J. A. Hodges *et al.*, PRL **88**, 077204 (2002)



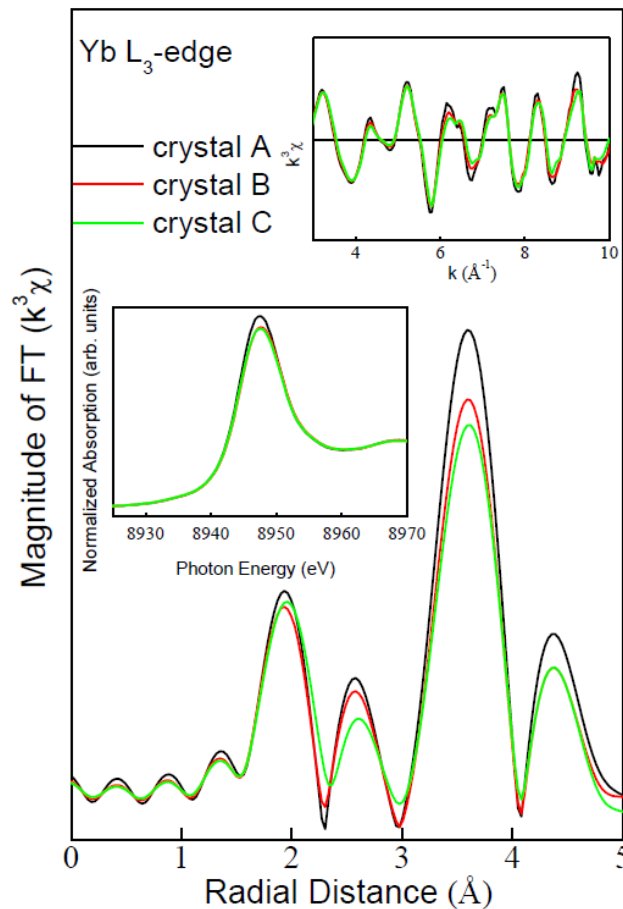
D. M. D'Ortenzio *et al.*, arXiv:1303.3850

Comments on the NMR results

We had carried out MuSR experiments on powder sample, long-ranged order crystal, and a crystal without HC peak.

- Emergence of static (<1 MHz) internal magnetic moments observed for powder and long-ranged order crystal.
- Temperature vs relaxation rate of the crystal without HC peak is close to that reported in the D. M. D'Ortenzio paper. \rightarrow magnetic interaction is weaker in this sample (small fraction of the crystal contributed to magnetic order)

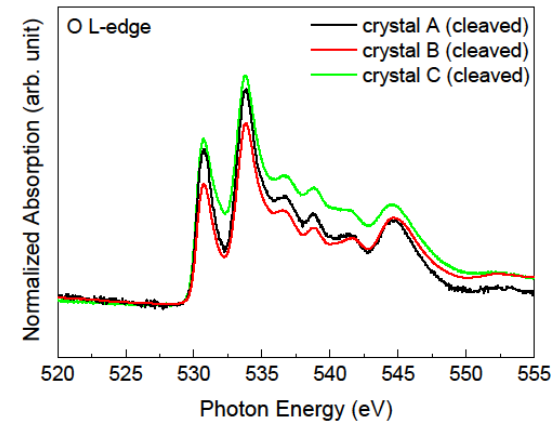
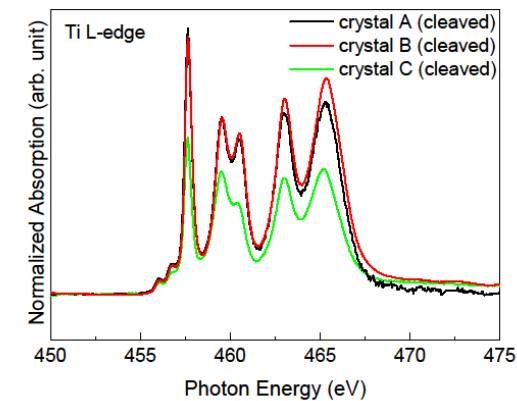
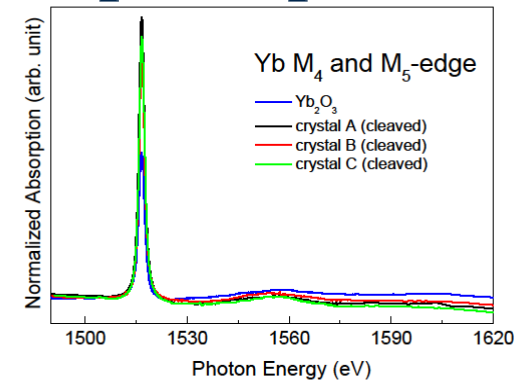
EXAFS



L. J. Chang/ S. Onoda *et al.*, Nat. Commun 3, 992 (2012).

K.A. Ross *et al.*, proposed “stuffed”
 $\text{Yb}_2(\text{Ti}_{2-x}\text{Yb}_x)\text{O}_{7-x/2}$ with $x = 0.046$
 PRB 86, 174424 (2012)

Sample dependent



No charge state variations