Coherent Neutron Scattering and its Implications to UCN Production Physics

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Good Candidate Material

- UCN density: $$\rho_{ucn} = P \times \tau \propto \sigma_{down} \left(\frac{1}{\sigma_{up}} + \frac{1}{\sigma_{\beta}} + \frac{1}{\sigma_{nucl.ab.}} + \ldots \right)$$

  (Limited by loss)

- The figure of merit:

$$\sigma_s / \sigma_a$$

Strong coherent scatterers

Isotop	σ_{coh}	σ_{inc}	σ_a	σ_s/σ_a	*purity*	*Debye T*
^{2}D	5.59	2.04	0.000519	1.47×10^{4}	99.82	110
^{4}He	1.13	0	0	∞		20
^{15}N	5.23	0.0005	0.000024	2.1×10^{5}	99.9999	80
^{16}O	4.23	0	0.00010	2.2×10^{4}	99.95	104
^{208}Pb	11.7	0	0.00049	2.38×10^{4}	99.93	105

Inspired by Young & Koppel (PRA, 135, 603, 1964), free H_2, D_2 gas

$$\left(\frac{d^2\sigma}{d\Omega dE'}\right)^{1\ \text{phonon}}_{J\rightarrow J'} = \frac{k'}{k}\frac{\hbar^2\kappa^2}{2M_{D_2}} e^{-2W(\kappa)} S_{JJ'}(2J'+1)$$

$$\times \sum_n \left(\frac{\hbar\kappa^2}{2M_{D_2}\omega}\right)^n \frac{1}{n!}$$

$$\times \sum_{l=|J'-J|}^{J'+J} |A_{nl}|^2 C^2(JJ'l;00)$$

$$\times \frac{Z(E_{\text{ph}})}{E_{\text{ph}}} \begin{cases} n(E_{\text{ph}})+1 & \text{if } E_{\text{ph}} >= 0 \\ n(E_{\text{ph}}) & \text{if } E_{\text{ph}} < 0, \end{cases}$$

Spin-dependent strong interaction

Molecular vibrational

Molecular rotational

Phonons

Note that this is using "incoherent approximation"

Liu et al.
(PRB, 62, R3581, 2000)
Extend the model to solid H_2, D_2

Molecular Form Factor:

(coherent sum of the scattering amplitudes from two atoms in each molecule.)

$$A_{nl} = \int_{-1}^{1} d\mu\, \mu^n \exp\left(-\frac{\hbar\kappa^2\mu^2}{4M_{D_2}\omega} + \frac{i\kappa a\mu}{2}\right) P_l(\mu)$$

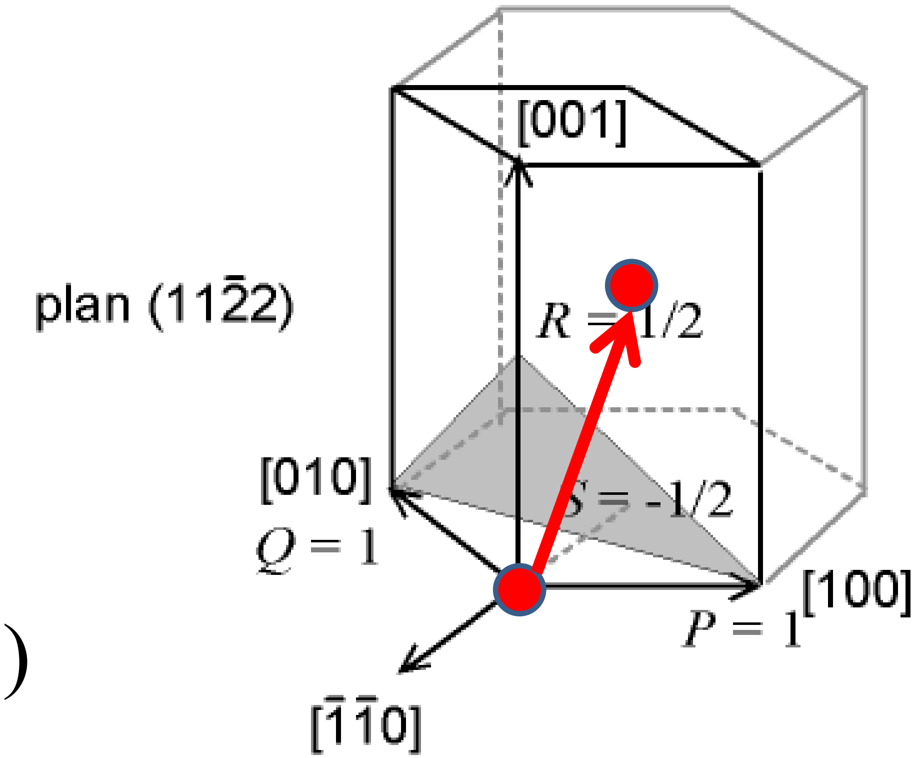
Question:

Couldn't we have a more updated scattering cross-section, taking into accounts of all the coherent effect?

Is it that difficult?

Neutron scatterers have long figured out how to describe coherent scattering, for both elastic and inelastic processes.

In solid D2,
we also need to account for the "interference between basis" in a unit cell.

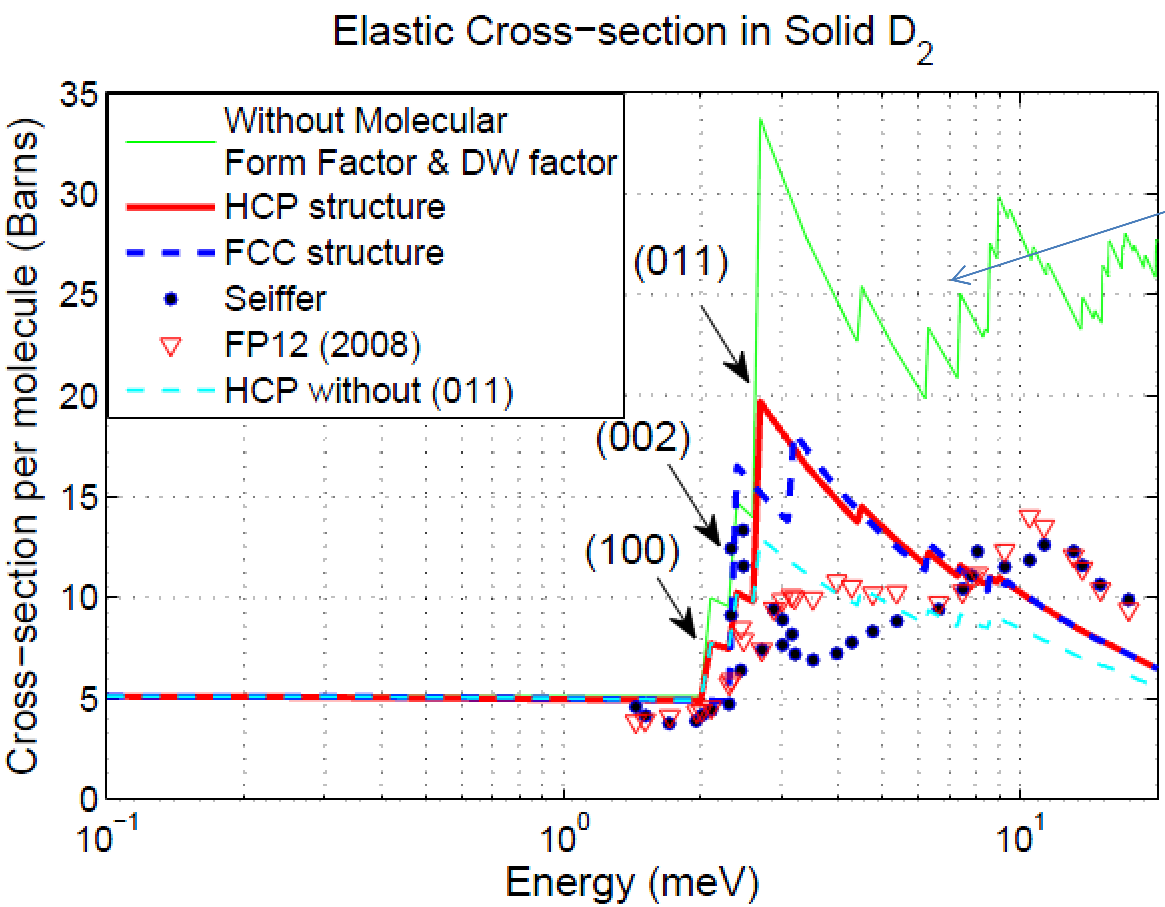


$$F_{cell} = 1 + \exp(iQ \cdot r_{basis})$$

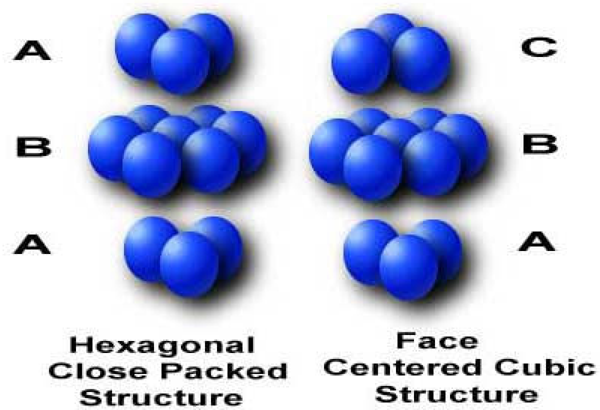
There are two basis in the primitive cell.

For ortho-D_2 (J=0), the molecular form factor is: $2\, j_0\,(Qa/2)$.

2 atoms per molecule.



Bragg Scattering of simple HCP structure.



Problem: missing the [011] peak!

Incoherent Approximation (widely used in previous calculations)

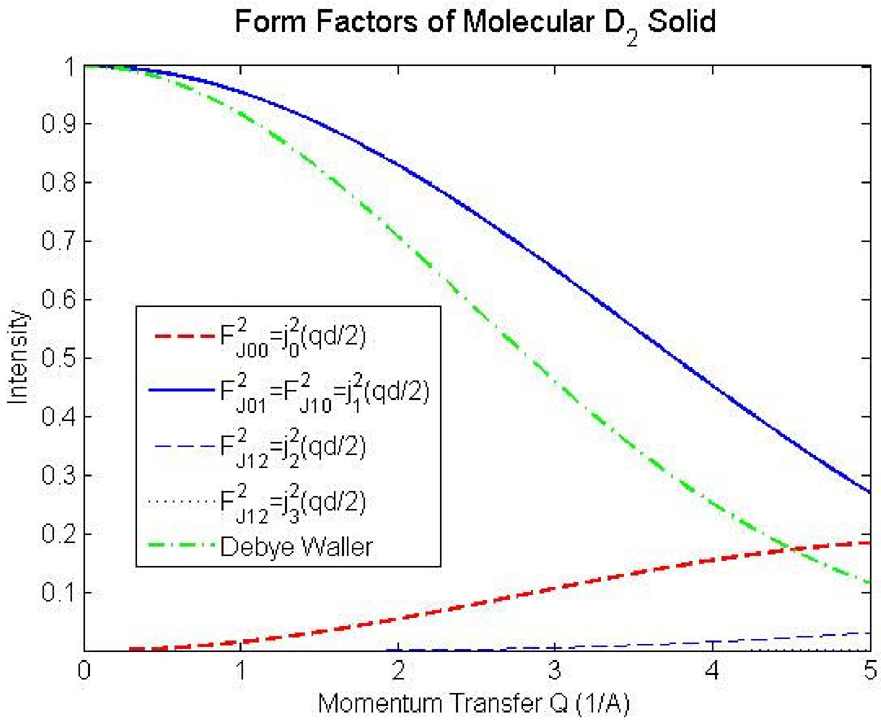
Formulism:

$$\left(\frac{d^2\sigma}{d\Omega dE'}\right)^{1\ \text{phonon}}_{J\to J'} = \frac{k'}{k}\frac{\hbar^2\kappa^2}{2M_{D_2}} e^{-2W(\kappa)} S_{JJ'}(2J'+1)$$

$$\times \sum_n \left(\frac{\hbar\kappa^2}{2M_{D_2}\omega}\right)^n \frac{1}{n!}$$

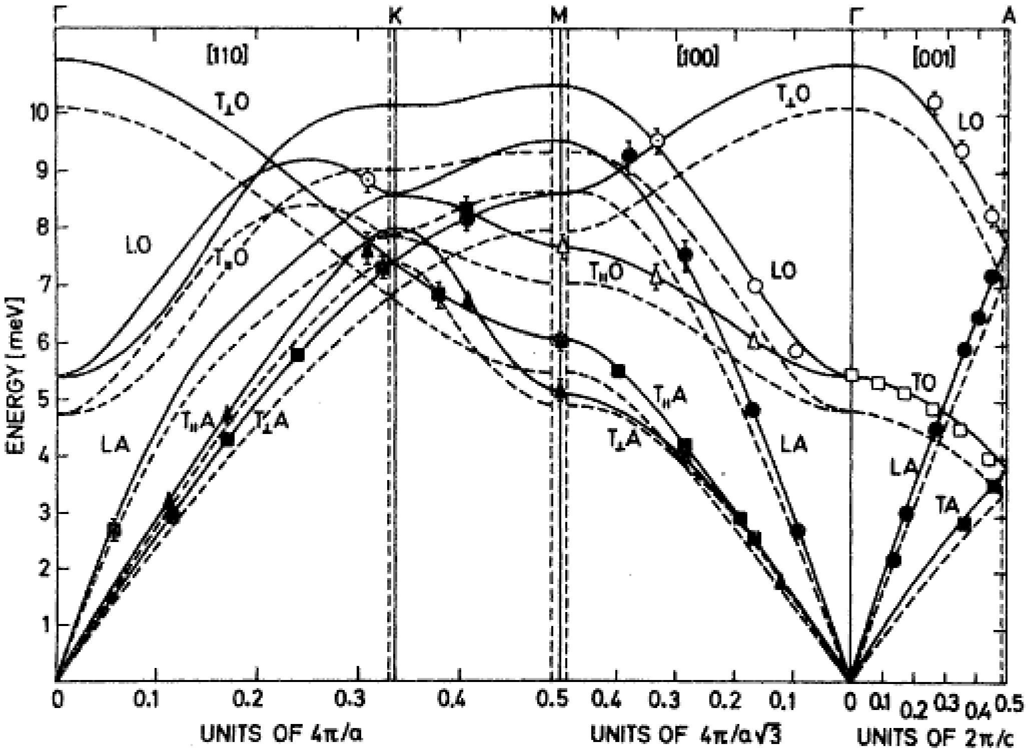
$$\times \sum_{l=|J'-J|}^{J'+J} |A_{nl}|^2 C^2(JJ'l;00)$$

$$\times \frac{Z(E_{\text{ph}})}{E_{\text{ph}}} \begin{cases} n(E_{\text{ph}})+1 & \text{if } E_{\text{ph}} >= 0 \\ n(E_{\text{ph}}) & \text{if } E_{\text{ph}} < 0, \end{cases}$$



Weak Q dependence
(through Debye-Waller factor, and the molecular form-factors.)

1628 M. NIELSEN 7



M. Nielsen, PRB, 7, 1626 (1973)

FIG. 1. Phonon dispersion relations for o-D_2' at 5 K and 275 bar. The full lines are the results of the Born–von Karman fit and the dashed lines are the dispersion relations for o-D_2 at 5 K and zero pressure.

Single Crystal

Disperson function of phonons in HCP lattice with axially symmetric force model: Solution of the force matrix (including coupling constants up to the 3rd nearest neighbors)

ω(vec q)

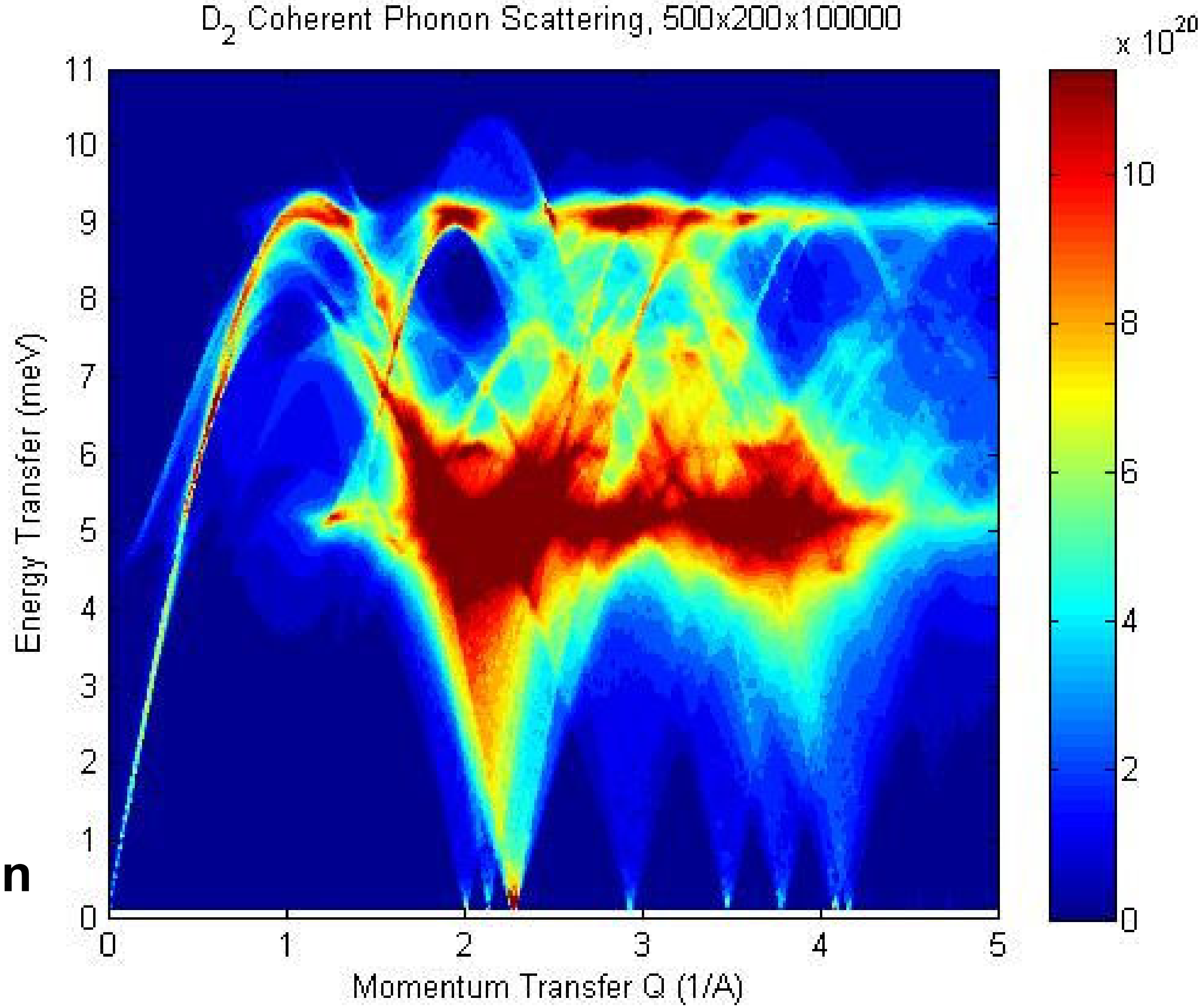
Through a Monte-Carlo angular average

Polycrystalline D_2

Results of our full treatment:

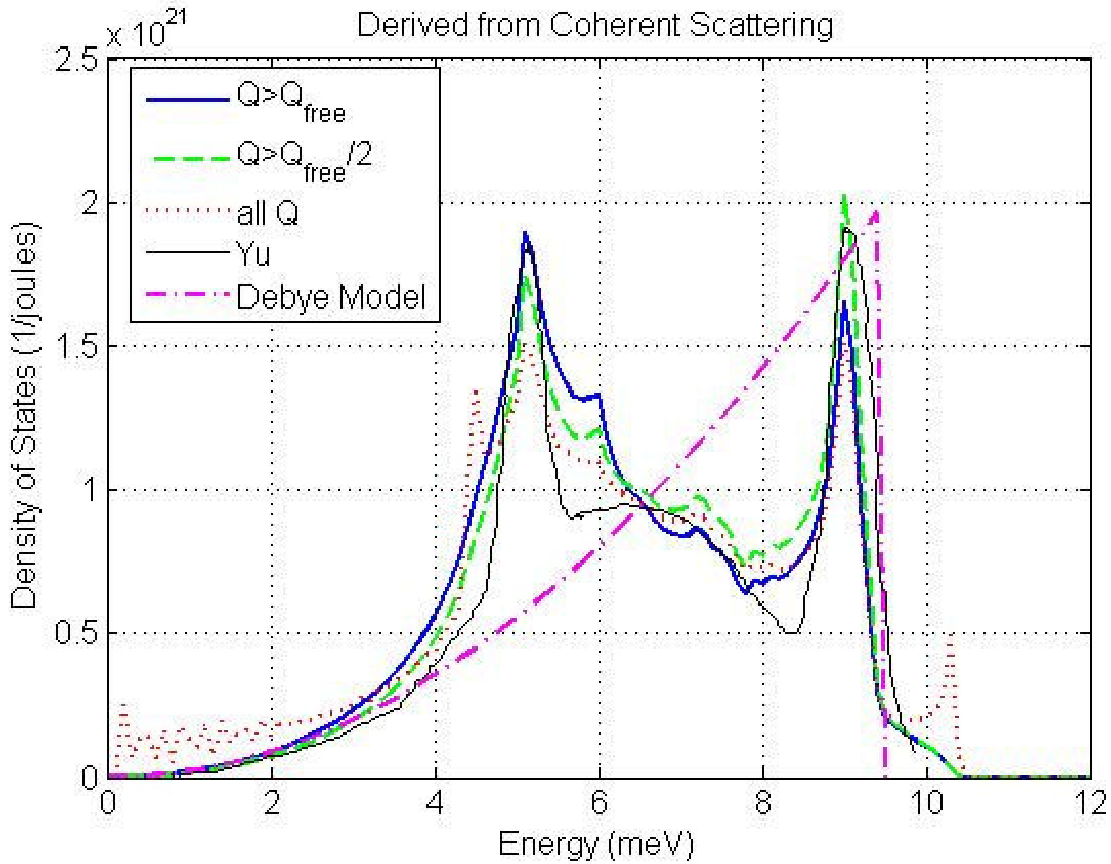
High Resolution Map of the Dynamic Structure Function S(Q,ω)

J: 0→0 only



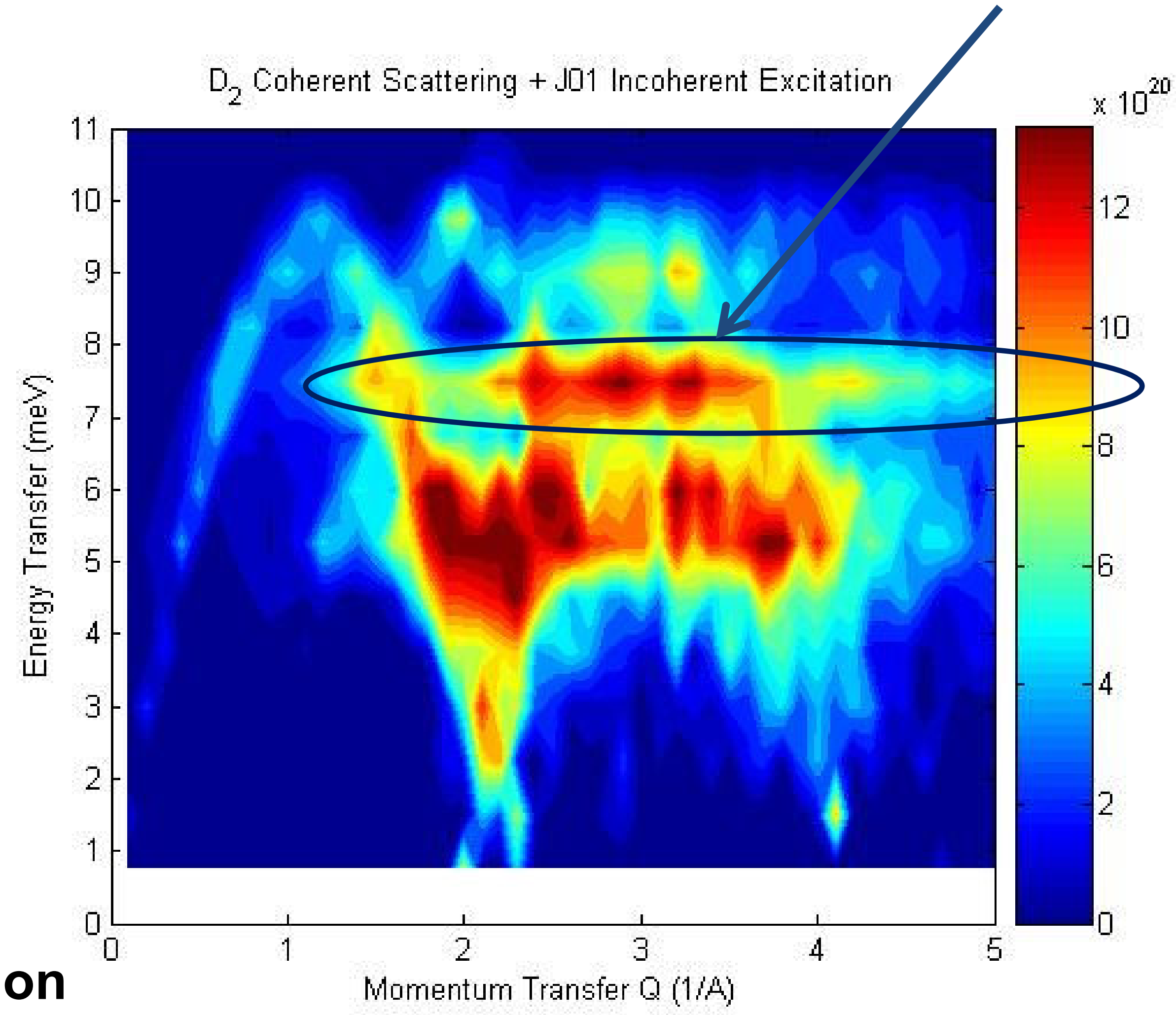
High resolution 500x200

Density of states, Z(ω)
Derived from the coherent scattering amplitude



Z(ω): not used in the actual coherent scattering calculation.
Plotted here just for fun!

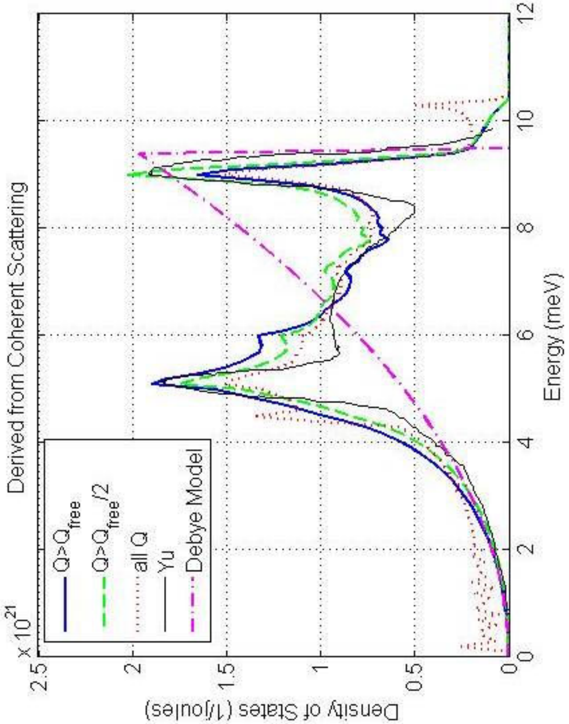
Include the rotational transition ($J=0\rightarrow1$), E_{01}=7.1 meV

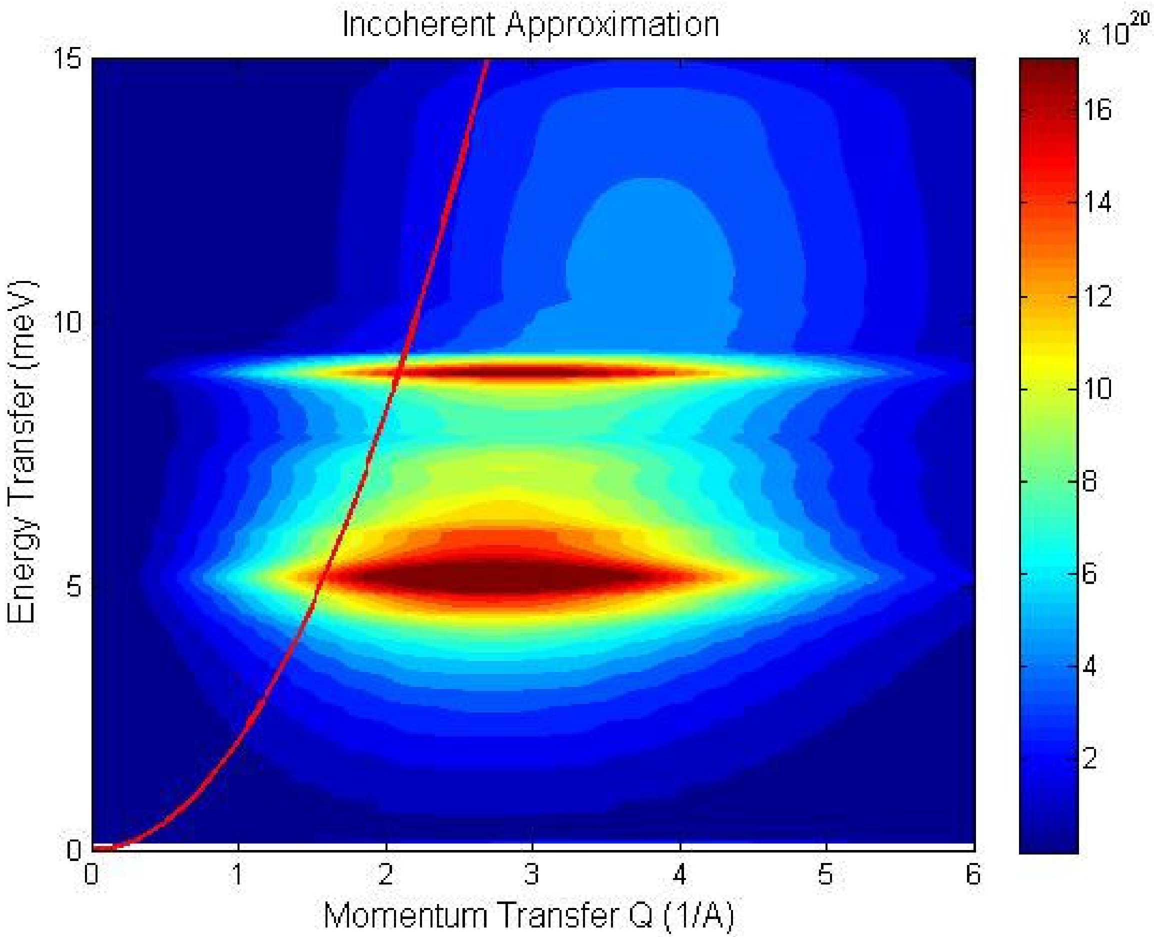


Low resolution
50x20

Compares pretty well with the Munich data.

Incoherent Approximation in treating the phonon contribution

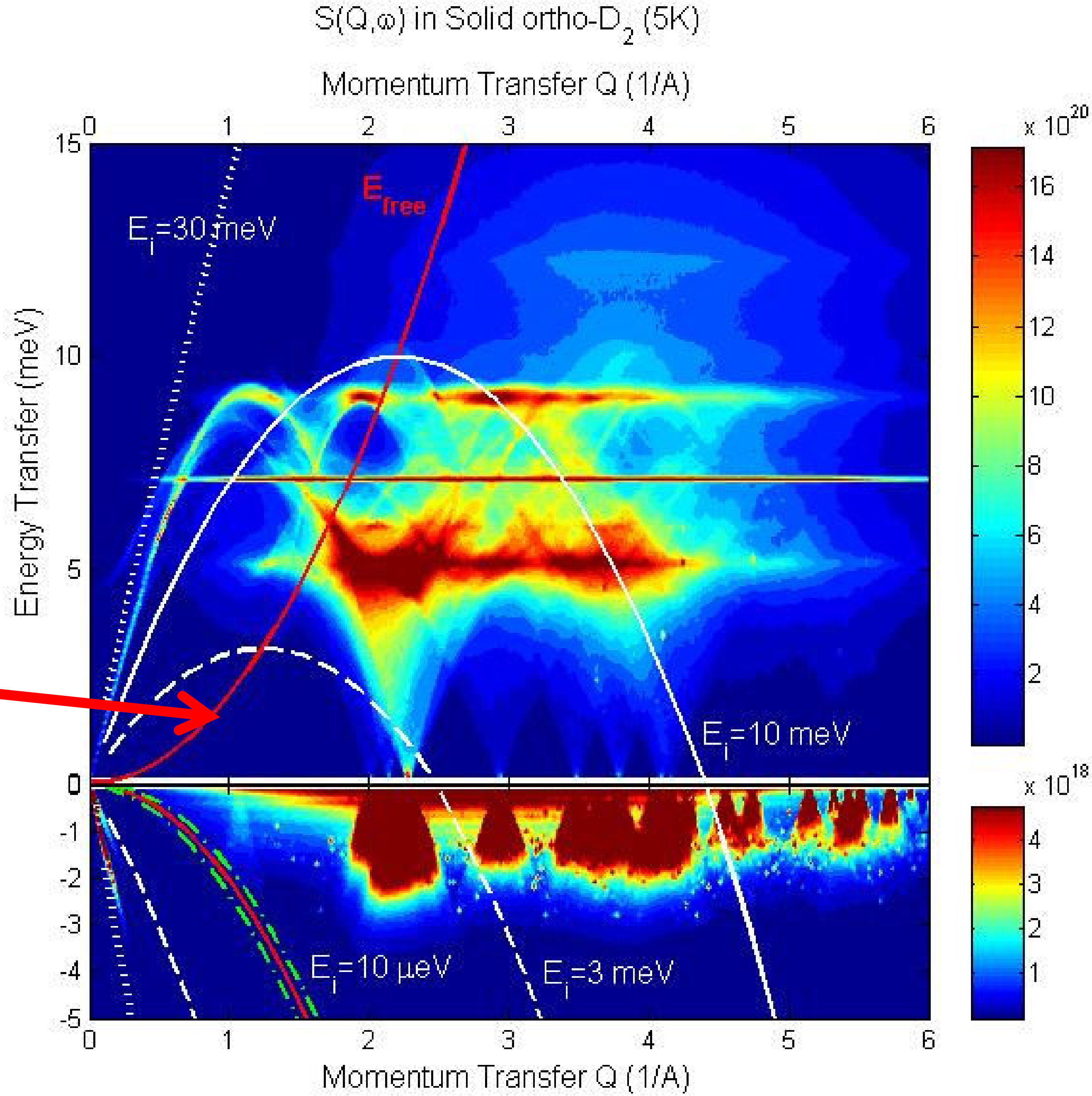




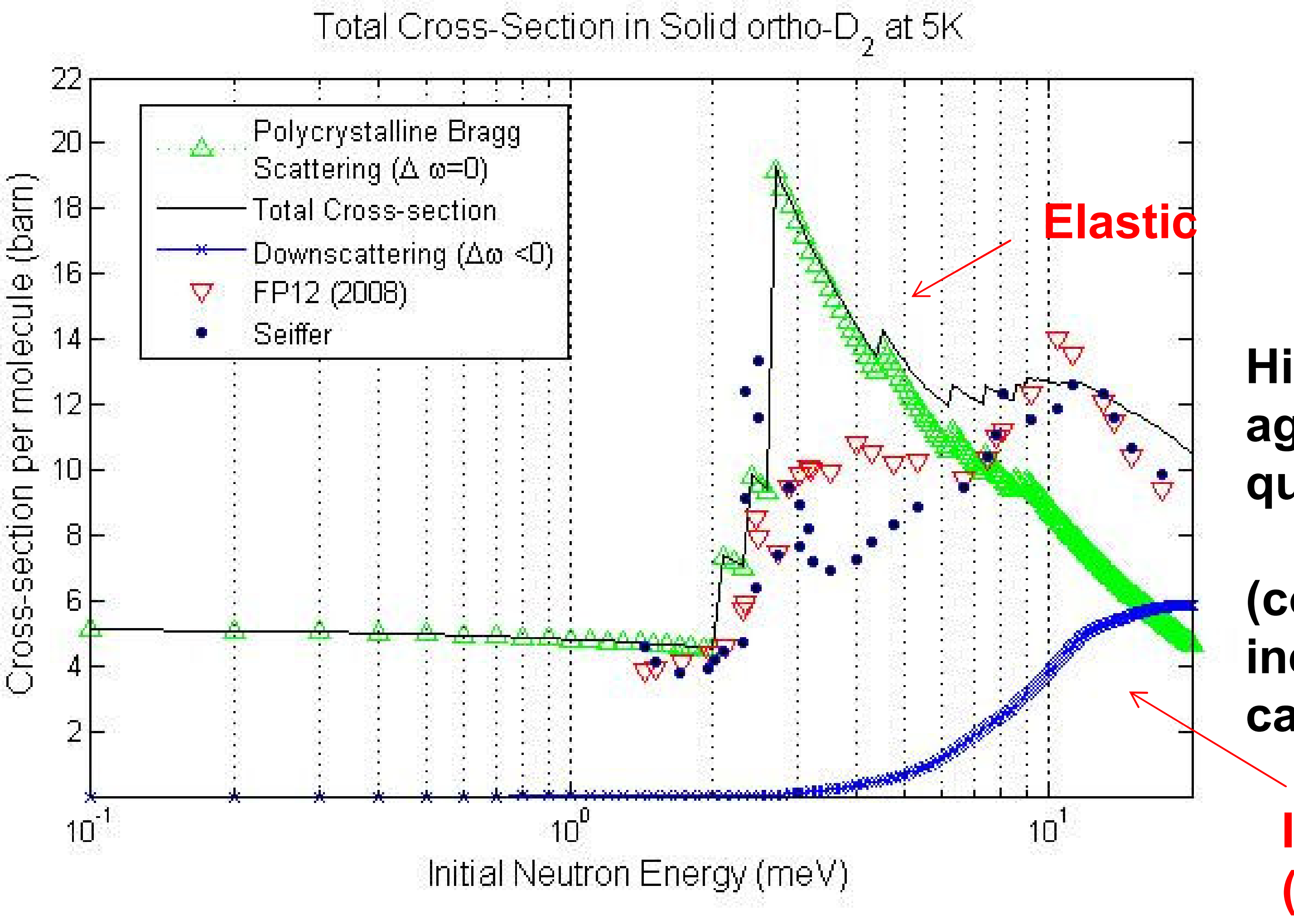
Lacking the detailed Q dependence.

UCN production:

The is not much intersection within the first Brioulloin zone.

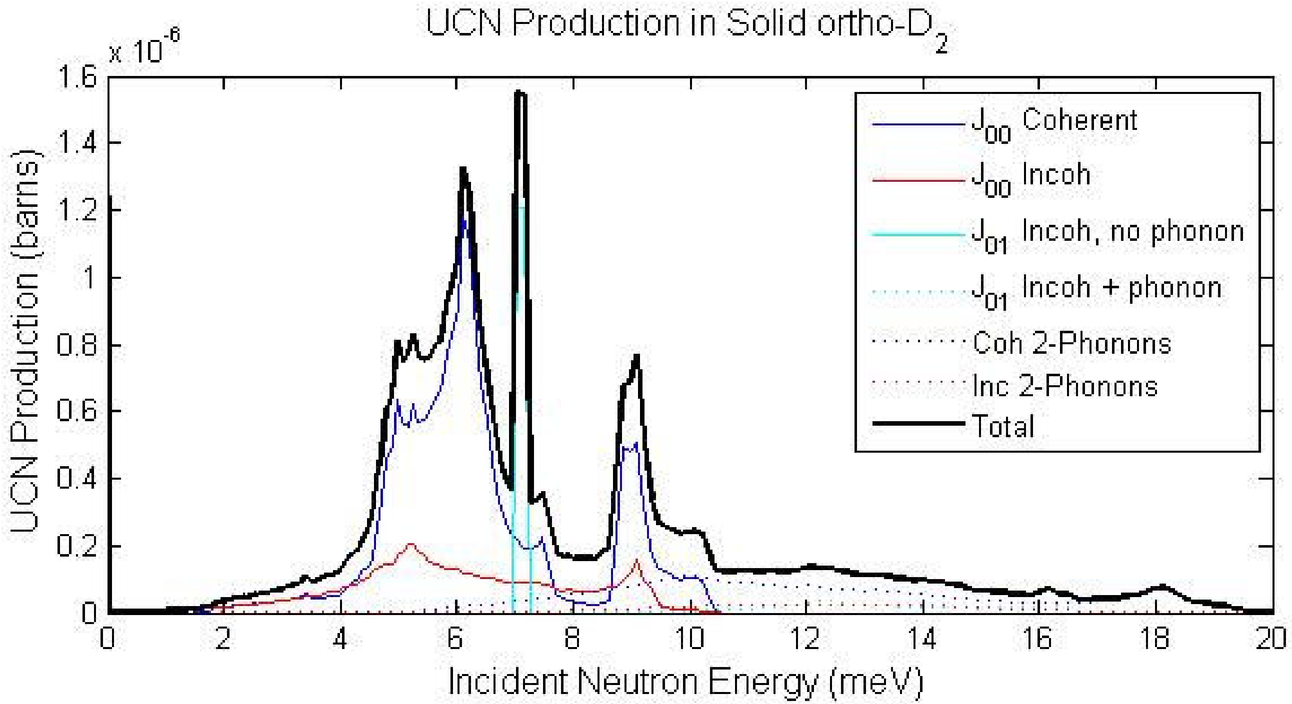


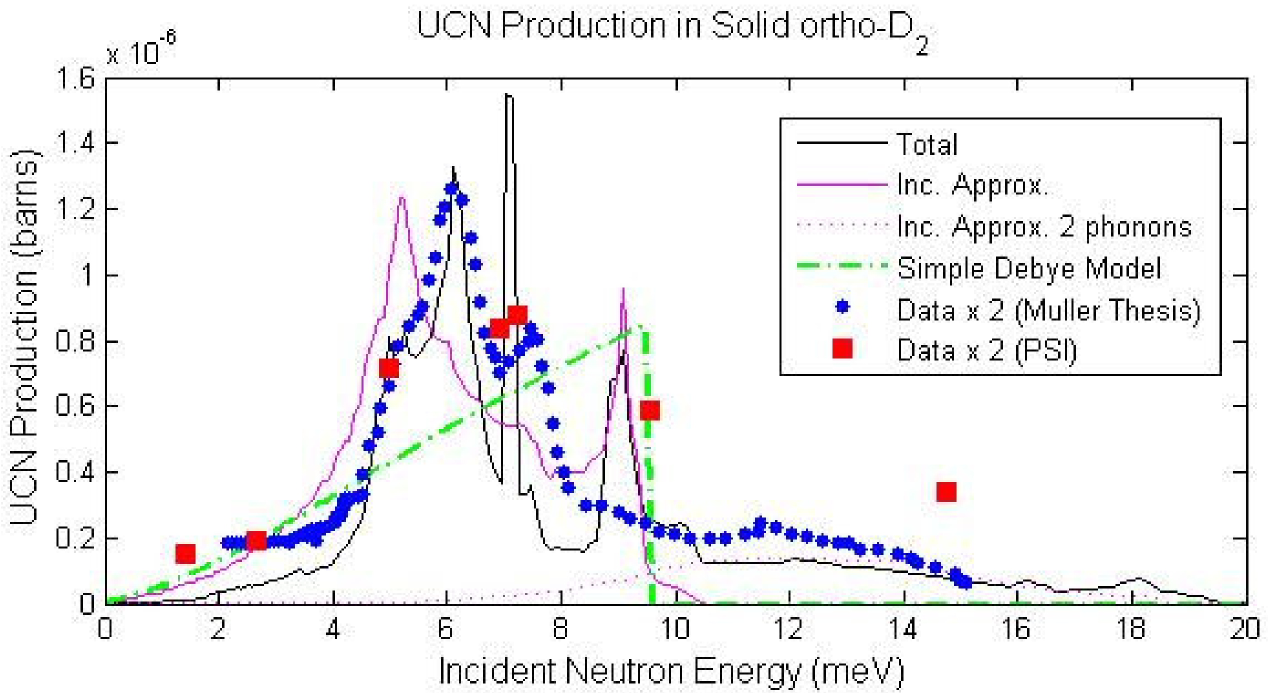
Total Cross-section in Solid ortho-D_2



High energy part agrees with data quite well!

(confidence in inelastic calculation).

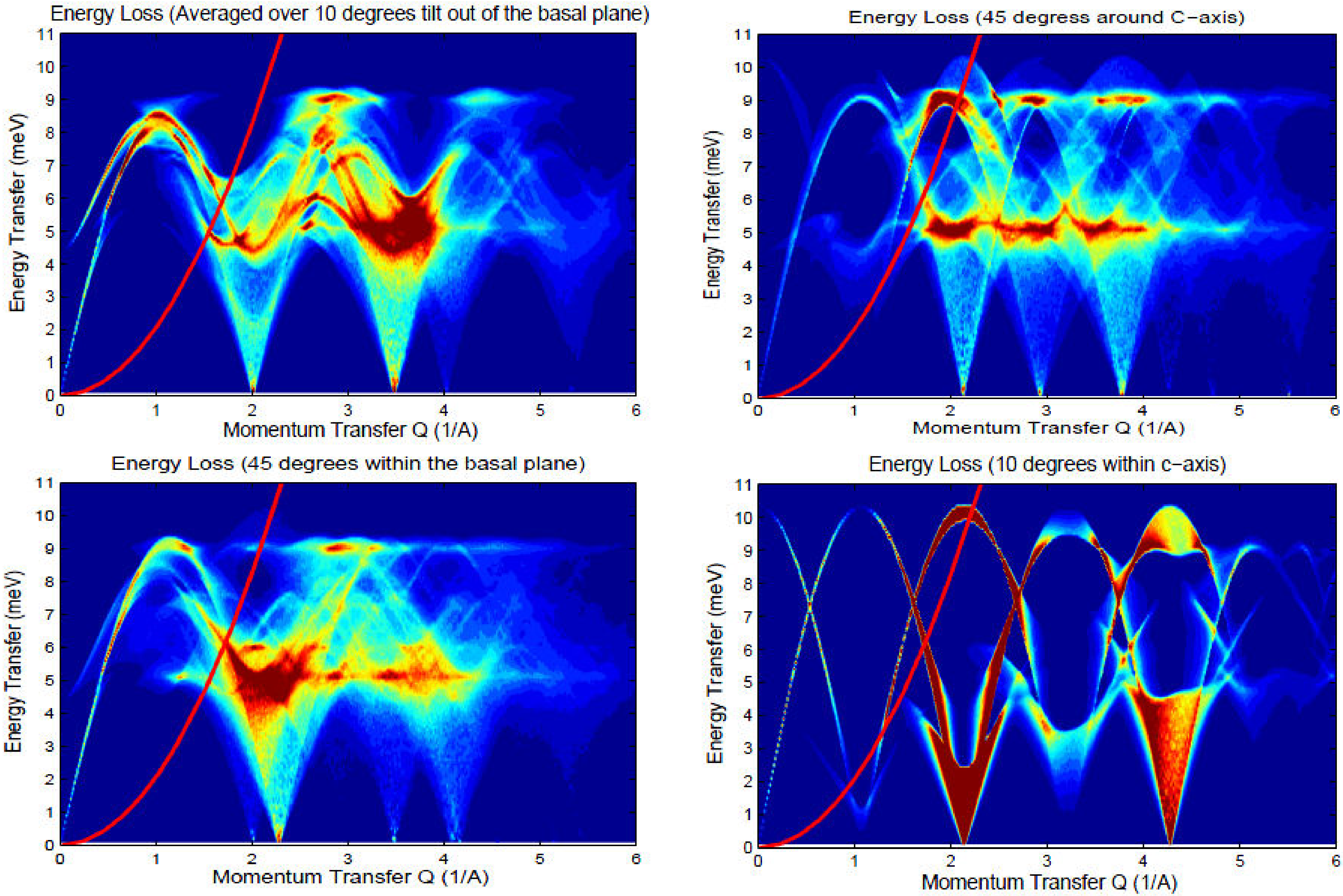




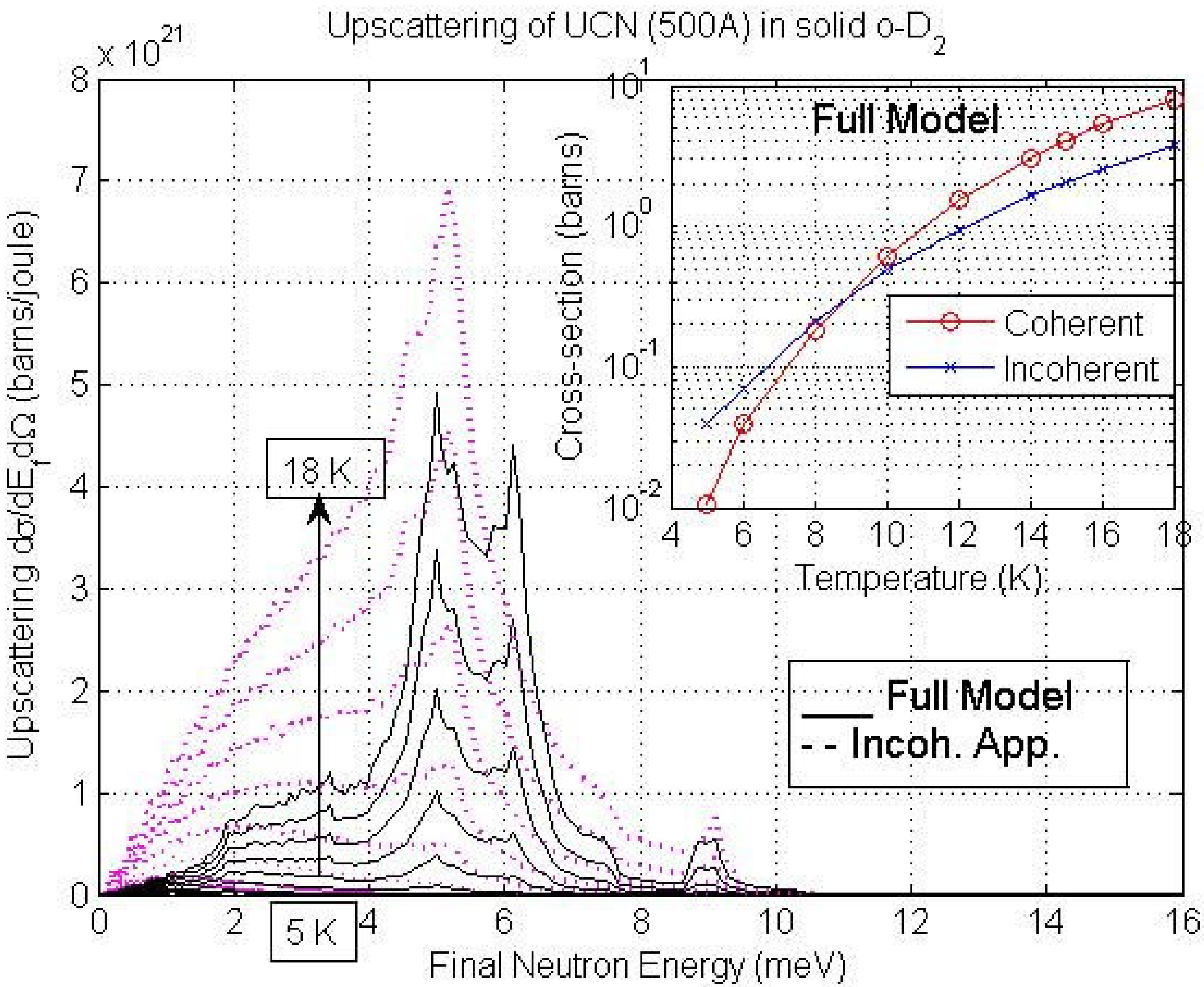
A.R.Muller Thesis
TUM, 2008

Atchison et al.,
PRL 99, 26250

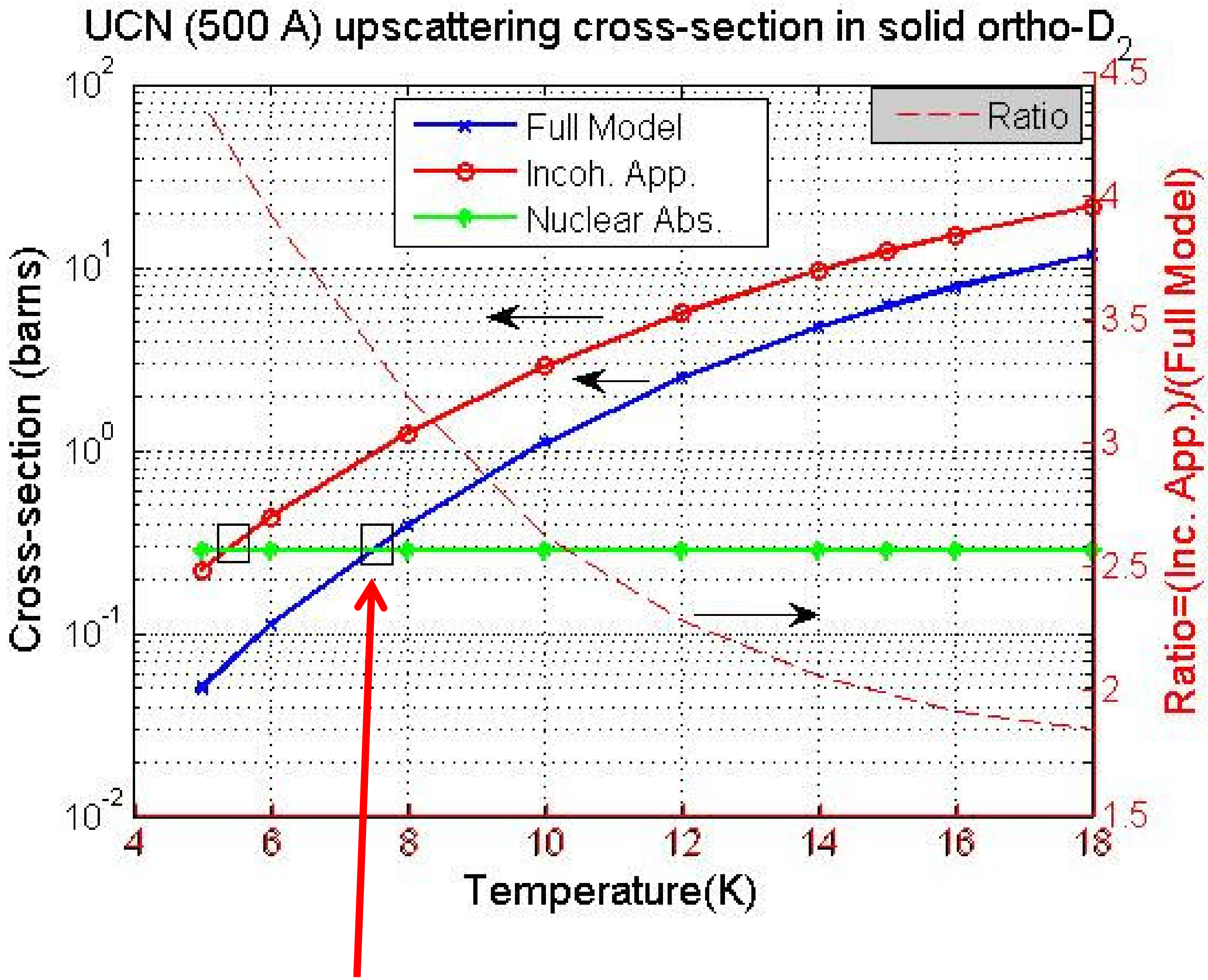
Relax from the polycrystalline limit



(coherent contribution only)

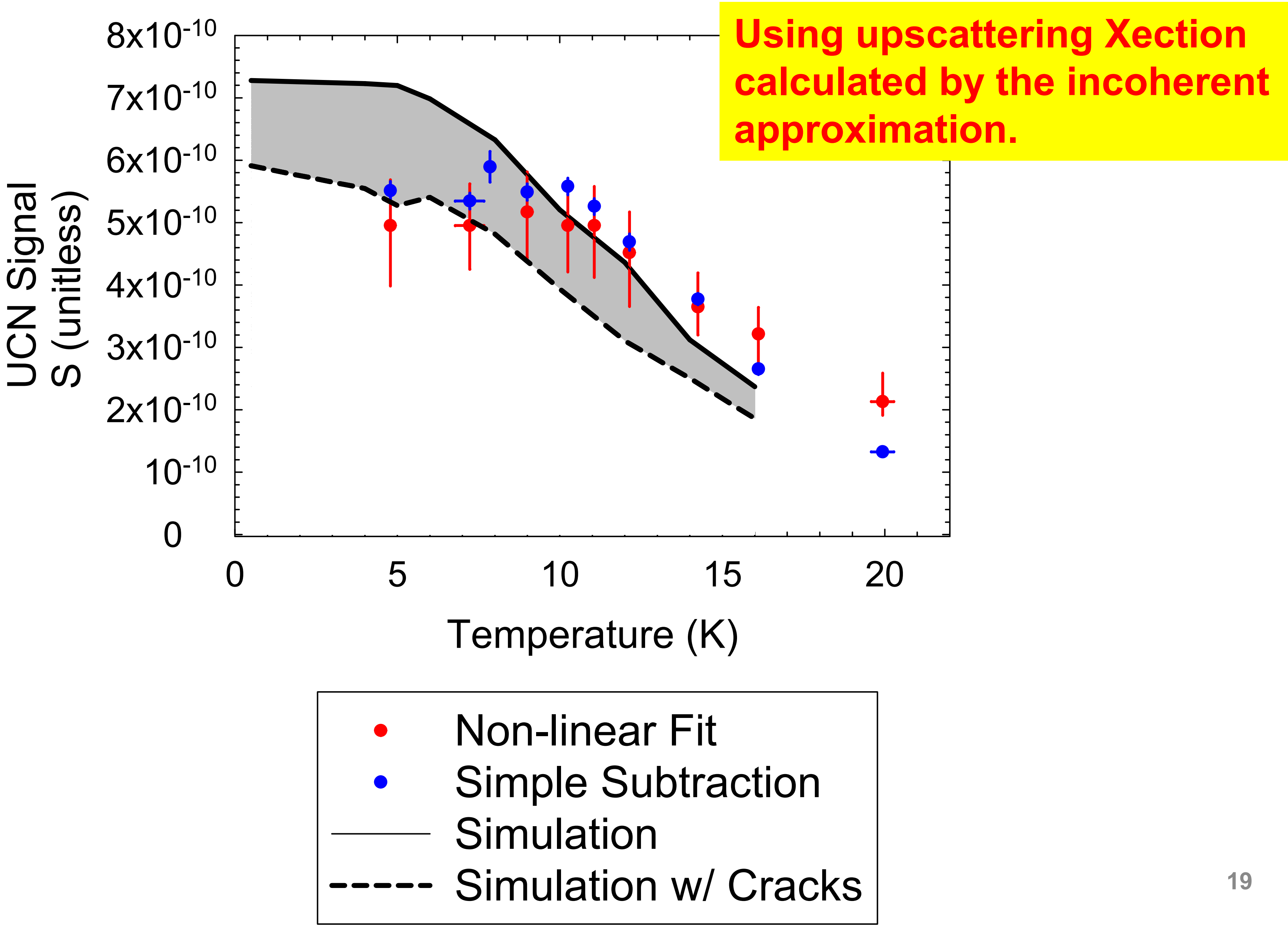


Upscattering of UCN (500A) in solid o-D2
x 10^21
Upscattering dσ/dE_f dΩ (barns/joule)
Final Neutron Energy (meV)
18 K
5 K
Full Model
- - Incoh. App.
Full Model
Cross-section (barns)
Temperature (K)
Coherent
Incoherent

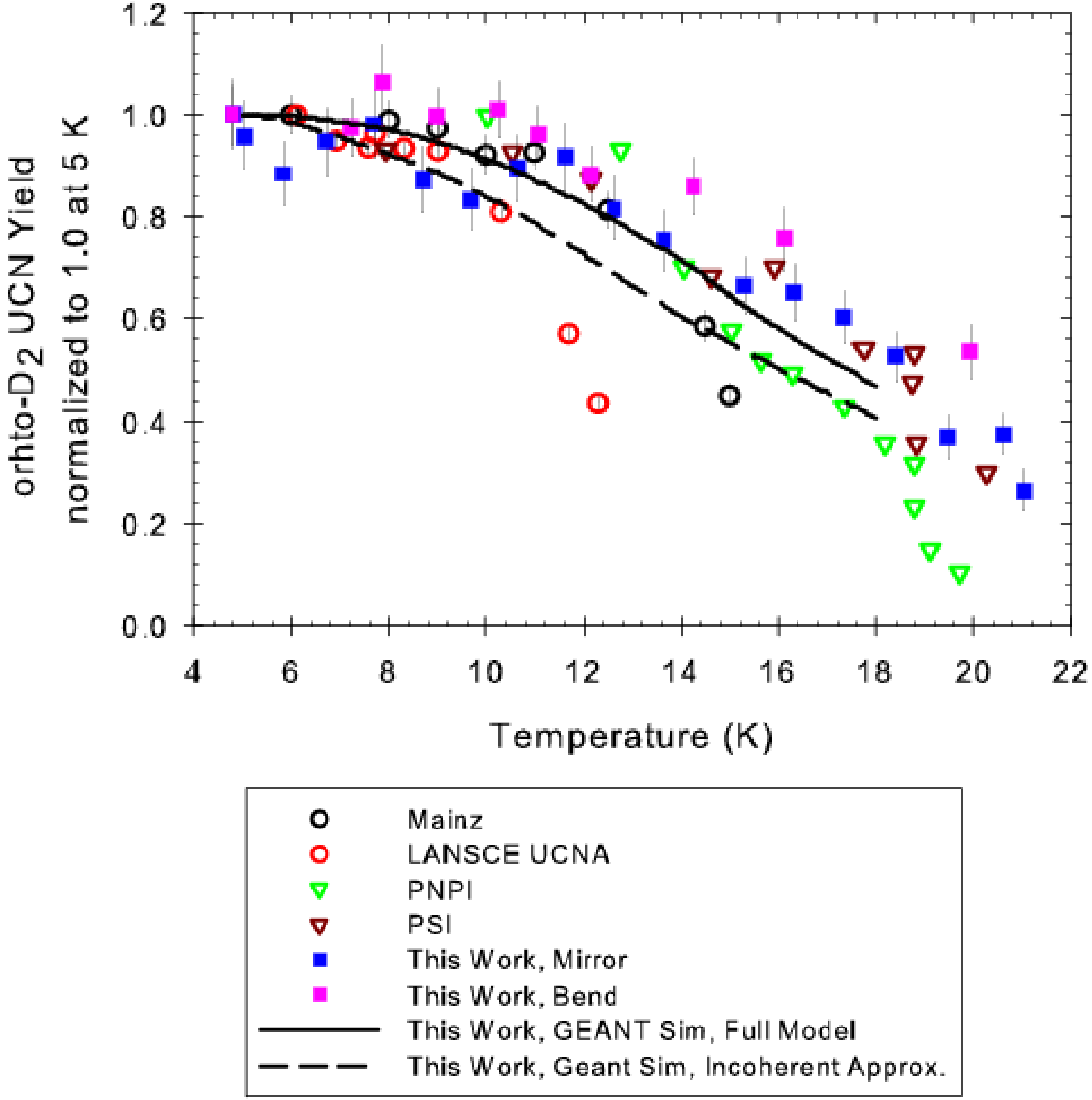


Higher saturation temperature!

D_2 data to validate the simulation



A survey of all the UCN production data using D_2

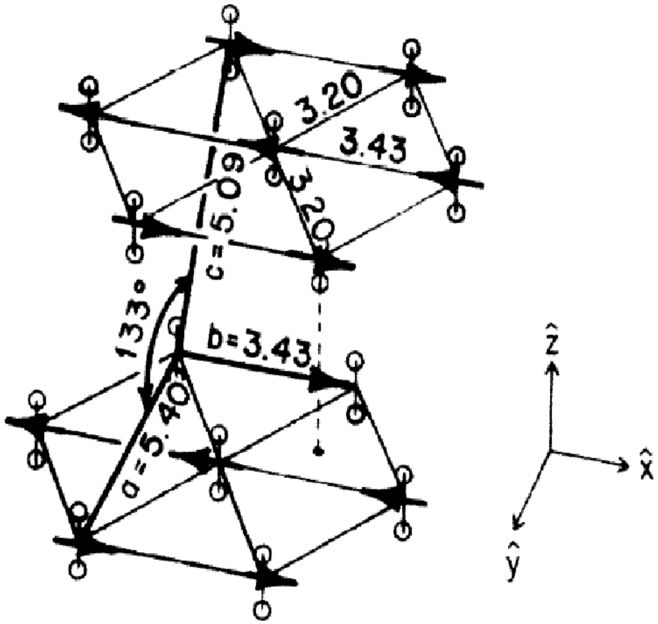


Solid Oxygen as a UCN Source

σ_{coh} =4.232 barn, σ_{inc} = 0 barn,
σ_{abs} = 0.0001 barn

- Electronic spin S=1 in O_2 molecules.
- Nuclear spin = 0 in $_{16}O$
- Collinear Anti-ferromagnetic in 2-D
  - α-phase, T < 24K.

Stephens & Majkrzak, PRB **33**, 1 (1986)

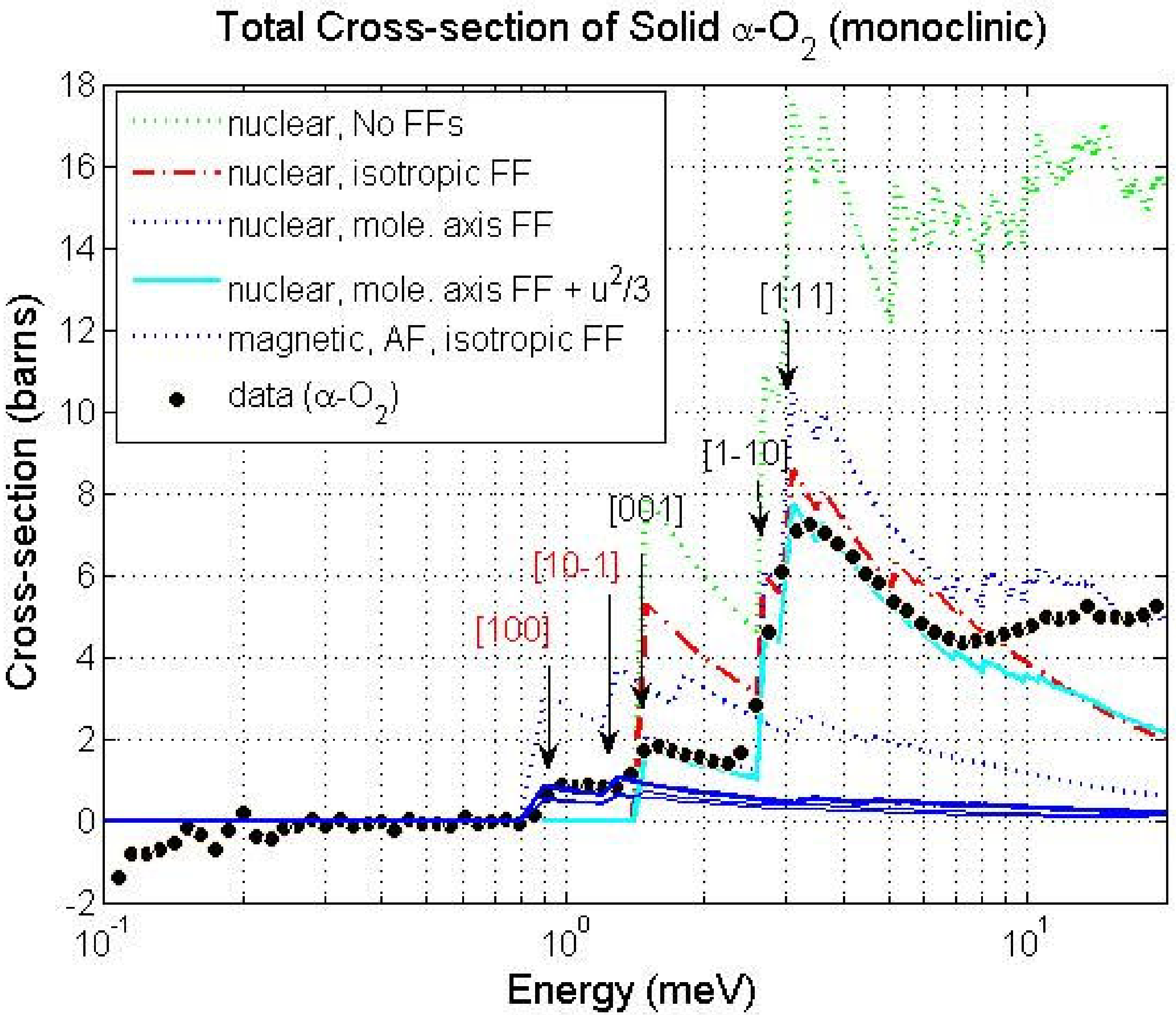


UCN Production in alpha S-O_2

- Produce UCN through magnon excitations.
  - Magnetic scattering length ~ 5.4 fm.
- Null incoherent scattering length.
- Small nuclear absorption probability.

$\Rightarrow$ A very large source possible.

Total cross-section (check form factors)

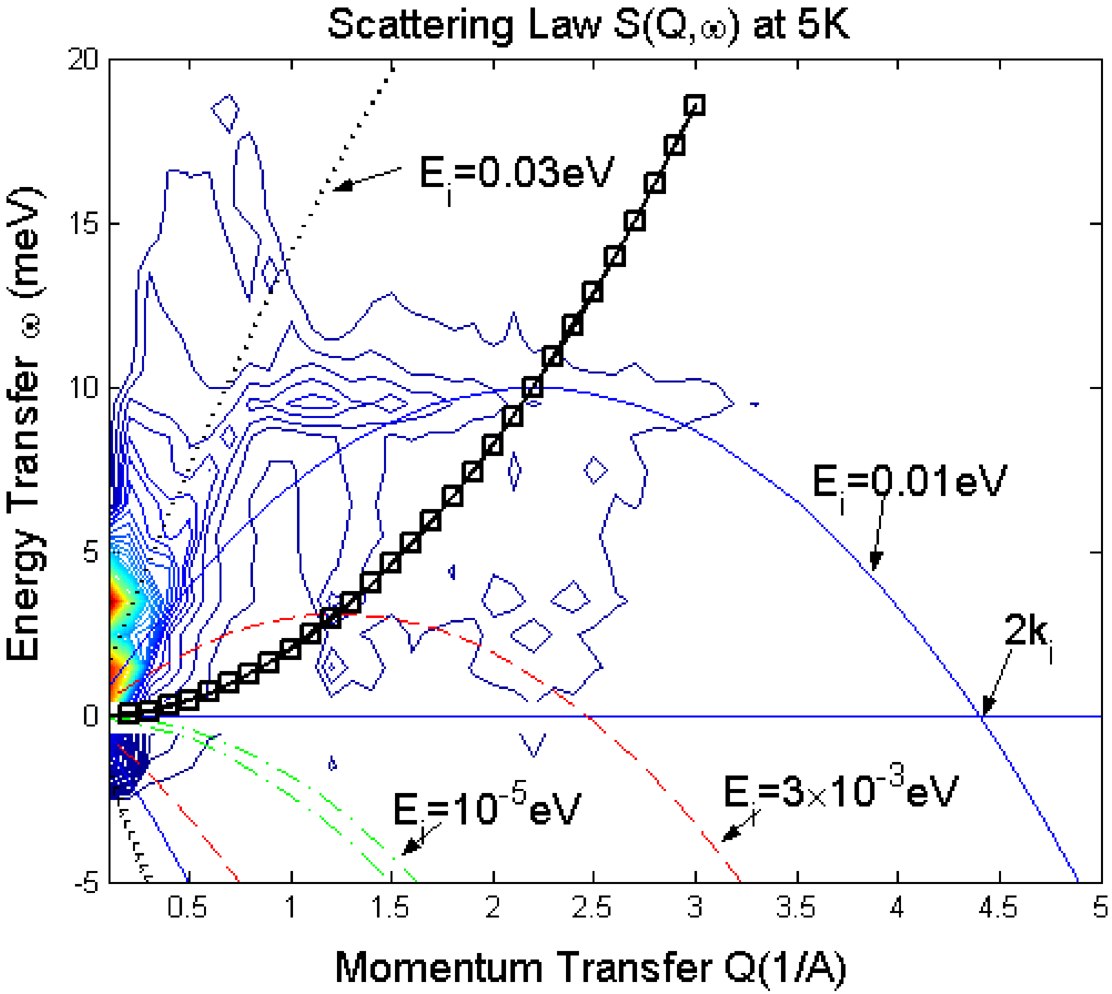


Again, there are some details that need to get right.

Molecular form factor is no longer isotropic, because the molecules are "oriented" in solid.

Calculated S(Q,ω) in α-O2

$$H = -2\sum_{\langle ij\rangle} J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j + \sum_i(-DS_{xi}^2 - D'S_{yi}^2 + D'S_{zi}^2)$$



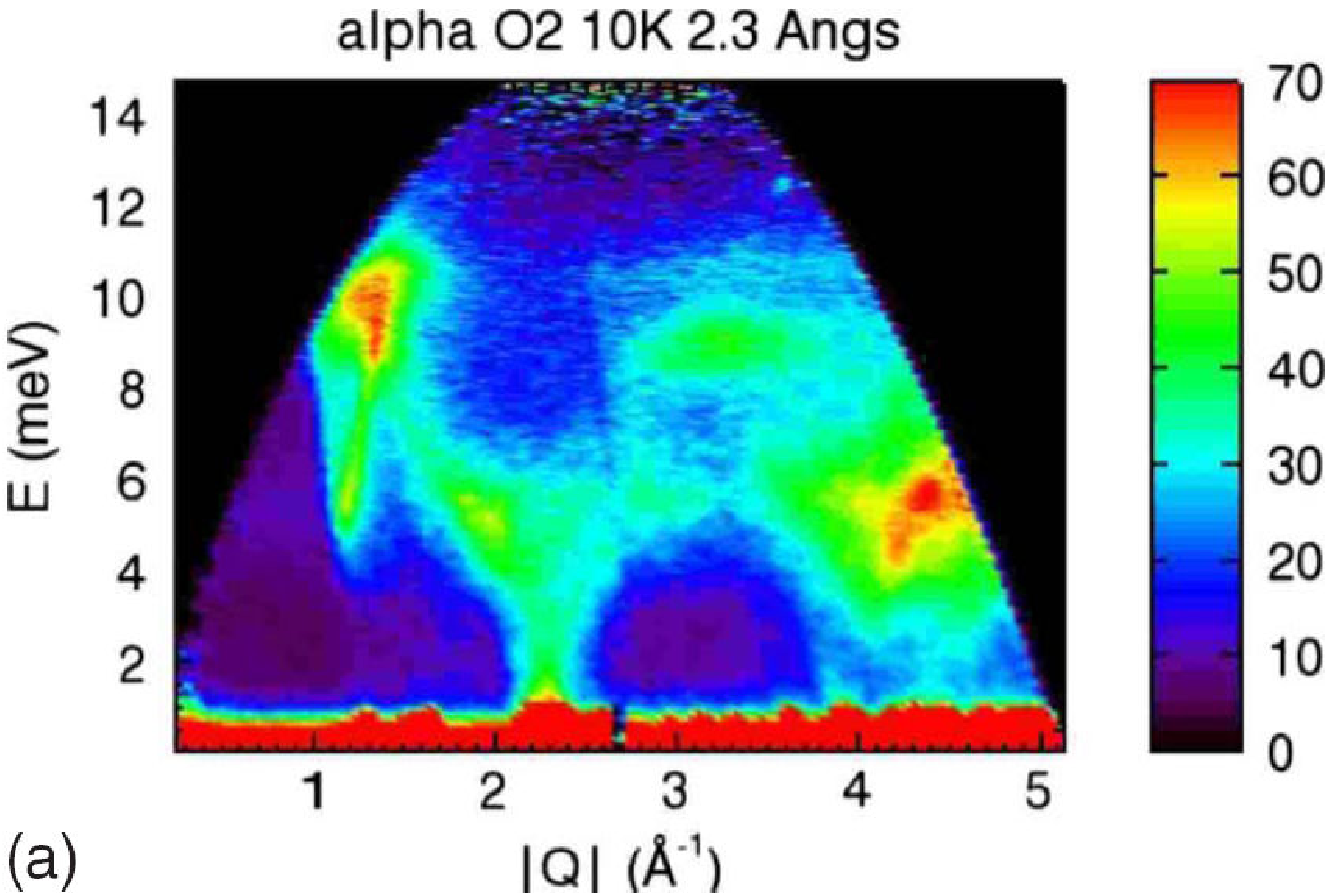
Range of coupling constants
J_{NN} = -3.32 (-2.44) meV
J_{NNN} = -0.91 (-1.22) meV
$J_{\perp}$ < 0(0) meV

J_{NN}=-2.44 meV
J_{NNN} = -1.22 meV

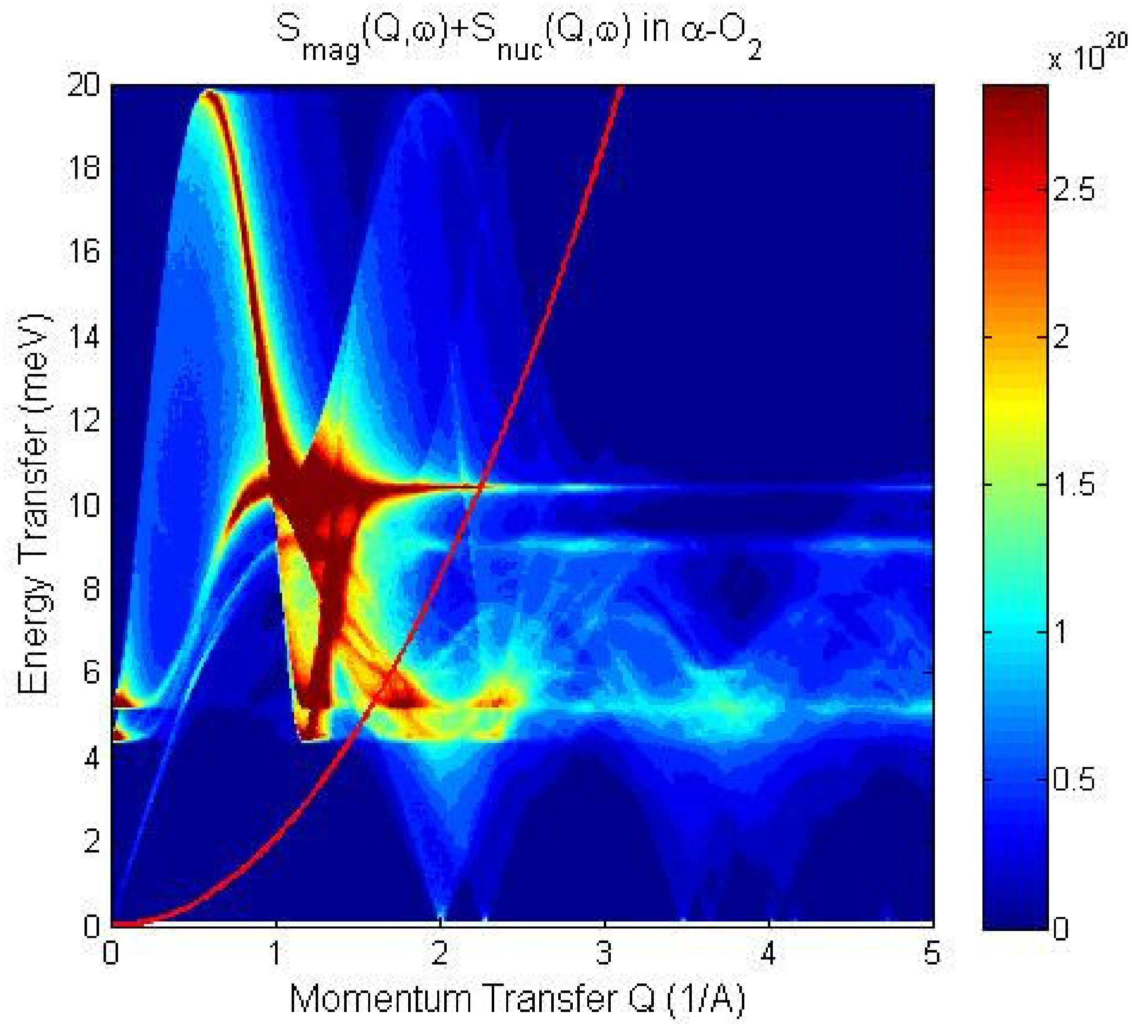
D=0.132 meV
D'=0.118 meV

Suggested in Stephens & Majkrzak, PRB **33**, 1 (1986)

Neutron scattering data



Updated S(Q,ω) in α-O2



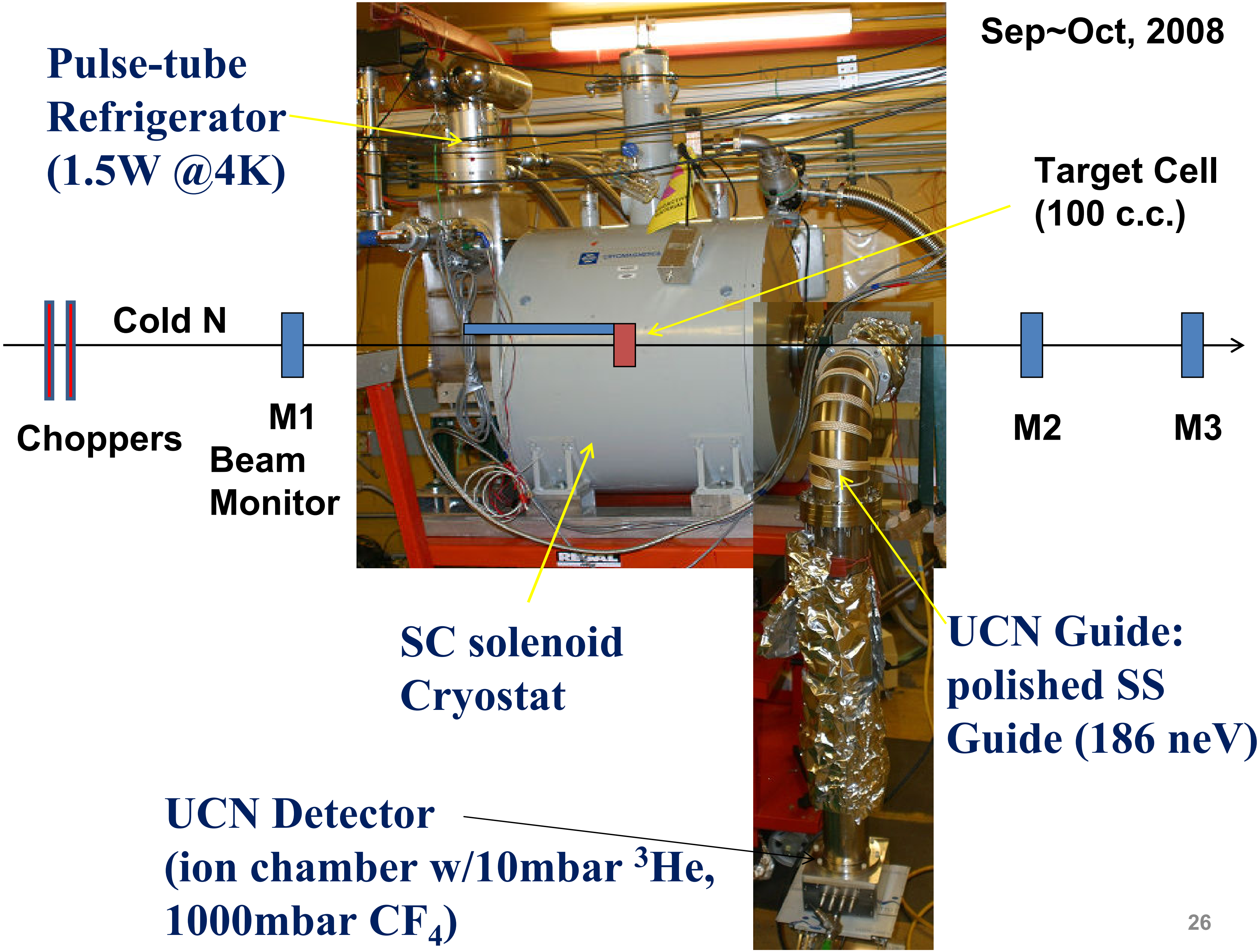
Jnn=-2.44 meV
Jnnn=-1.22 meV

D=0.6 meV (updated)
D'=0.1 meV

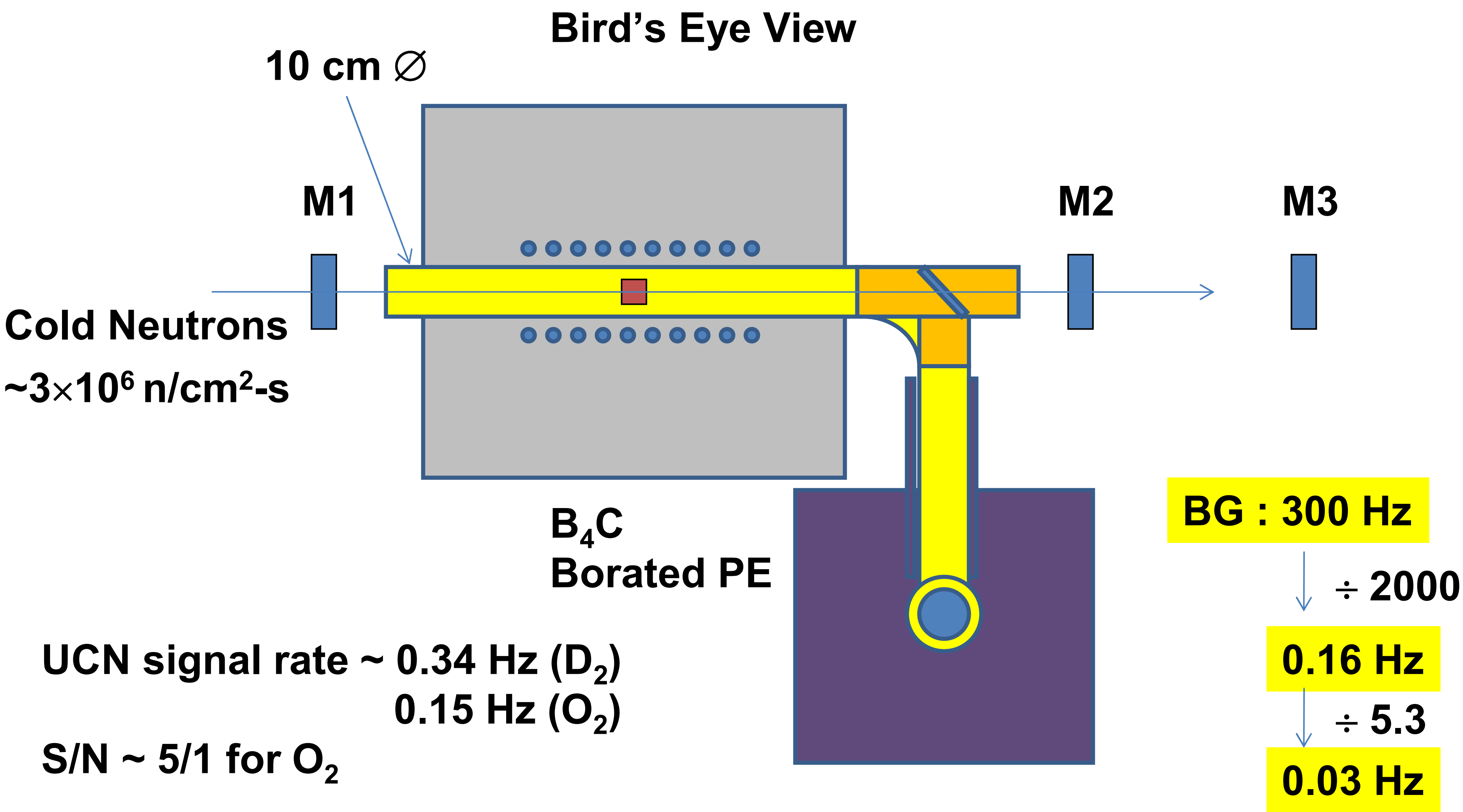
Also, there was a sign error.

Spin self-energy is very strong along the direction of spin alignment!

Sep~Oct, 2008


Pulse-tube
Refrigerator
(1.5W @4K)
Target Cell
(100 c.c.)
Cold N
Choppers
M1
Beam
Monitor
M2
M3
SC solenoid
Cryostat
UCN Guide:
polished SS
Guide (186 neV)
UCN Detector
(ion chamber w/10mbar ^{3}He,
1000mbar CF_4)

Low Statistics Measurements



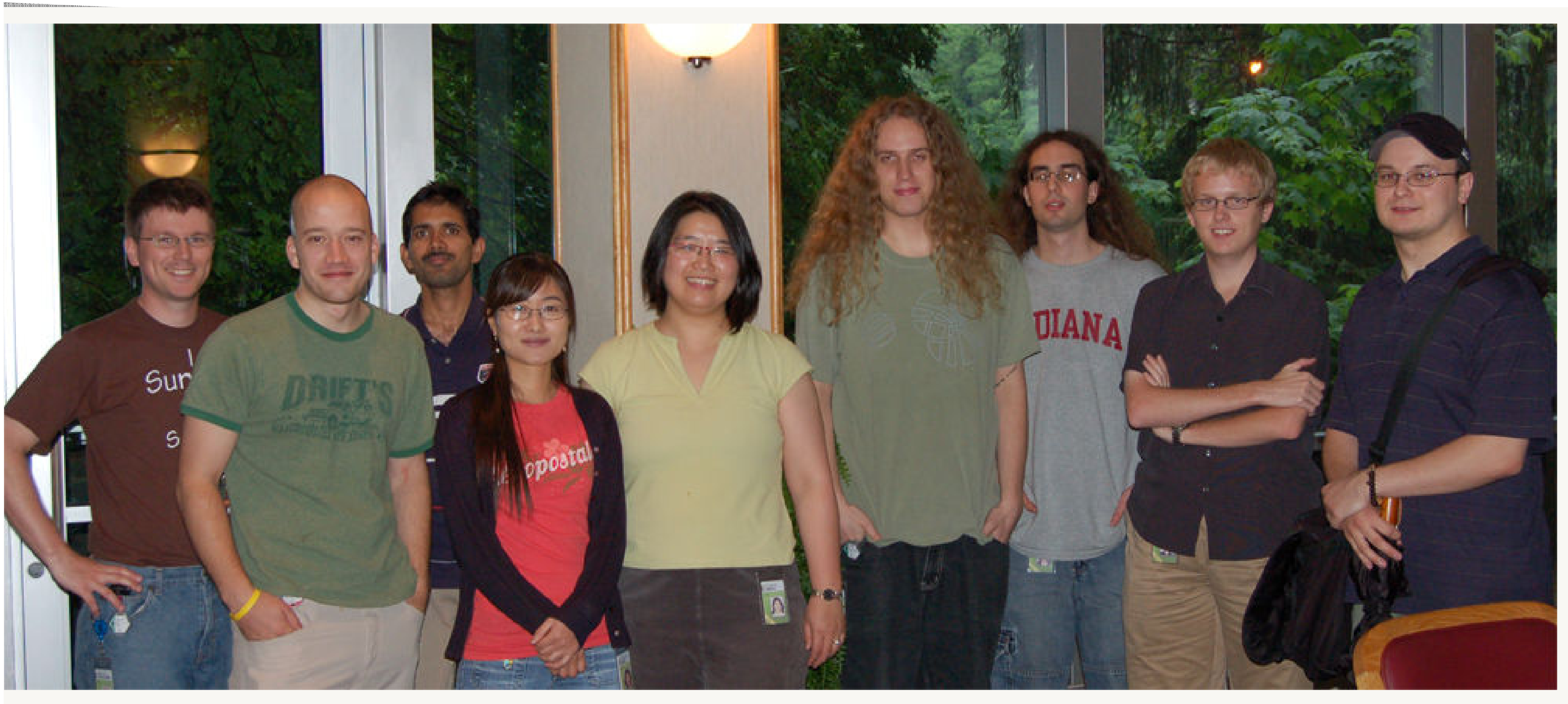
Summary

- First complete treatment of neutron cross-section in solid D_2.
  - UCN downscattering cross-sections need to be updated.
  - UCN upscattering cross-sections also need to be updated.

  Have not yet include very likely effects of quantum solids, might lead to quasielastic scattering from enhanced diffusion.

- UCN production in solid α-O_2 revisited.
  - Several problems have been fixed, i.e., stronger self-spin constant and a sign error.
  - Should be able to interpret the experimental data on UCN production from solid O_2.

Our Group at IUCF



Ultra-Cold Neutrons, Neutron EDM, Electron EDM