

- Relationship between structure and property

$((=B\ddot{u}4\text{\textcircled{S}} X \hat{a}(= \hat{u})$

- Why neutrons: neutron characteristics and neutron scattering

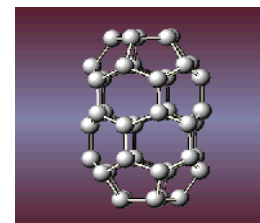
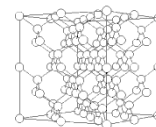
$(\text{ " } L\hat{O}?U \text{ \$ } \ddot{O} \text{ \$}(M\&\bullet \hat{a} \text{ \$ } 7 \emptyset \quad)$

- Coupling between lattice, orbital and spin in manganites studied by neutron scattering

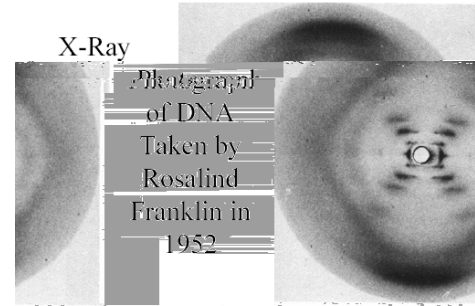
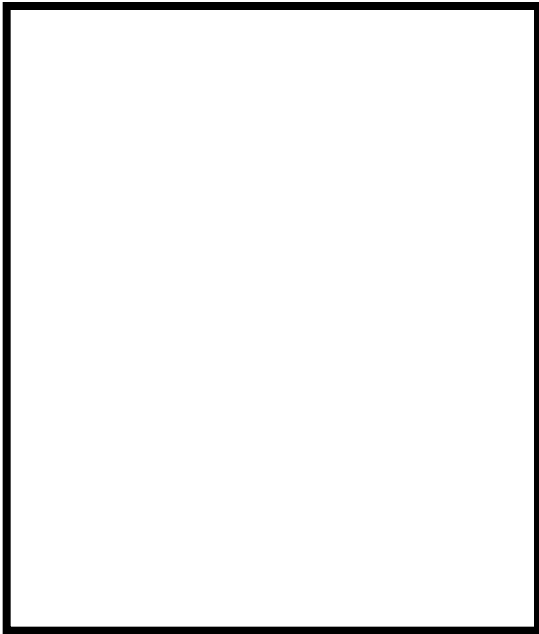
$(K !\hat{u} \hat{e}(= \text{ J } \tilde{A}E<F' \text{ `7}\frac{3}{4} \ddot{Y},\grave{\text{I}} \text{ f } 0*\ddot{u},X \text{ \$ } 7 \emptyset\text{-}\grave{e}0J \quad)$

- Target Station of spallation neutron sources

$(7>\text{-- } \text{\textdollar}\text{\textdollar}d \text{)}$



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Ÿ ã _4§ X È J b1958 H ¢ î Z —"© í Ä

James Watson and Francis Crick

结构模型

认识相互
作用

晶体和分
子构型

说明物
质性质

磁、电、光、热等基本物性

- Relationship between structure and property

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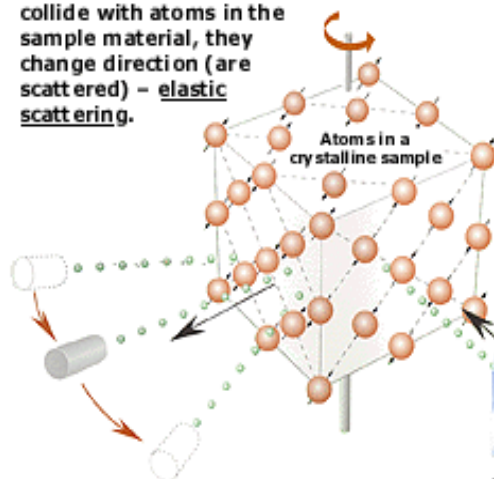
$(K \text{ !}\hat{u} \hat{e}(= \text{ J } \tilde{A}E<F' \text{ `}7\frac{3}{4} \ddot{Y},\grave{\text{I}} \text{ f } 0^*\ddot{u},X \text{ \$ } 7 \emptyset\text{-}\grave{e}0J \quad)$

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When the neutrons collide with atoms in the sample material, they change direction (are scattered) – elastic scattering.



Detectors record the directions of the neutrons and a diffraction pattern is obtained.

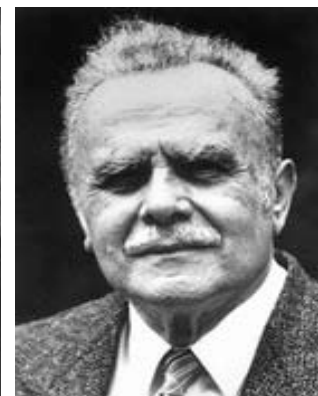
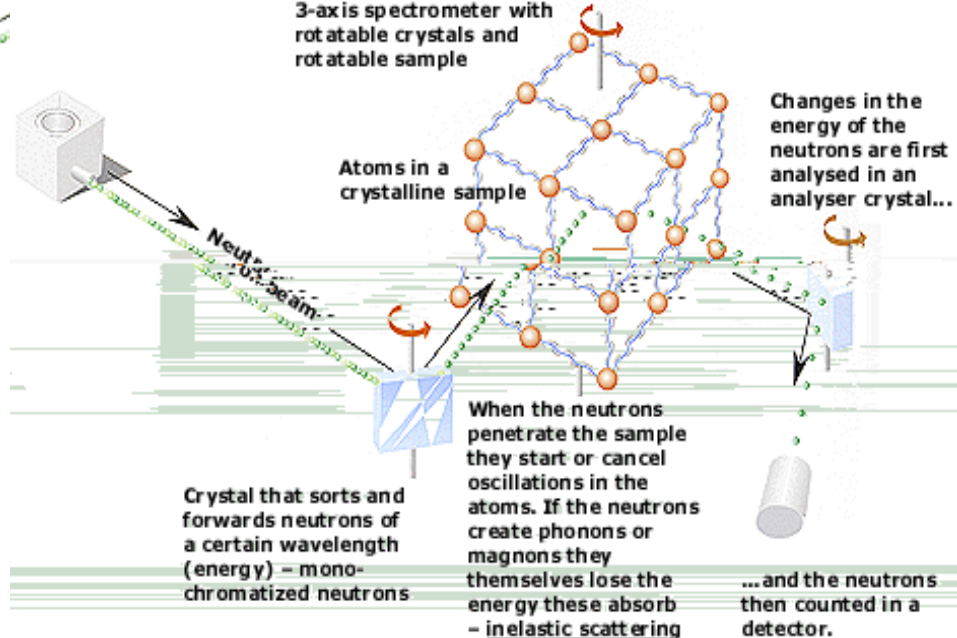
The pattern shows the positions of the atoms relative to one another.

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Research reactor



Crystal that sorts and forwards neutrons of a certain wavelength (energy) – monochromatized neutrons



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Charge = 0

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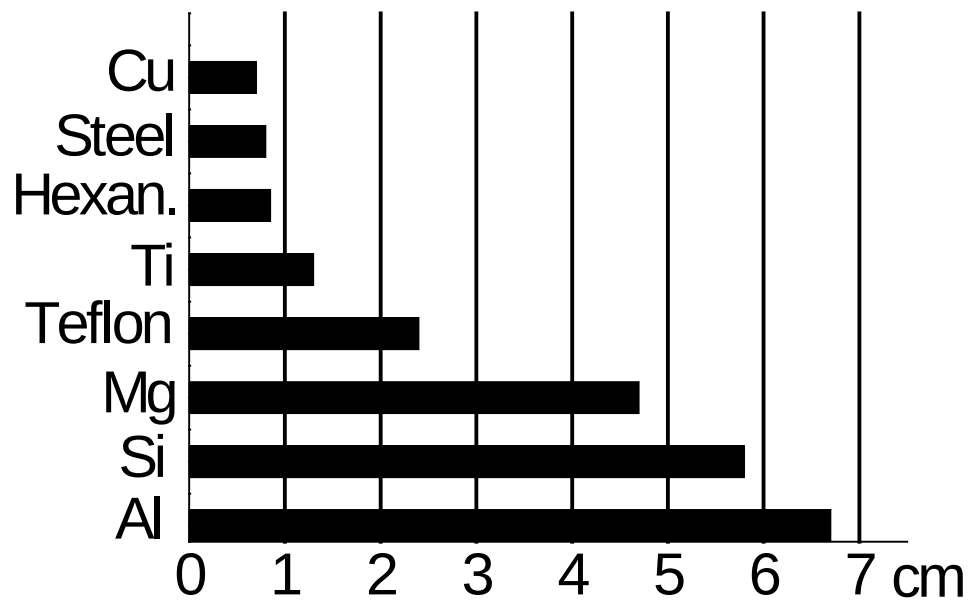
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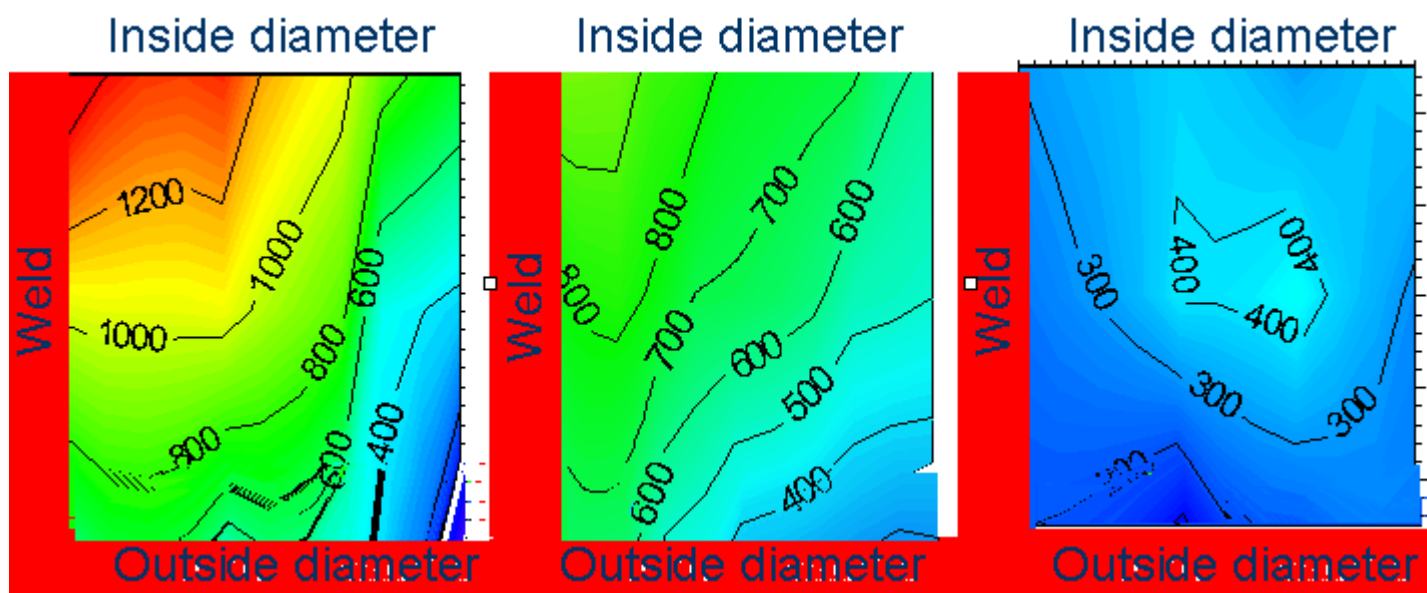
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 o < Ž2O S*ü 3000 H
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Vision 21



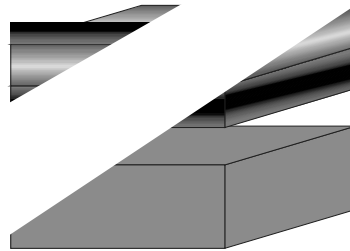
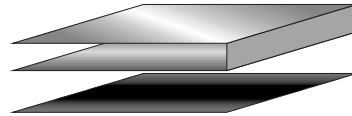


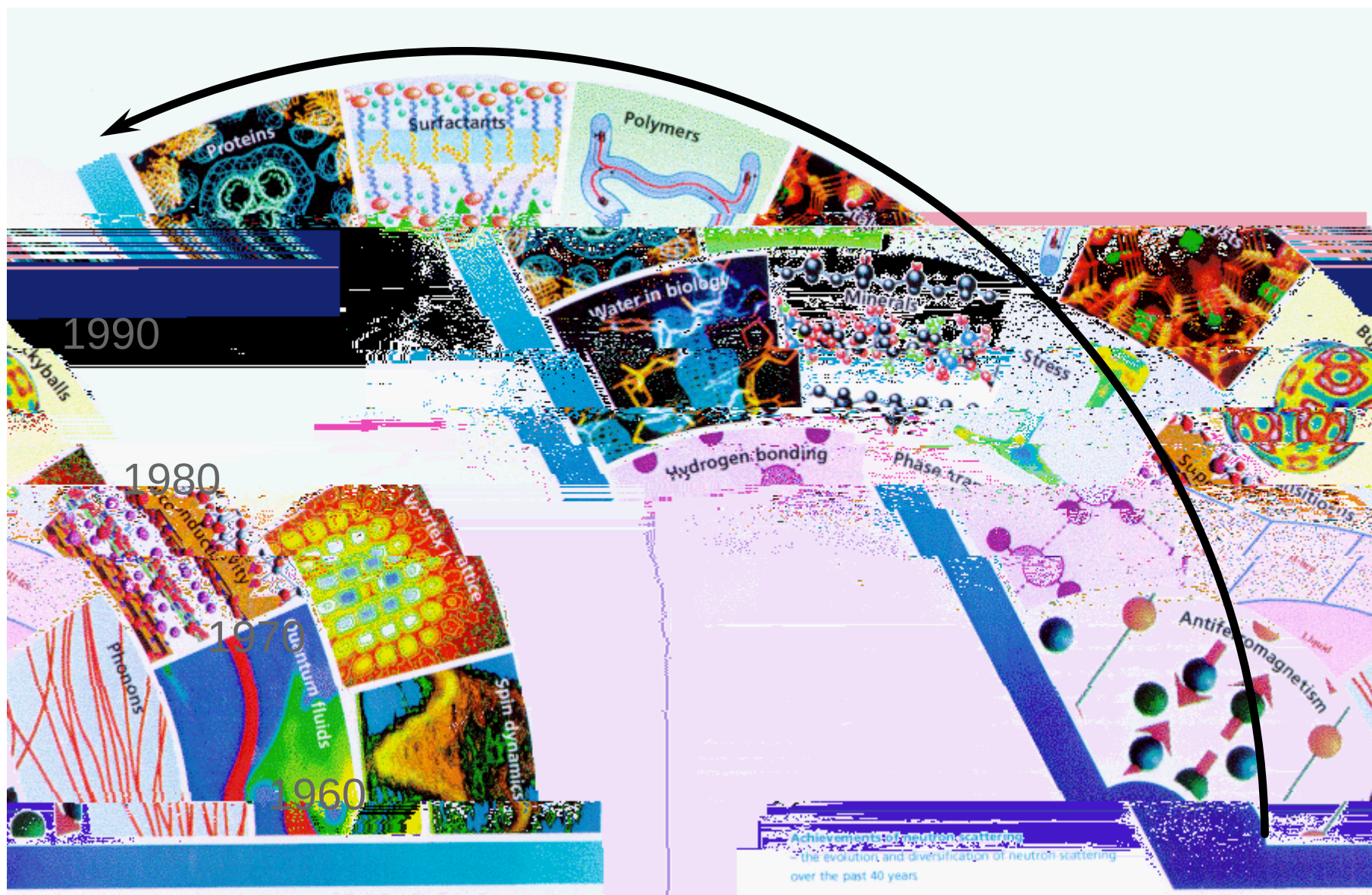


Spin = $\frac{1}{2}$

$n = -$

N





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- Target Station of spallation neutron sources

$(7>\text{-- } \$\$d \text{)}$

Collaborators:

LLB, France :

A. Gukasov

F. Moussa

M. Hennion

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LPCES/Univ. Paris Sud, France:

M. Apostu

R. Suryanarayanan

A. Revcolevschi

IOP/CAS, China:

Lunhua He

Zhaohua Cheng

- Introduction to CMR manganites
 - Structure, CMR effect, interplay between the degrees of freedom, application of neutron scattering
- Coupling demonstrated by neutron scattering
 - Magnetic properties of $(\text{La}_{0.4}\text{Pr}_{0.6})_{1.2}\text{Sr}_{1.8}\text{Mn}_2\text{O}_7$ single crystal
 - Lattice and spin by neutron diffraction
 - Charge and spin by inelastic and diffusion neutron diffraction
 - Orbital and spin by polarized neutron diffraction

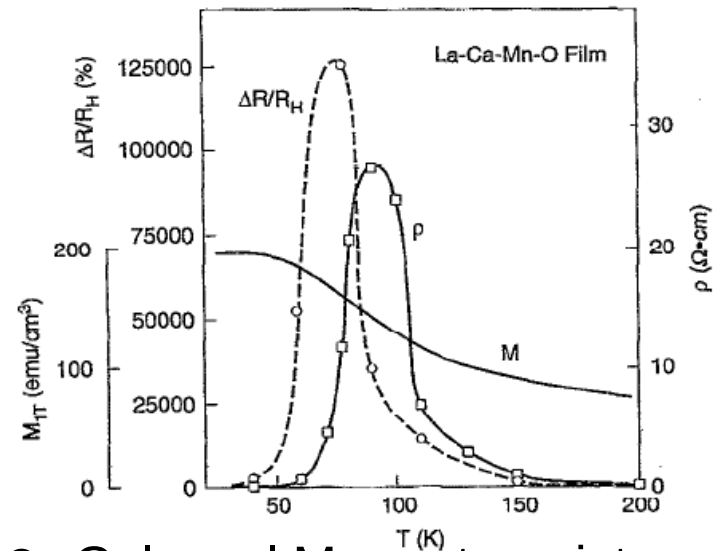
(From A. P. Ramirez, J. Phys.:Condens.Matter 39, (1997) 8171)

n: the number of connected layers
of vertex-sharing MnO_6 octahedra

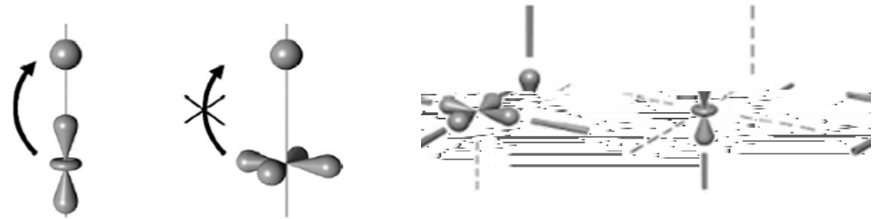
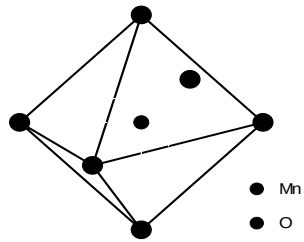
n=1: $(\text{La,Sr})_2\text{MnO}_4$

n=2: $(\text{La,Sr})_3\text{Mn}_2\text{O}_7$

n= ∞ : $(\text{La,Sr})\text{MnO}_3$



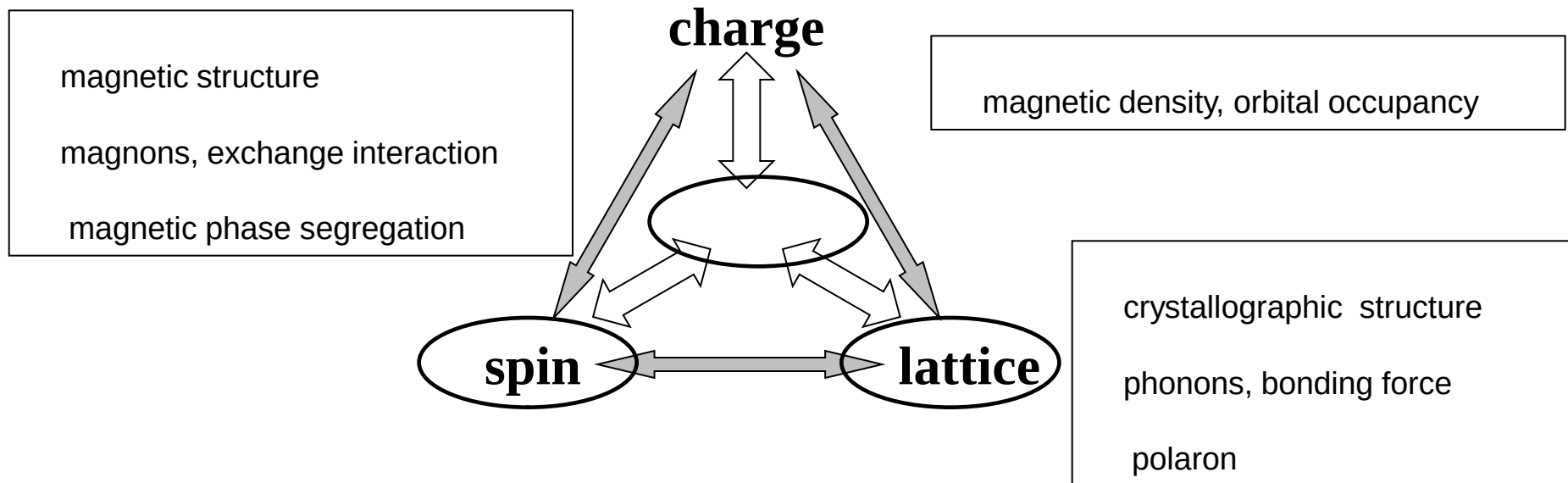
- Colossal Magnetoresistance
- Metal insulator transition
- Jahn -Teller effect
- Phase separation
- Charge ordering
- Orbital ordering
-



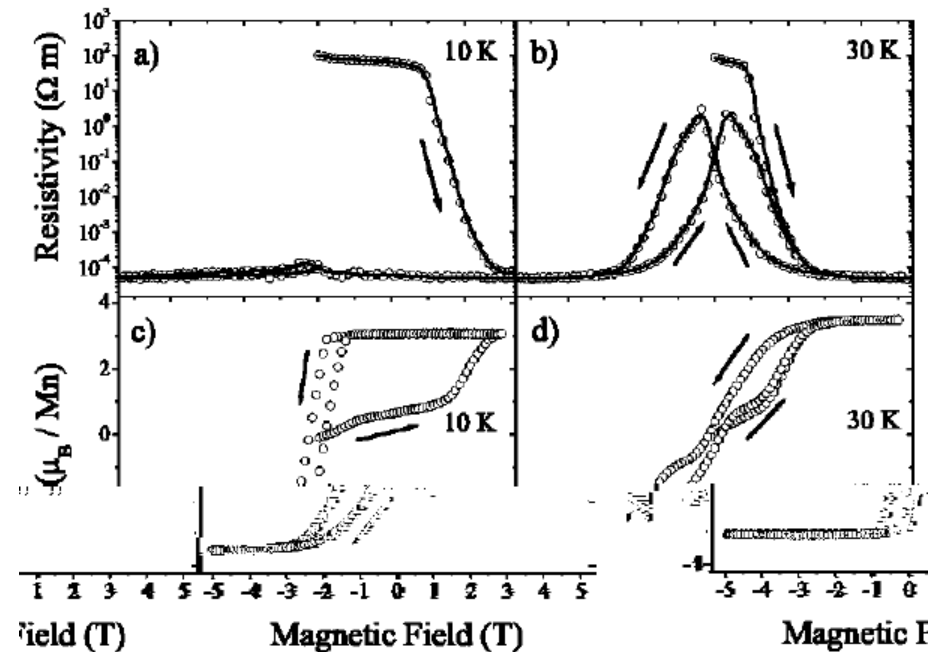
G. Khalillin and R. Kilan, Phys. Rev. B 61 3494 (2001)
 D. Khomskii and K. Kugel, Phys. Rev. B 67 134401 (2003)

Tokura et al. Science 288, 462(2000))

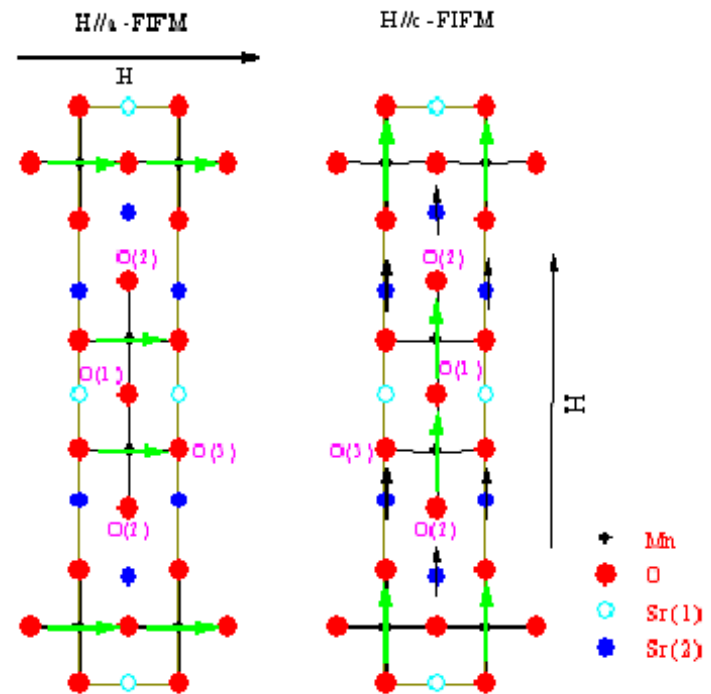
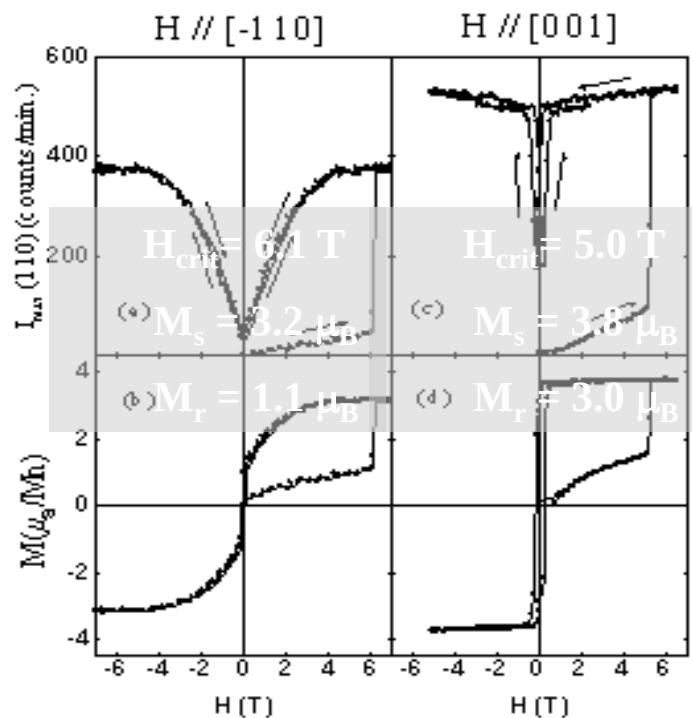
- Competition and co- operation between lattice, charge, spin and orbital of Mn- ion 3d electrons.
- Energies of those degrees of freedom are comparable.
- Ground state is easily tuned by environment, such as chemical doping, temperature, pressure, field and so on, leading richness of physical phenomena.



- 2D characteristics: strong anisotropy
- Similar physical phenomena: CMR, MIT, PS, CO, OO...
- Twin-free single crystal



- Magnetic moments are aligned to the direction of the applied field.
- Different critical fields for the transition para- to ferromagnetism.
- Different saturation magnetization due to ordering of Pr moment.



site	atom	variable	FIFM(ab)	FIFM(c)
4e(00z)	Sr2	z	0.3175(1)	0.3144(6)
		$\mu_{Pr}(\mu_B)$		2.8(3)
4e(00z)	Mn	z	0.0968(2)	0.0962(7)
		$\mu_{Mn}(\mu_B)$	3.29(6)	3.4(1)
4e(00z)	O2	z	0.1973(1)	0.2008(6)
8g(01/2z)	O3	z	0.09590(8)	0.0957(2)
		$R_{F2}(\%)$	6.79	6.93
		χ^2	10.2	16.7
		No. of observed reflections	212	146
		$d_{Mn-O1}(\text{\AA})$	1.951(4)	1.94(1)
		$d_{Mn-O2}(\text{\AA})$	2.025(5)	2.10(2)
4(2)		$d_{Mn-O3}(\text{\AA})$	1.987(6)	1.937(2)
5(7)		$\angle Mn-O3-Mn(^{\circ})$		178.9(3)
3(6)		Δ_{JT}		1.026(2)

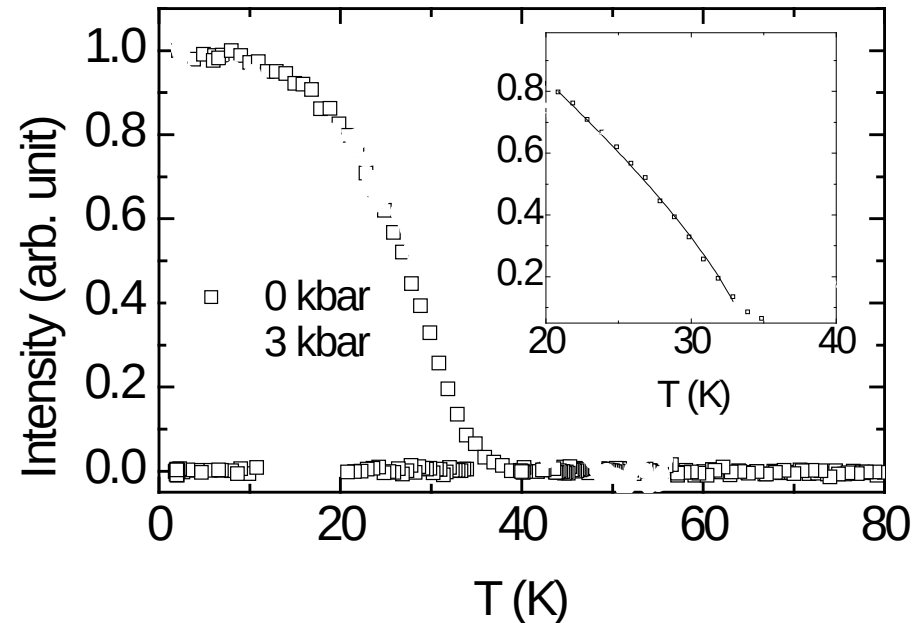
- Decreases the critical field of PM-FM transition
- Narrows the hysteresis loop
- Broadens the field transition region

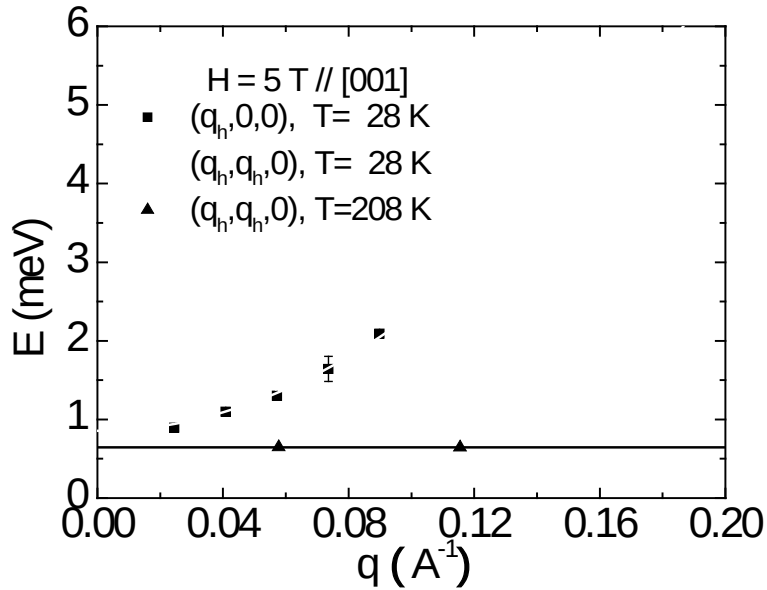
$$I/I_0 = (1-T/T_C)^{2\beta}:$$

P = 0 kbar: $T_C=33.9(2)$ K; $\beta=0.37(2)$

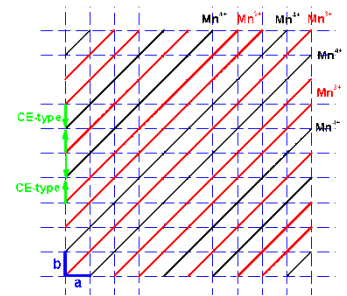
P = 3 kbar: $T_C=39.6(4)$ K; $\beta=0.24(1)$

Decrease of β : weakness of interlayer super -exchange interaction.
Increase of T_C : Strength of intralayer double exchange interaction.





- i) Spin wave:** FIM at low temperature
- ii) Spin gap:** 2D-anisotropy
- iii) Same dispersion:** isotropy in the plane
- iv) $D \sim 148 \text{ meV\AA}^2$:**
metallic state



- i) Insulated State ($H = 0$ T) :
(0.2, -0.2, 0) diffuse scattering: Electron ordering
- ii) Metallic State ($H = 5$ T):
No diffuse scattering : Electron order melting

- $$((=B\ddot{u}4\S X \hat{a}(= \hat{u}))$$

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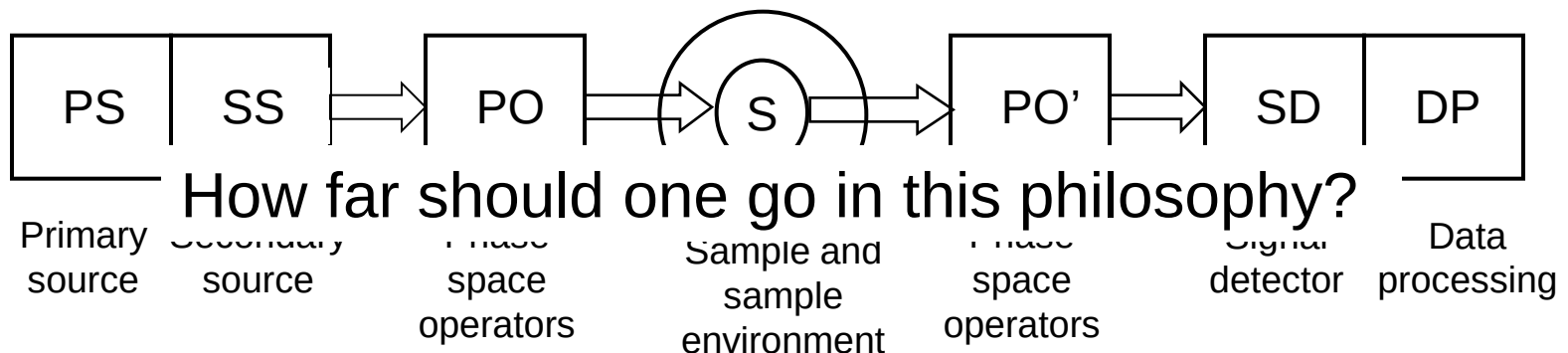
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- Coupling between lattice, orbital and spin in manganites studied by neutron scattering

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- Neutron scattering instruments can be designed to work in continuous mode or in time of flight mode.
- There is no one instrument that can cover most of the Q - ω space with sufficient resolution and flexibility.
- Instruments have varying requirements with respect to spectral properties and time structure.
- This is why instrument and source designers have come to interact ever more closely in conceiving new systems (not so in the early days of reactor development).



Nuclear process	Example	Neutron yield	Heat release (MeV/n)
D-T in solid target	400 keV deuterons on T in Ti	$4 \cdot 10^{-5}$ n/d	10 000

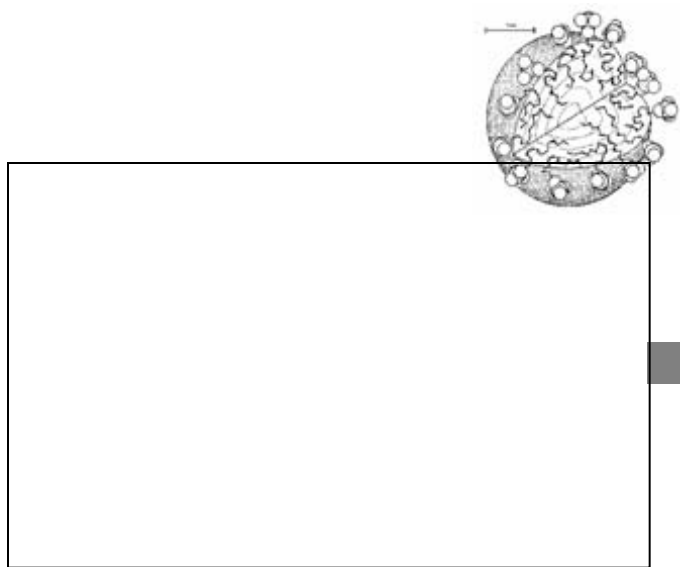
•Spallation

- no chain reaction
- pulsed operation
- 35 neutrons/proton
- ~45 MeV/neutron

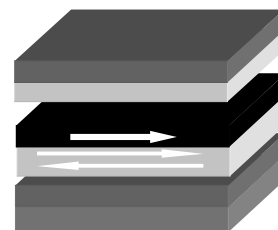
•Fission

- chain reaction
- continuous flow
- 1 neutron/fission
- 180 Mev/neutron





$P-E$ $\$d$

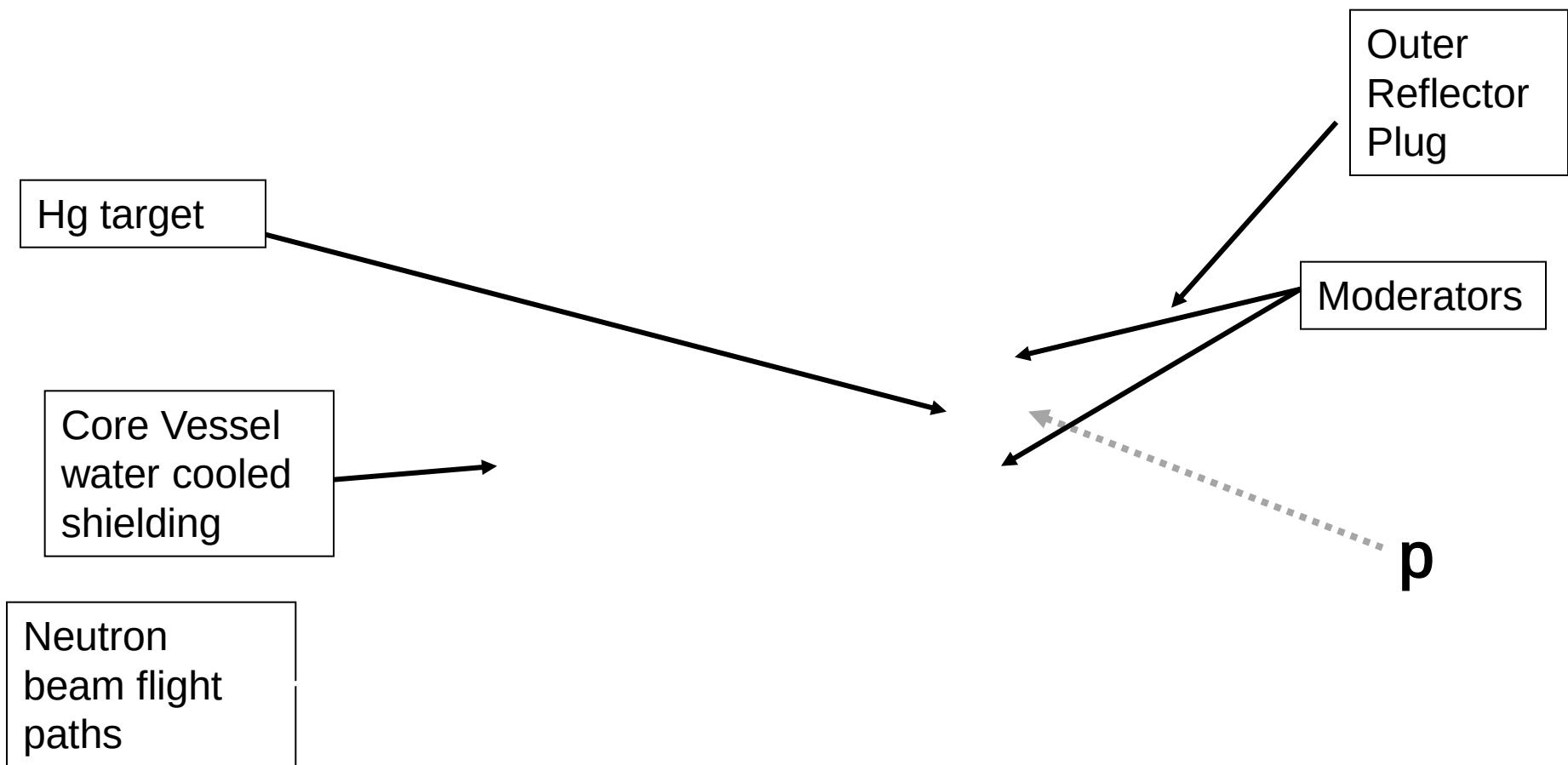


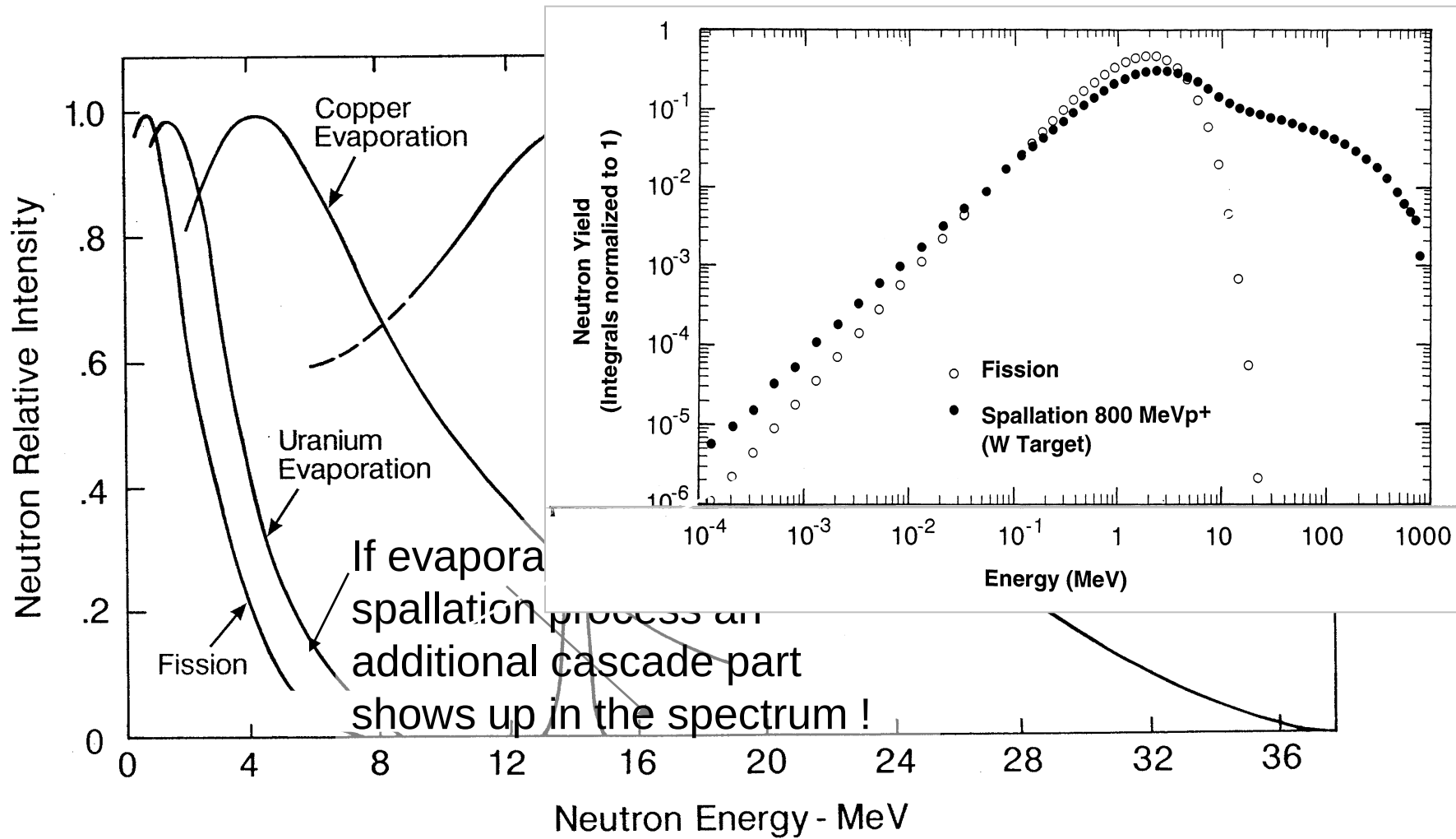
- 2006 HEα>
- 2 MW Ê ÈÊÊG£ Ö~12x ISIS È ÊKÈ G ÊÊG£ Ö½ ILL
- Ä &Á \$ÊÊG£ Ö ~50-100x ILL
- ê+ Ô Q,X 7>-\$d È),,0 nEα> ü 800kW

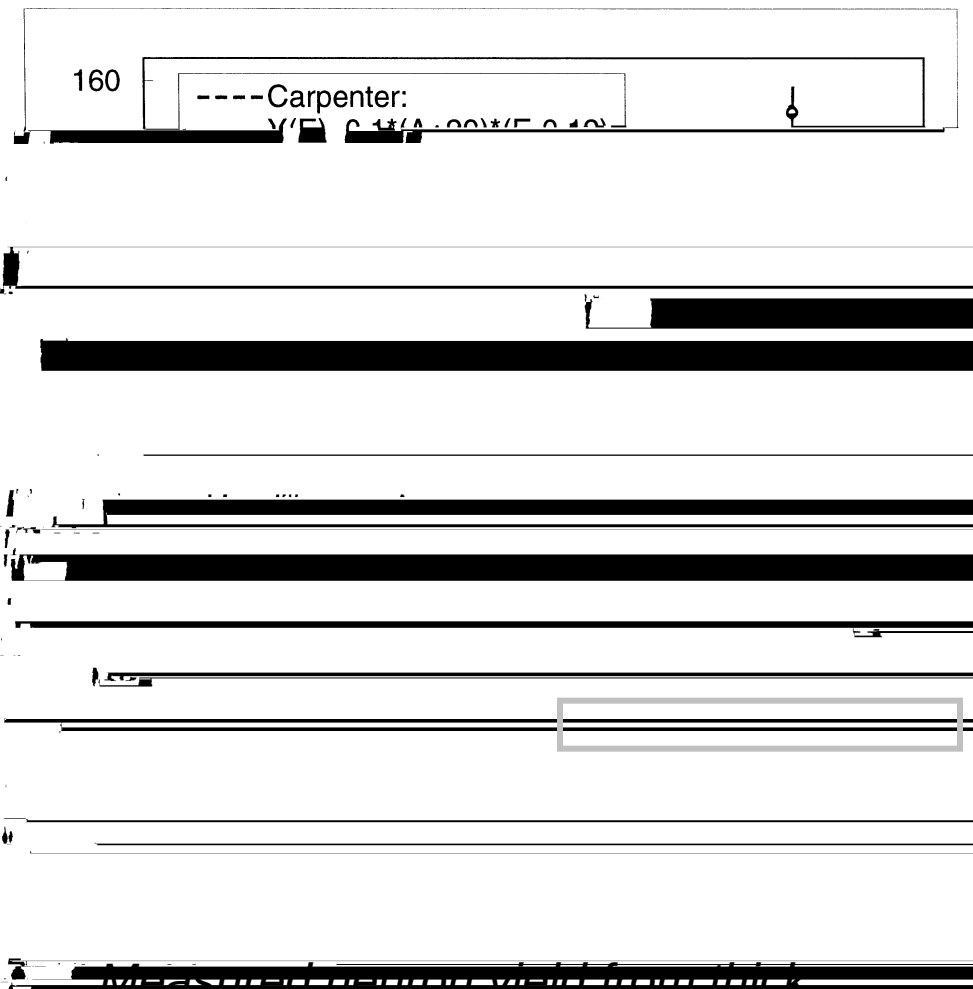
• 7³/2001 H $\ddot{Y}$ È Ô ó iC 1527 “¹ Ñ ` ó?~ æ 363 “¹ È

2009 H Î äEα>

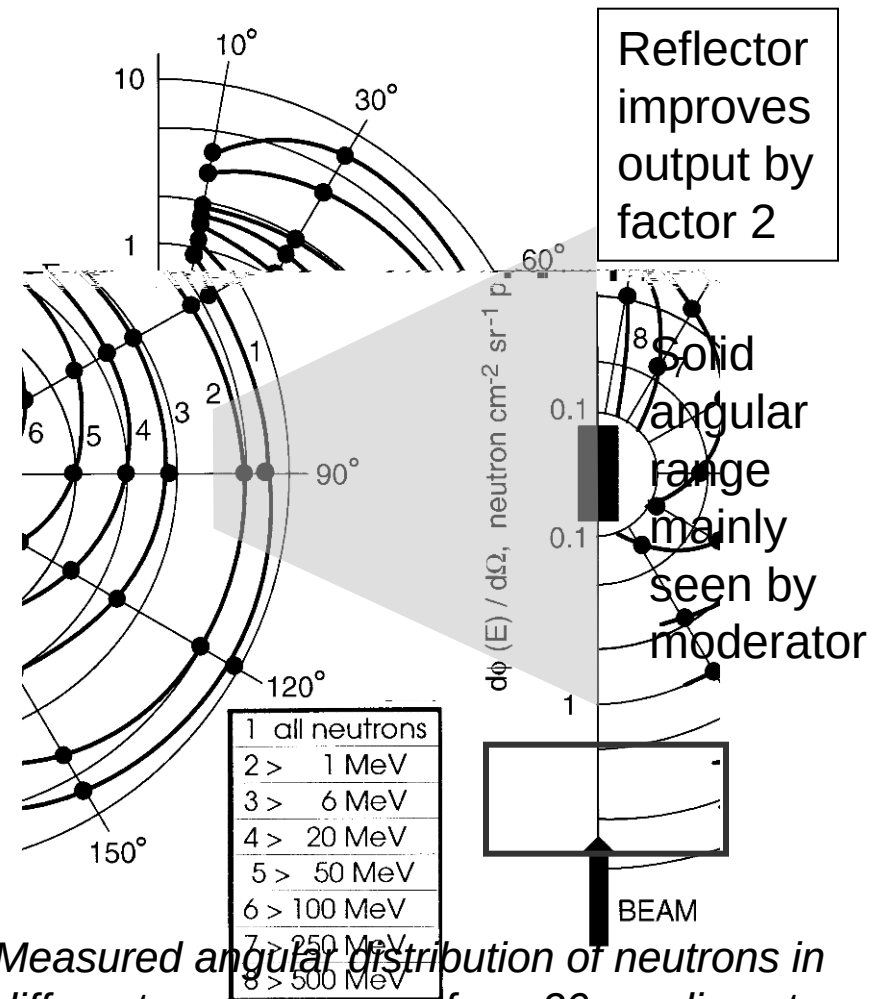
• 1MW È 25Hz, 3GeV



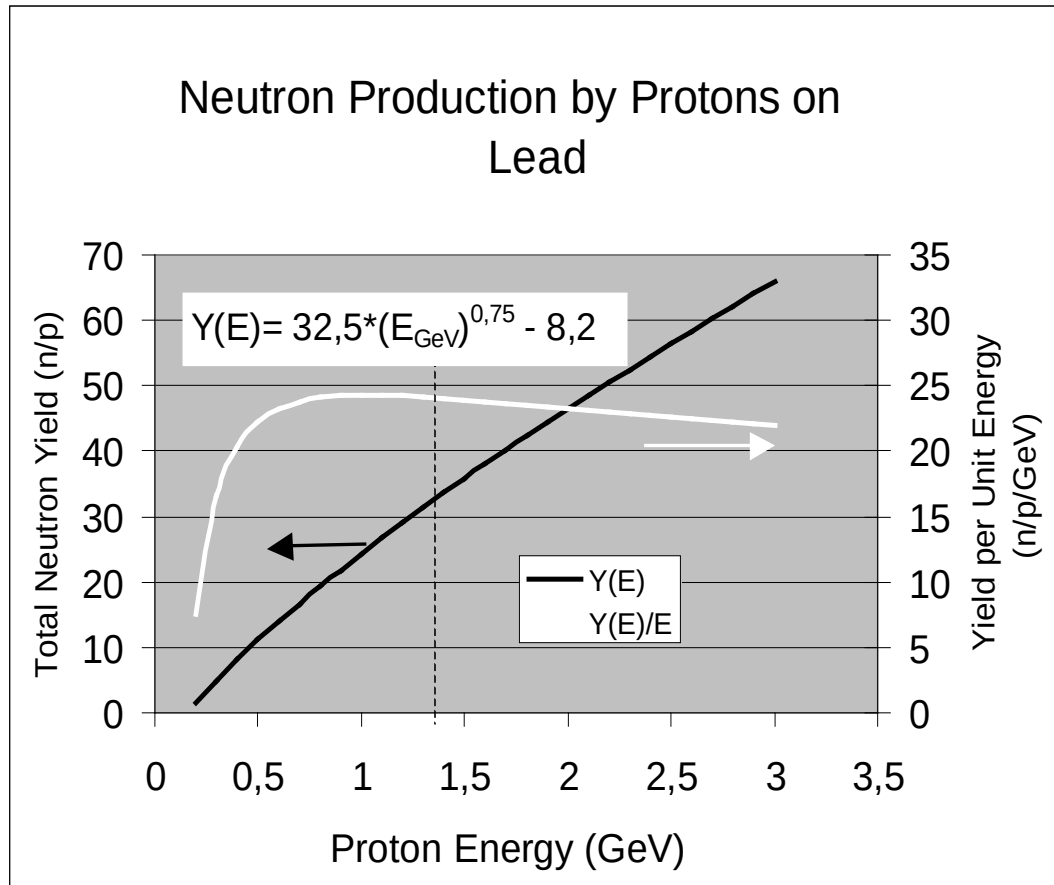




Measured neutron yield from thick lead targets



Measured angular distribution of neutrons in different energy groups for a 20 cm diameter lead target bombarded by protons of 2 GeV

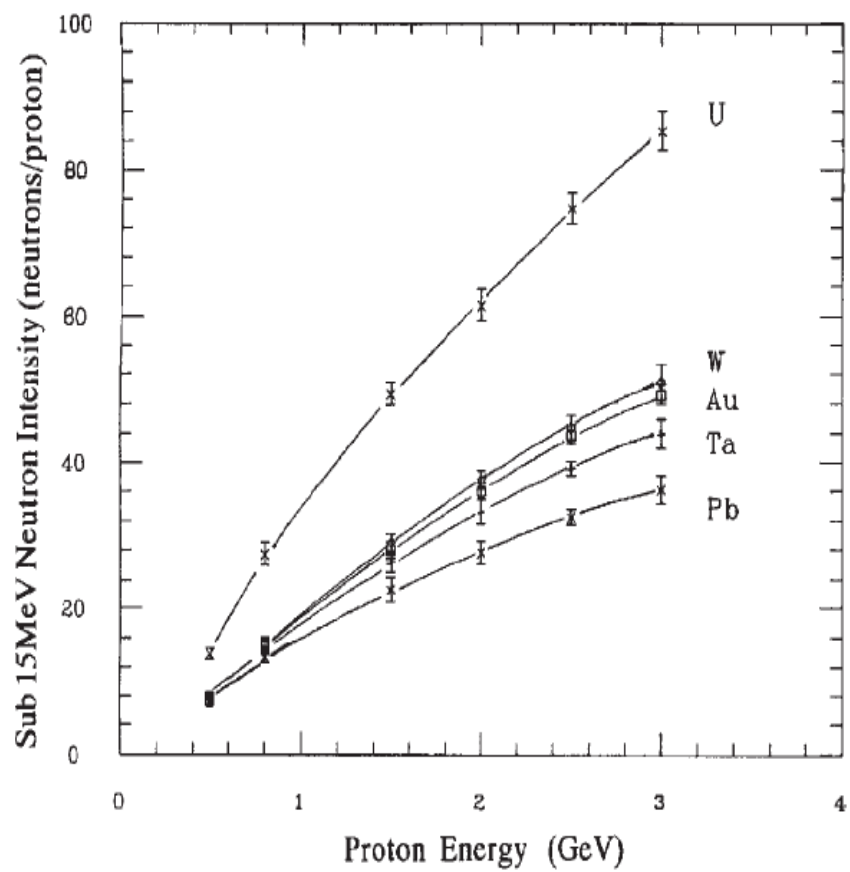


Arguments for higher proton energy :

Easier to accelerate to higher energy than to increase current (in particular with circular accelerators)

No Bragg peak above 600 Mev

Radiation damage in target and window materials scales roughly with number of protons per unit area, not with beam power.



- Moderation of neutrons occurs by collisions with moderator atoms

• “•

$$\xi = \ln E_1 - \ln E_2 \quad \left\{ \begin{array}{l} = 1 \text{ for } A=1 \\ \approx 2/(A+2/3) \text{ for } A > 1 \end{array} \right. \quad \begin{array}{l} A \text{ is the atomic} \\ \text{number of the} \\ \text{moderator atom} \end{array}$$

- Number of collisions x required to slow down from energy E_0 to E_f
 $x = 1/\xi * \ln(E_0/E_f)$ for $E_0 = 2\text{MeV}$ and $E_f = 1\text{ eV}$: $x = 14.5/\xi$

Parameter	Element						
	H	D	Be	C	O	Hg	Pb
A	1	2	9,01	12,01	16	200,6	207,19
$\sigma_{fr} (10^{-24} \text{ cm}^2)$	20,51	3,40	6,18	4,73	3,75	26,53	11,01
$\rho (\text{g/cm}^3) (*)$	0,07	0,163	1,85	2,3	1,13	13,55	11,3
$\Sigma_{fr} = N * \sigma_{fr} (\text{cm}^{-1})$	0,86	0,17	0,76	0,55	0,16	1,08	0,36
ξ	1,000	0,725	0,206	0,158	0,120	0,010	0,010
$x (2\text{MeV} \rightarrow 1\text{eV})$	14,5	20,0	70,3	92,0	121,0	1460,1	1507,9

- Similar physical procedure to moderation of neutrons, i.e. reflection occurs by collisions with moderator atoms
- Requirements:
 - Large scattering density
 - Large-angle scattering: larger mass than that of a neutron
 - Large energy loss to shorten the slowing-down time: not too larger mass

	$\rho(\text{gcm}^{-3})$	Mol mass	$\sigma_s(10^{-28}\text{m}^2)$	$N\sigma_s(\text{cm}^{-1})$	ξ
H2O	1.0	18.01	44.4	1.485	0.925
polyethylene	0.918	14.01	45.3	1.765	0.913
D2O	1.1	20.03	10.5	0.347	0.505
Be	1.85	9.013	6.1	0.754	0.206
Graphite	1.6	12.01	4.7	0.377	0.158
Fe	7.86	55.847	11.5	0.930	0.035

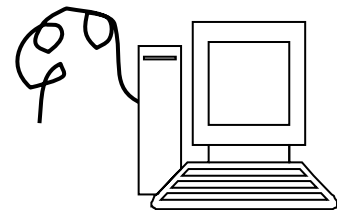
scattering function $\ddot{O}$

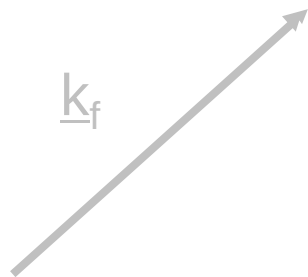
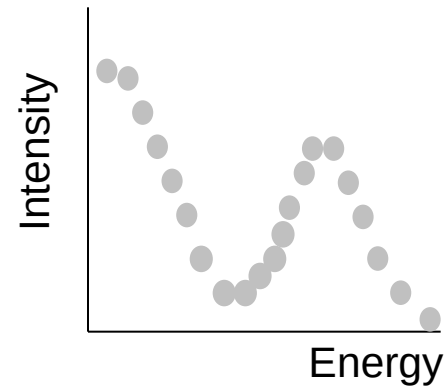
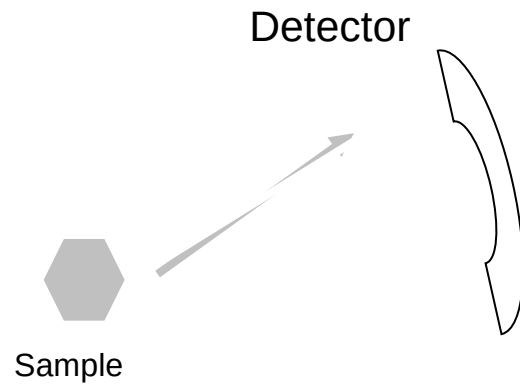
$$\frac{d^2\sigma}{d\Omega dE} \propto S(Q, E)$$

$$S(Q, E) = \frac{1}{N} \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} \sum_{ii'}^{i \neq i'} \left\langle e^{-iQ \cdot R_i(0)} e^{iQ \cdot R_{i'}(t)} \right\rangle e^{-iEt/\hbar} dt$$

$$I(Q, E) = \iint R(Q - Q', E - E') S(Q', E') dQ' dE'$$

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$$= \underline{k}_f -$$

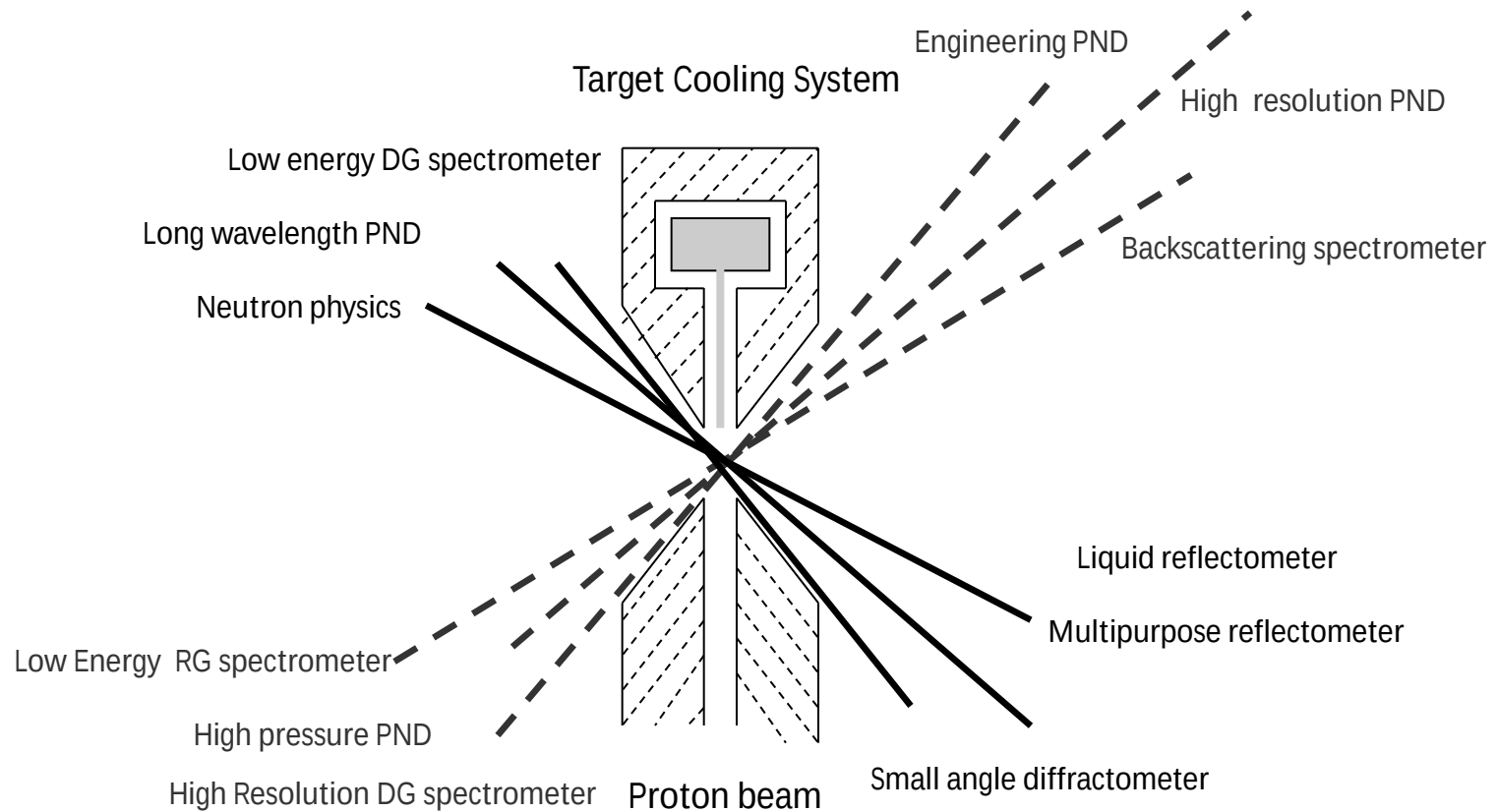
Wavevector transfer

$$\hbar\omega = \underline{E}_f -$$

Energy transfer

“Inelastic” scattering , ω

Parameters	Phase I	Phase II	PHASEIII		



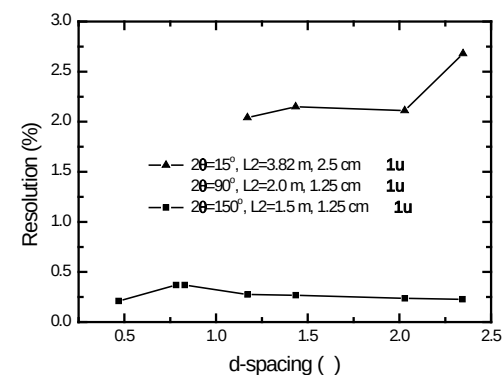
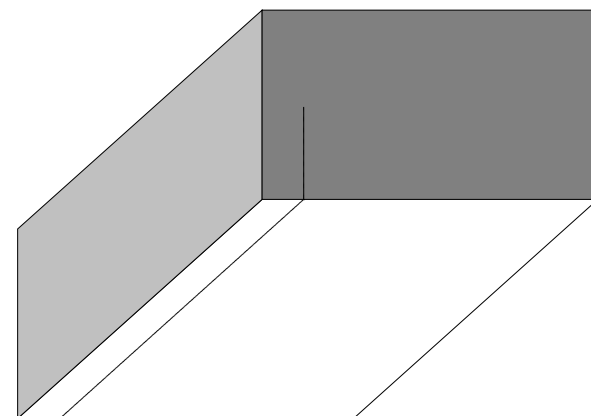
(PND: Powder Neutron Diffractometer; RG/DG: Reversal/Direct Geometry)

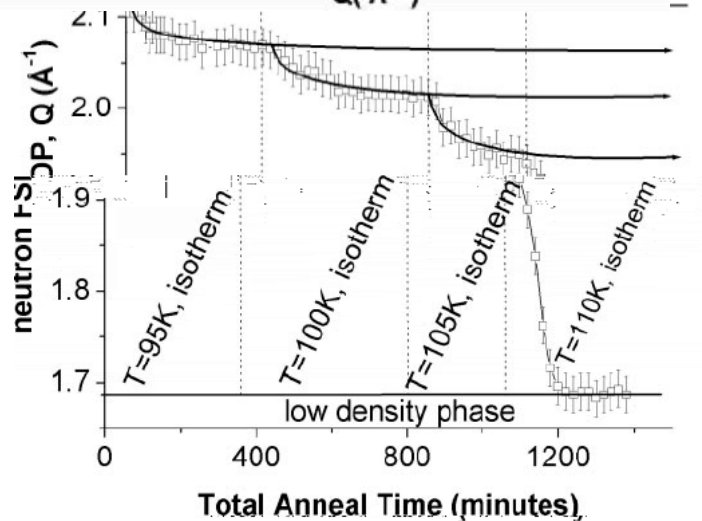
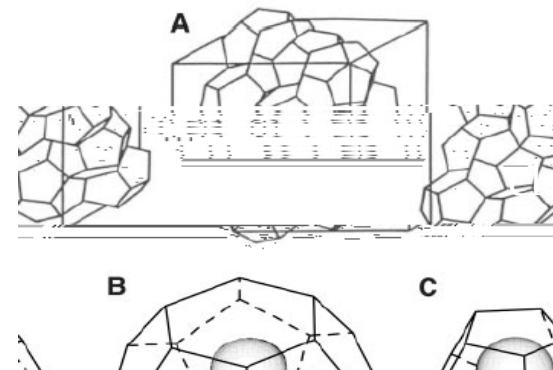
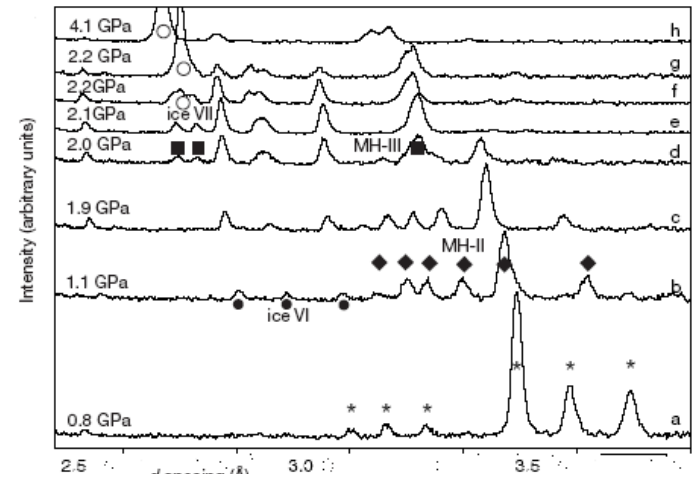
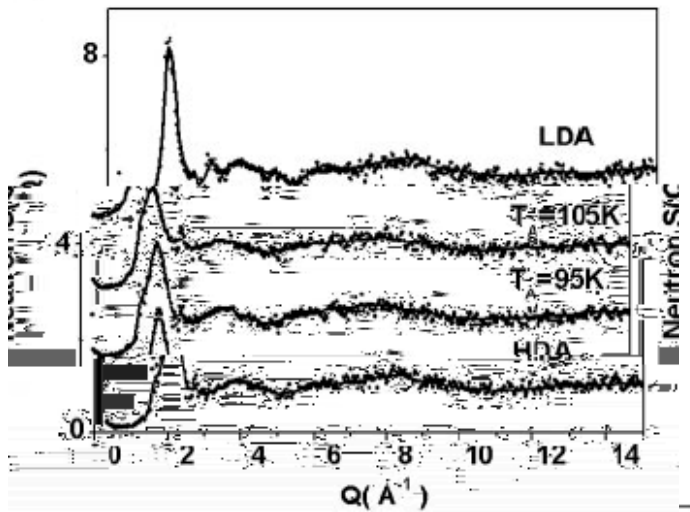
Moderator $\ddot{O}$

— — — D+P, LH2
(20K Å)

———— C, LH2
(20K)

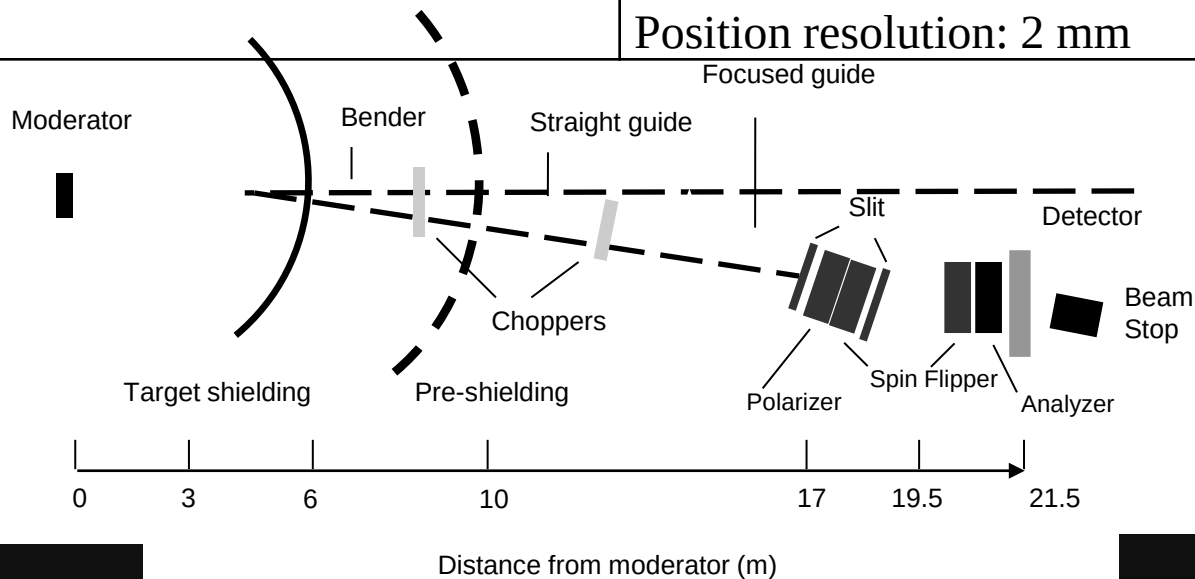
Moderator		decoupled water moderator $\text{\AA}300 \text{ K } \text{\AA}$
Bandwidth($\Delta\lambda$)		4.5 $\text{\AA}$
Max. Beam Size		40(h) $\times$ 20(w) mm
Flux at sample position		$\sim 10^7 \text{ n/cm}^2/\text{s}$
Best Resolution($\Delta d/d$)		0.2 % at $2\theta = 150^\circ$
Guide		Taper focus, m=3
Source to sample distance L1		30 m
Sample- detector distance L_2	$2\theta = 150^\circ$	1.5 m
	$2\theta = 90^\circ$	2.0 m
	$2\theta = 15^\circ$	3.8 m

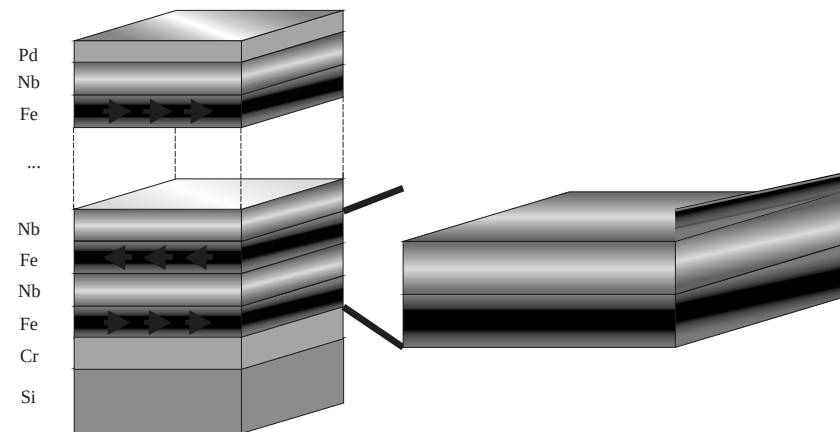




J. S. Loveday et al., Nature 410, 661 (2001);
W. L. Mao et al., Science 297, 1320 (2002)

Moderator	Coupled liquid H ₂ (20 K)
Bandwidth $\Delta\lambda$ Å	6 Å
Guide	Bender+Sraight+Taper $40 \times 60 \rightarrow 20 \times 30 \text{ mm}^2$
Source to sample distance L1	19.5 m
Sample to detector distance L2	2 m
Sample table	6-axis movements
Polarizer/analyzer	Supermirror type
Detector	2D position-sensitive detector Position resolution: 2 mm





Exchange coupling energy
 $J \sim \sin(2 k_F t_{Nb})$

Moderator	Coupled hydrogen $\lambda 20\text{K } \text{\AA}$
Moderator to sample distance	14 m
Sample to detector distance	5 m
Detector	
Effective area	$50 \times 50 \text{ cm}^2$
Resolution	1 cm (FWHM)
Distance to sample	1~5 m
Working wavelength range	0.4-8 $\text{\AA}$
q range	0.004-3.4 $\text{\AA}^{-1}$

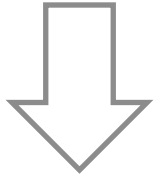


SANS diffraction patterns of the vortex lattice in $\text{La}_{1.83}\text{Sr}_{0.17}\text{CuO}_4$. As the applied field is increased, the vortex lattice changes from hexagonal (left) to square (right) coordination

- Five CSNS User Meetings/Workshops on Application of Spallation Neutron Source have been held since 2004
 - User Committee has been set up
 - discuss and review the design of 3 instruments for CSNS phase- 1 project
 - a better understanding of special needs from the potential users
- CSNS started to support some users for training at foreign neutron sources in 2005.
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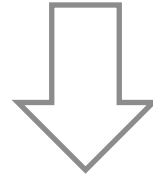
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- D: Democracy
- S: Science



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- D: Dynamics
- S: Structure



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