

中子散射与散裂中子源

Neutron Scattering & Spallation Neutron Source

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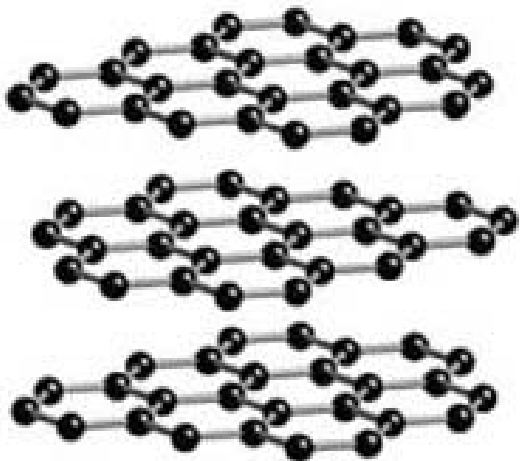


(CSNS靶站谱仪中心, 中科院物理研究所)

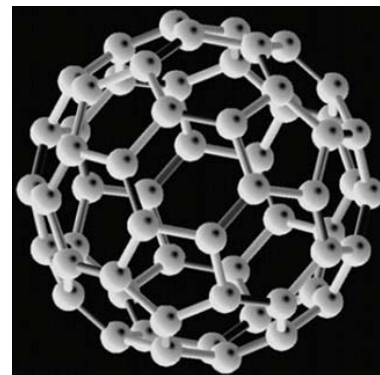
outline

- **Relationship between structure and property**
(物质结构与物性)
- **Why neutrons: neutron characteristics and neutron scattering**
(为什么需要中子：中子特点与中子散射)
- **Coupling between lattice, orbital and spin in manganites studied by neutron scattering**
(锰氧化物中晶格、轨道和自旋相互作用的中子散射研究)
- **Target Station of spallation neutron sources**
(散裂中子源)

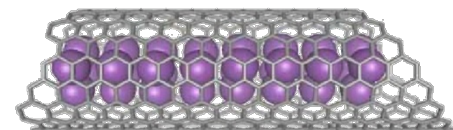
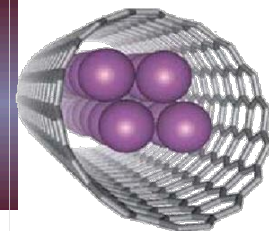
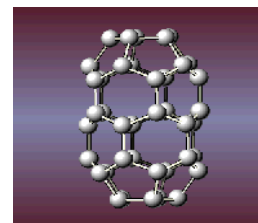
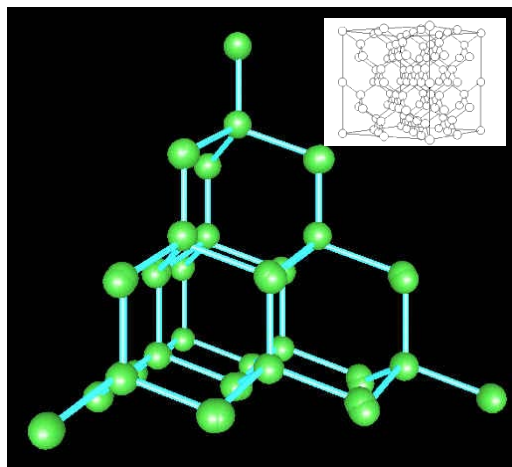
物质结构决定物质性质



玻璃刀头上镶的金刚石用来裁玻璃

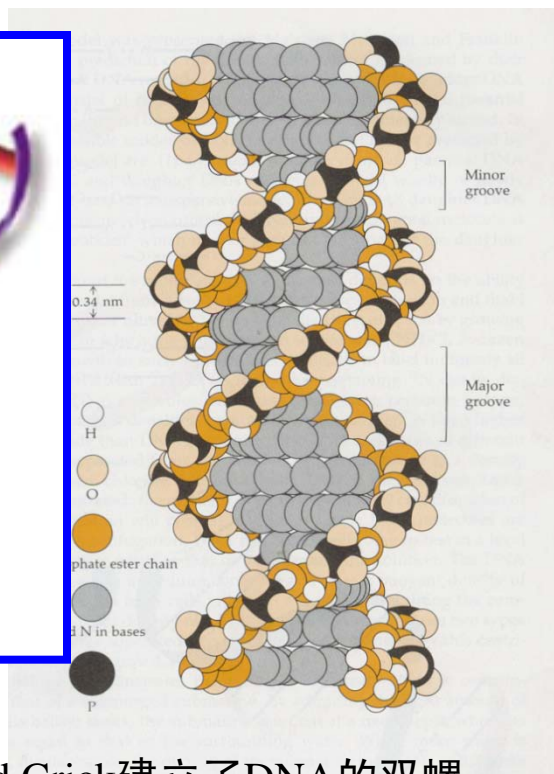


石墨可用于制铅笔芯



物质结构决定物质性质

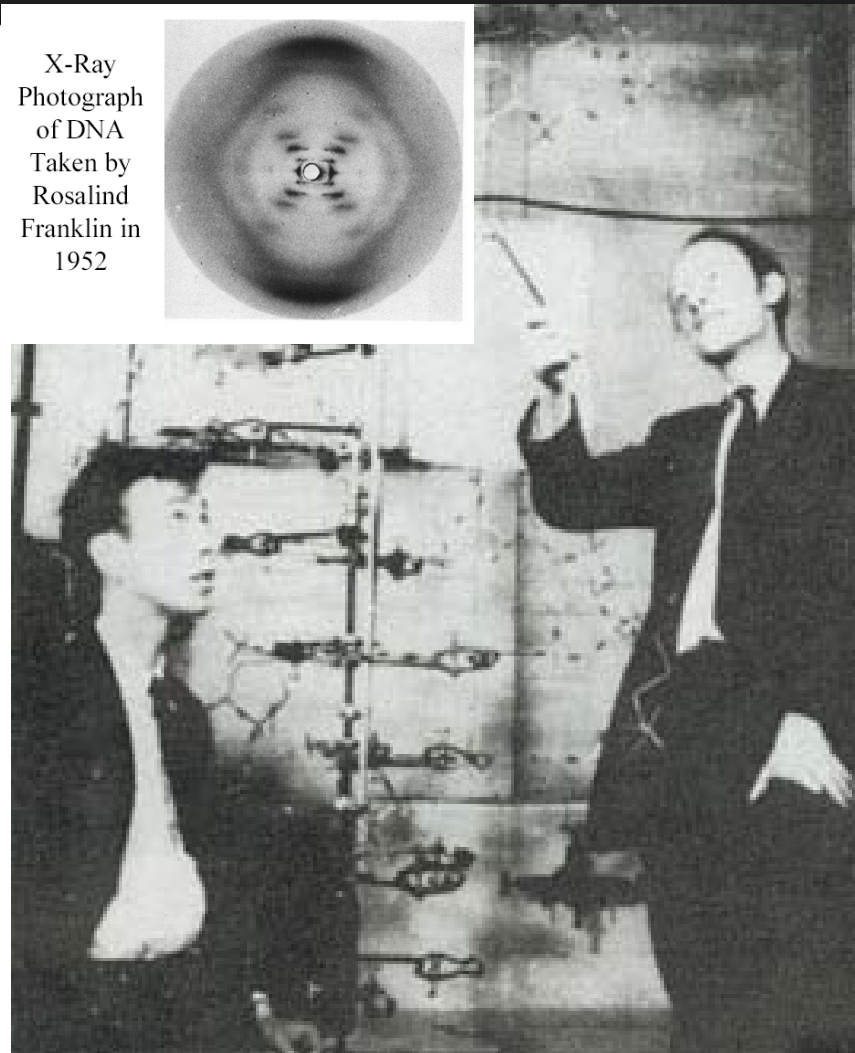
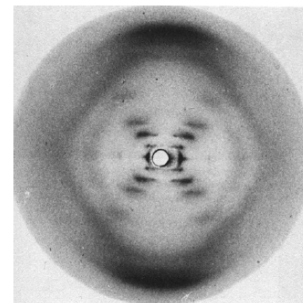
- DNA双螺旋结构：分子生物学



1953年Watson and Crick建立了DNA的双螺旋模型结构，并于1958年提出了中心法则。

获1962年度诺贝尔奖

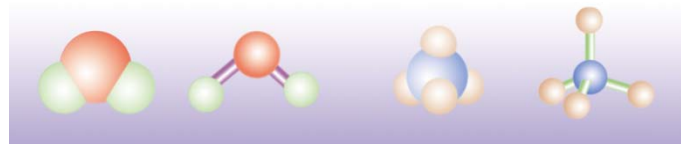
X-Ray
Photograph
of DNA
Taken by
Rosalind
Franklin in
1952



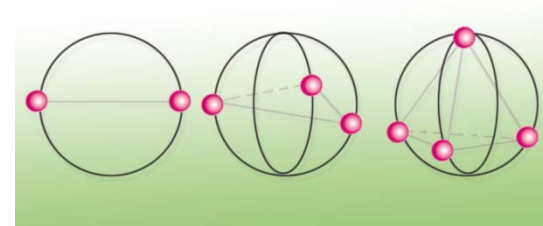
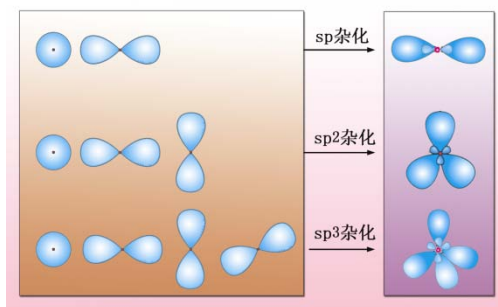
James Watson and Francis Crick

物质结构决定物质性质

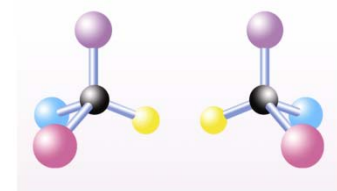
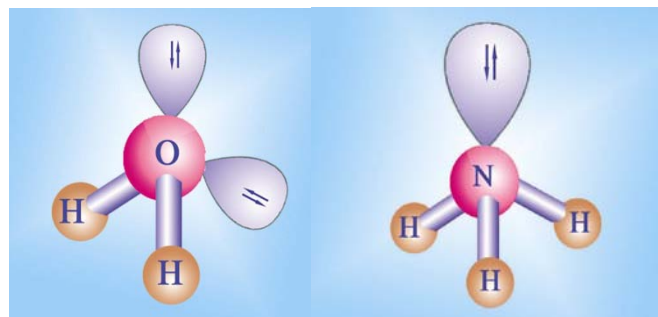
结构模型



认识相互作用



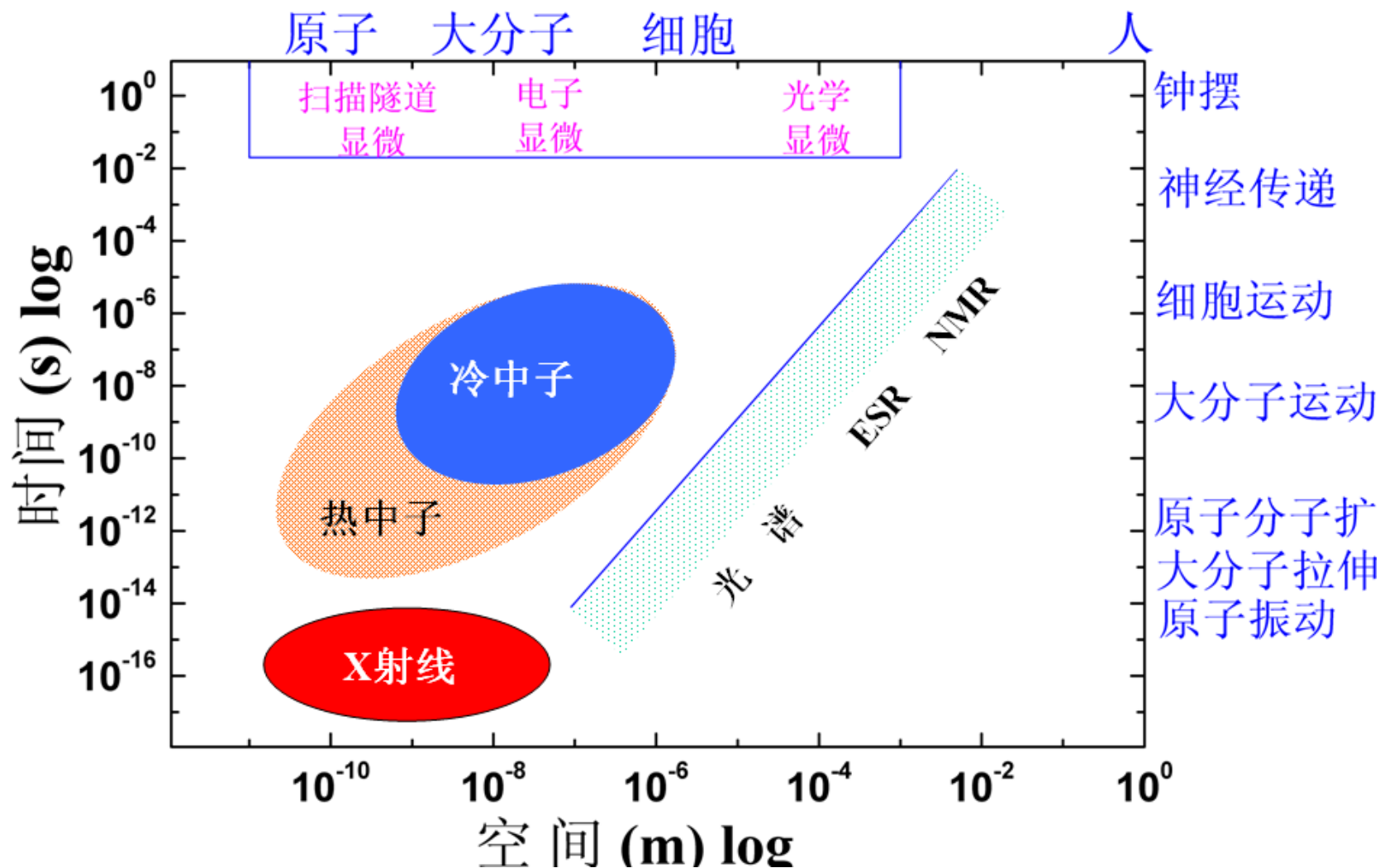
晶体和分子构型



说明物质性质

磁、电、光、热等基本物性

中子散射在各种微观结构研究手段中的地位



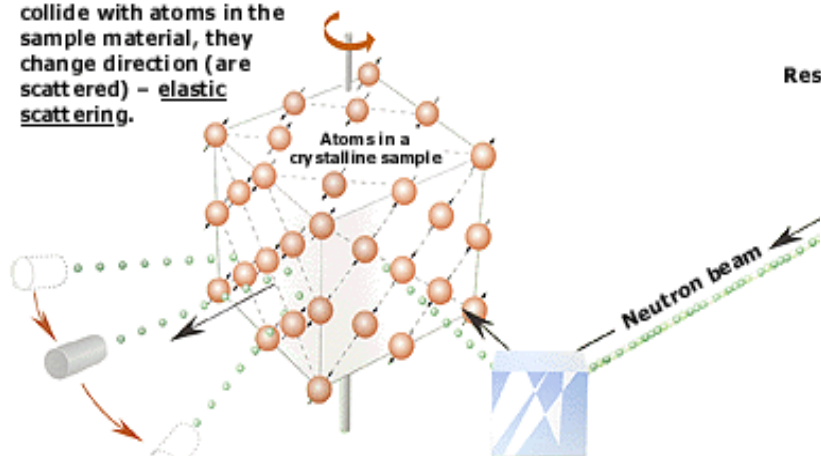
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(散裂中子源)

中子散射是探测物质结构的重要手段

中子散射可探测原子、分子和原子分子团簇的位置...

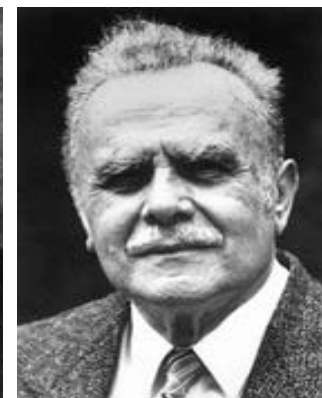
When the neutrons collide with atoms in the sample material, they change direction (are scattered) - elastic scattering.



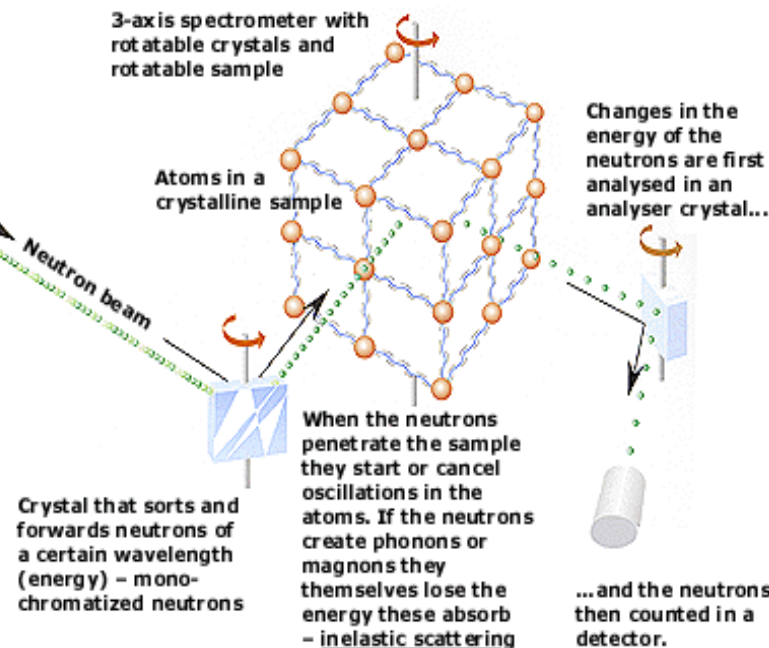
Detectors record the directions of the neutrons and a diffraction pattern is obtained.

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

Research reactor



3-axis spectrometer with rotatable crystals and rotatable sample



Atoms in a crystalline sample

Changes in the energy of the neutrons are first analysed in an analyser crystal...

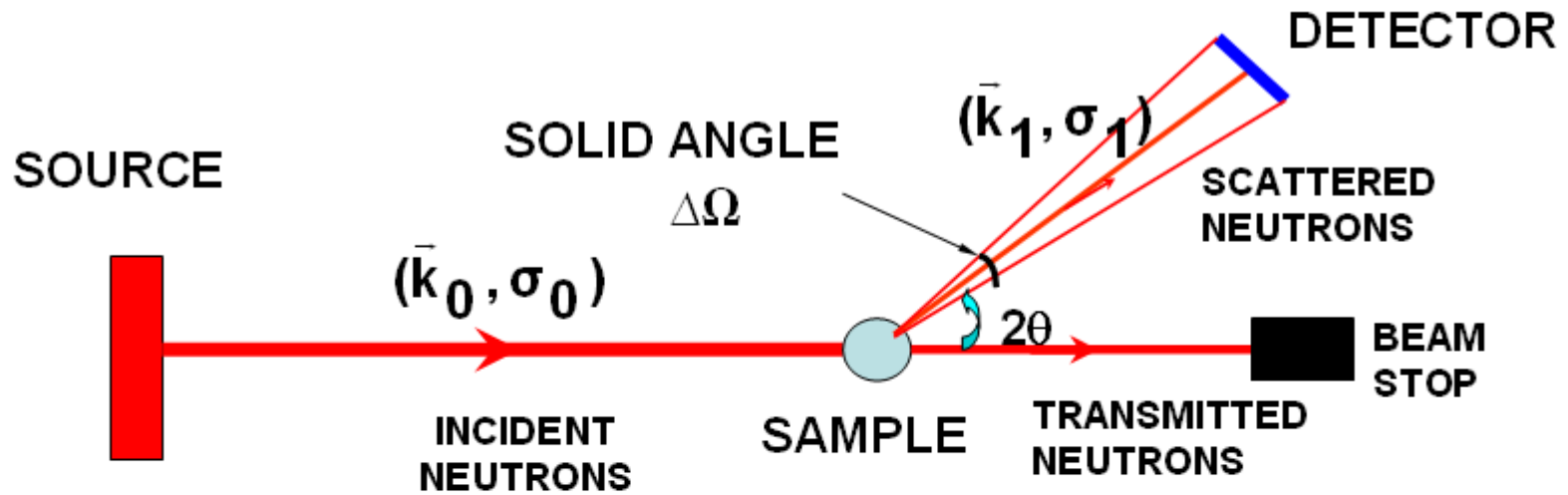
Crystal that sorts and forwards neutrons of a certain wavelength (energy) - monochromatized neutrons

When the neutrons penetrate the sample they start or cancel oscillations in the atoms. If the neutrons create phonons or magnons they themselves lose the energy these absorb - inelastic scattering

... and the neutrons then counted in a detector.

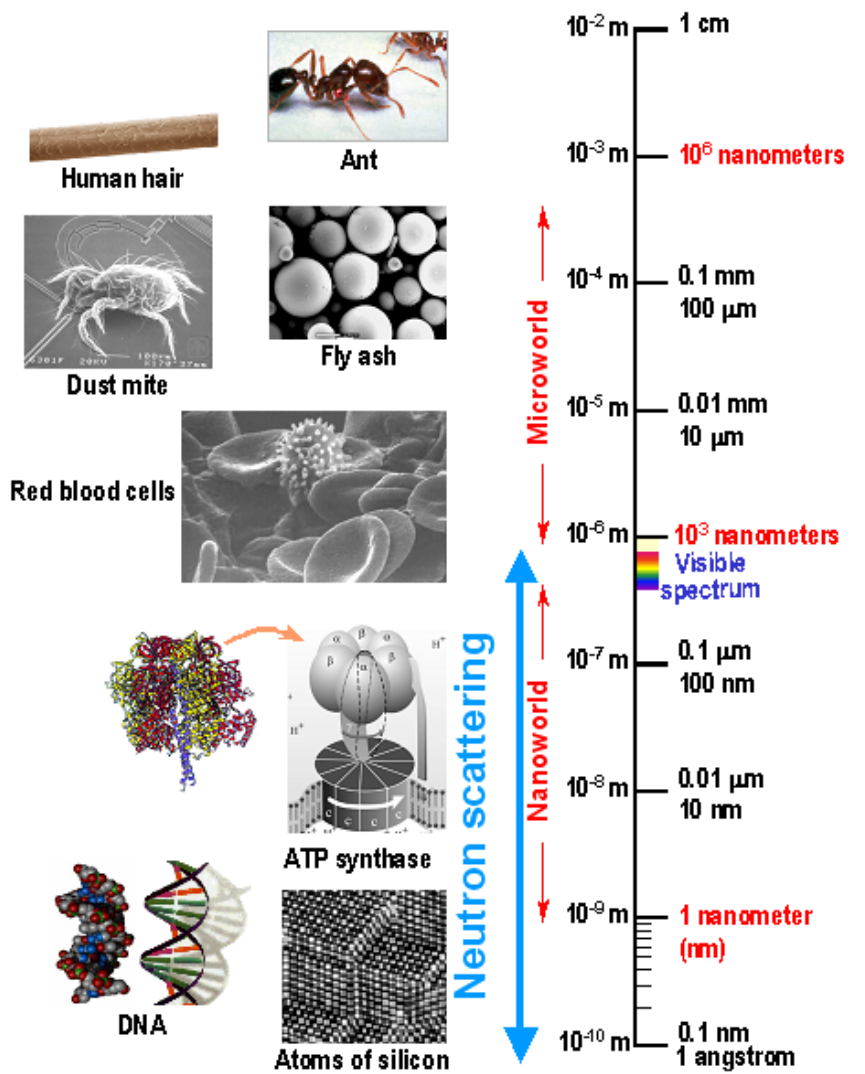
... 以及它们是如何运动的

中子散射基本概念



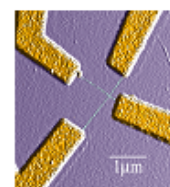
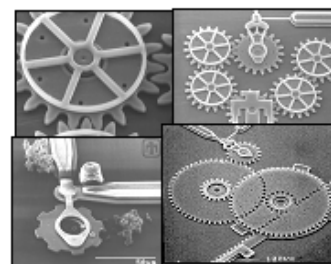
$$C = \eta \Phi N \left(\frac{d^2 \sigma}{d\Omega dE} \right) \Delta\Omega \Delta E$$

中子特性—波长覆盖宽的微观尺度

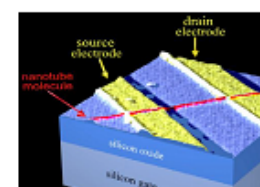


Head of a pin

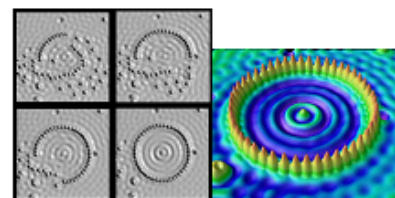
Microelectromechanical Devices



Nanotube electrode



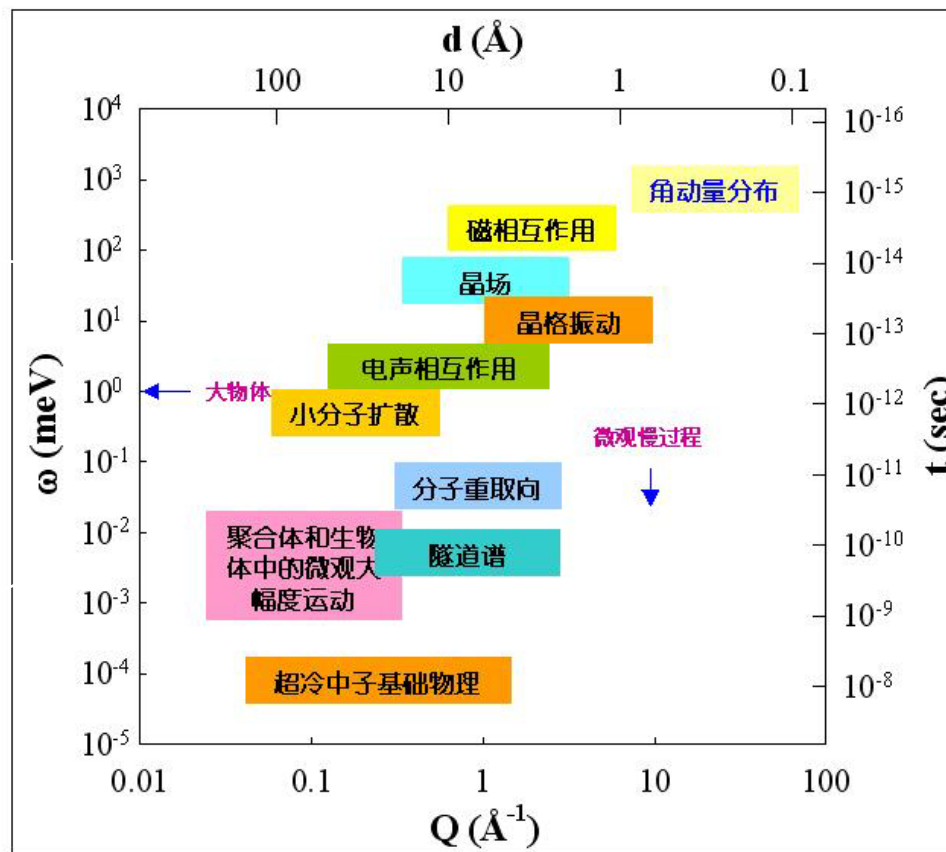
Nanotube transistor



Quantum corral of 48 iron atoms

中子特性—适合的能量范围

波长 (nm)	X射线 (eV)	中子 (meV)
0.1	12400	82
1	1240	0.82
10	124	0.0082



热中子能量与物质中许多动态过程的激发能量相当

中子特性—电中性

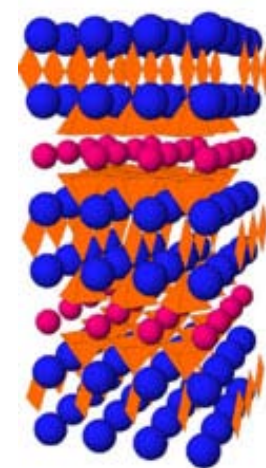
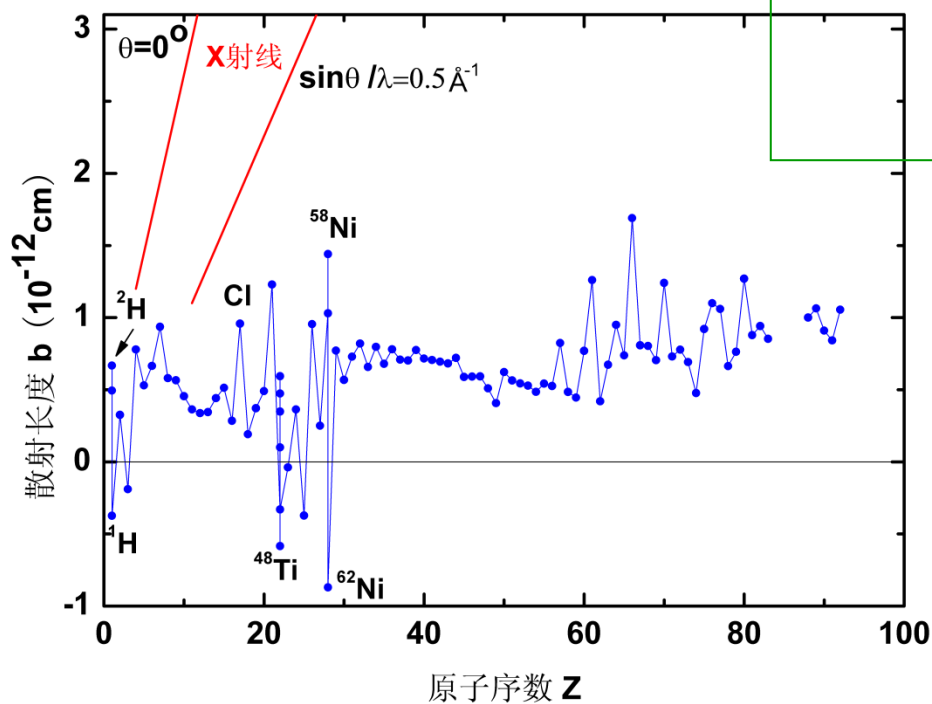
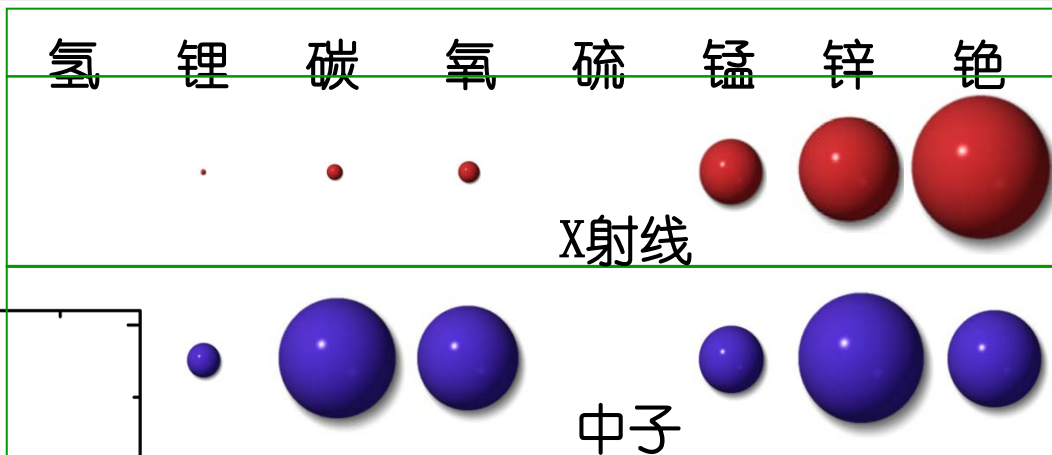
 Charge = 0

与物质相互作用时，中子几乎不受原子核外电子的影响，被散射的可能性主要取决于原子核的性质。这些带来四个优势：

- 中子对轻元素敏感，并可区分同位素。
- 中子的穿透能力较强。研究的是体效应，更容易接近研究对象本质；易于开展极端条件下物质结构和动态的研究。
- 中子散射结果可在量子力学一级微扰的框架内得到合理的解释，便于与分子（晶格）动力学的数值模拟比较。
- 中子对物质的破坏很小，更有利于研究生物活性体系。

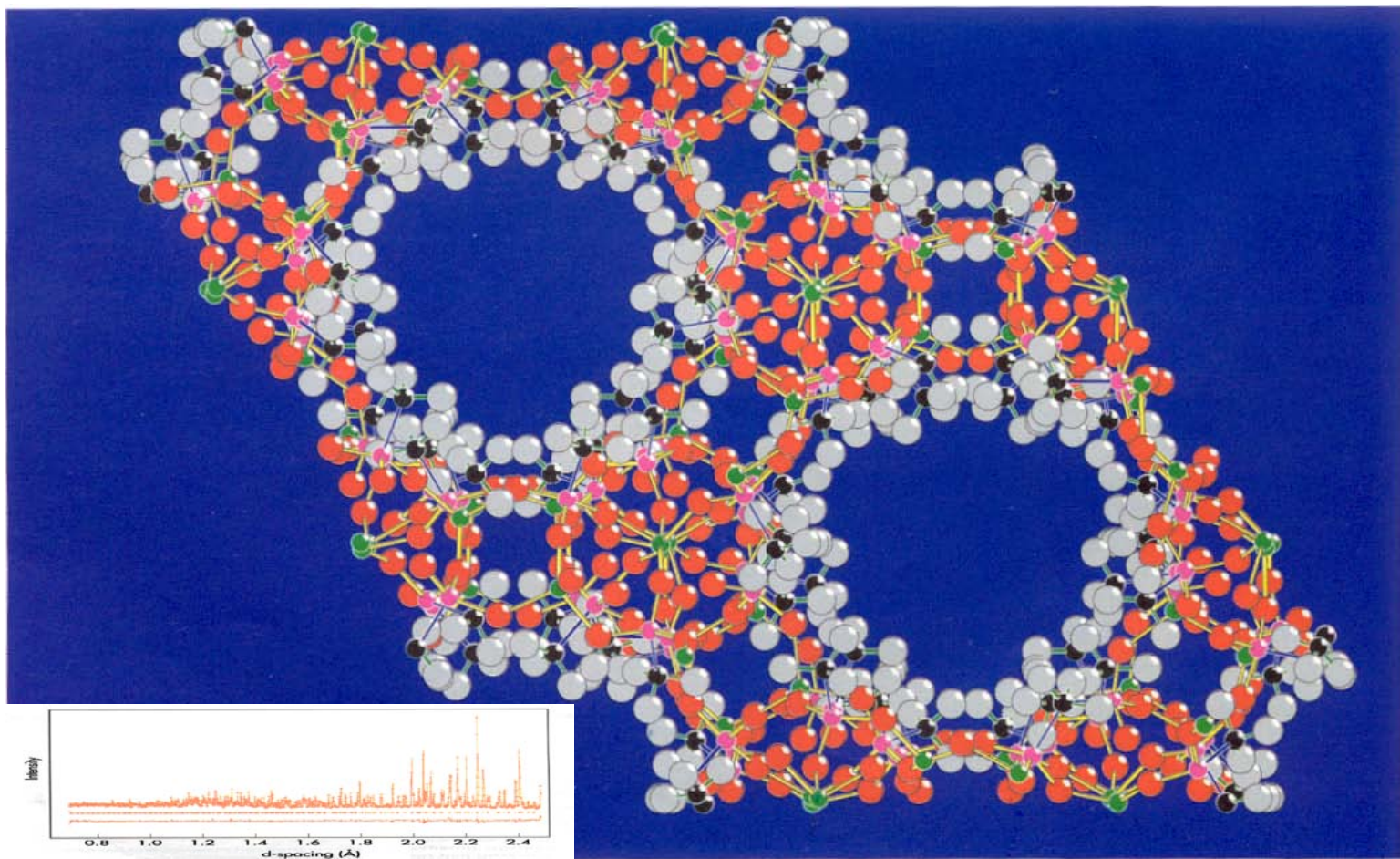
相对于X射线或同步辐射，中子源能提供的中子通量相对较低，局限了中子散射的研究范畴，通常研究能获得**较大样品量**的材料体系。

中子探针特性—对较轻的原子灵敏



高温超导体中氧的位置和占有率

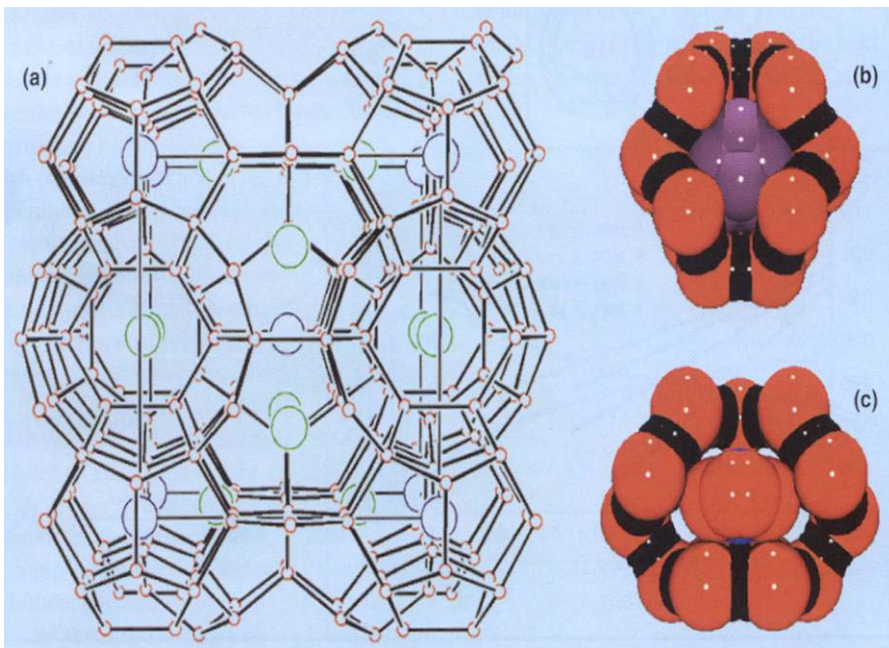
中子与同步辐射在物质结构研究上互补



$\text{Al}_2(\text{PO}_3\text{CH}_3)_3$ (甲基沸石) 的结构

红, 白色部分分别是X射线, 中子散射的结构分析结果

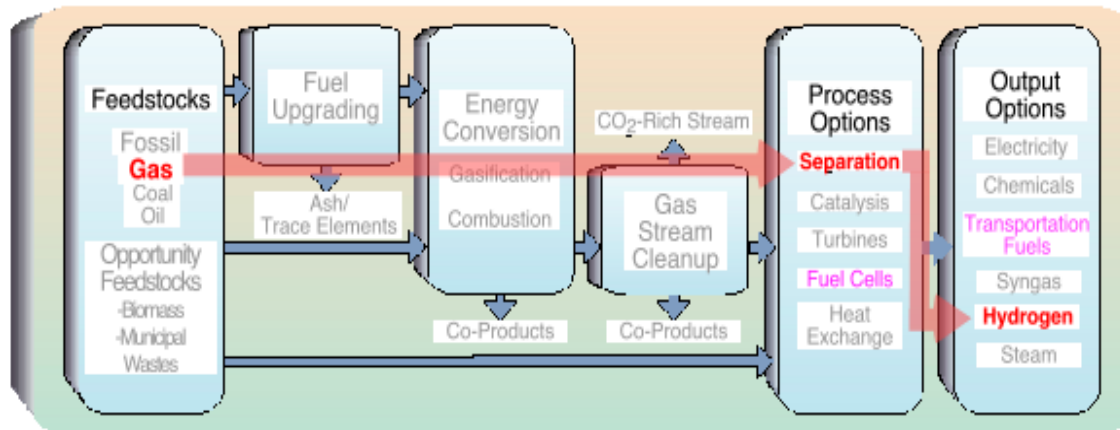
中子对轻元素敏感：可燃冰研究



- 美国科学家估计，储存于墨西哥湾海底的可燃冰可供美国使用**2000**年
- 预计全世界海底的可燃冰可供全人类使用**3000**年
- 高压、低温下中子散射实验可研究可燃冰性能及形成机制

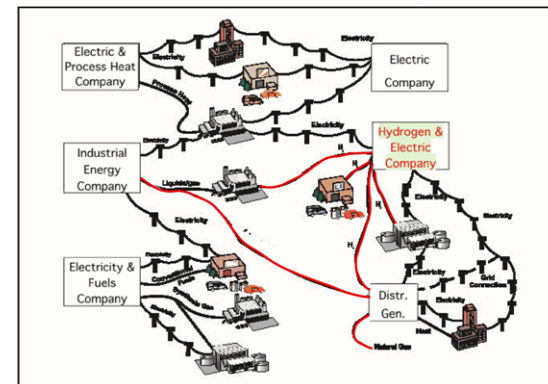
深海可燃冰的中子散射研究
(海底能源－水合天然气)

中子对轻元素敏感：氢能源

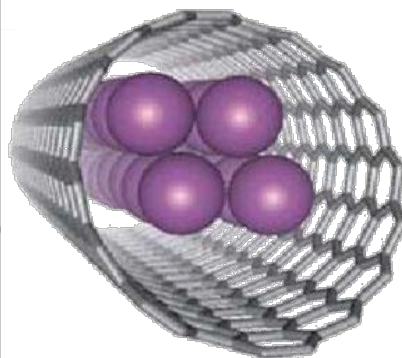
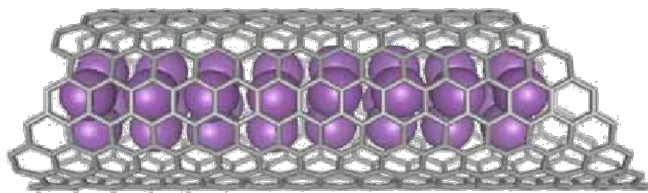


Roadmap: R&D Today -----> Realization ~2010

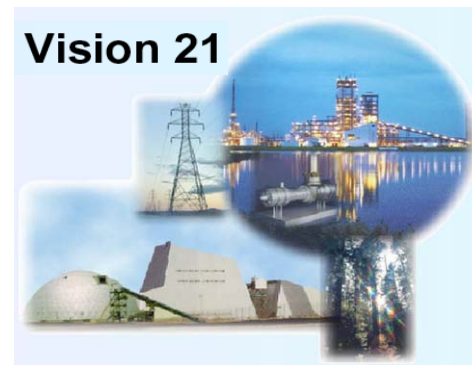
路线图：今天的研发，明天的应用（~2010）



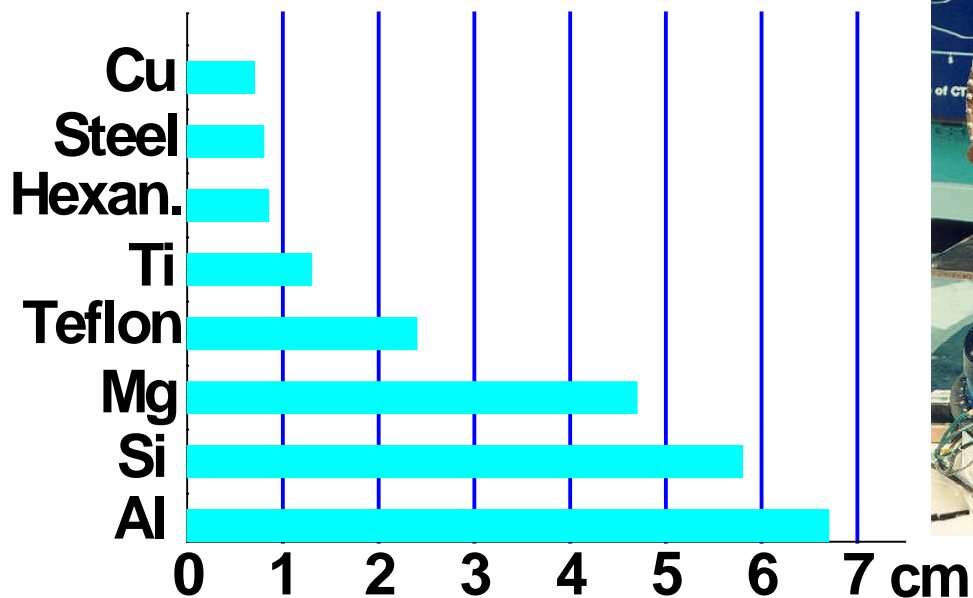
- 美国能源部的21世纪新能源方案
- 石油经济向氢经济过渡
- 相应的科技开发和储备工作
- 需要散裂源这样的大科学平台



储氢纳米管的中子散射研究



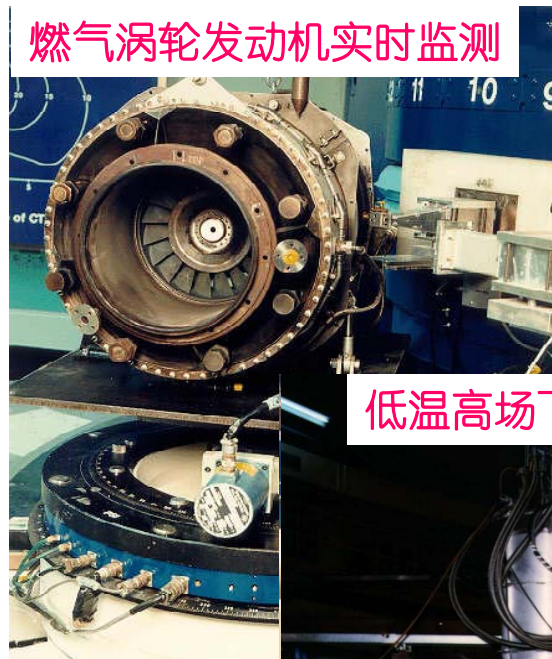
中子探针特性—强穿透能力



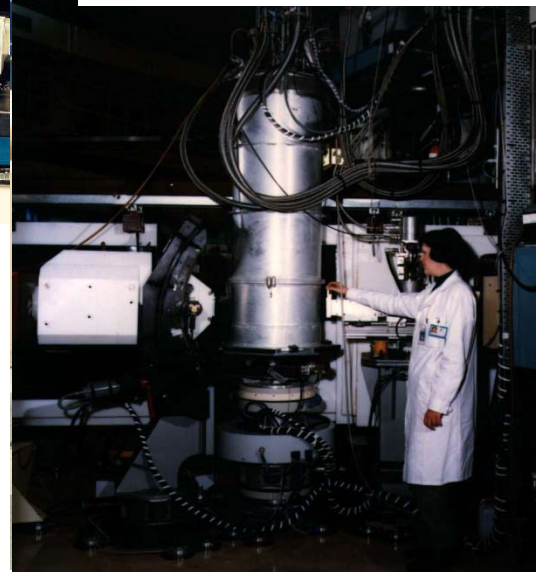
热中子在不同材料中的穿透深度

穿透能力强，可以对较大的部件进行非破坏性测量，利于加载高温高压及强场等极端条件设备。

燃气涡轮发动机实时监测



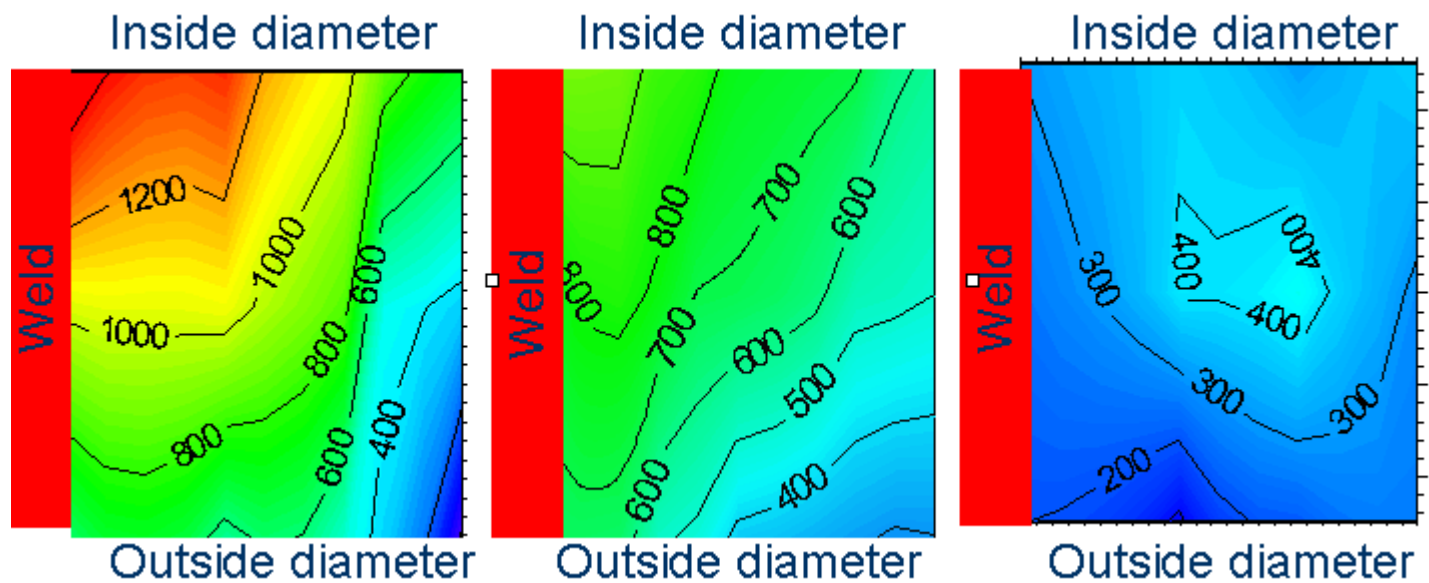
低温高场下的中子散射



中子探针特性—强穿透能力



飞机涡轮的叶片与轮盘的焊接应力测量

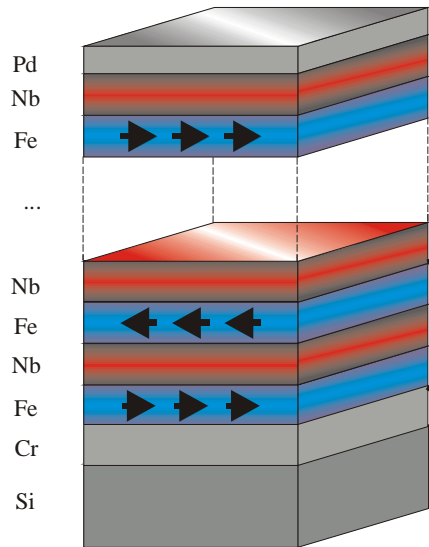
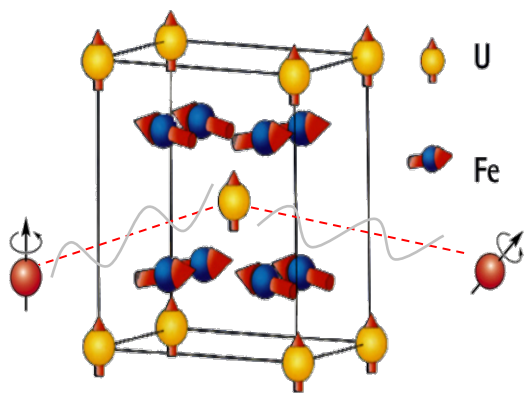


中子探针特性—具有磁矩

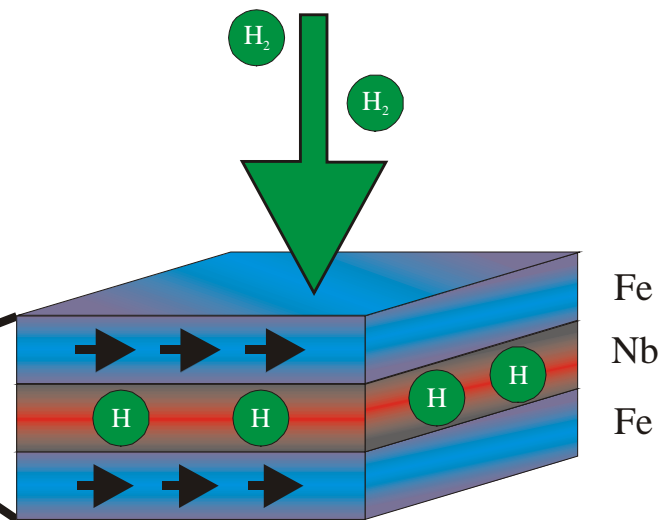


Spin = $\frac{1}{2}$

$\mu_n = -1.913 \mu_N$



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

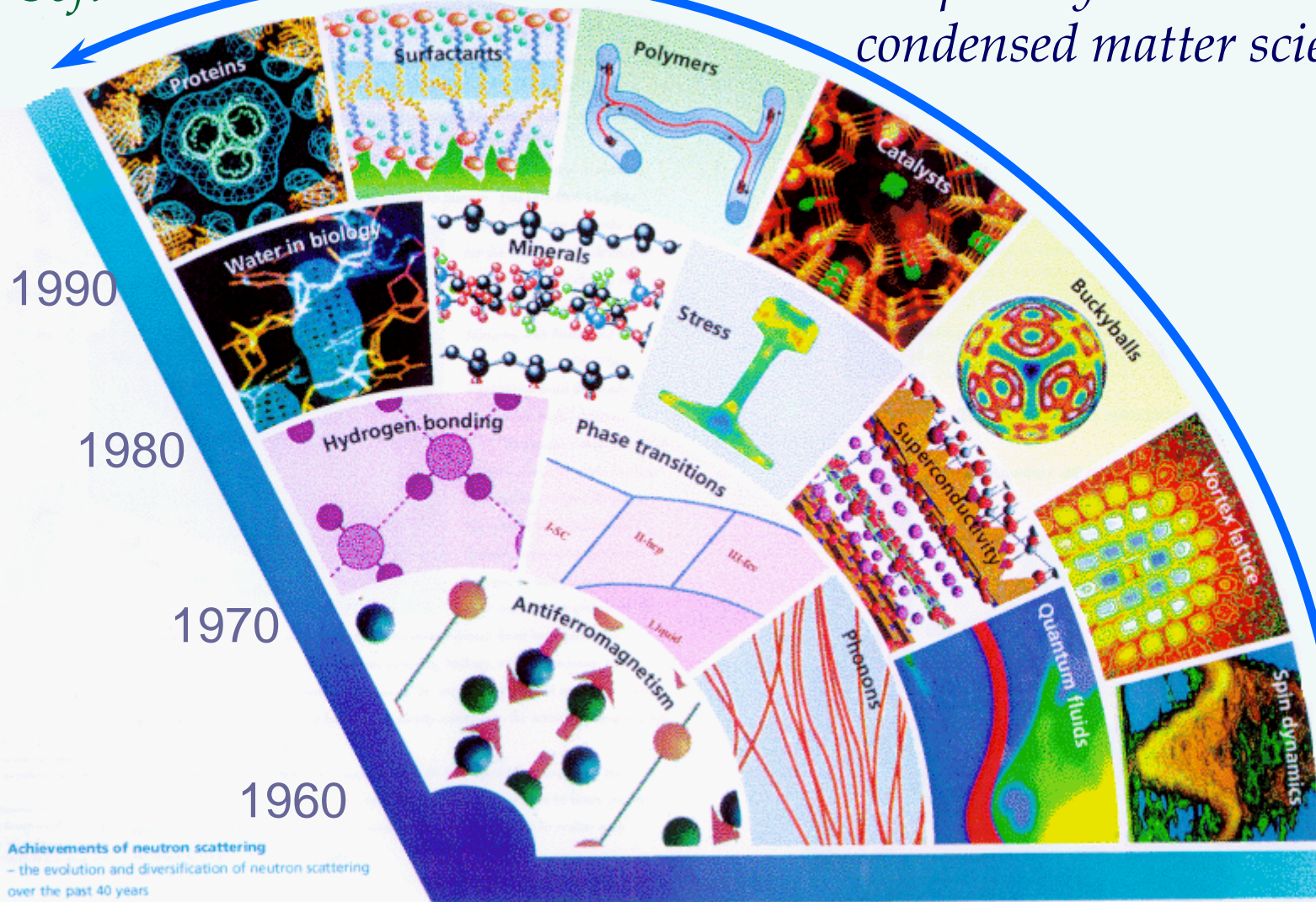


Modification of the exchange coupling via hydrogen absorption

中子是研究材料中磁结构和磁涨落的特有工具

Soft

*multidisciplinary
condensed matter science*



Hard

Achievements of neutron scattering
– the evolution and diversification of neutron scattering
over the past 40 years

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

Collaborators:

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A. Gukasov

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LPCES/Univ. Paris Sud, France:

M. Apostu

R. Suryanarayanan

A. Revcolevschi

IOP/CAS, China:

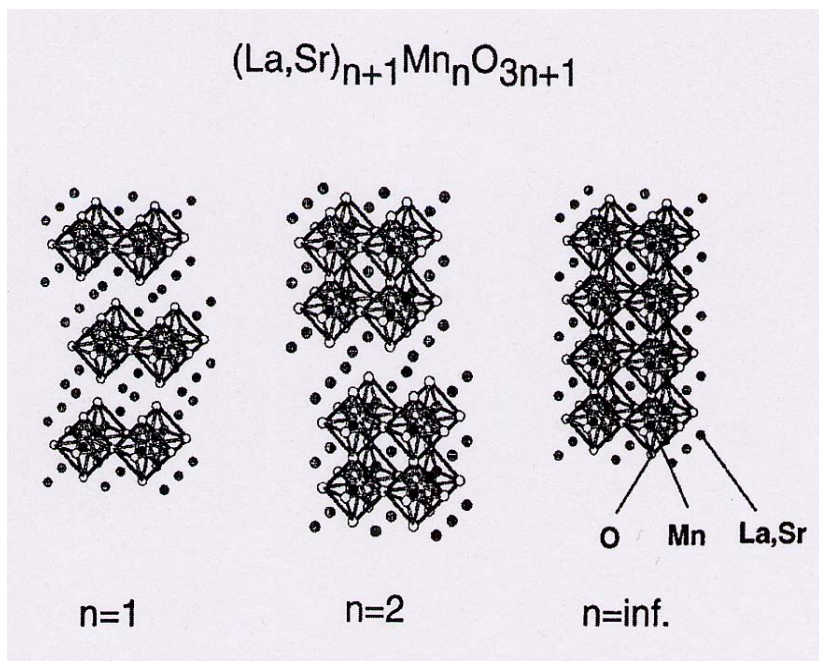
Lunhua He

Zhaohua Cheng

Outline

- **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

Ruddlesden-Poper-type Perovskite Manganites and CMR



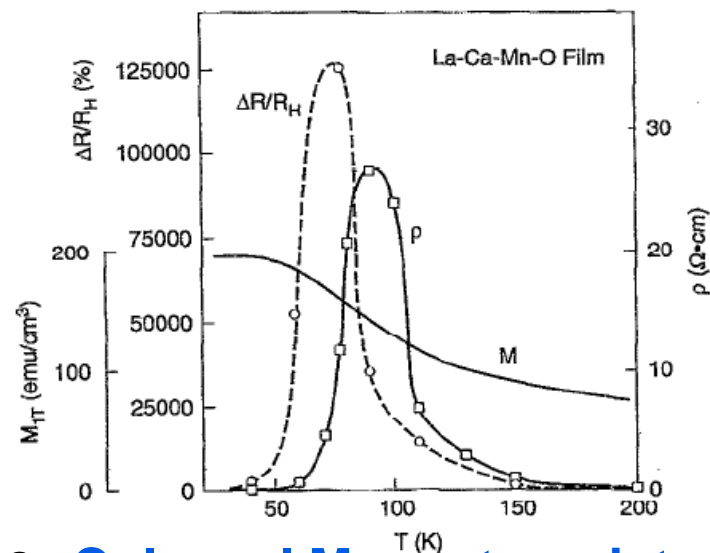
(From A. P. Ramirez, J. Phys.:Condens.Matter 39, (1997) 8171)

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

n=1: $(La,Sr)_2MnO_4$

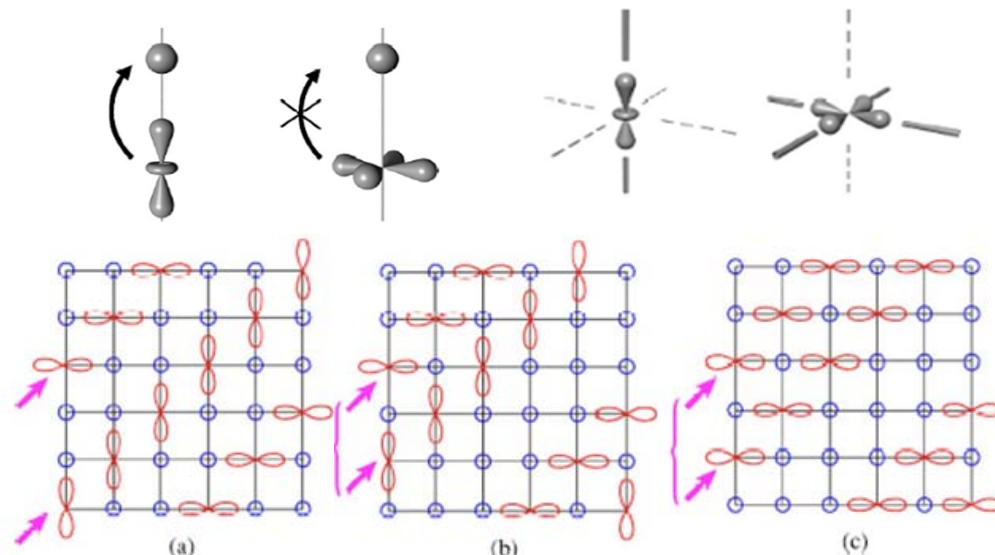
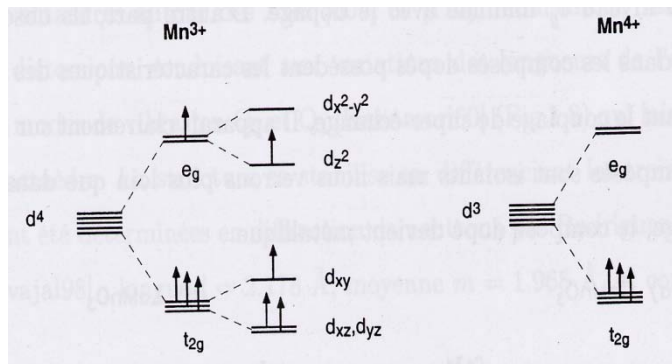
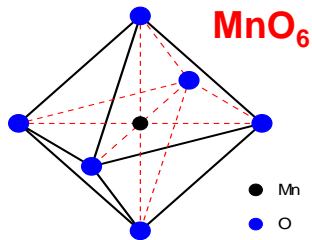
n=2: $(La,Sr)_3Mn_2O_7$

n=∞: $(La,Sr)MnO_3$



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

Interplay between the degrees of freedom

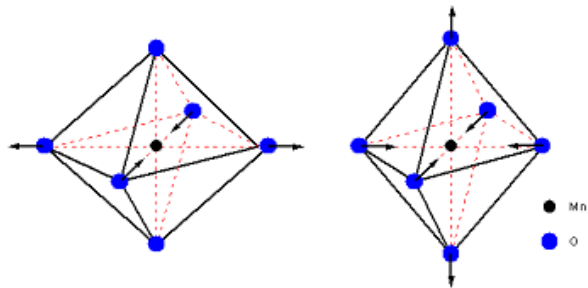


G. Khalillin and R. Kilan, Phys. Rev. B 61 3494 (2001)

D. Khomskii and K. Kugel, Phys. Rev. B 67 134401 (2003)

Q_2 mode

Q_3 mode

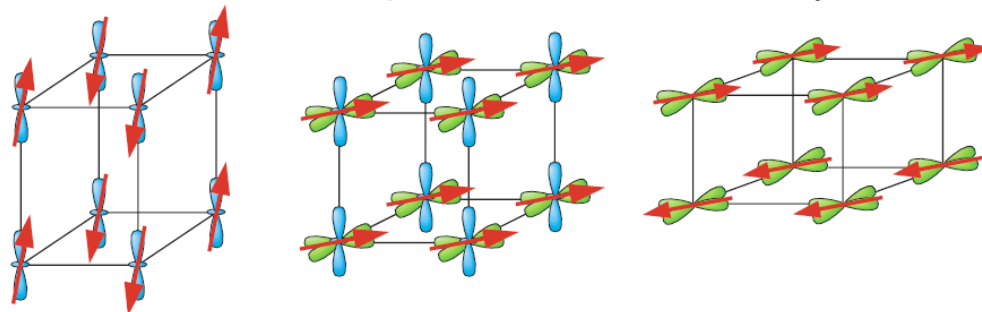


$$H_{JT} = -g(T_x Q_2 + T_z Q_3)$$

$3z^2-r^2$

x^2-y^2 & $3z^2-r^2$

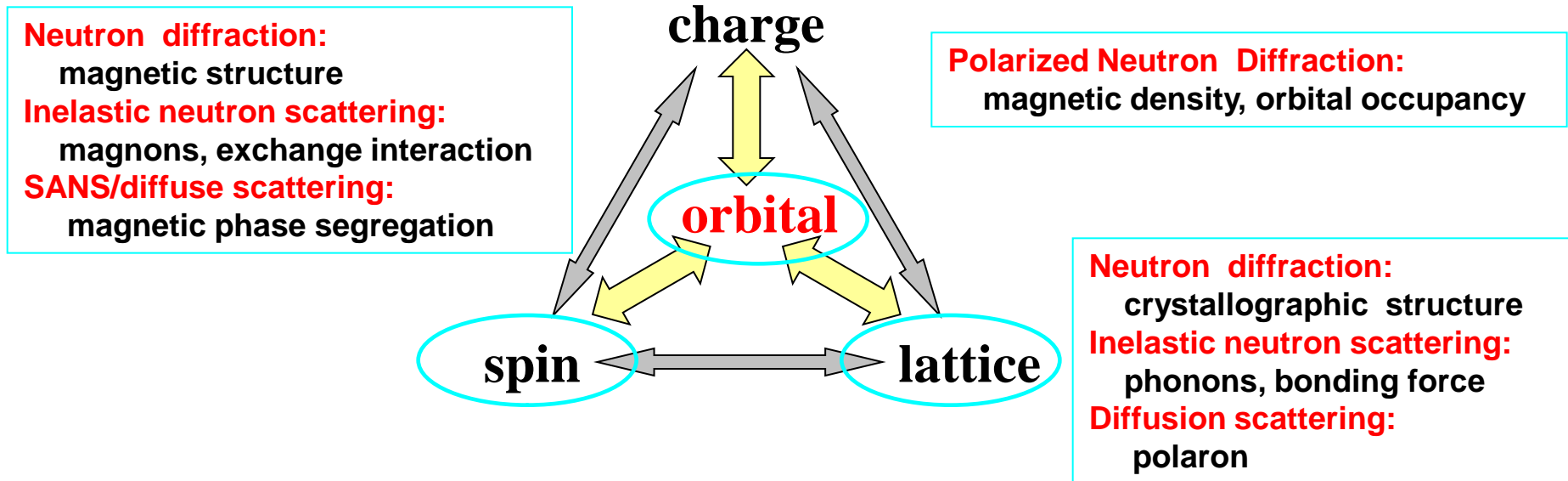
x^2-y^2



Tokura et al. Science 288, 462(2000)

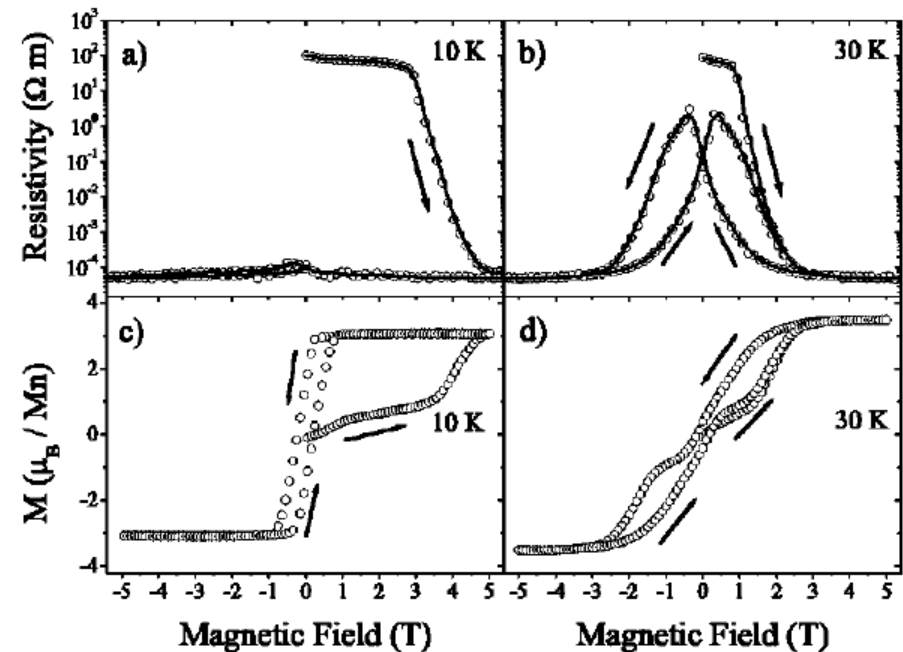
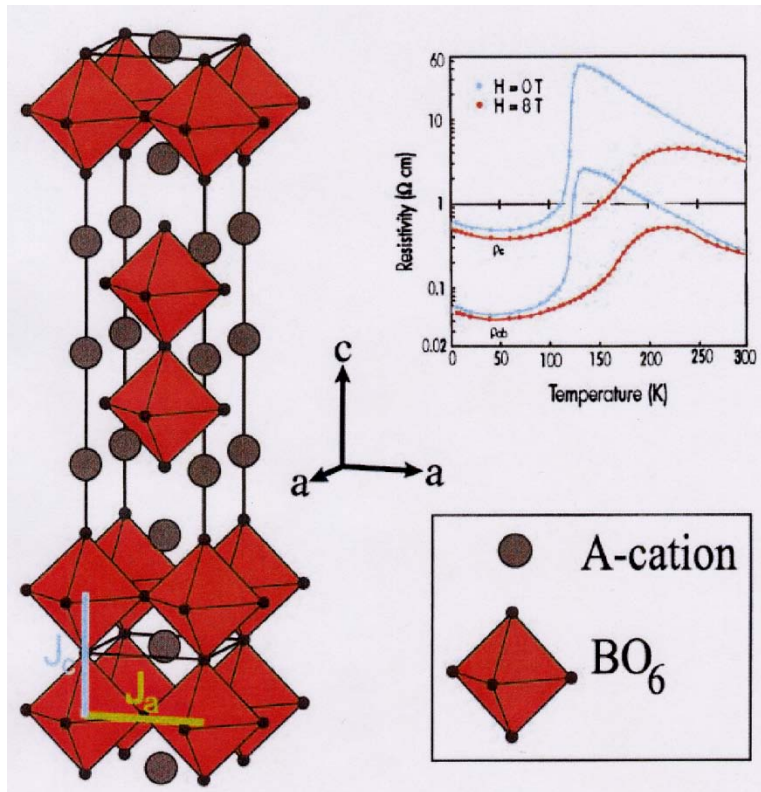
Neutron scattering for Interplay between the degrees of freedom

- **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.**



Bilayer RP manganites: typical system studied

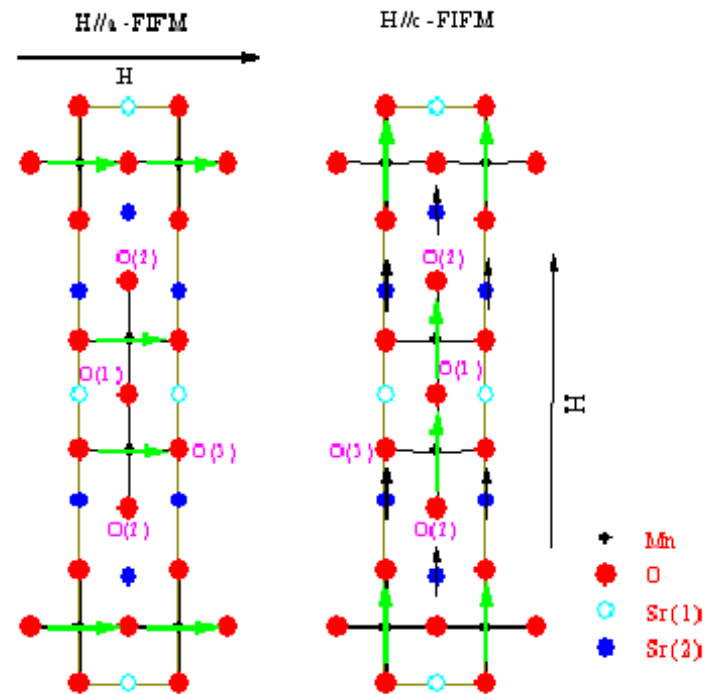
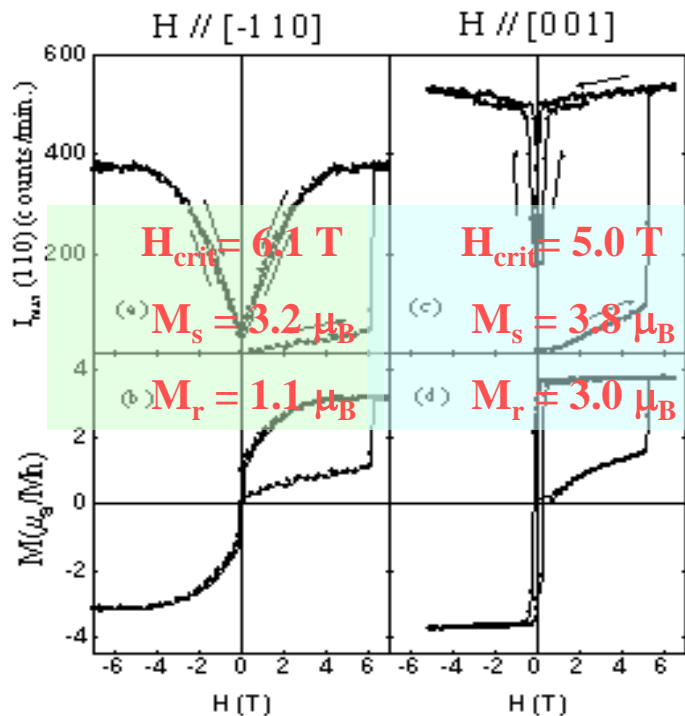
- 2D characteristics: strong anisotropy
- Similar physical phenomena: CMR, MIT, PS, CO, OO...
- Twin-free single crystal



Crystallographic and magnetic structures

Two different ferromagnetic states induced by the field applied in or perpendicular to the ab-plane:

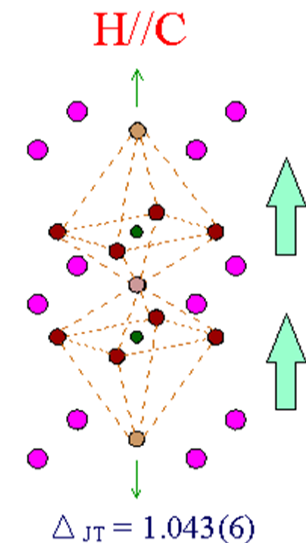
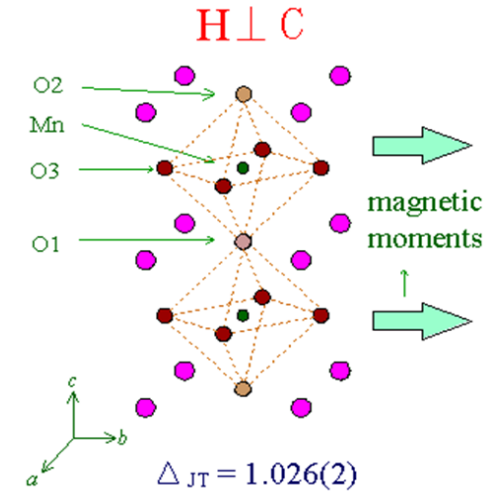
- Magnetic moments are aligned to the direction of the applied field.
- Different critical fields for the transition para- to ferromagnetism.
- Different saturation magnetization due to ordering of Pr moment.



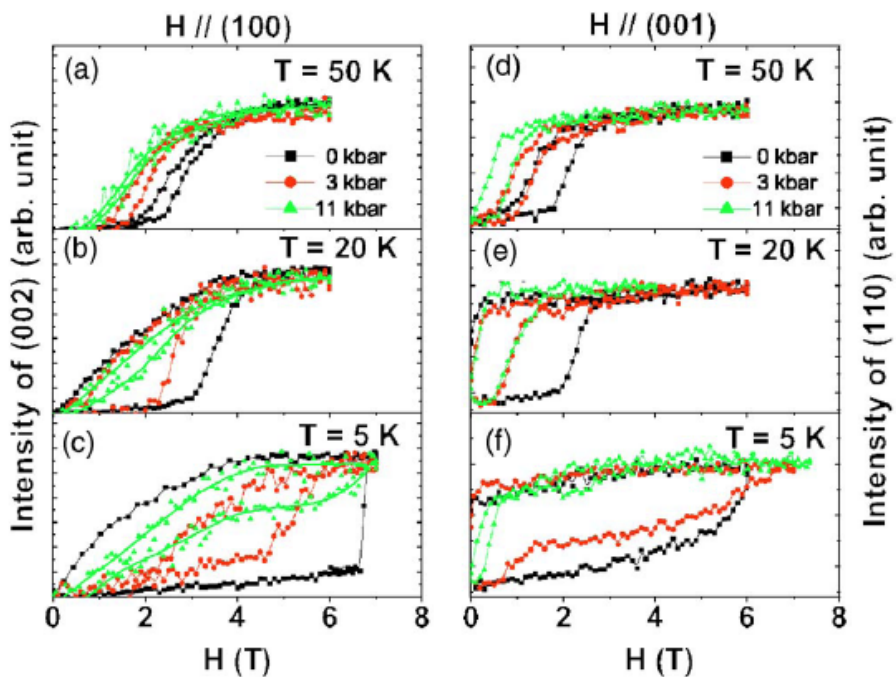
Interplay between spin and lattice

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)
$d_{Mn-O3}(\text{\AA})$			1.937(2)	1.937(2)
$\angle Mn-O3-Mn(^{\circ})$			178.9(3)	179.5(7)
Δ_{JT}			1.026(2)	1.043(6)

$$\Delta_{JT} = (d_{Mn-O1} + d_{Mn-O2}) / 2d_{Mn-O3} \quad \text{PM: } \Delta_{JT} = 1.028(3)$$



Interplay between spin and lattice: Pressure effect



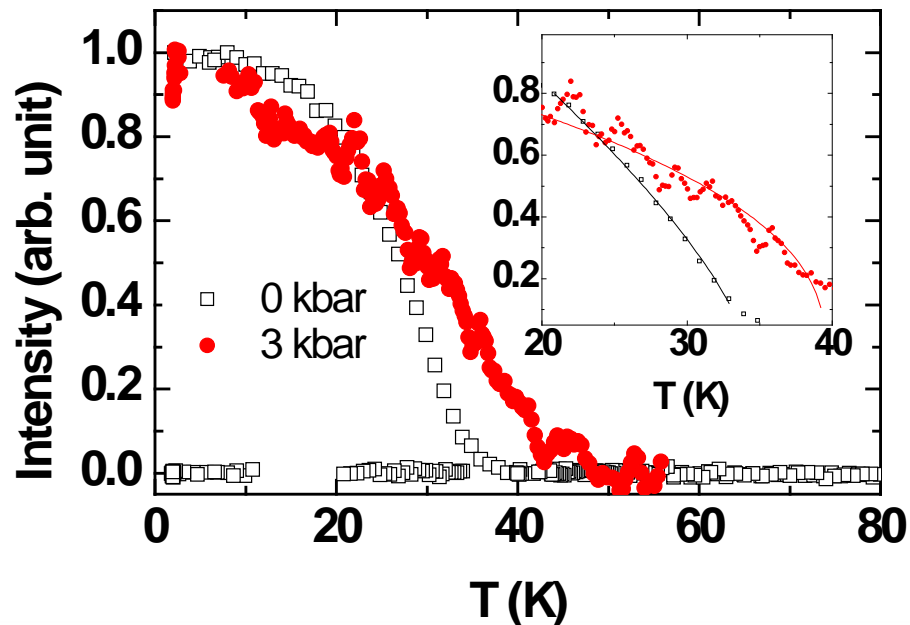
- Decreases the critical field of PM-FM transition
- Narrows the hysteresis loop
- Broadens the field transition region

Pressure facilitates FIM state in both cases

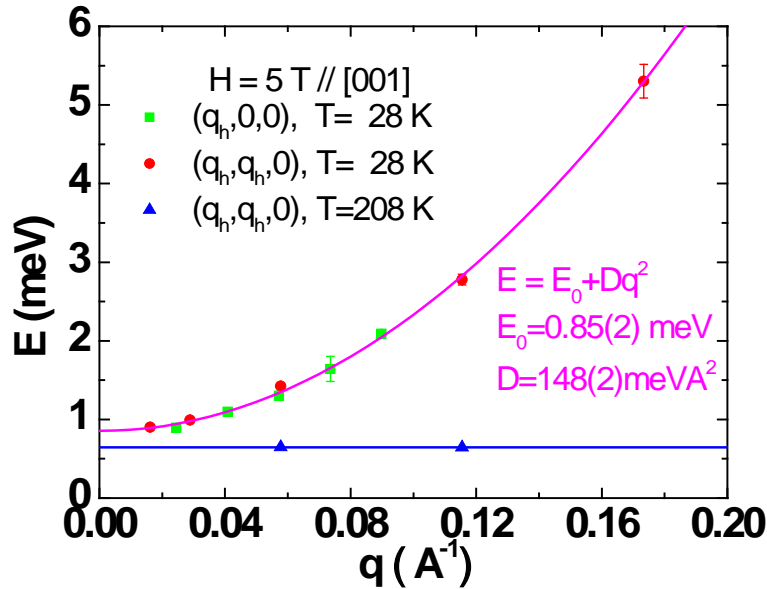
$$I/I_0 = (1-T/T_C)^{2\beta}$$

$P = 0 \text{ kbar: } T_C = 33.9(2) \text{ K; } \beta = 0.37(2)$
 $P = 3 \text{ kbar: } T_C = 39.6(4) \text{ K; } \beta = 0.24(1)$

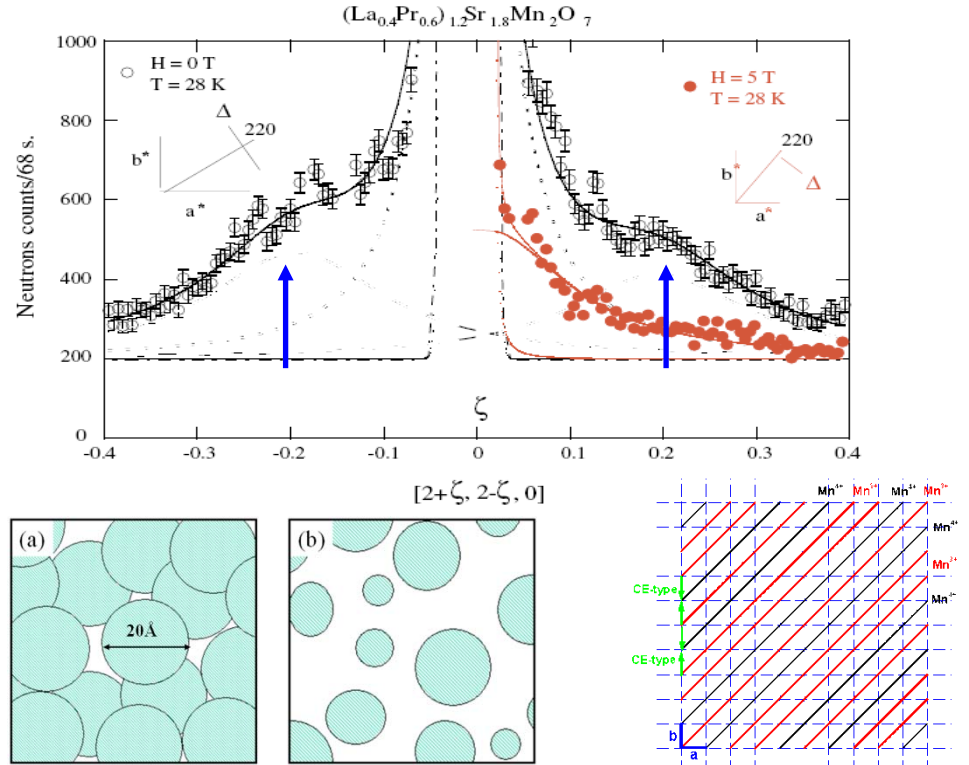
Decrease of β : **3D \Rightarrow 2D**, weakness of interlayer super-exchange interaction. $J_{\perp} \downarrow$
 Increase of T_C : Strength of intralayer double exchange interaction. $J_{\parallel} \uparrow$



Phase transition and phase separation: Spin vs Charge

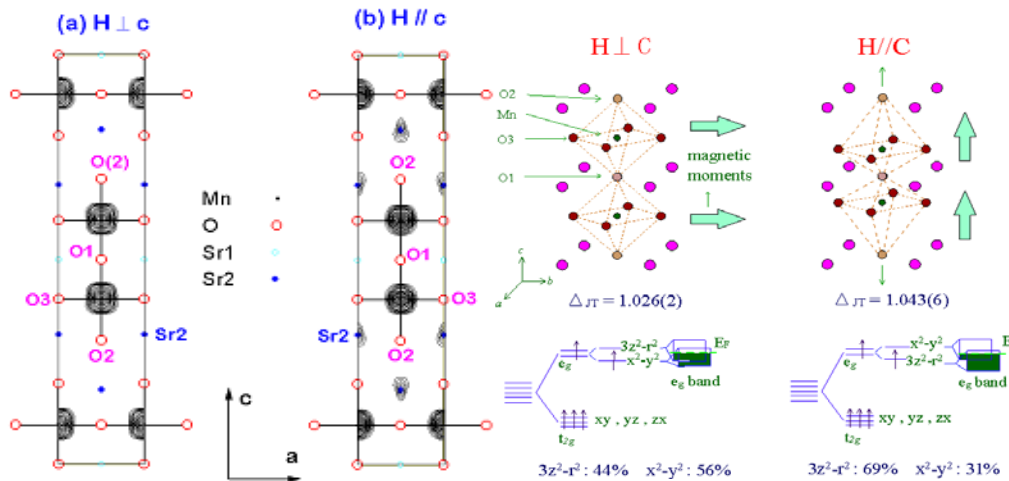
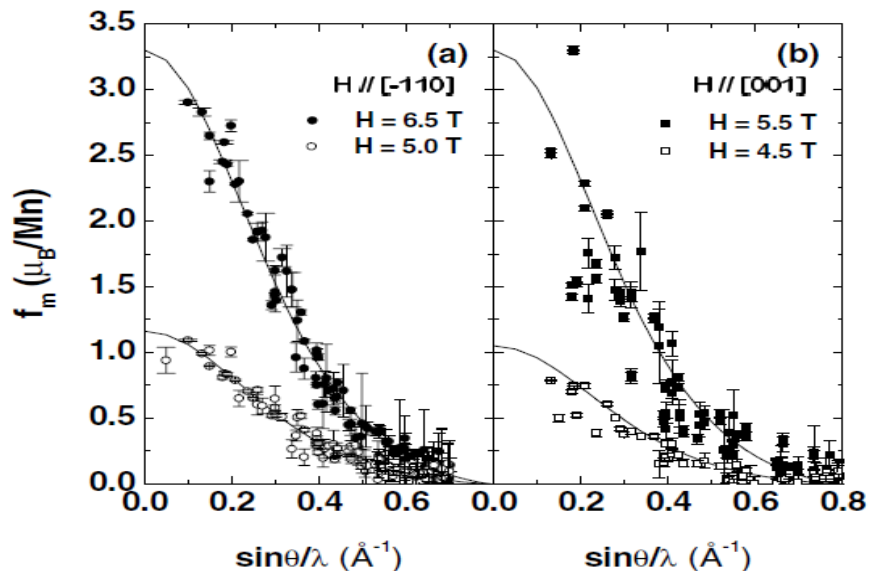


- i) Spin wave: FIMF at low temperature
- ii) Spin gap: 2D-anisotropy
- iii) Same dispersion: isotropy in the plane
- iv) $D \sim 148 \text{ meV}\text{\AA}^2$:
metallic state



- i) Insulated State ($H = 0 \text{ T}$) :
(0.2, -0.2, 0) diffuse scattering: Electron ordering
Cluster size $\sim 20\text{\AA}$
- ii) Metallic State ($H = 5 \text{ T}$):
No diffuse scattering : Electron order melting

Interplay between spin and orbital: polarized neutron diffraction



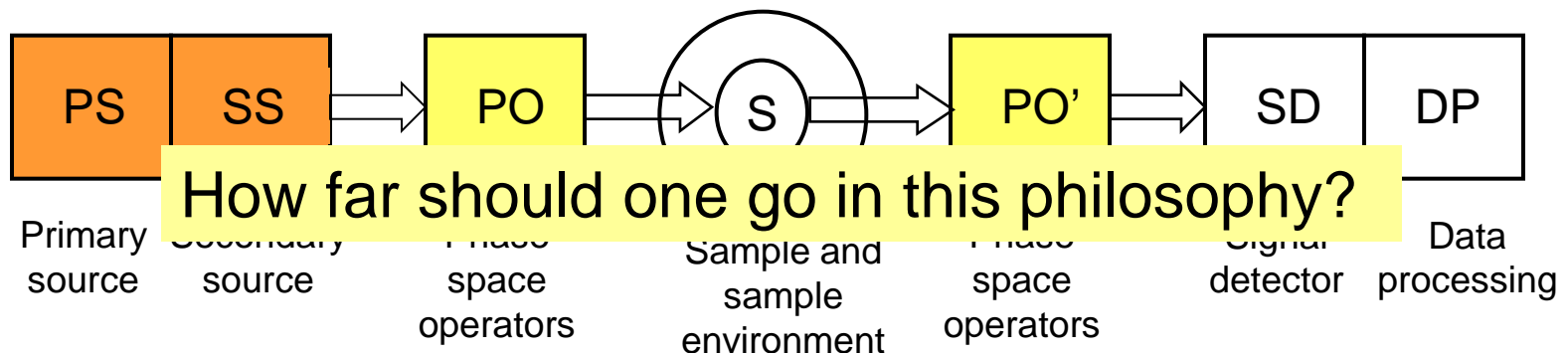
Data set	$H = 6.5 \text{ T} \parallel ab$	$H = 5.5 \text{ T} \parallel c$
No. of observ.	295	174
Spherical model: two variables		
χ^2	7.42	54.4
R_w	6.1	32.2
Mn $(\mu_S + \mu_L)\langle j_0 \rangle$	3.32(2)	2.9(1)
Mn $\mu_L\langle j_2 \rangle$	-0.38(5)	-0.6(2)
Spherical model: four variables		
χ^2	7.42	10.9
R_w	6.0	13.2
Mn $(\mu_S + \mu_L)\langle j_0 \rangle$	3.32(2)	2.9(1)
Mn $\mu_L\langle j_2 \rangle$	-0.38(5)	-0.6(2)
Sr2 $(\mu_S + \mu_L)\langle j_0 \rangle$	0.00(2)	0.48(2)
Sr2 $\mu_L\langle j_2 \rangle$	-0.01(2)	0.77(4)
Multipole model		
χ^2	4.20	5.68
R_w	4.3	8.8
Mn $Y_{00}\langle j_0 \rangle$	3.36(3)	3.12(5)
Mn $Y_{20}\langle j_2 \rangle$	0.03(2)	0.01(5)
Mn $Y_{44+}\langle j_4 \rangle$	-0.18(9)	-0.35(6)
Mn $Y_{40}\langle j_4 \rangle$	-0.50(7)	0.1(1)
Mn $\mu_L\langle j_2 \rangle$	-0.48(4)	-0.58(7)
Sr2 $(\mu_S + \mu_L)\langle j_0 \rangle$...	0.50(3)
Sr2 $\mu_L\langle j_2 \rangle$...	0.77(4)
O1 $Y_{00}\langle j_0 \rangle$	0.15(2)	-0.3(1)
O2 $Y_{00}\langle j_0 \rangle$	0.03(2)	-0.2(1)
O3 $Y_{00}\langle j_0 \rangle$	-0.05(1)	0.05(5)
Orbital occupancies from multipole model (%)		
Mn $d_{x^2-y^2}$	14(3)	9(4)
Mn $d_{3z^2-r^2}$	11(3)	20(4)
Mn d_{xy}	23(3)	30(4)
Mn d_{zx+zy}	52(3)	41(4)

outline

- **Relationship between structure and property**
(物质结构与物性)
- **Why neutrons: neutron characteristics and neutron scattering**
(为什么需要中子：中子特点与中子散射)
- **Coupling between lattice, orbital and spin in manganites studied by neutron scattering**
(锰氧化物中晶格、轨道和自旋相互作用的中子散射研究)
- **Target Station of spallation neutron sources**
(散裂中子源)

Neutron Source Design

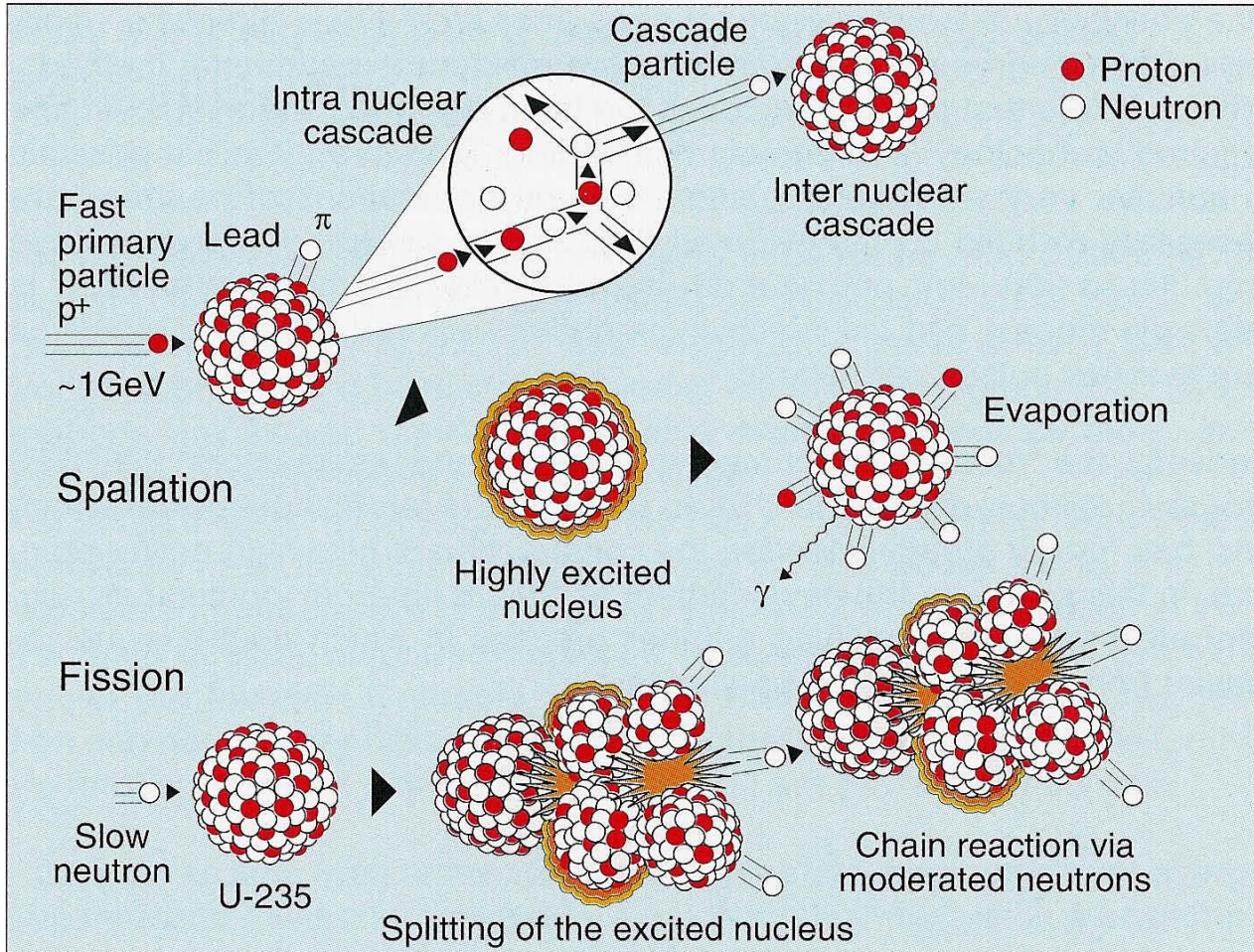
- Neutron scattering instruments can be designed to work in continuous mode or in time of flight mode. (中子散射谱仪：连续模式与飞行时间模式)
- There is no one instrument that can cover most of the Q - ω space with sufficient resolution and flexibility. (任何谱仪只能在特定的分辨率下覆盖特定的 Q - ω 空间)
- Instruments have varying requirements with respect to spectral properties and time structure. (针对所测量的中子谱和时间结构，谱仪就有不同的需求)
- 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). (中子散射谱仪的设计者与中子源的设计者需要紧密合作)



Neutron Yield of Different Nuclear Reactions

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
Deuteron stripping	40 MeV deuterons on liquid Li	$7 \cdot 10^{-2}$ n/d	3 500
Nuclear photo effect from e^- -bremsstrahlung	100 MeV e^- on ^{238}U	$5 \cdot 10^{-2}$ n/ e^-	2 000
^9Be (d,n) ^{10}Be	15 MeV d on Be	1 n/d	1 000
^9Be (p,n;p,pn)	11 MeV p on Be	$5 \cdot 10^{-3}$ n/p	2 000
Nuclear fission	fission of ^{235}U by thermal neutrons	1n/fission	180
Nuclear evaporation (spallation)	800 MeV p^+ on ^{238}U on Pb	27 n/p 17 n/p	55 30

Visualisation of the Spallation and Fission Processes



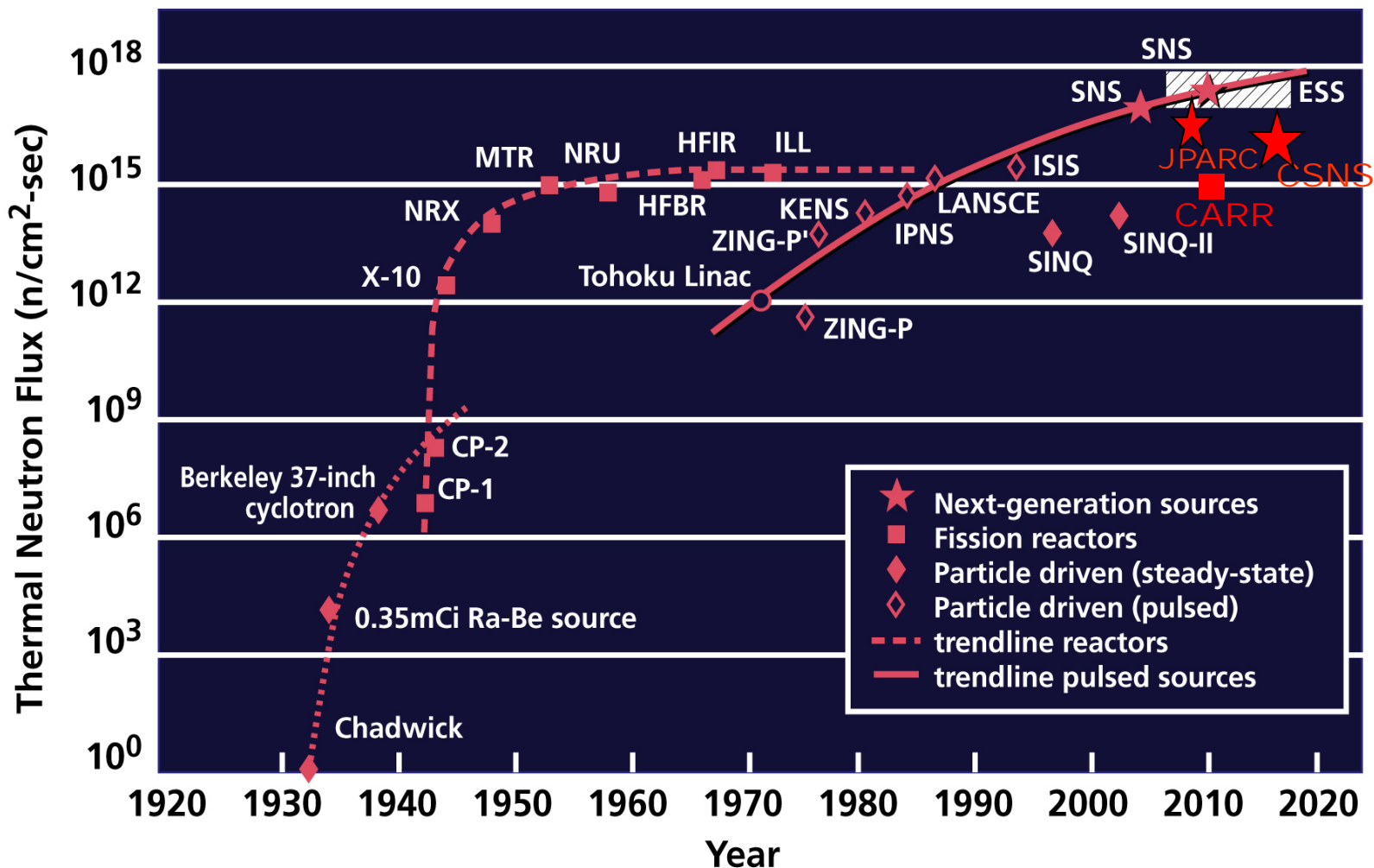
• Spallation

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

• Fission

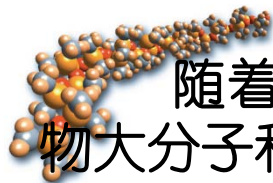
- chain reaction
- continuous flow
- 1 neutron/fission
- 180 MeV/neutron

中子源发展趋势



(Updated from *Neutron Scattering*, K. Skold and D. L. Price: eds., Academic Press, 1986)

Why spallation neutron sources?



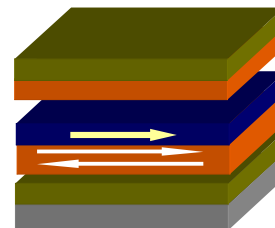
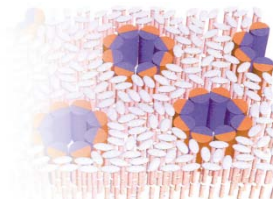
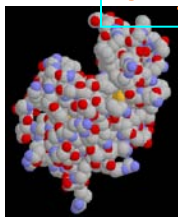
随着科学技术的飞速发展，薄膜、纳米团簇、生物大分子和蛋白质等研究体系成为研究的主要对象。



- 周期结构单元更大
- 样品体积更小
- 结构形态变化更快



高通量中子源



美国散裂中子源-SNS



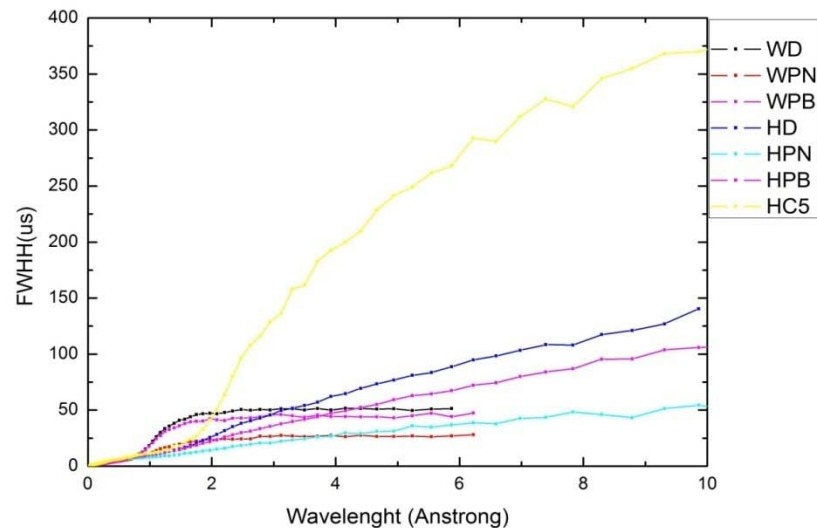
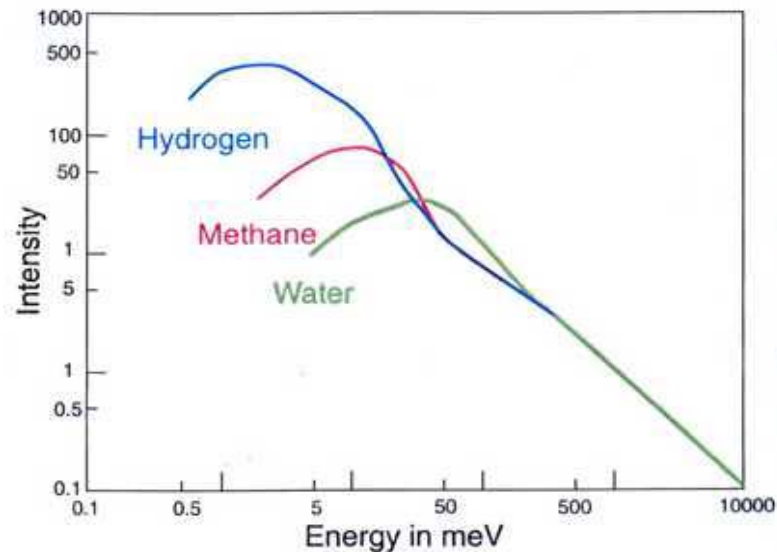
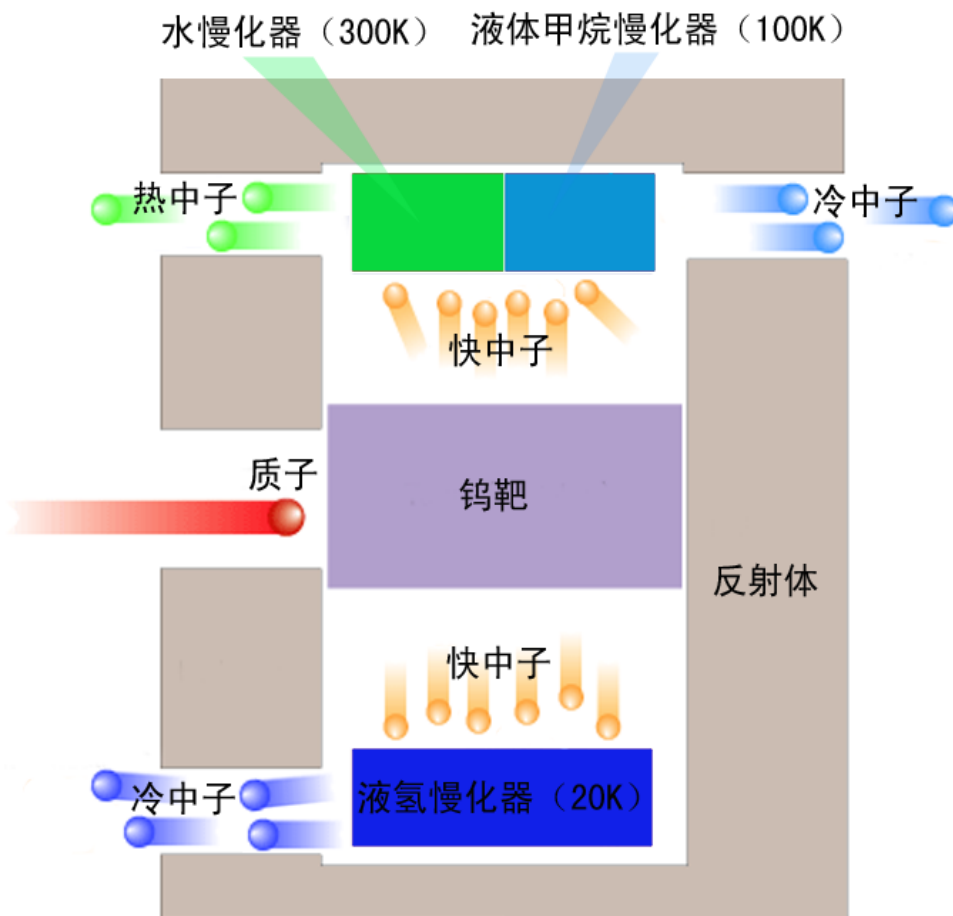
- 2 MW时，通量：~12x ISIS，时间平均通量： $\frac{1}{2}$ ILL
- 峰值热中子通量：~50-100x ILL
- 世界最好的散裂源，现稳定运行在800kW

日本散裂中子源-JSNS

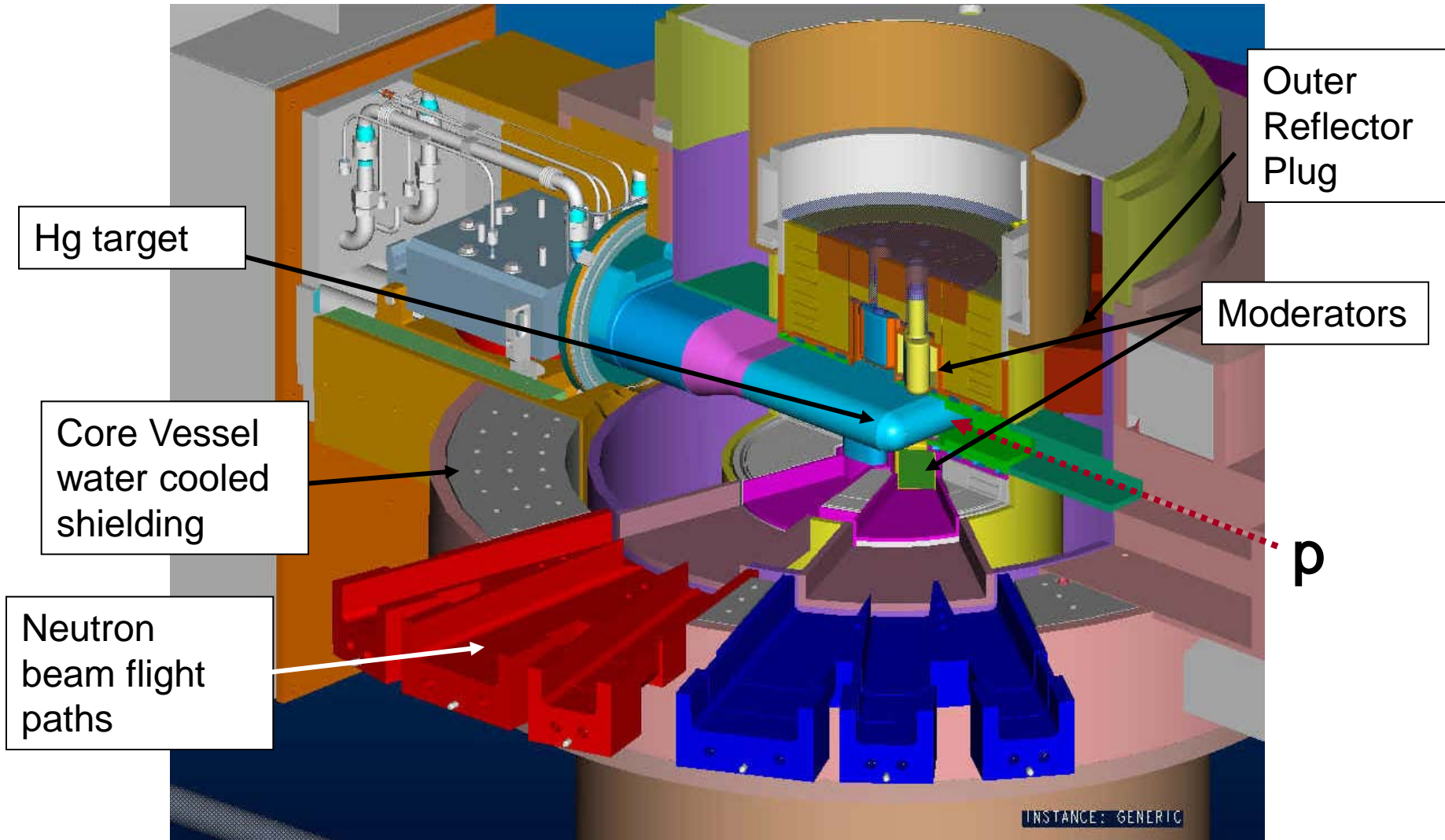
- 自2001年始，一期投资1527亿日元、二期规划363亿日元，2009年建成运行
- 1MW, 25Hz, 3GeV



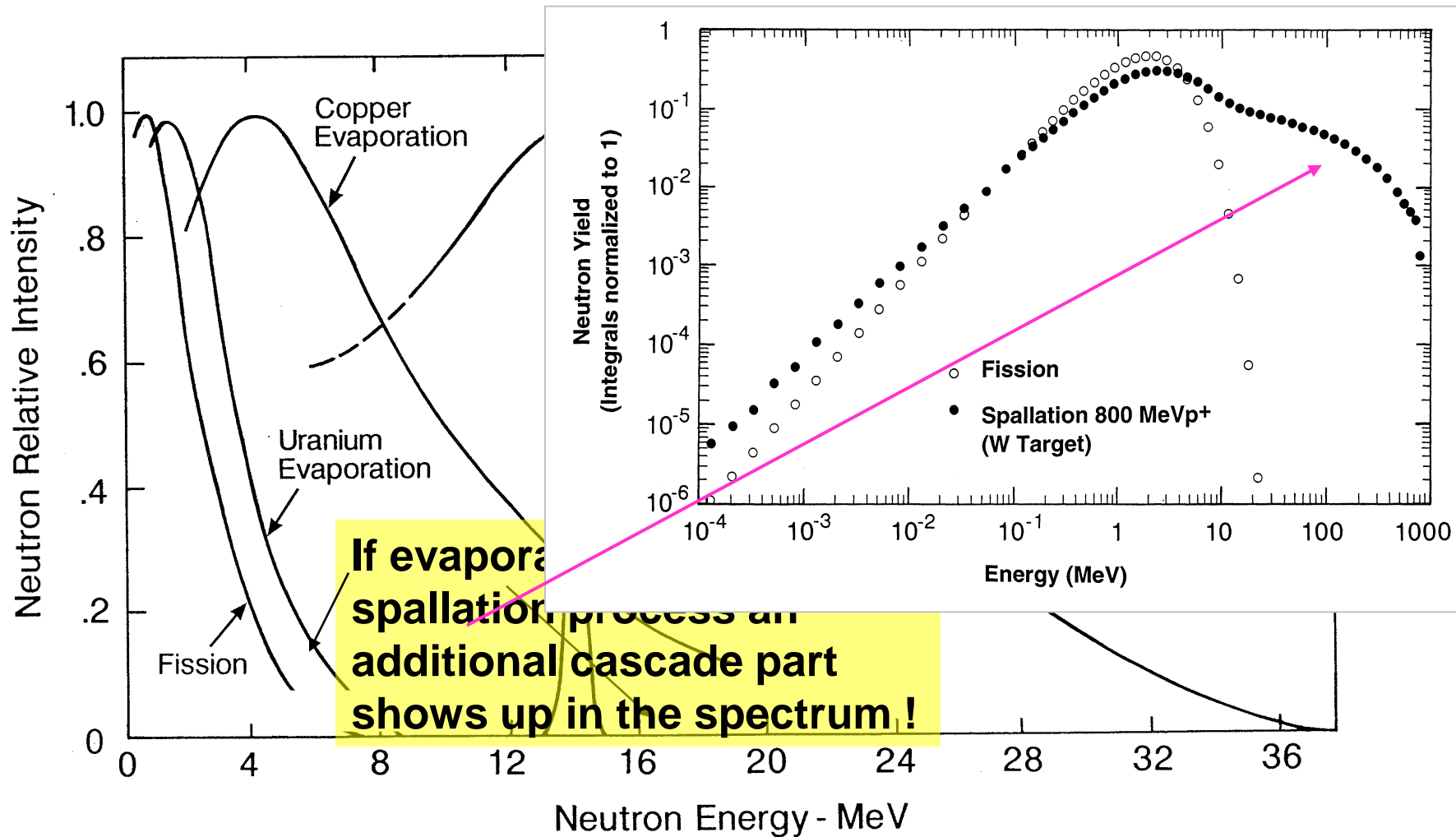
散裂中子源原理



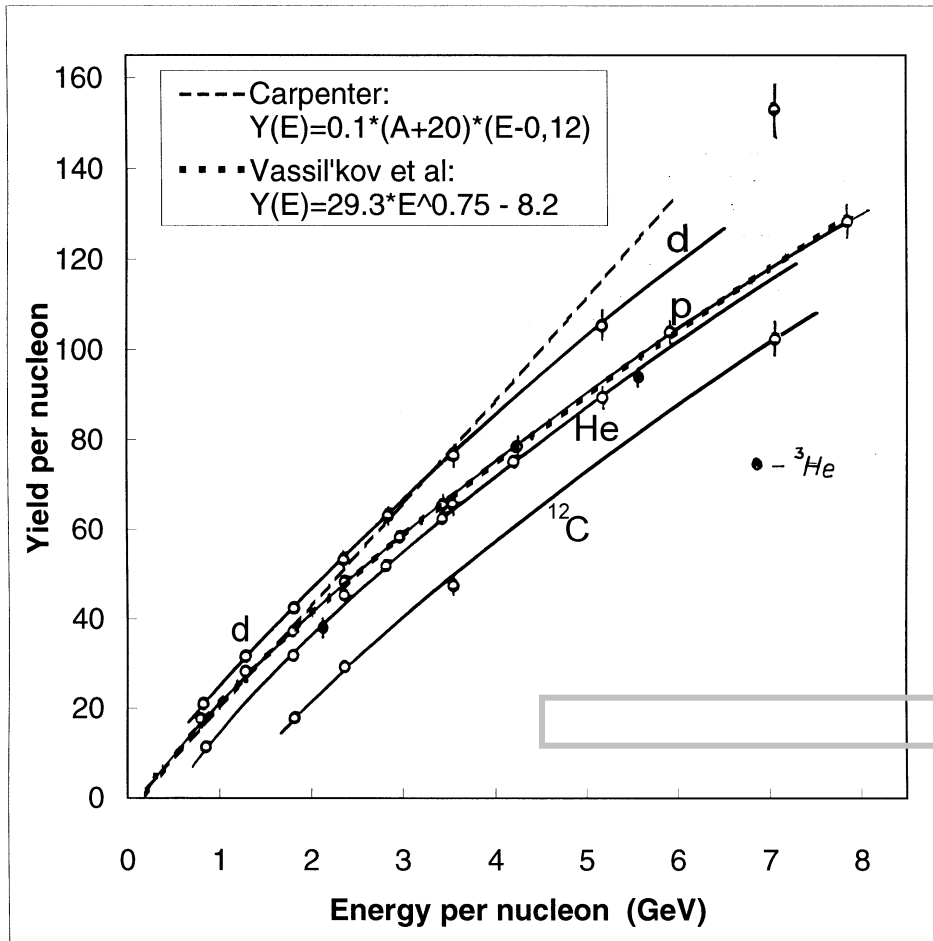
SNS Target System



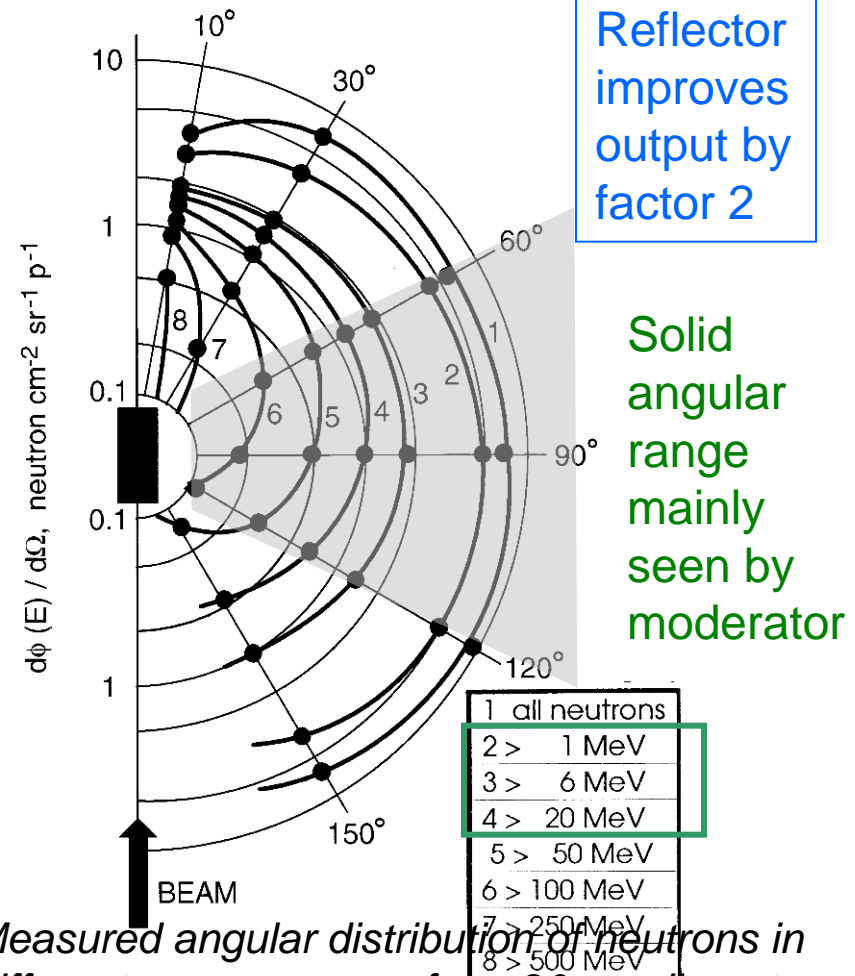
Neutron Spectra from Different Nuclear Reactions



Spallation neutron yield and angular distribution

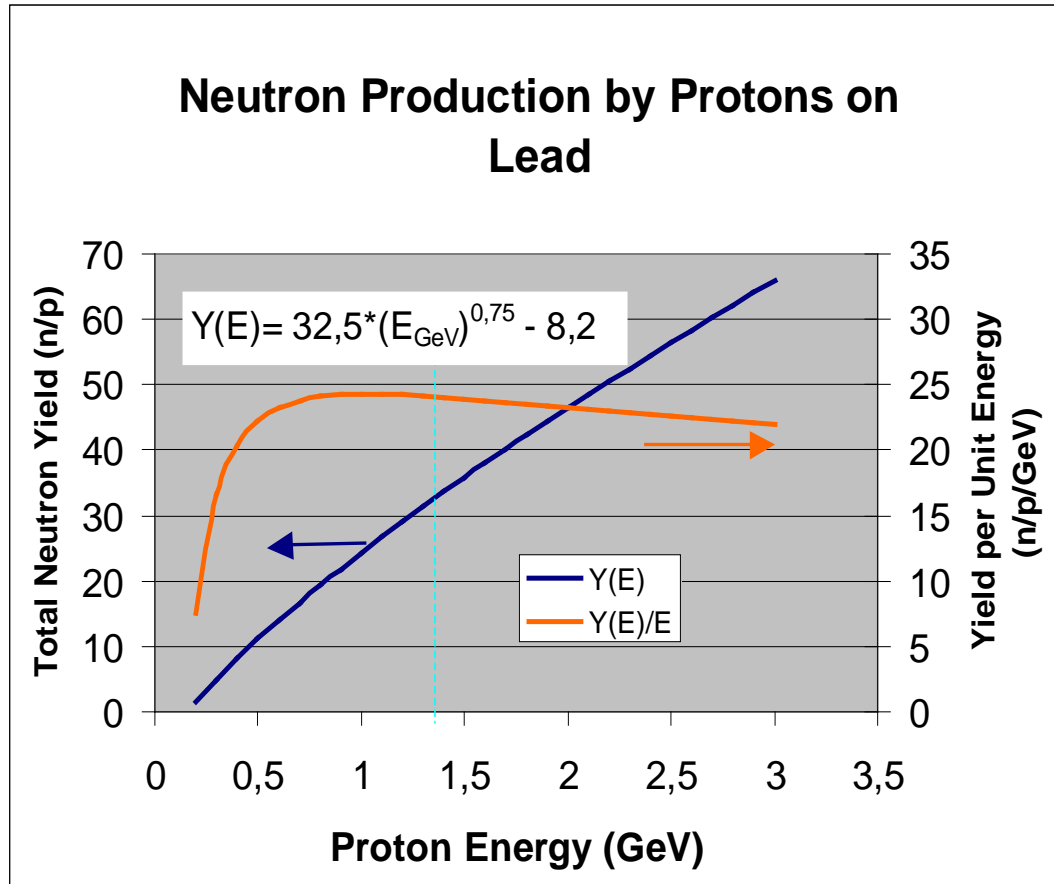


Measured neutron yield from thick lead targets



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

Choice of proton and its energy



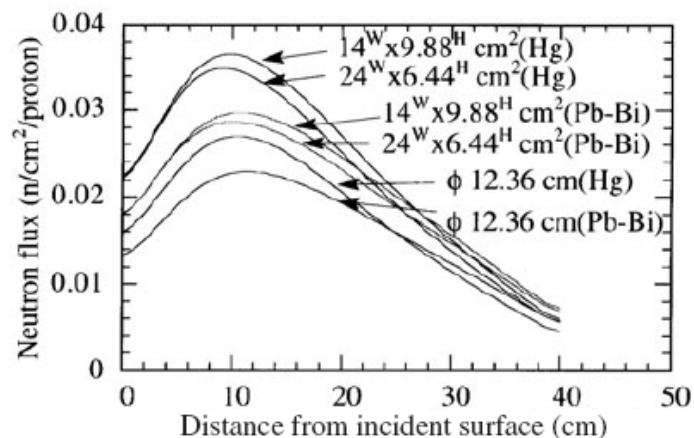
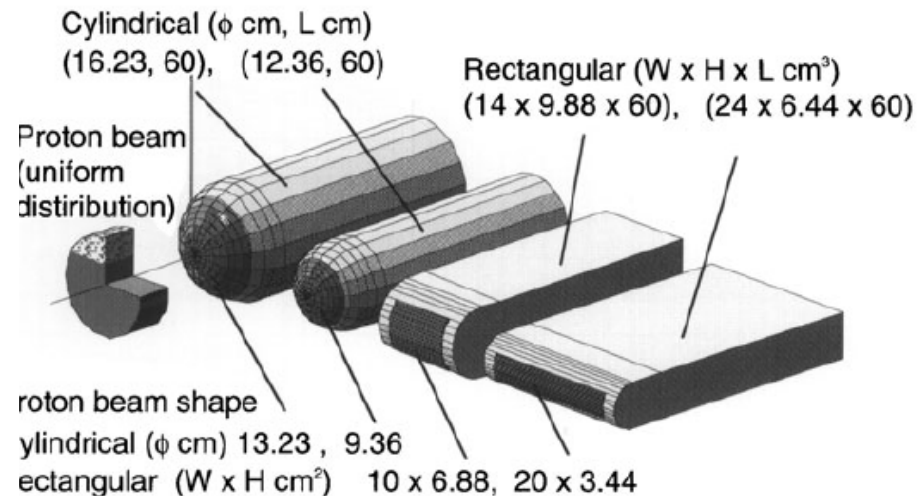
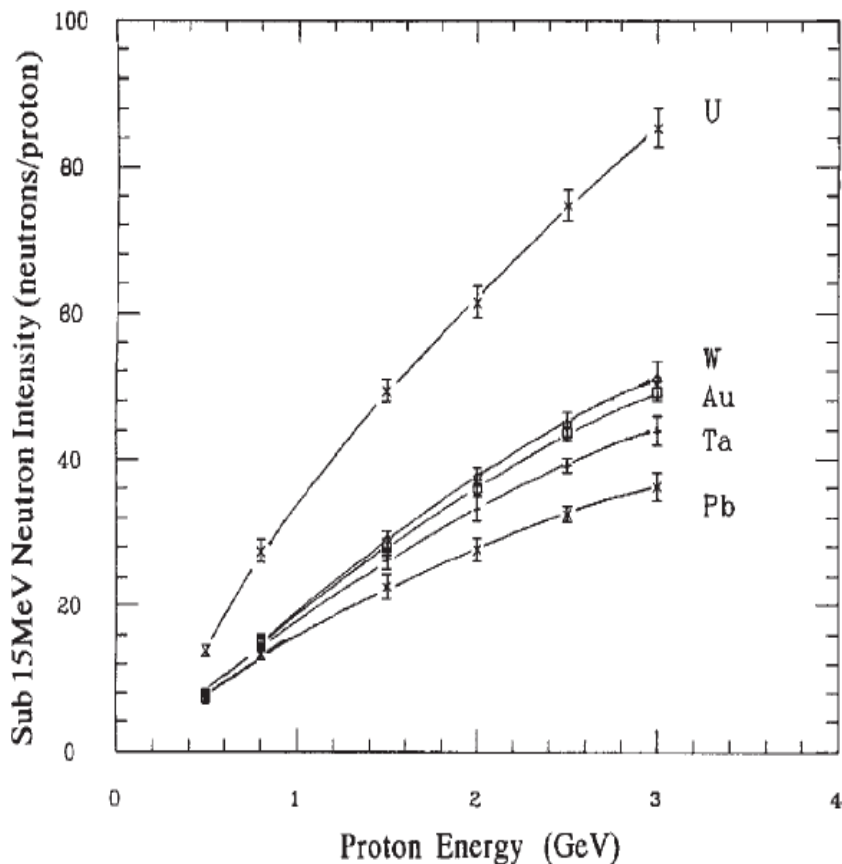
Arguments for higher proton energy:

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.

Target Material and Shape



Neutron Moderation

- Moderation of neutrons occurs by collisions with moderator atoms
- In each collision a constant fraction of the energy is lost
- “Logarithmic energy decrement”:

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

A is the atomic number of the moderator atom
- 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 $E_f = 1\text{ eV}$: $x = 14.5/\xi$

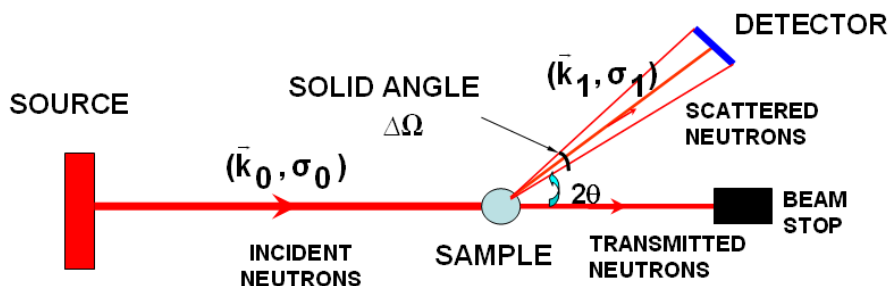
Parameter	Element						
	H	D	Be	C	O	Hg	Pb
A	1	2	9,01	12,01	16	200,6	207,19
$\sigma_{fr} (10^{-24} \text{ cm}^2)$	20,51	3,40	6,18	4,73	3,75	26,53	11,01
$\rho (\text{g/cm}^3)$ (*)	0,07	0,163	1,85	2,3	1,13	13,55	11,3
$\Sigma_{fr} = N * \sigma_{fr} (\text{cm}^{-1})$	0,86	0,17	0,76	0,55	0,16	1,08	0,36
ξ	1,000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

Neutron Reflector

- 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

中子散射基本概念



scattering function:

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

$$C = \eta\Phi N \left(\frac{d^2\sigma}{d\Omega dE} \right) \Delta\Omega \Delta E$$

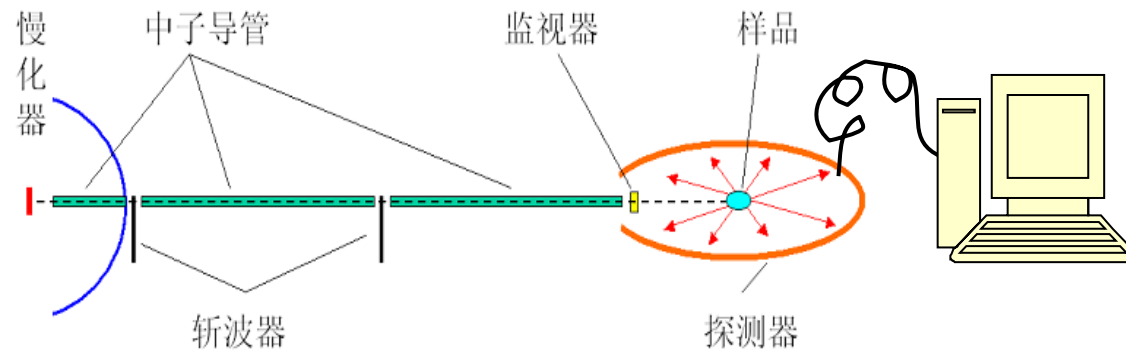
$$S(Q, E) = \frac{1}{N} \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} \sum_{ii'}^{i \neq i'} \langle e^{-iQ \cdot R_i(0)} e^{iQ \cdot R_{i'}(t)} \rangle e^{-iEt/\hbar} dt$$

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

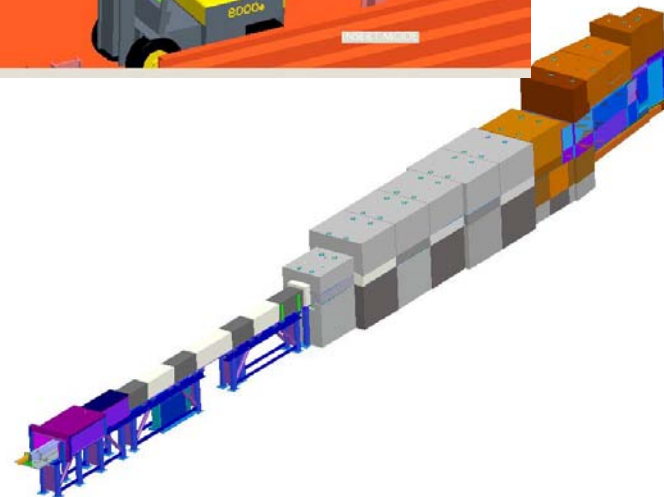
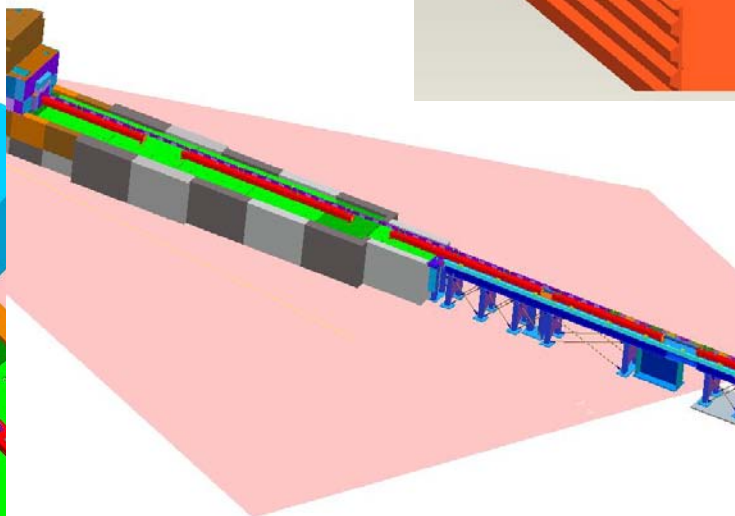
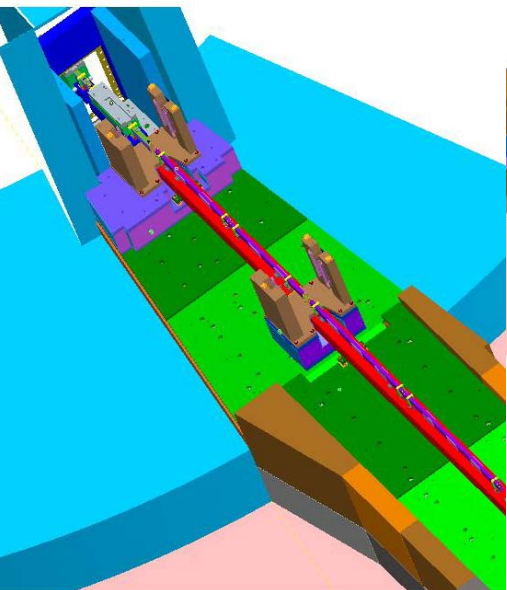
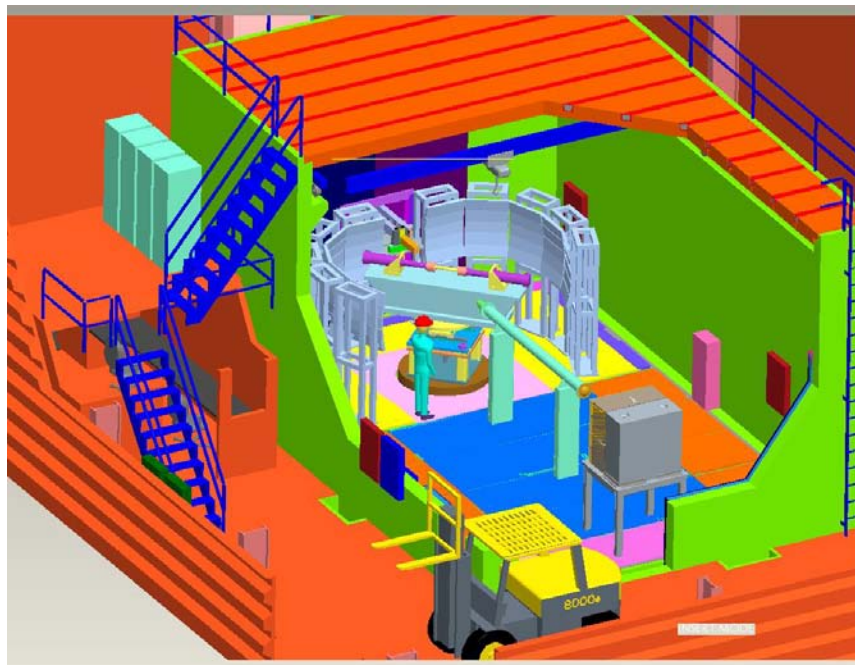
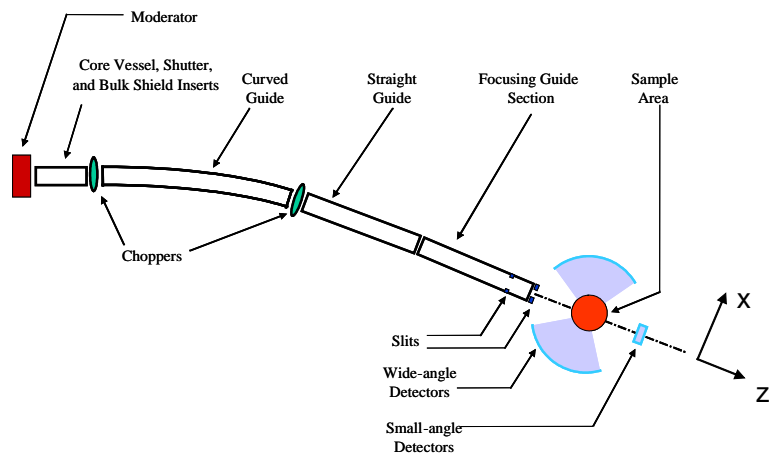
仪器分辨率函数所表达的物理意义是：当谱仪被设定测量动量转移为 Q ，能量转移为 E 的散射过程时，在相近的动量、能量空间中探测到中子的概率。

Basic components of TOF spectrometer

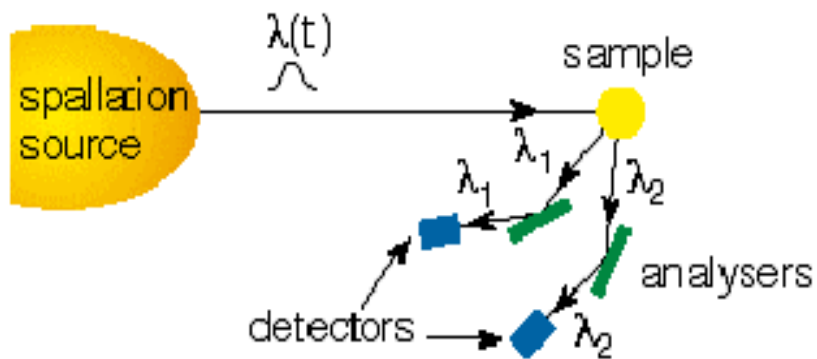
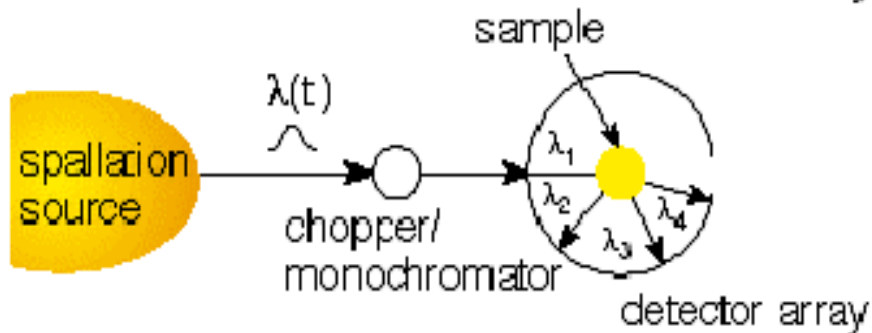
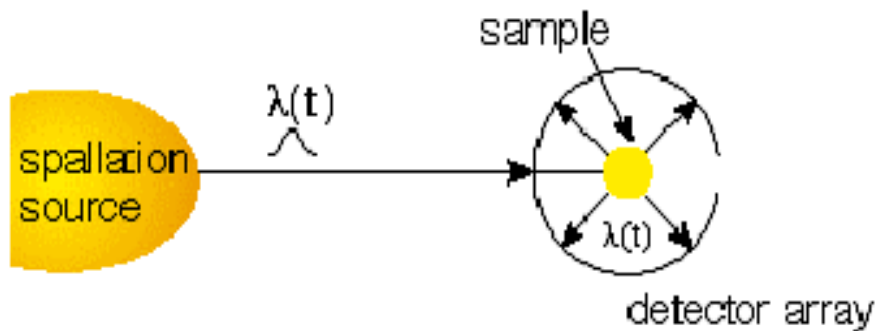
- 转子 (Chopper): 又称斩波器、中子能量选择器
 本底转子、盘状转子和费米转子
- 中子导管
- 探测器
- 数据采集和分析系统
- 准直器
- 监测器
- 样品台
- 屏蔽体



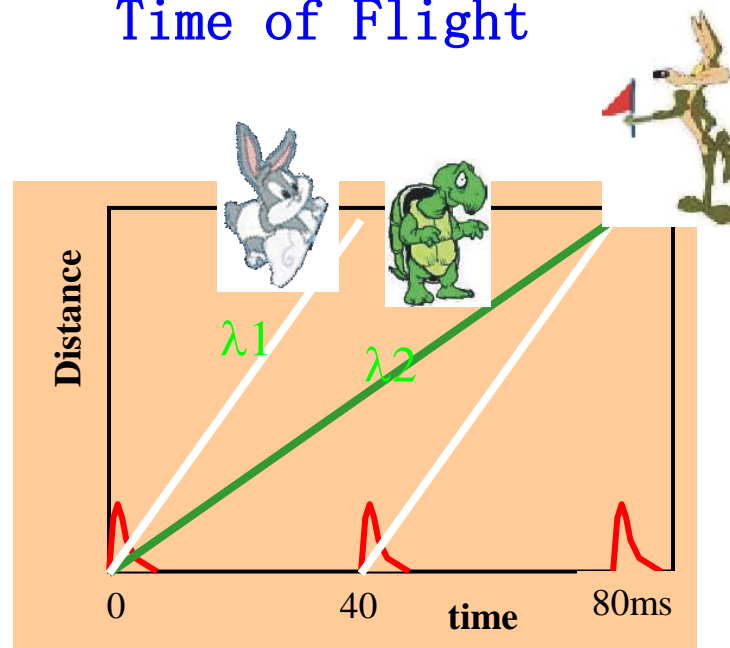
VULCAN (SNS)



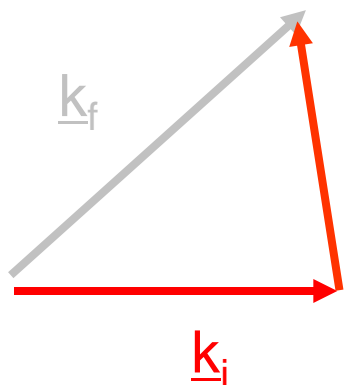
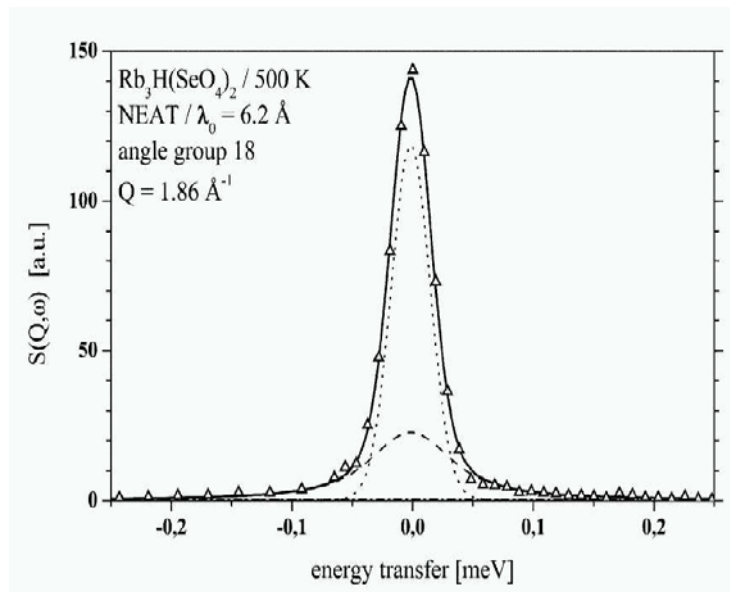
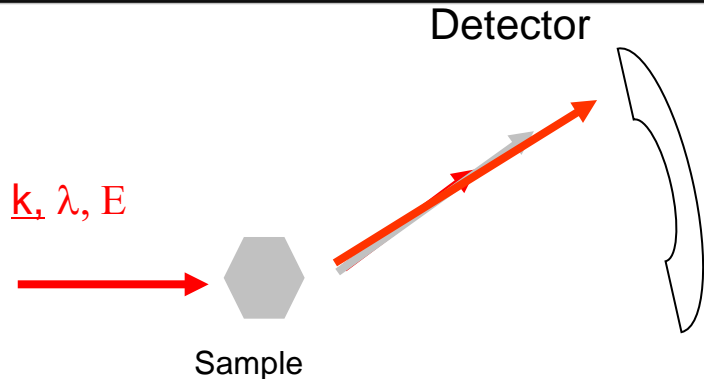
Schematic instrument layout at pulse source



Time of Flight



TOF data collection



$\underline{Q} = \underline{k}_f - \underline{k}_i$ Wavevector transfer

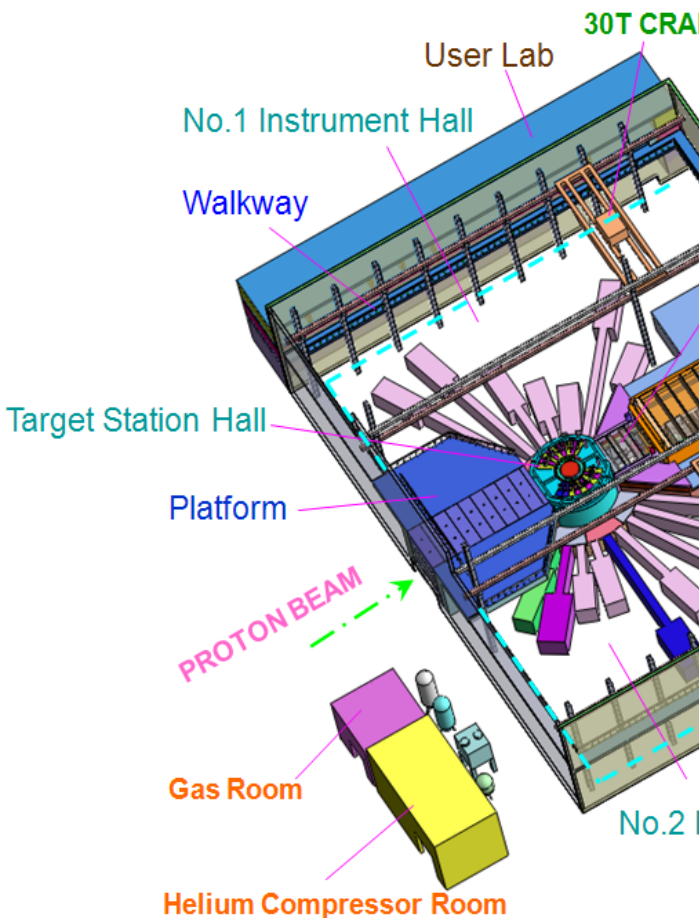
$\hbar\omega = \underline{E}_f - \underline{E}_i$ Energy transfer

$|\underline{k}_f| \neq |\underline{k}_i|$ “Inelastic” scattering $I(\underline{Q}, \omega)$

中国散裂中子源-CSNS

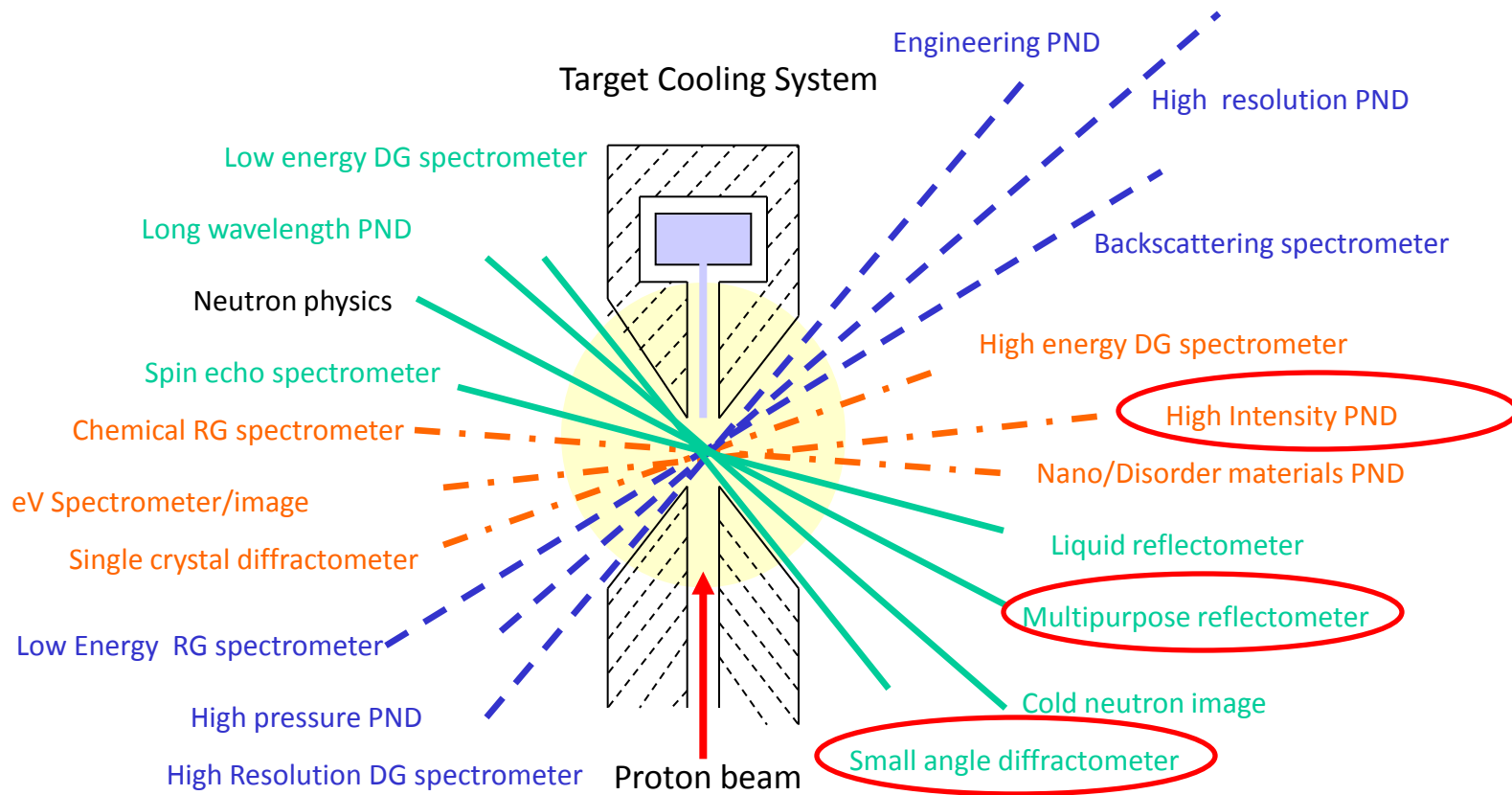


Design parameters



Parameters	Phase I	Phase II	PHASEIII
Beam power on target (kW)	100	200	500
Proton energy on target (GeV)	1.6		
Average beam current (μA)	62.5	125	
Pulse repetition rate (Hz)	25		
Target	1; Tungsten		1 or 2
Moderators	3; LH2(C), LH2(DP), H2O(D)		
Reflector	Be		
Beam ports	20		
Neutron instruments	3	20	
Dose control in hall ($\mu\text{Sv/h}$)	2.5		
Operation (hrs/yr)	5000		

CSNS instrument layout



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

Moderator:

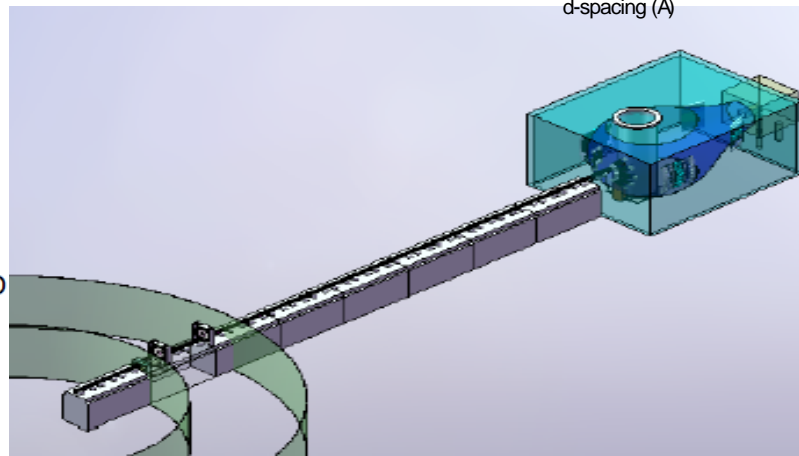
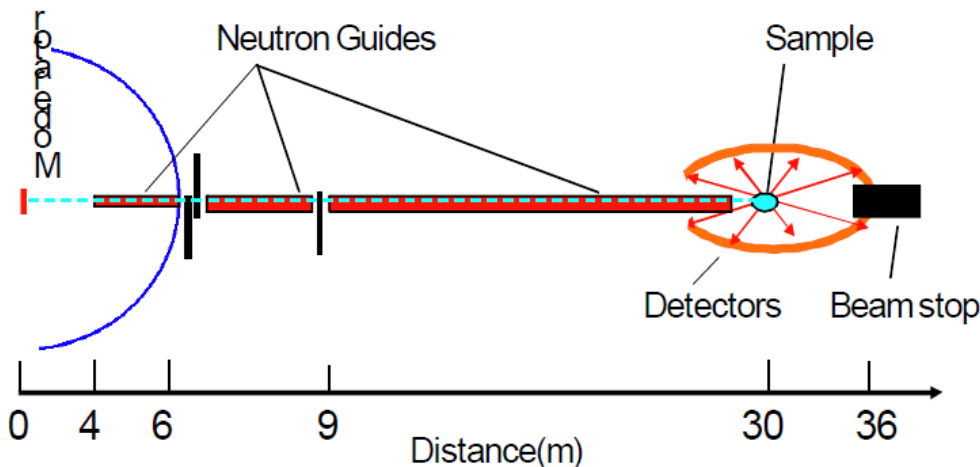
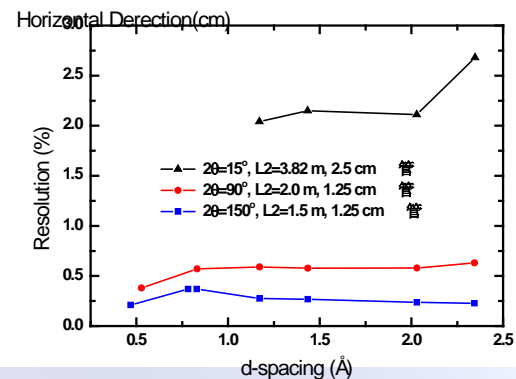
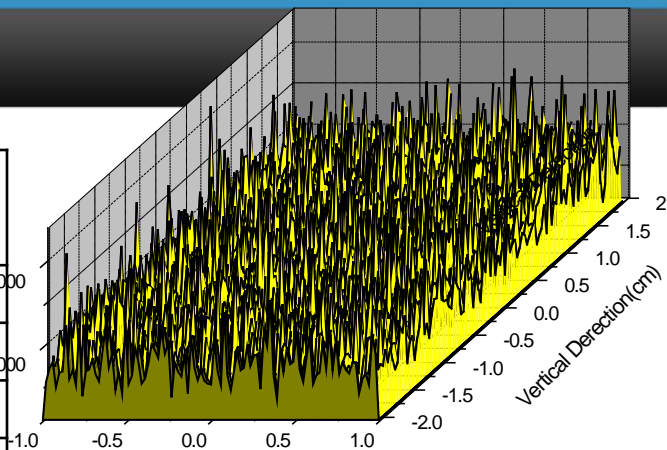
— — — D+P, LH2
(20K)

— — — C, LH2
(20K)

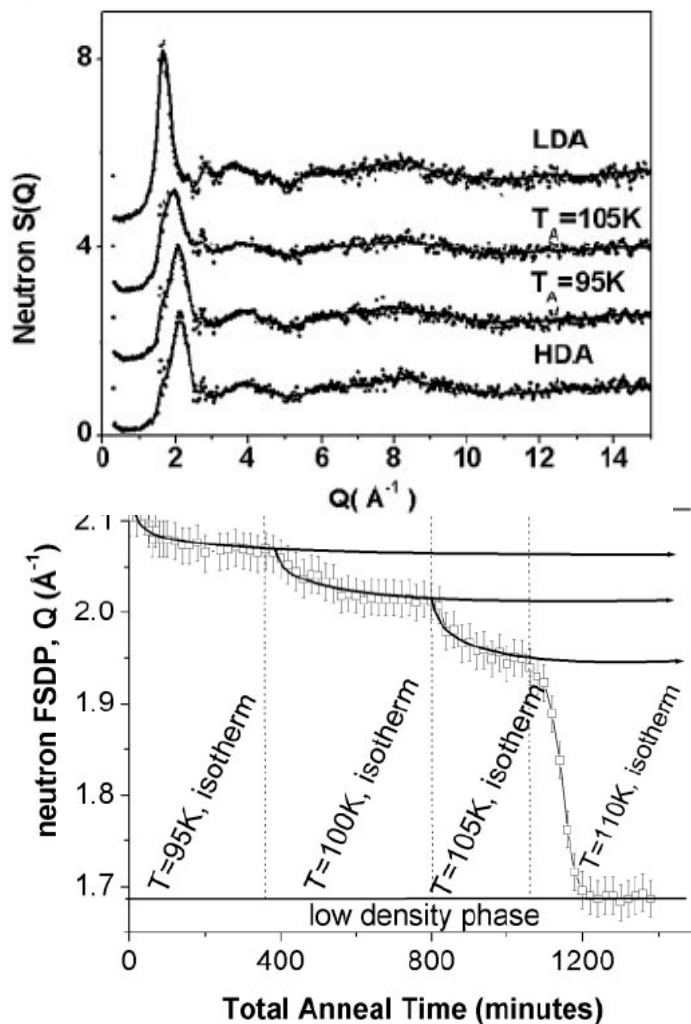
— — — D, Water
(300K)

Neutron instrument: HIPD design

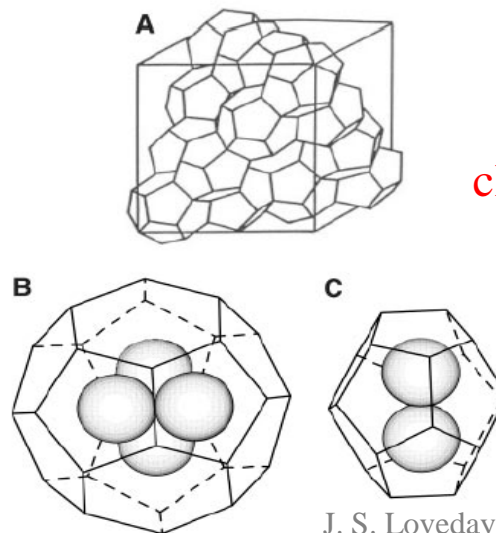
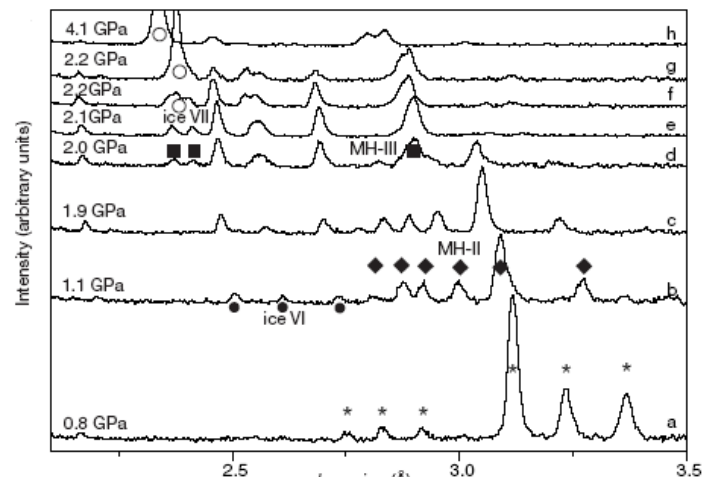
Moderator	decoupled water moderator (300 K)	
Bandwidth($\Delta\lambda$)	4.5 Å	
Max. Beam Size	40(h) × 20(w) mm	
Flux at sample position	$\sim 10^7$ n/cm ² /s	
Best Resolution($\Delta d/d$)	0.2 % at $2\theta = 150^\circ$	
Guide	Taper focus, m=3	
Source to sample distance L1	30 m	
Sample-detector distance L₂	$2\theta = 150^\circ$	1.5 m
	$2\theta = 90^\circ$	2.0 m
	$2\theta = 15^\circ$	3.8 m



小样品的结构研究—高通量粉末衍射仪应用



Several distinct metastable forms of amorphous Ice



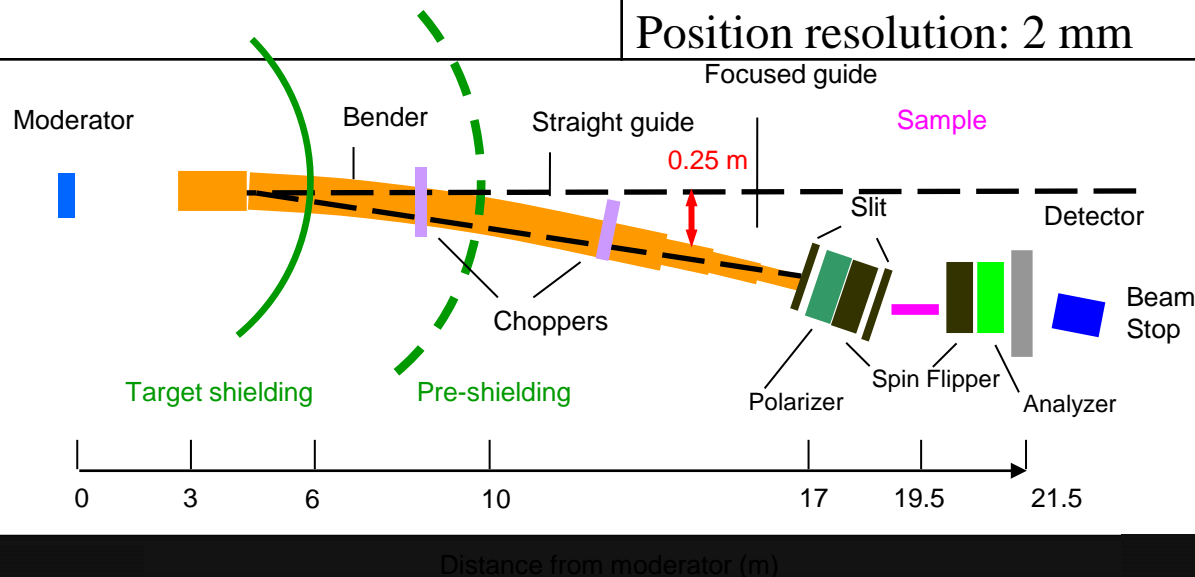
Methane and hydrogen in clathrate hydrate

C. A Tulk et al., Science 297, 1320 (2002)

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

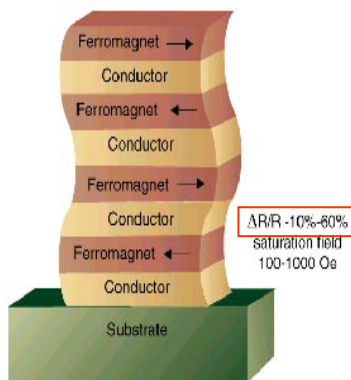
Neutron instruments: REFL design

Moderator	Coupled liquid H ₂ (20 K)
Bandwidth ($\Delta\lambda$)	6 Å
Guide	Bender+Sraight+Taper 40 × 60 → 20 × 30 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

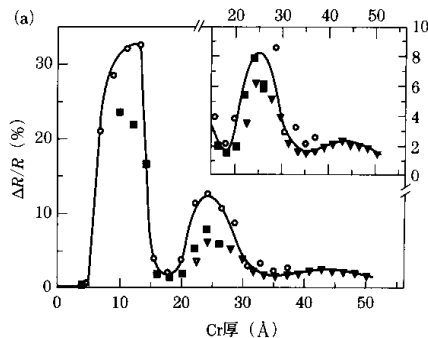
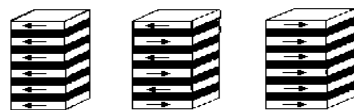
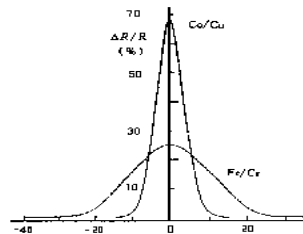


磁性多层膜的层间耦合和层内涨落——反射仪应用

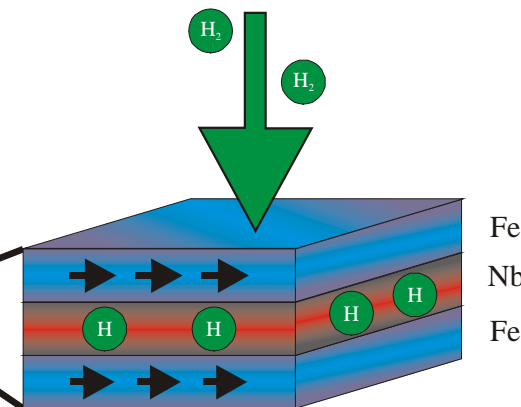
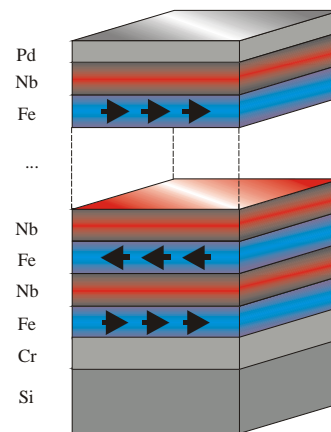
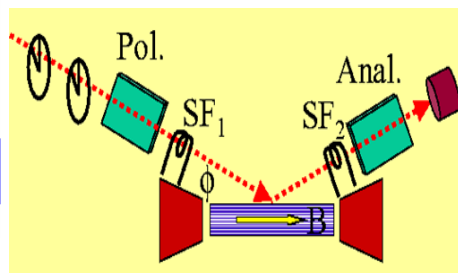
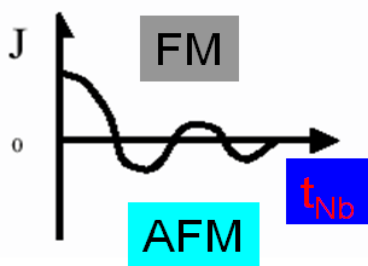
GMR Multilayer



$\Delta R/R$ ~10%-60%
saturation field
100-1000 Oe



Hydrogen Loading of Fe/Nb Multilayers



Modification of the
exchange coupling
via hydrogen absorption

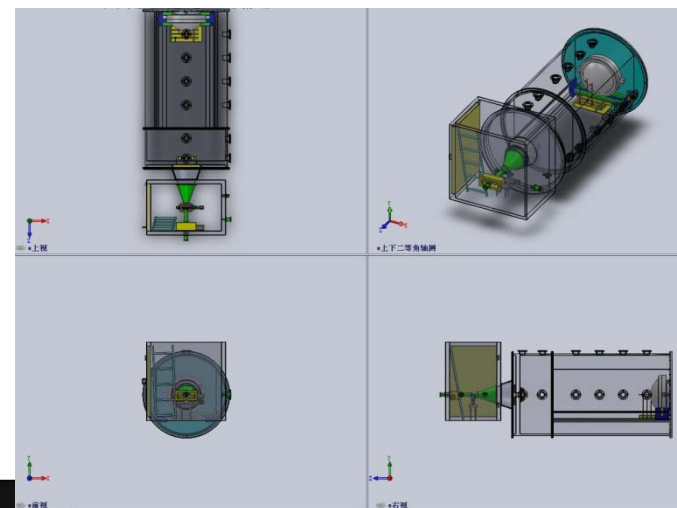
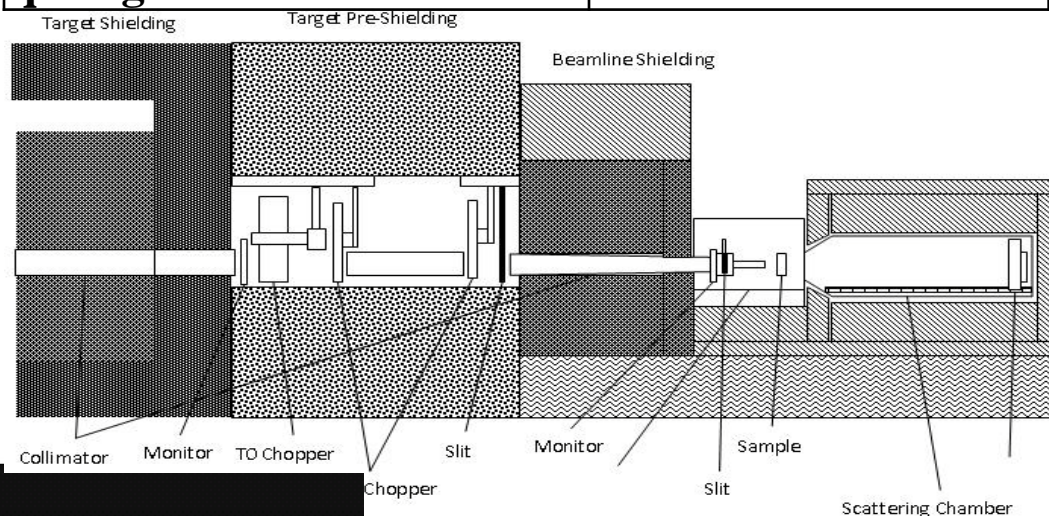
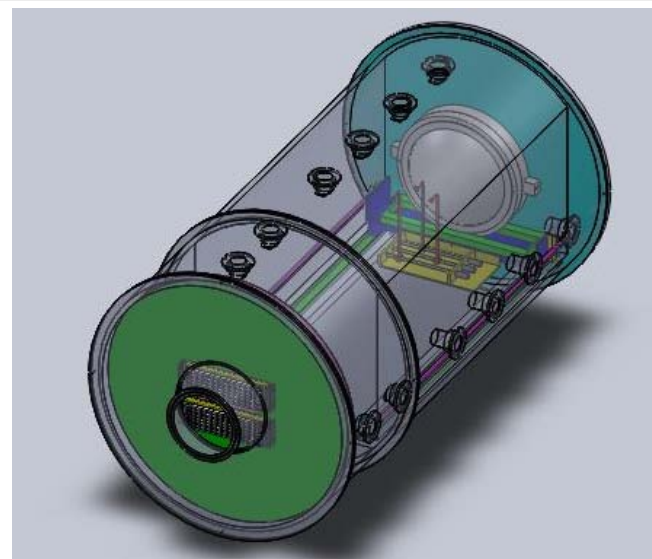
Exchange coupling energy
 $J \sim \sin(2k_F t_{Nb})$

Exchange coupling energy:

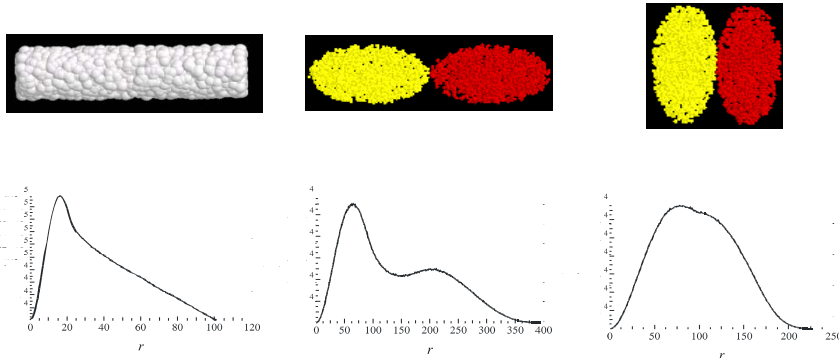
$$J \sim \sin(2k_F t_{Nb}) / t_{Nb}^2$$

Neutron instruments: SANS

Moderator	Coupled hydrogen (20K)
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 Å
q range	$0.004\text{-}3.4 \text{ \AA}^{-1}$

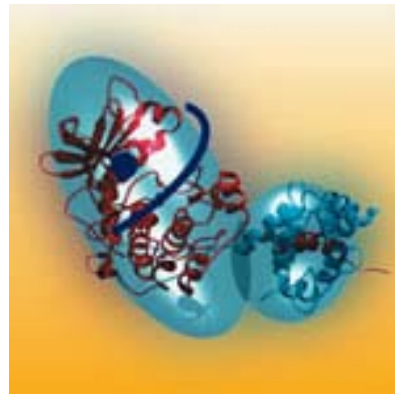
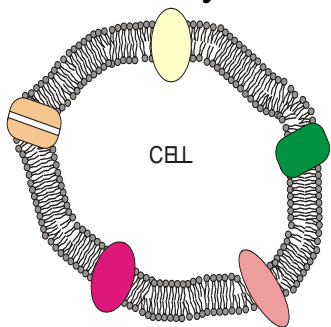


小角中子散射谱仪的应用

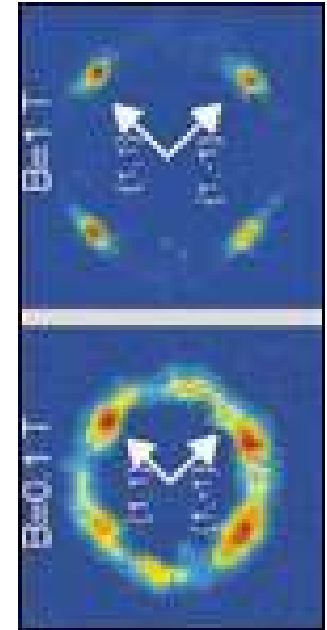
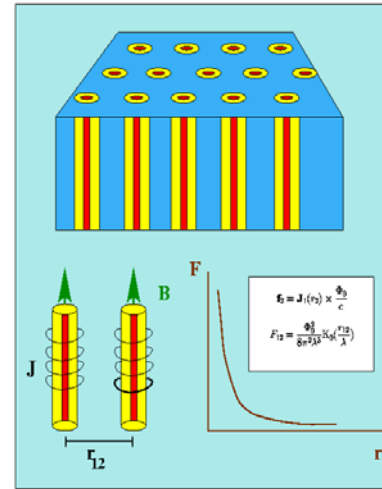


Neutron scattering provides lower-resolution information on the shapes and arrangements of these subunits in solution.

~30% proteins are membrane proteins, difficult to crystallize



The enzyme CAM kinase II and its activator protein calmodulin



R. Gilardi et al., Phys. Rev. Lett. 88, 217003 (2002).

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

Users Development

- **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.**
- **User Meeting 2010 will be held in December 6-8, at Zhuhai, Guangdong.**

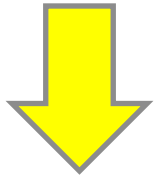
结束语

- 中子散射是研究位置微观结构与相互作用的不可替代的工具。
- **CSNS**是目前我国投资最大的多学科研究平台，与同步辐射光源（如上海、北京和合肥光源）及反应堆（原子能研究院、绵阳九院）互补，以其独特性能服务于生命、环境、材料、医药、物理、化学等学科及工业界。
- 期待用户独立或联合申请其他途径的经费，建造更专业化的、世界水平的中子散射谱仪。
- **CSNS**是一项艰巨、复杂但值得付出的工程建设和科学研究项目，期待更多的青年才俊。

结束语

- **D: Democracy**

- **S: Science**

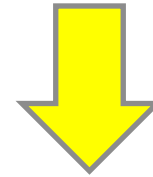


- **PRC**

**People's Republic of
China matter**

- **D: Dynamics**

- **S: Structure**



- **PRC**

**Property Research of
Condensed matter**

THANK YOU!

中子散射基本概念

Radius of nuclear force: $10^{-12} \sim 10^{-13}$ cm

Wavelength of neutron: 10^{-9} cm

Atomic distance in sample: $\geq 10^{-8}$ cm

Fermi potential: $U(\mathbf{r}) = \frac{2\pi\hbar^2}{m} b\delta(\mathbf{r} - \mathbf{R})$

$$U(\mathbf{Q}) = be^{i\mathbf{Q}\cdot\mathbf{R}}$$

$$\frac{d\sigma}{d\Omega} = b^2$$

a spherical symmetry

b: the scattering length, a property only of the nucleus of the the scattering atom and its spin state.

scattering function:

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

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