INTRODUCTION TO NEUTRON OPTICS

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Introduction to Neutron Optics

- The Neutron
- The Neutron Source at ILL
- Reflective Optics Neutron guides
- Diffractive Optics Neutron Monochromators
- Polarized Neutrons





Neutron Properties & Neutron Source (ILL)



Neutrons have both particle-like and wave-like properties



Neutrons	E	λ (Å)	photons	E	λ
Hot	900 - 80 meV	0.3 - 1 Å	Gamma Ray	$\sim 1 \text{ MeV}$	< 0.0124 Å
Thermal	80 - 5 meV	1 - 4 Å	X-Ray	~ 0.5 - 500 keV	25 - 0.025 Å
cold	5 - 0.03 meV	4 - 50 Å	Visible Light	~ 1.6 - 3 eV	0.4 - 0.8 μm

Neutron interactions with matter

The scattering length describes the strength and character of the interaction of low-energy neutrons with the individual nuclei and atomic structures.

- Neutron Scattering : Interaction with the individual nuclei via short range forces
- **Coherent scattering length** b_{coh} (depends on the direction of scattering vector Q = $k_i k_f$)
- Incoherent scattering length **b**_{inc} (uniform scattering)
- > Neutron capture (absorption cross section)

- \rightarrow diffraction, reflection, refraction
- ightarrow background ...
- \rightarrow Activation of materials gamma rays
- □ Magnetic scattering : Interaction with unpaired electrons via a dipole interaction
- > Magnetic scattering length $p \approx 0.269 \mu_{at}$ (10⁻¹² cm/µ_B) ~ $b_{coh} \rightarrow polarized$ neutron beams



Neutron scattering vs X-Ray scattering





Apparent cross-section σ of some elements $\sigma = 4\pi b^2$

Neutron interact with the individual nuclei via short range forces

The neutron scattering power varies in a quasi-random manner

X-Rays interact with matter via electromagnetic interaction

The X-Ray scattering power is proportional to the atomic number Z



Scattering lengths of some important elements



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Neutron production

$^{235}U + n (meV) \rightarrow F.P. + 2 \text{ or } 3n (MeV)$

- Fast neutrons (~ MeV) are slowed down to meV Energy by collisions in a thermal bath (liquid D₂O) => 1 n sustains the reaction and 1n available
- Neutrons must be moderated to give optimized flux distributions <E> = k_bT
 - **Cold source is liquid Deuterium at T = 20 K**
 - □ Thermal Source is liquid D_20 at room temperature T = 300 K $\lambda = 1 \rightarrow 4$ Å
 - □ Hot source is graphite at T = 2000 K (heated by radiation)



Fission



 $\lambda = 4 \rightarrow 20 \text{ Å}$

 $\lambda = 0.3 \rightarrow 1\text{\AA}$

Neutron Extraction

The neutrons stream out of the reactor through a series of tubes which conduct beams of **hot**, cold or thermal neutrons.



Neutron transport & Neutron Guides

Reflective Optics Mirrors and Super-Mirrors



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Neutron Transport – Neutron Guides

- Neutron Guides are used to transport neutrons over long distances (L ~ 100 m)
- Guides can increase the neutron flux at the sample by bringing more "divergence" to the sample.





Neutron Mirrors

Reflection/Refraction at Surfaces



Material	Nb (x 10 ³⁸ /m²)	θ_{c} (mrad)	
⁵⁸ Nickel	13.31	2.03	
Nickel	9.41	1.7	
Iron	8.2	1.62	
Copper	6.7	1.39	
Silicon	2.08	0.81	
Aluminium	2.08	0.81	





Increasing the angular acceptance of Mirrors

Single layer





Increasing the angular acceptance of Mirrors



Increasing the angular acceptance of Mirrors







Increasing the angular acceptance of Mirrors

- \rightarrow Significant increase in critical angle ($\theta_c = \lambda / 2d_{min}$)
- m Super-Mirror
- Gain in neutron flux
- Neutron Reflectivity

High contrast \rightarrow high reflectivity !









Ni/Ti Super-Mirrors

Still the most efficient

Neutron Reflectivity R \propto (N₁b₁-N₂b₂)²

- Ni Nb = 9.40 (10⁻⁶Å⁻²)
- Ti Nb = $-1.95 (10^{-6} \text{\AA}^{-2})$





Performances

- R > 80% for m = 4 Ni/Ti SM
- Gain factor m=4 / Ni mirror = 16 (2D)
- \succ but transmission T \propto Rⁿ !!

eg : for a 100 m long guide , at least ten reflections

 \rightarrow Transmission < 10% ...



- Neutron Guide at ILL
- Neutron guides are typically made by depositing the coating (Ni/Ti supermirror) on smooth glass substrates
- After coating, these substrates are joined together and aligned to make up the desired guide profile
- Curved guides are used in preference to avoid direct line of sight and then fast neutrons are not transmitted (small critical angle)

Production of Neutron Super-Mirrors

Deposition : Reactive DC Magnetron Sputtering



Sputtering machine (ILL) - Production 0.8 m² / day

Production

- > m= 4 : 1600 layers !
- Substrate : 0.5 cm thick Si wafers or
 0.2 cm thick Glass/Si/Sapphire







Diffractive Optics Crystal Monochromators





Crystal for neutron monochromator

- > To select a given wavelength band according to the Bragg's Law $2 d_{hkl} \sin \theta_B = n \lambda_0$
- \blacktriangleright To match the neutron beam divergence α which is typically 0.2°-1°
- Perfect crystal is not suitable since reflection range is in the order of 0.005° << α



- The neutron flux is proportional to integrated reflectivity $R(\lambda_0)$. β (*R* : neutron peak reflectivity at λ_0)
- The Resolution is given by $\Delta \lambda / \lambda_0 = \cot \theta_{\rm B} \cdot \Delta \theta \sim \cot \theta_{\rm B} \cdot \beta$
- \succ Choice of mosaic β is always a compromise between flux and resolution !

Mosaic crystals for neutron monochromators at ILL

- Mosaic crystals should have high neutron reflectivity, low background and small attenuation
- \succ Large single crystals must be available \rightarrow ILL production !

Crystal	orientation	Crystal Mosaic	Neutron Energy	Application	Supplier
C (graphite) d ₀₀₂ = 3.35 Å	HOPG(002)	0.5°- 3°	Cold Thermal	High flux	Momentive
Cu d ₁₁₁ = 2.08 Å	(111) (220) (200) (331)	0.05° - 3°	Hot Thermal	High resolution or high flux	ILL
Si d ₁₁₁ = 3.13 Å	(111) (113)	bent 0.2°- 0.5°	Cold Thermal	High resolution	ILL
Ge d ₁₁₁ = 3.26 Å	(111) (113) (115)	< 0.25°	Cold Thermal	High resolution	ILL
Heusler Cu₂MnAl	(111)	0.2°- 0.6°	Thermal	Polarized Neutrons	ILL



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Production of mosaic crystals at I.L.L. Control of the mosaic distribution by plastic deformation



- Growth of large Cu single (8 kg) crystals performed at ILL
- Production of high quality Cu(220) and Cu(200) single crystals with a controlled mosaic distribution



Production of "mosaic" Si crystals at I.L.L. Si crystal exhibits excellent properties for neutrons applications

- \blacktriangleright No $\lambda/2$ contamination, low attenuation factor, no parasitic scattering
- Use of elastically bent perfect crystals to produce effective mosaic distribution



Stack of thin Si blades to allow bending

- wafer thickness = 1 mm
- 10 wafers to get t = 10 mm (or more)
- Curvature : flat to $R_H \approx 2 \text{ m}$



Effective mosaic δ (rad) $\delta = \cot(\theta_{\rm B}) t / R$

t = total crystal thickness R = radius of curvature $\theta_{\rm B}$ = Bragg angle (ex: $\theta_{\rm B}$ = 30°, t=10mm, R=2m -> δ = 0.5°)







We need also Focusing Devices ...



➢ Focusing devices are used to increase the neutron flux at the sample position. However, the increase of neutron flux implies a degradation of the angular resolution (Liouville's theorem !)





A Neutron Monochromator is a big device...



Double Focusing Cu Monochromator

- Effective Area 300 x 165 mm²
- 165 Cu mosaic crystals
- Crystal size = 20 x 19.8 mm2
- ¹⁰B₄C plate is used to reduce background and activation





Monochromator for neutron diffractometers... Elastic Scattering



Double face monochromator Cu(200) and HOPG

Cu(200) - λ = 1.2 Å crystal mosaic = 0.25 °

HOPG (002) - λ = 2.4 Å crystal mosaic = 0.5 °

HOPG monochromator

- Total Area : 120 x 84 mm²
- Crystal dimensions : 42 x 8 mm²
- Neutron flux **5.10⁶ n/cm²/s** (at 2.4 Å)
- Low Resolution $\Delta \lambda / \lambda = 3\%$

Cu monochromator

- Total Area : 120 x 84 mm²
- Crystal dimensions : 42 x 8 mm²
- Neutron flux 2.10⁶ n/cm²/s (at 1.2 Å)
- Good Resolution $\Delta \lambda / \lambda = 1\%$



Monochromator for triple axis spectrometers Inelastic Scattering experiments

- Optimization of instrument performances for a wide energy range
- Double variable Focusing monochromator is used in combination with virtual source



Monochromator

- Optimization of the neutron flux
- Optimization of the Energy Resolution
- L₁ = L₂ (Rowland Geometry)

Analyzer

- Energy Analysis after Inelastic Scattering
- \blacktriangleright $\Delta E = E_i E_f = \hbar \omega$

Monochromator and analyzer should be composed of the same material (i.e. HOPG-HOPG or Cu-Cu)



Monochromator for triple axis spectrometers

Double variable Focusing Monochromators



Cu(220) monochromator Effective Area 300 x 165 mm² hot and thermal neutrons flux : 5.10⁸ n/cm²/s at (at 1.5 Å)



HOPG monochromator Effective Area 300 x 165 mm² cold and thermal neutrons flux : 10⁹ n/cm²/s at (at 1.5 Å)



Si monochromator Effective Area 250 x 200 mm² cold and thermal neutrons flux : 10⁸ n/cm²/s at (at 2 Å)



Polarized neutron beams



Polarizing Devices

- Polarization efficiency P
- Good Transmission of the desired spin state
- Angular acceptance, absorption and reflection
- Guide field is necessary to transport the polarization to the sample area



 $P = \frac{N_{+} - N_{-}}{N_{+} + N_{-}}$

Principal methods

- Fe/Si and Co/Ti super-mirrors (reflection, transmission)
- Heusler Cu₂MnAl crystal (diffraction)
- ³He3 spin filters (absorption by polarized ³He nuclei)



 N_+ neutrons with $|\uparrow>$

 N_{-} neutrons with $|\downarrow>$

Polarizing crystal monochromators Heusler Cu₂MnAl single crystal



Bragg reflection

from a ferromagnetic crystal

• $|\uparrow > : I^+ \propto [F_N(Q) + F_M(Q)]^2$

$$|\downarrow > : I^{-} \propto [F_{N}(Q) - F_{M}(Q)]^{2}$$

 $F_N(Q)$ nuclear structure factor $F_M(Q)$ magnetic structure factor

Polarization $F_N(Q) = \pm F_M(Q)$



Polarizing crystal monochromators Heusler Cu₂MnAl single crystal





Cubic structure L₂₁

- Structures Factors reflection(111)
- Nuclear: $F_{111N} = 4 (b_{Mn}-b_{Al})$ ($F_{111N} = -2.8 \ 10^{-12} \ cm$)
- Magnetic: $F_{111M} = 4 p_{Mn}$ ($F_{111M} = 2.78 \ 10^{-12} \ cm$)





• (111) reflection	$F_{111N} = - F_{111M}$		
• mosaic	0.2° < fwhm < 0.6°		
Reflectivity	$R_{experimental} \approx R_{theoretical}$		
 Polarization 	P > 92 %		



Polarizing Super-Mirrors Co/Ti & Fe/Si Super-Mirrors





Polarizing Super-Mirrors

- Co/Ti Super-Mirrors
- $|\uparrow>: N(b+p)_{Co} = 6.55;$ $|\downarrow>: N(b-p)_{Co} = -2.00 ≈ Nb_{Ti} = -1.95$
- m= 3.2 Super-Mirrors

but Activation of Cobalt ! (lifetime 5 Years)

- can be used only for polarization analysis
- Fe/Si Super-mirrors

 $|\uparrow>: N(b+p)_{Fe} = 13.04;$

- $|\downarrow>: N(b-p)_{Fe} = 3.08 \approx Nb_{Si} = 2.08$
- m = 4 super-Mirrors
- \rightarrow Polarizer in reflection / Transmission geometry





Fe/Si Polarizer

An advanced super-mirror solid state polarizer





Sputtering machine at ILL



Stack of Fe/Si SMs

Provides a "perfectly" polarized neutron beam

- Active area : 64 cm² (80 x 80 mm²)
- 800 m=3.2 Fe/Si/Gd Super-Mirrors coated on both sides of Sapphire substrate (t=0.2mm)
- Optimized magnet to provide a strong and homogeneous magnetic field of 0.4 T
- V geometry to ensure at least two reflections on the polarizing SMs (2 stacks of 400 SMs)
- ▶ P ≈ 99.7 % for the full bandwidth λ = [3-20 Å]
- > Transmission ≈ 30% (good spin state)

Neutron spin-Filters

³He spin filters

Absorption cross section of ³Helium nuclei

- > If the nuclear spin of He and the neutron spin are parallel, $\sigma_{a\uparrow\uparrow} \approx 0$
- > If the nuclear spin of He and the neutron spin are anti-parallel, $\sigma_a \uparrow \downarrow \approx 6000$ barns

For fully polarized gas ³He ($P_{He} = 1$), one spin state goes through the filter with zero absorption. The other spin state is almost fully absorbed since $\sigma = 6000$ barns \rightarrow **polarized neutron beam**







³He spin filter cell



Glass cell with Si windows (Small angle neutron scattering)







Production of ³He spin filters Metastability Exchange Optical Pumping (MEOP)





polarization of ³He nuclei using MEOP

³He filling station at I.L.L.



Production of ³He spin filters Metastability Exchange Optical Pumping (MEOP)







Optical Pumping Cells

³He Compressor

³He Cell place



Neutron spin-Filters ³He spin filter cells

- Polarization of ³He is time dependent: $P(t) = exp(-t/T_1)$
 - *T_w* : *Relaxation due to interactions with the cell*
 - T_d : Dipolar relaxation among ³He nuclear spins
 - *T_m* : *Relaxation due to field gradients*

$$\frac{1}{T_1} = \frac{1}{T_d} + \frac{1}{T_w} + \frac{1}{T_m}$$

$$T_m[h] = \frac{P[b]}{7000} \left(\frac{\partial B / \partial r[cm]}{B}\right)^{-2}$$

- The total relaxation time T_1 must be in the order of 100 hours to perform high quality neutron experiments
- \succ High quality ³He spin filter cells (Polarization, T_w)
- > High quality magnetic devices to produce homogeneous magnetic field : $\left(\frac{\partial B / \partial r}{B}\right) < 10^{-3} cm^{-1}$



Conclusion

Neutron Optics define beam properties

- Direction, Divergence, Wavelength, Energy, Polarization
- Angular Resolution, Wavelength resolution, Energy resolution
- Vertical focusing devices allow the optimization of the neutron flux at the sample position
- Double variable focusing devices allow the optimization of instrument performances for a wide energy range
- Since the power of the source is low and neutron beams are divergent , neutron optical components must be of high quality and properly designed
- Neutron Optics obey to Liouville's Theorem : It costs flux to increase resolution and it costs resolution to increase flux

The optimization of instrument performances is always a compromise between flux and resolution



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Thank you for your attention



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