PAUL SCHERRER INSTITUT


Markus Strobl :: Applied Materials Group :: LNS :: Paul Scherrer Institut

# Some thoughts concerning condensed matter science instrumentation with VCN

VCN/UCN HighNESS workshop, ESS, Feb 2022

PAUL SCHERRER INSTITUT

# Outline

- Introduction
- Previous workshops
- SANS
- NR
- QE/INS
- NSE
- Imaging

# Optics

**basic properties of VCNs making their use appealing if they can be generated in significant quantities**

- The index of refraction *n* of neutrons approaches significant deviations from 1 only in the VCN range. The **refracting power of a material *n*-1 (~ $\lambda^2$) is typically in the range of $10^{-6}$ for thermal neutrons, but $10^{-4}$ in the VCN range**

  - total **angle of reflection from a surface is proportional to $\lambda$**
  - **deflection angle in a prism is proportional to $\lambda^2$**
  - **focal length of a focusing lens is proportional to $1/\lambda^2$**
  - The extreme absorption of VCNs for certain isotopes (6 Mbarn for $^{157}$Gd) combined with the very low absorption for elements like Si, Al, and O (around or less than 1 barn at 20 Å) allow the **design of highly precise optical components similar to light optics**. Near-perfect null-scattering highly-absorbing mixtures can be made.

# Scattering

**basic properties of VCNs making their use appealing if they can be generated in significant quantities**

- VCNs, with their **kinetic energies in the sub-meV range**, are well-suited for exploring the **dynamics of soft matter**, as their typical energies of motion are in the same range, thereby enhancing the relative change in energy upon scattering as compared to using thermal or cold neutrons.

- The correlation lengths of beams scale with $\lambda$ in the lateral direction and with $\lambda^2/\Delta\lambda$ in longitudinal direction, where $\Delta\lambda$ is the $\lambda$-bandwidth of the beam. The longitudinal correlation length prepared in **NSE** instruments is proportional to $\lambda^3$; and the lateral correlation length in **SESANS** is proportional to $\lambda^2$

# Scattering

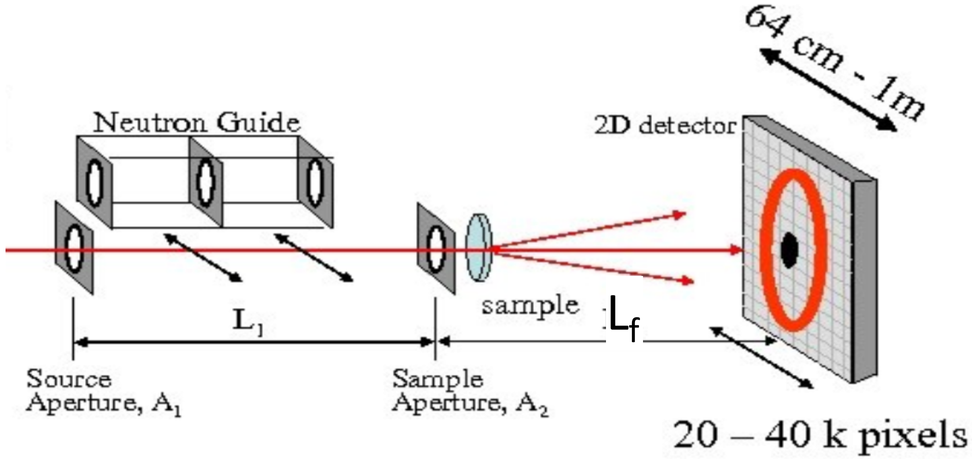
**basic properties of VCNs making their use appealing if they can be generated in significant quantities**

• VCNs, with their kinetic energies in the sub-meV range, are well-suited for exploring the dynamics of soft matter, as their typical energies of motion are in the same range, thereby enhancing the relative change in energy upon scattering as compared to using thermal or cold neutrons.

• The correlations lengths of beams scale with $\lambda$ in the lateral direction and with $\lambda_2/\Delta\lambda$ in longitudinal direction, where $\Delta\lambda$ is the $\lambda$-bandwidth of the beam. The longitudinal correlation length prepared in **NSE** instruments is proportional to $\lambda^3$; and the lateral correlation length in **SESANS** is proportional to $\lambda^2$

• Their wavelength makes VCNs very powerful for the exploration of the structure of the nanometer-scaled world. **Larger complexes in biology** will be a main target for new VCN instruments → **smaller Q**

# SANS




Sizes of interest = "large scale structures" = 1 – 300 nm or more

$0.02 < Q \sim 2\pi/d < 6$

$Q = 4\pi \sin\theta / \lambda$ 3-5< $\lambda$ <20A and 0.1 < $\theta$ <20

Generally long wavelength flux = efficiency limitation

$$Q_{min} = \frac{8\pi r_s}{\boxed{\lambda_{max}} L_f}$$

What about gravity?

$r_s$ sample aperture radius, $L_f$ final flight path, $\lambda_{max}$ maximum wavelength

$$Q_{max} = \frac{2\pi r_{max}}{\boxed{\lambda_{min}} L_f}$$

$r_{max}$ distance center of the scattering pattern to farthest detector pixel $\lambda_{min}$ minimum wavelength

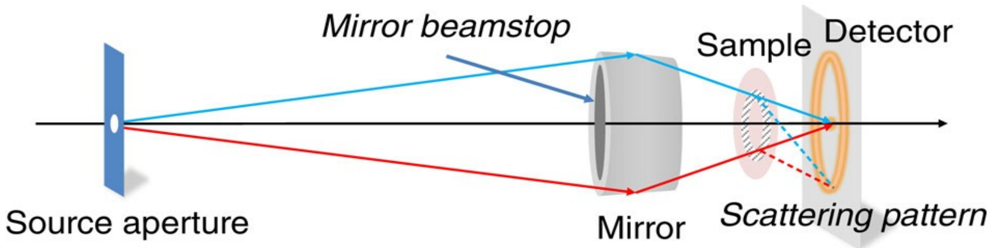
# REMINDER: Optics

**basic properties of VCNs making their use appealing if they can be generated in significant quantities**

- The index of refraction *n* of neutrons approaches significant deviations from 1 only in the VCN range. The **refracting power of a material *n*-1 (~ $\lambda^2$) is typically in the range of $10^{-6}$ for thermal neutrons, but $10^{-4}$ in the VCN range**

  - total **angle of reflection from a surface is proportional to $\lambda$**
  - **deflection angle in a prism is proportional to $\lambda^2$**
  - **focal length of a focusing lens is proportional to $1/\lambda^2$**
  - The extreme absorption of VCNs for certain isotopes (6 Mbarn for $^{157}$Gd) combined with the very low absorption for elements like Si, Al, and O (around or less than 1 barn at 20 Å) allow the **design of highly precise optical components similar to light optics**. Near-perfect null-scattering highly-absorbing mixtures can be made.

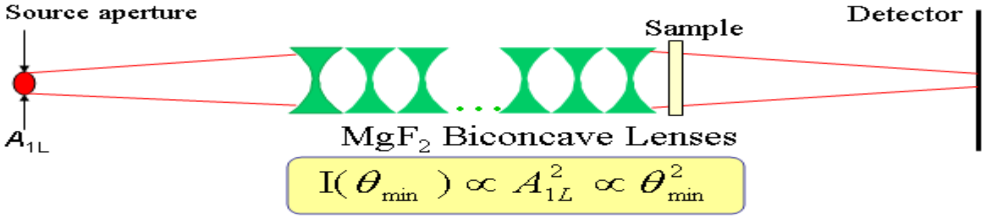
# Focusing SANS




Sizes of interest = "large scale structures" = 1 – 300 nm or more

$0.02 < Q \sim 2\pi/d < 6$

$Q = 4\pi \sin\theta / \lambda$ 3-5< $\lambda$ <20A and $0.1 < \theta < 20$




+ VCN higher divergence transported
+ More efficient optics

$$Q_{min} = \frac{\boxed{8\pi r_s}}{\boxed{\lambda_{max}} L_f}$$

$r_s$ sample aperture radius, $L_f$ final flight path, $\lambda_{max}$ maximum wavelength

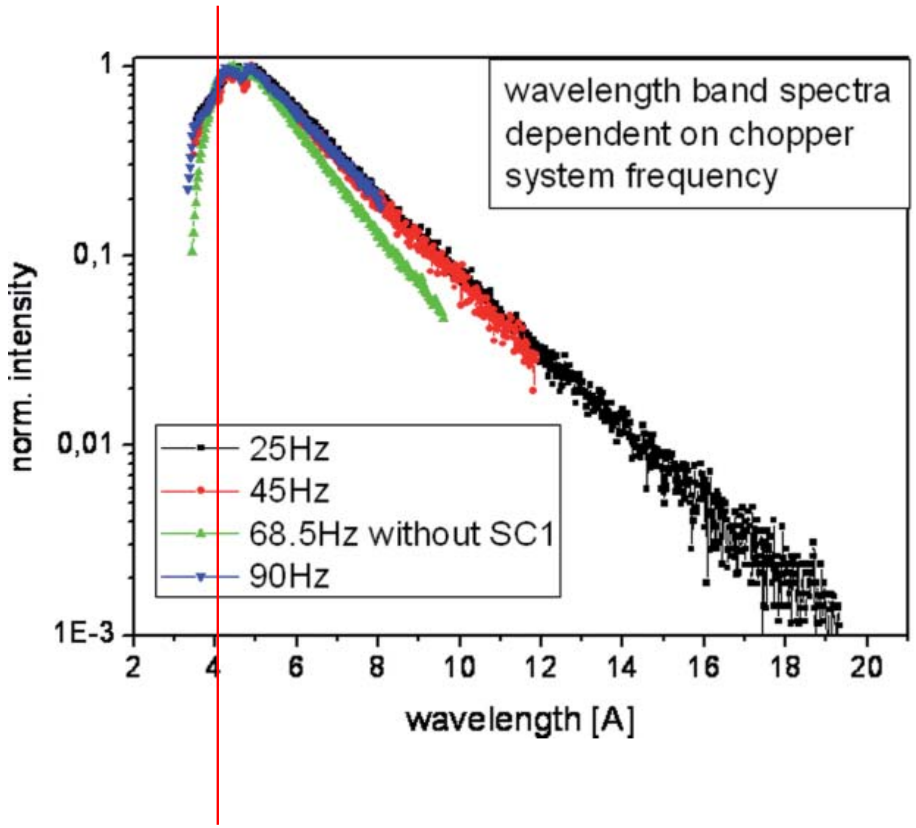
What about gravity?

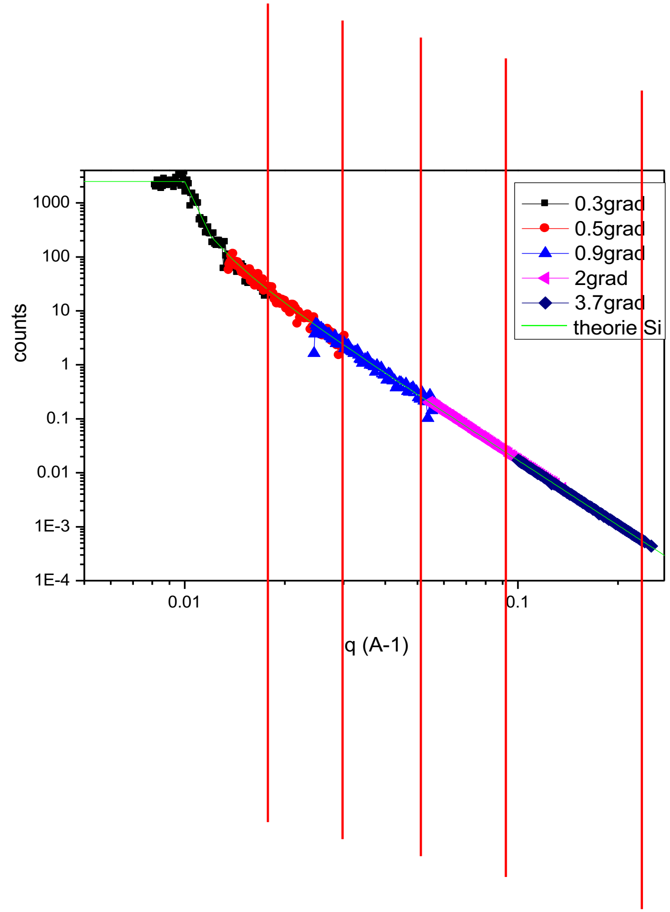
$$Q_{max} = \frac{2\pi \boxed{r_{max}}}{\boxed{\lambda_{min}} L_f}$$

$r_{max}$ distance center of the scattering pattern to farthest detector pixel $\lambda_{min}$ minimum wavelength

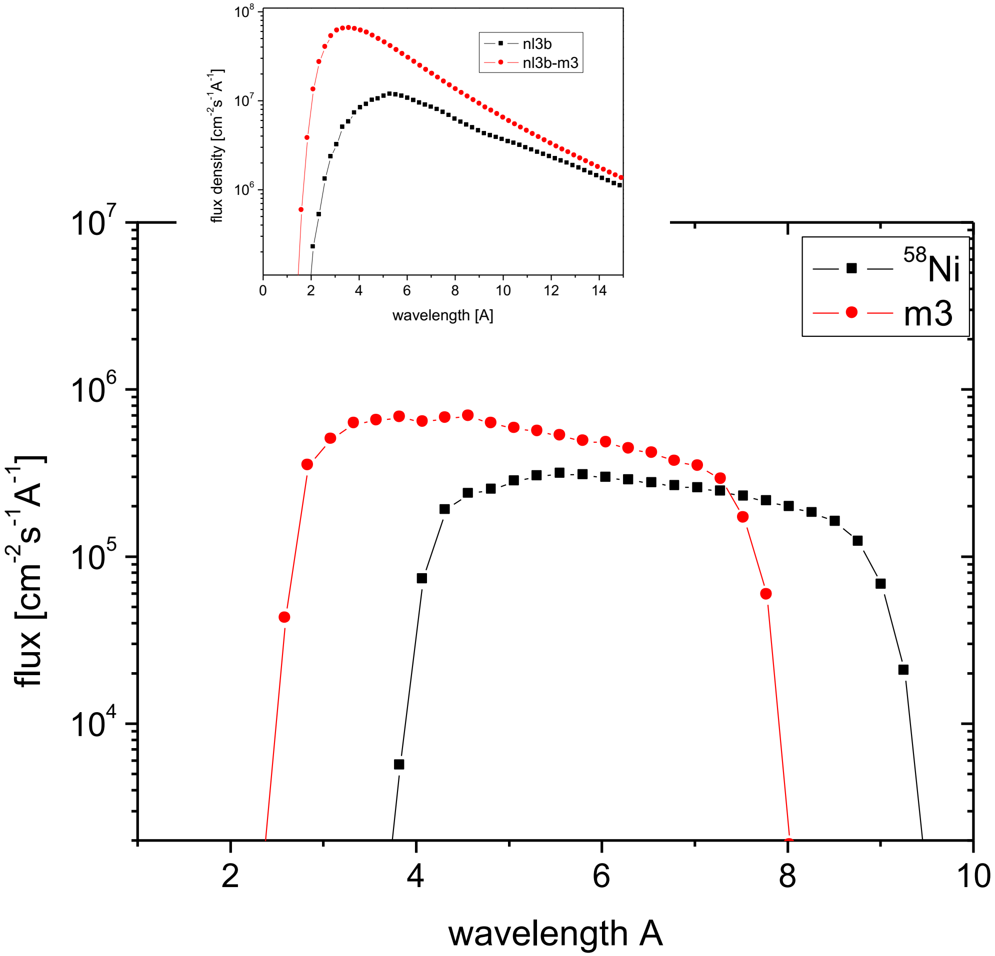
# Reflectometry

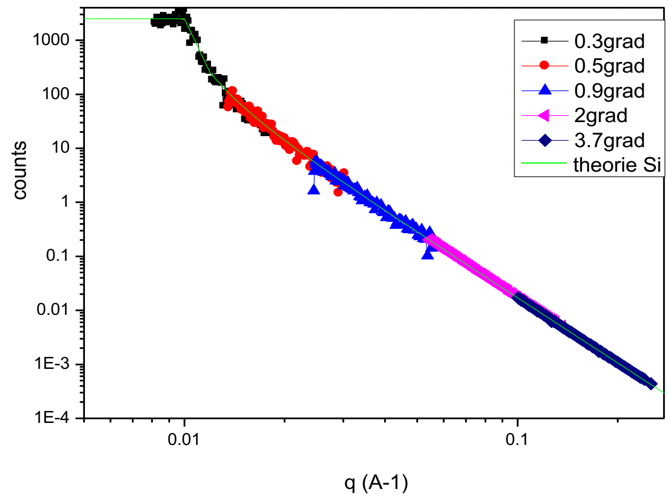
## Efficiency cut-off

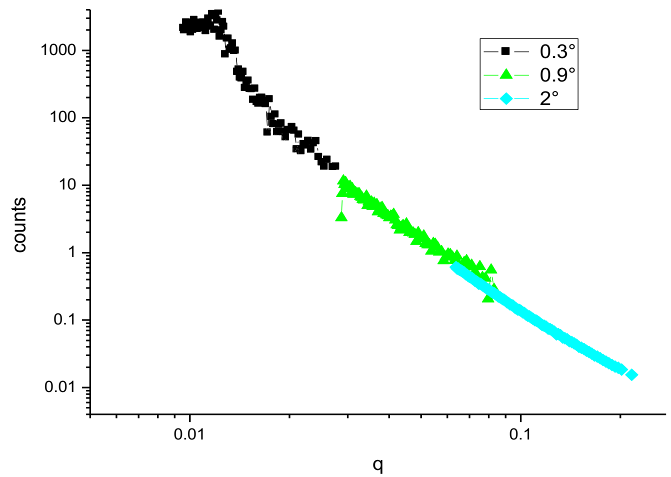


# Reflectometry



# Gains

- Gains calculated in ANL work shop VCN long pulse vs CN continuous
- Excessive resolution at very long wavelengths not considered

- This and bandwidth require e.g. a very short instrument → limitations

Shielding
Installations
background

# VCN workshop at ANL 2005

Very cold neutrons (VCNs, with temperatures around 1 – 10 K or wavelengths λ around 14 – 40 Å) are not typically used to explore matter

existing neutron sources: their spectral temperatures are either in the thermal range near 300 K or in the cold range near 30 K so that the phase space density of the Maxwellian distribution of wavelengths decreases as $1/\lambda^5$

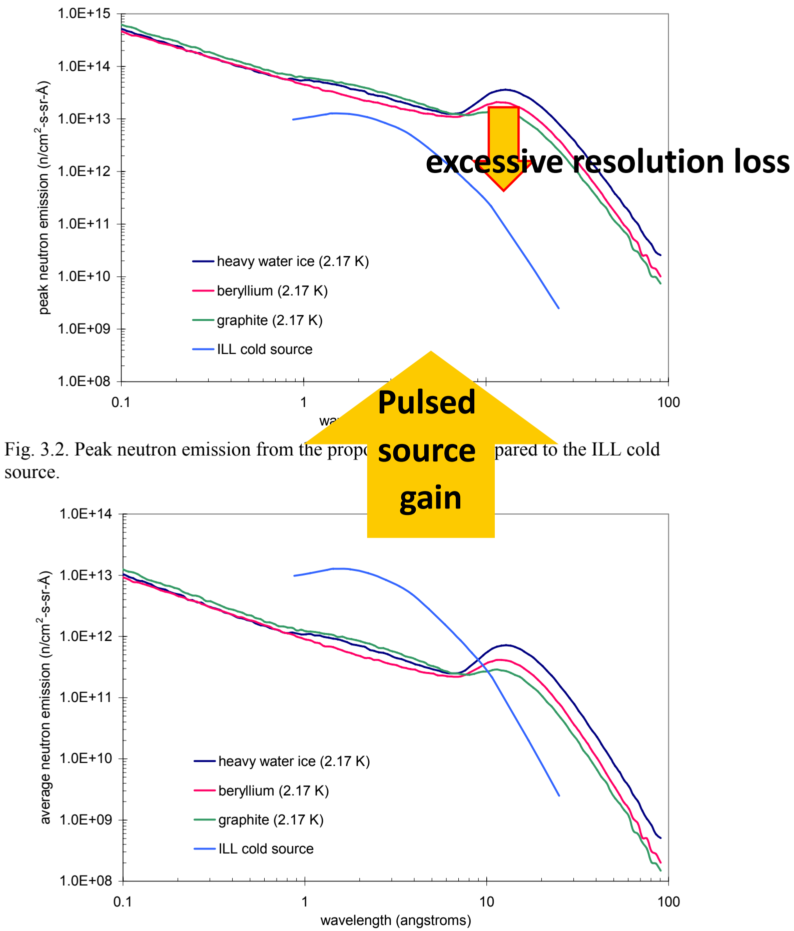
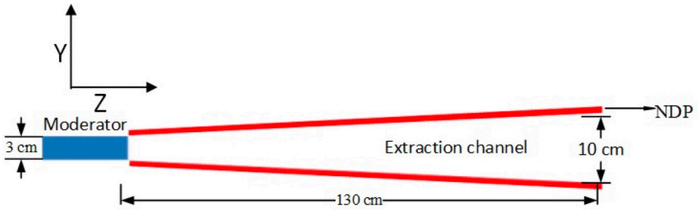


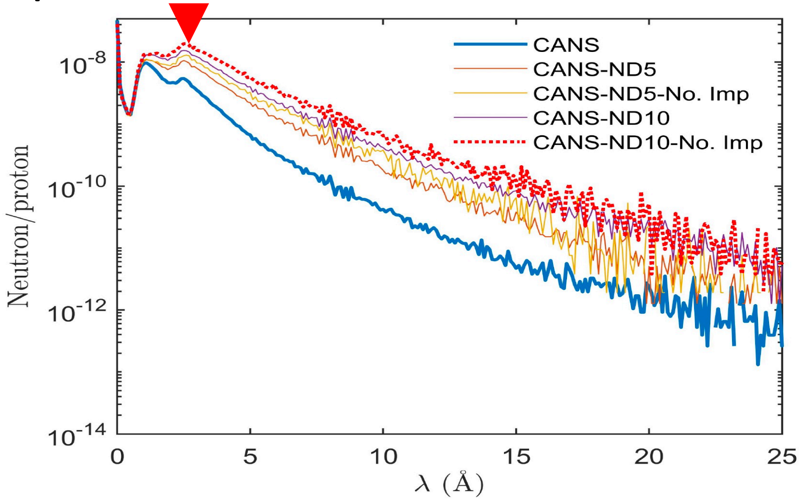

Fig. 3.3. Time-average neutron emission from the proposed VCNS (operating at 5 Hz) compared to the ILL cold source.

# VCN workshop at ANL 2005

## In contrast: HighNESS
## e.g. nano-diamond extraction reflector




**Cold spectral peak remains**



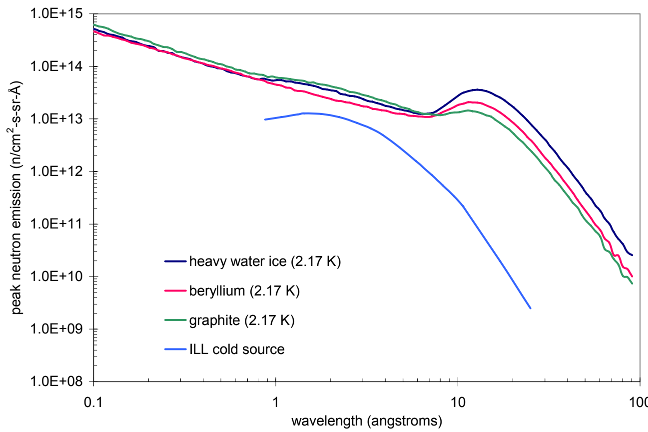




Fig. 3.2. Peak neutron emission from the proposed VCNS compared to the ILL cold source.

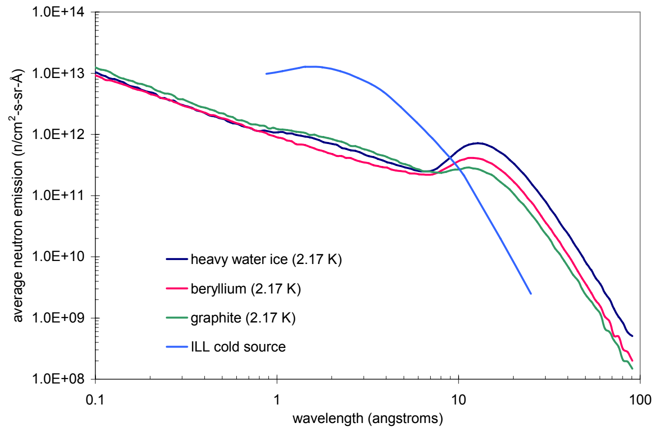



Fig. 3.3. Time-average neutron emission from the proposed VCNS (operating at 5 Hz) compared to the ILL cold source.

# VCN workshop at ANL 2005

Assuming 0.3 MW source power and an order of magnitude gain in VCN production efficiency at 20 Å

estimated gains in experimental efficiency of

- 5 for SANS and NSE compared to present, best-in-class instruments at ILL. Similarly, we expect a gain of
- 30 for quasielastic and low-energy TOF-INS.

A source with a repetition rate in the range of **1 to 5 Hz** and an accelerator pulse width of a **few ms** is well-adapted to the use of VCNs in a pulsed mode for many instruments.

→ however, now we need compare to ESS 1st moderator, but 5MW

# VCN workshop at ANL 2005

We consider the following existing instrument types as the ones that can benefit most from being used at a VCN source:

- long-baseline SANS instruments,
- reflectometers (for both horizontal and vertical geometry),
- high-resolution TOF instruments
- spin-echo spectrometers
- SESANS techniques

The gain factors for inelastic instruments like **TOF- INS and NSE scale with $\lambda^2$**;

however, for **elastic instruments like reflectometers and SANS instruments, gain factors generally are independent from $\lambda$**, as long as the wavelength distribution follows the $1/\lambda_5$ tail of a cold spectrum.

→ SANS resolution

# Conclusion

For pulsed VCN sources, the following gains can be assumed for resolution and intensity:

| | resolution at fixed geometry | Intensity at fixed resolution |
|---|---|---|
| SANS | $\lambda^{-1}$ | $\lambda^{0}$ |
| Reflectometry | $\lambda^{-1}$ | $\boxed{\lambda^{2}}$ doubt it |
| TOF-INS | $\lambda^{-3}$ | $\lambda^{2}$ |
| NSE | $\lambda^{-3}$ | $\lambda^{2}$-$\lambda^{4}$ |

**Other more speculative techniques** that may benefit from the use of VCNs are correlation spectroscopy with waveguides, VCN interferometry, VCN tomography, and neutron microscopy. Funding should be provided to explore these and other possibilities.

PAUL SCHERRER INSTITUT

# PSI 2006
# Quasi/In-elastic scattering

## A time lens for high resolution time of flight

*K. Baumann*, P. Grigoriev⁺, E. Kats⁺#, R. Gähler#,* **PRA 2005**

**TU München; #ILL Grenoble*
*⁺Landau Institute f. Theor. Phys. Moscow*

## Bunching of continuous polychromatic beams

*R. Golub*, R. Gähler#, K. Habicht⁺, S. Klimko#* **PLA 2005**

**Raleigh, North Carolina; #ILL Grenoble; HMI Berlin*

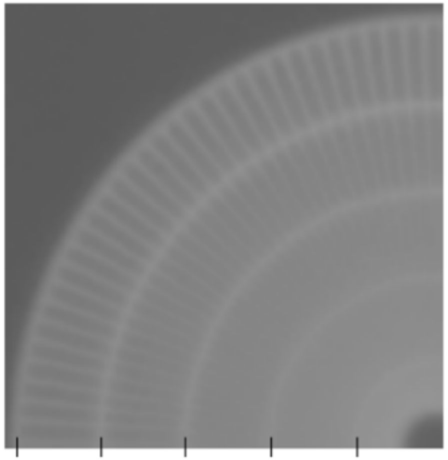
# PSI workshop 2006

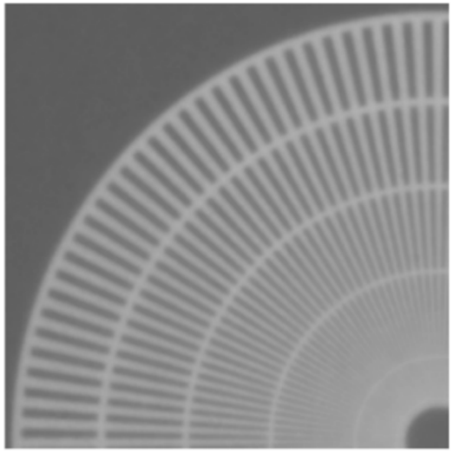
**2005 “more speculative techniques”**

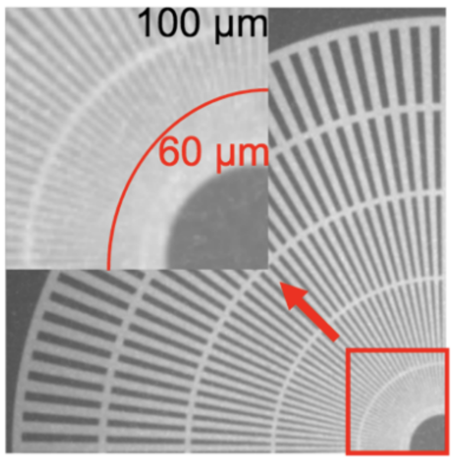
- This would also enable more detailed studies of VCN optics for applications in the complementary wavelength range below 30 Å. This later is the target of VCNS: to make optimal use of the extensions of neutron scattering methods in the wavelength range beyond 10 Å. **The most important applications would be: neutron microscopy (at the 50-100 nm scale) of biomolecular systems and nanocomposites with complex surfaces and buried structures;** holography of hydrogenous minerals and biological materials; nanoscale self-organization in geometrically frustrated magnets; spectroscopic studies of solar absorption in photoelectrochemical cells; structures of biological membranes and devices based on nanodots and nanotubes.

# Imaging Resolution

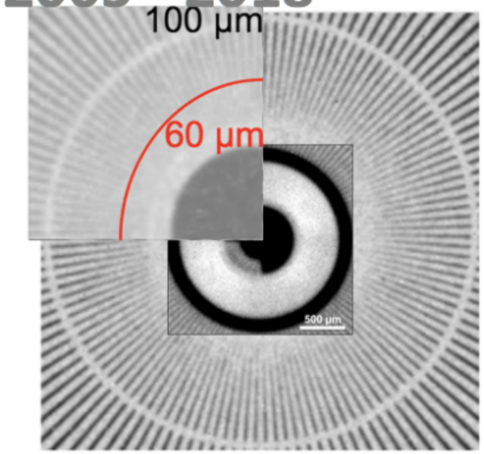
## 2000 - 2010

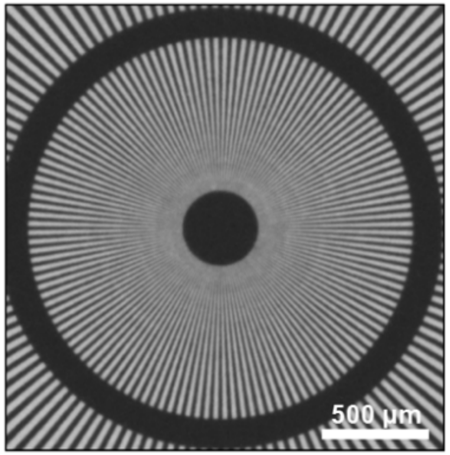


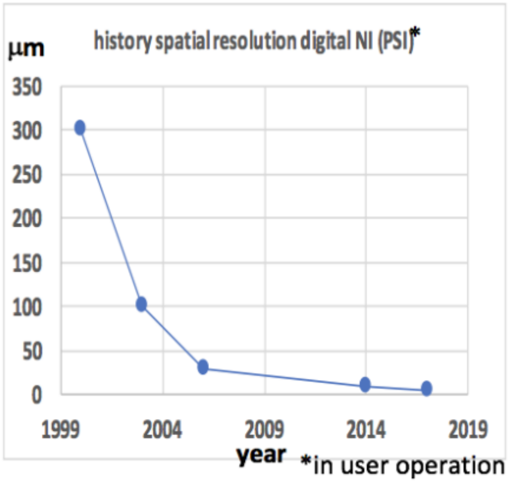




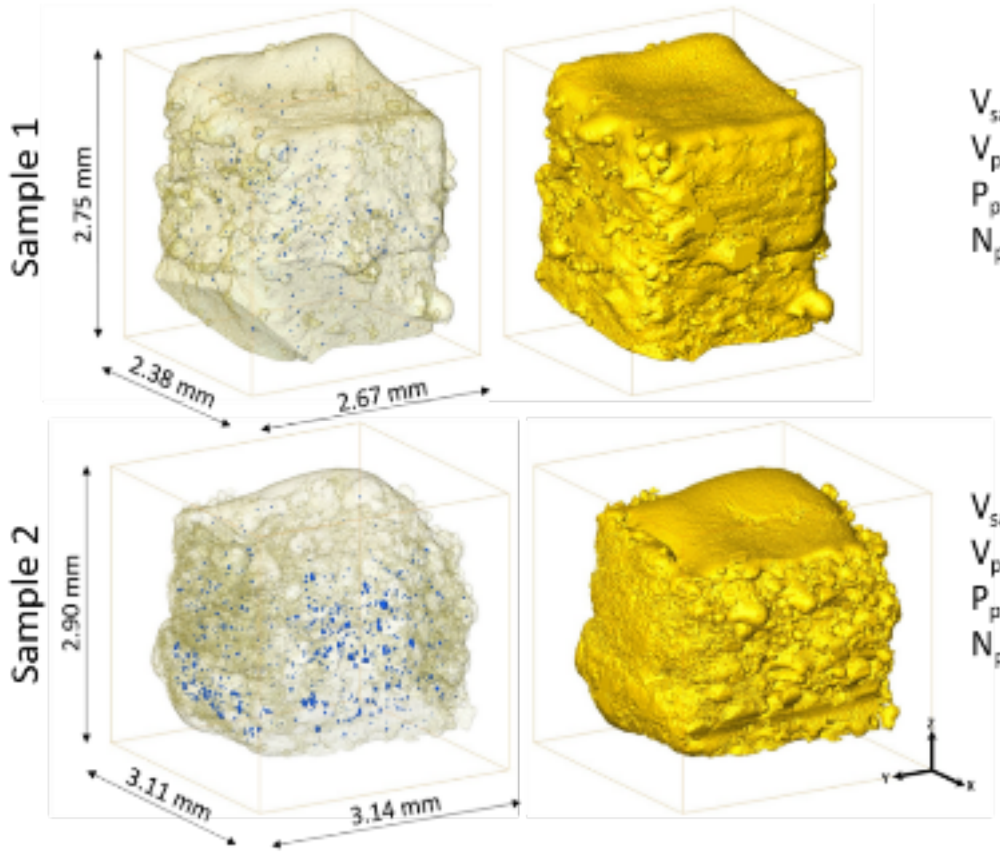

## 2005 - 2018



# Neutron Imaging → microscopy

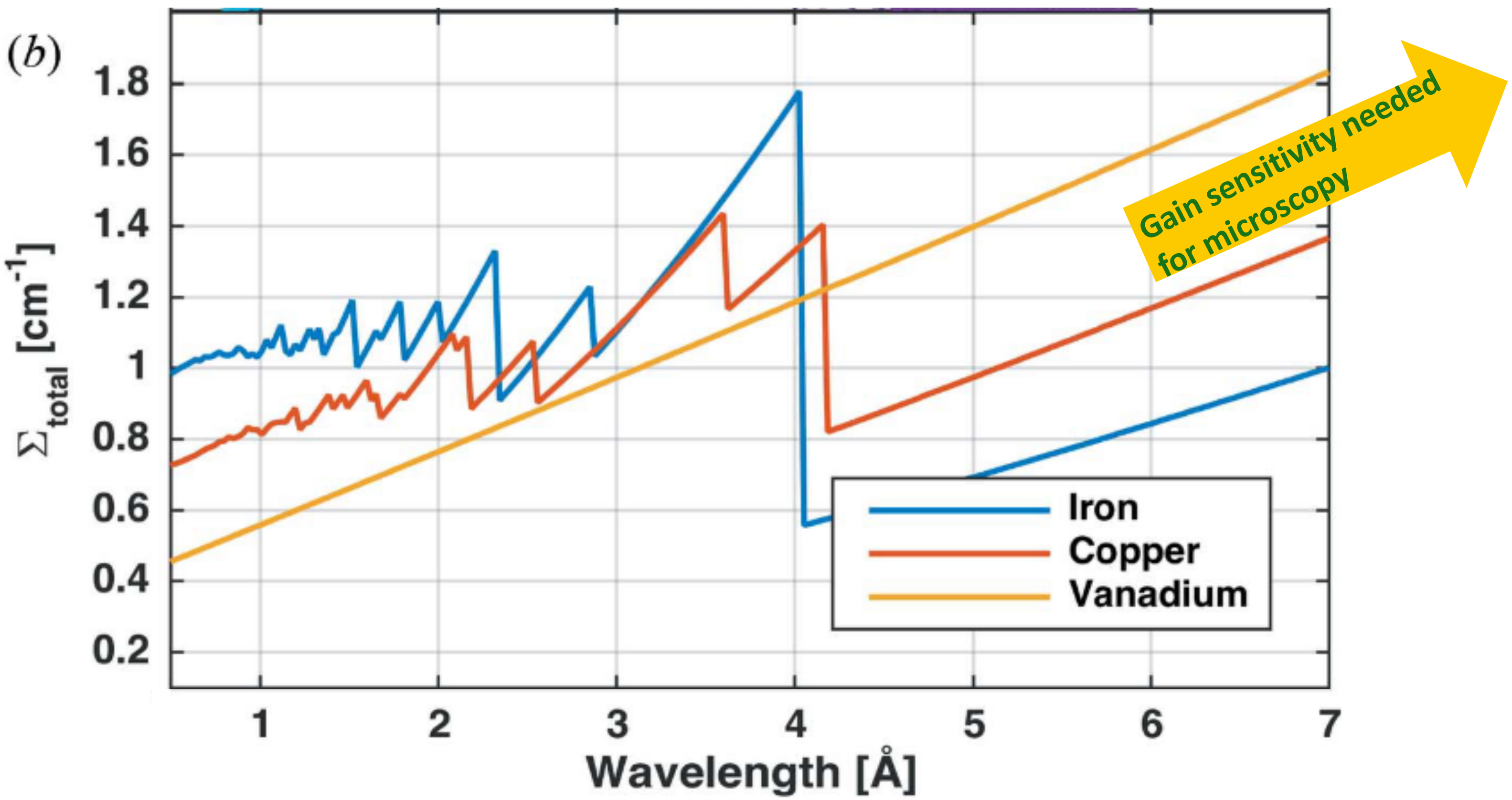



$V_{sample}$ = 9.5585 $mm^3$
$V_{pores>10\mu m}$ = 0.0012 $mm^3$
$P_{pores>10\mu m}$ = 0.012 %
$N_{pores>10\mu m}$ = 625

$V_{sample}$ = 13.2211 $mm^3$
$V_{pores>10\mu m}$ = 0.0062 $mm^3$
$P_{pores>10\mu m}$ = 0.047 %
$N_{pores>10\mu m}$ = 1226

H. Ghasemi-Tabasi et al. Applied Sciences 202 (2021) 1512

# Neutron Imaging



# Neutron Imaging → microscopy

Currently only highest absorbing materials suited for microscopy

→ VCN significant improvements

→ In addition potential neutron microscopy optics

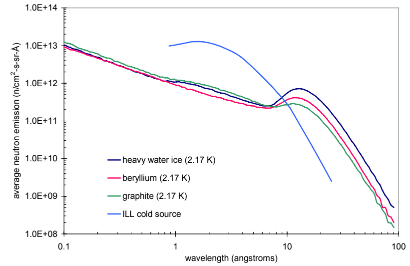
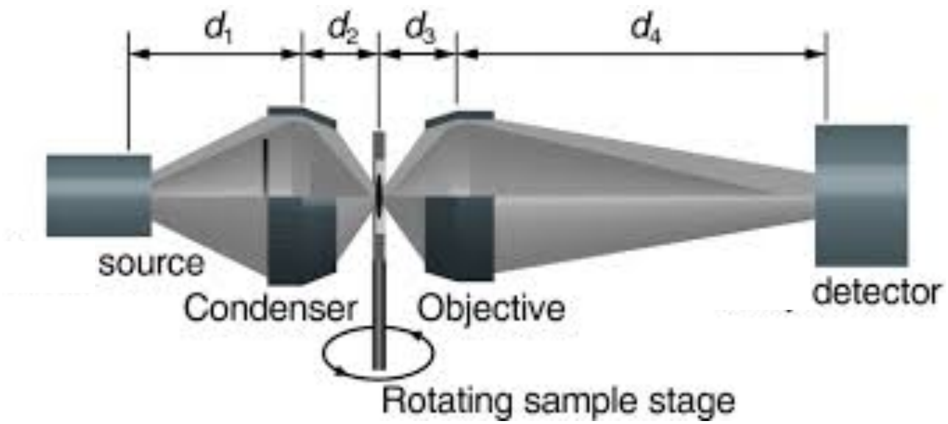
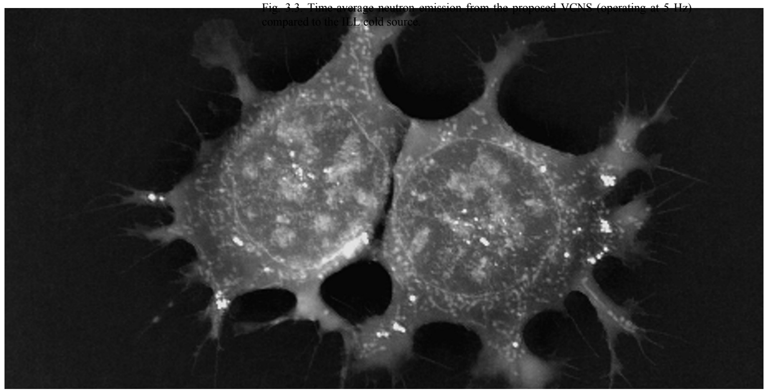



Fig. 3.3. Time average neutron emission from the proposed VCNS (operating at 5 Hz) compared to the ILL cold source.



PAUL SCHERRER INSTITUT

# Wir schaffen Wissen – heute für morgen