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- I Nanoscience and neutron fluxes**
  - a) What neutrons cannot do**
  - b) What neutrons can do**
  
- II Some scientific and experimental perspectives**
  
- III Some far-future perspectives**



# GENNESYS



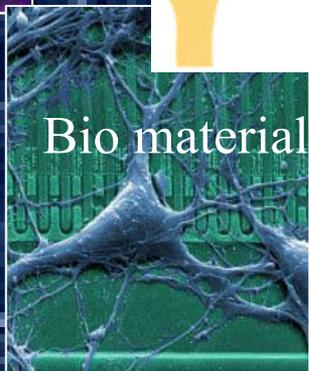
Grand European Initiative on Nanoscience and Nanotechnology using Neutron and Synchrotron Sources



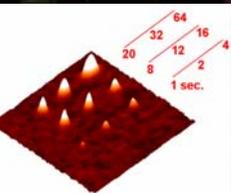
Aerospace



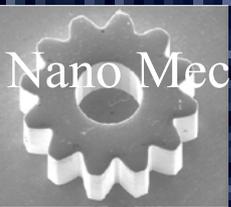
Functional materials



Bio materials



Nanomaterials  
Nanotechnology



Nano Mechanics

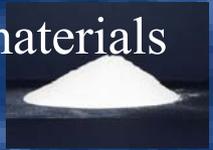


Nano Devices



Nano Synthesis

Struct. materials

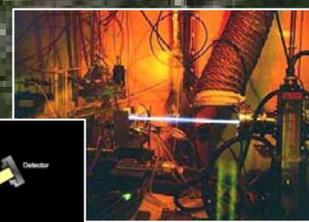
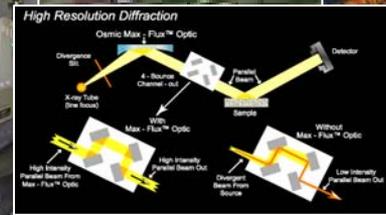
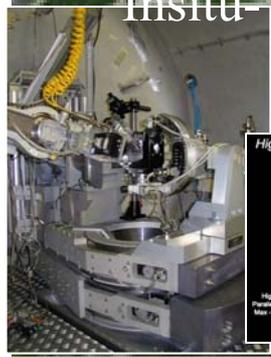


GAP



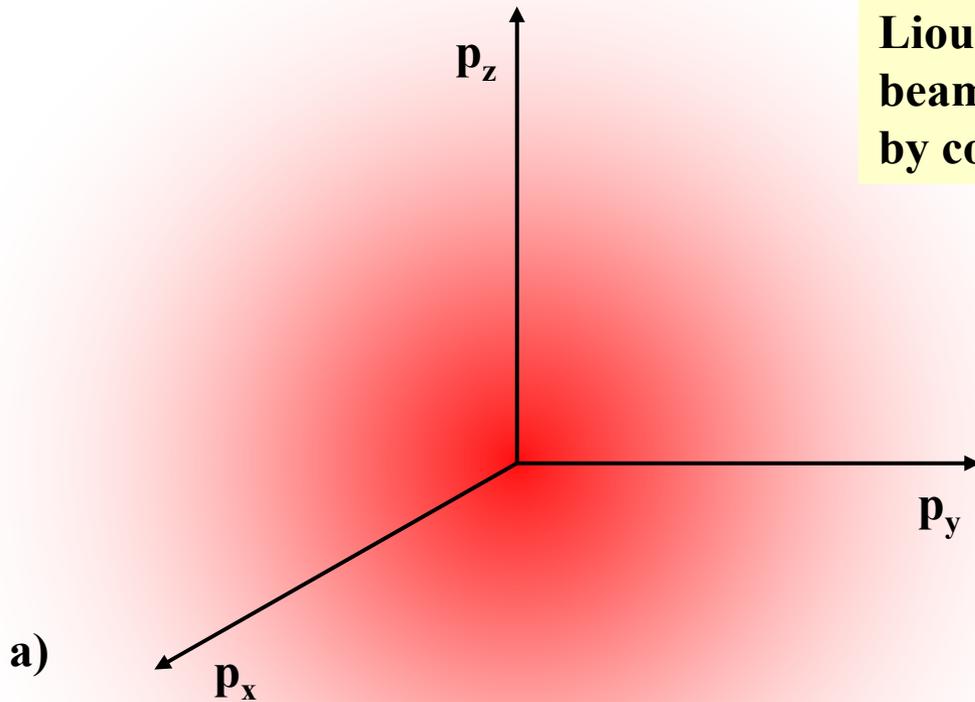
Infrastructures  
Synchrotron Radiation  
and  
Neutron Facilities

Detection  
Monitoring  
High-resolution analysis  
Insitu-control



The phase space density (in 6D) of a thermal source is constant in the centre.  
 It drops with  $\exp(-E/kT)$ ;  $E = p^2/2m$

**Liouville's theorem: The phase space density of a beam of non-interacting particles can't be increased by conservative forces acting on the ensemble.**

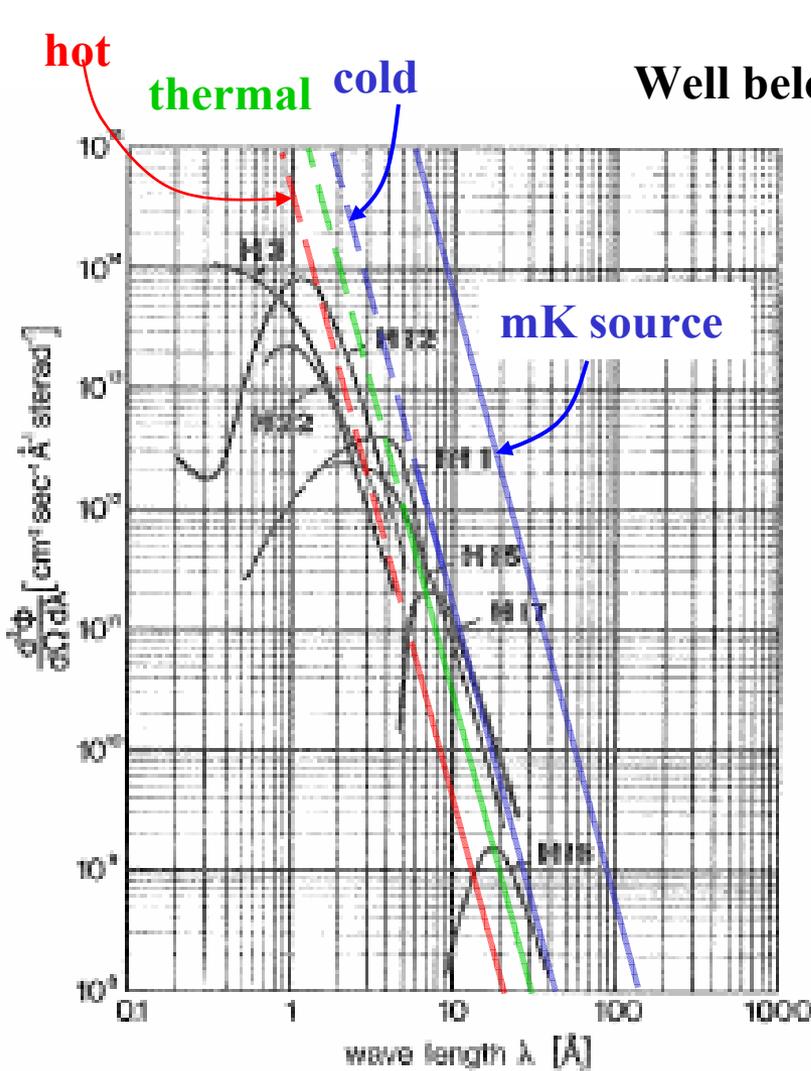


**Constant phase space density:**

- a) Imaging ( $|P| = \text{const.}$ )
- b) Acceleration ( $P_2^2 = P_1^2 + 2mE$ )

**Increase of phase space density**

- c) Cooling !
- d) Non-equilibrium production



The brilliance of ILL Grenoble

Well below  $kT$ : 
$$B = \frac{d^2\Phi}{d\lambda d\Omega} \approx \left(\frac{\lambda_0}{\lambda}\right)^5 \times N \left[ \frac{\text{neutrons}}{\text{cm}^2 \text{ s } \text{Å} \text{ sterad}} \right]$$

- $\approx 8 \cdot 10^{15}$  for cold source  $\lambda \odot 5\text{Å}$ ;
- $\approx 2 \cdot 10^{15}$  for thermal source  $\lambda \odot 3\text{Å}$ ;

$\lambda_0 = 1\text{Å}$

### Implications of Liouville's theorem:

- a) Imaging ( $|P| = \text{const.}$ ):  
Stay at the point of B where you are;
- b) Acceleration ( $P_2^2 = P_1^2 + E \cdot 2m$ ):  
Move along  $1/\lambda^5$  line;  $N = \text{constant}$ ;
- c) Cooling !  
Move the  $1/\lambda^5$  line to the right; increase N;

**\* Gain brightness by starting with a colder source and accelerating the beam;**

The mean brilliance of SNS will be less by a factor of  $\approx 3$   
the peak brilliance of SNS will be higher by a factor  $\leq 100$ ;

Can we examine single nanoparticles with neutrons?

The brilliance of a beam of non-interacting particles can't be changed if  $\langle \lambda \rangle = \text{const.}$

2 examples (for ILL brilliance):

**Diffraction:** Collimated beam of  $3 \text{ \AA} \pm 10\%$  and  $10^{-5}$  sterad :  
An area of  $10 \times 10 \text{ nm}^2$  is passed by **0.00005 n/s.**

**Imaging:** Focused microbeam of  $5 \text{ \AA} \pm 10\%$  and 1 sterad :  
An area of  $10 \times 10 \text{ nm}^2$  is passed by **2.6 n/s.**

The typical interaction probability along 10 nm is in the range of  $\approx 10^{-5}$ ;

**$\Rightarrow$  Direct examination of a single nano-particle is not possible at present neutron sources;**

The brilliance of a synchrotron (FEL) is  $\approx 14$  (17) orders of magnitudes above a n-source.

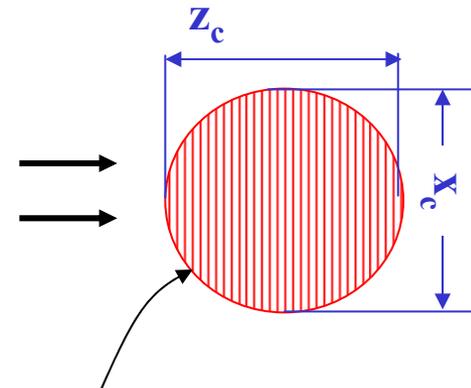
Neutron beams have just the right coherence volumes to observe the internal structure and the space/time correlations of ensembles of nanoparticles. But  $\mu\text{g} - \text{mg}$  are needed

**Lateral:**  $x_c = \frac{L}{k \cdot a} = \frac{\lambda}{2\pi} / \alpha$ ;  $\alpha = \text{'backward beam divergence'}$ ; **Longitudinal:**  $z_c = \lambda^2 / (2\pi \Delta\lambda)$ ; steady state beam

$$V_c \cdot \Delta p^3 = \text{const}^3$$

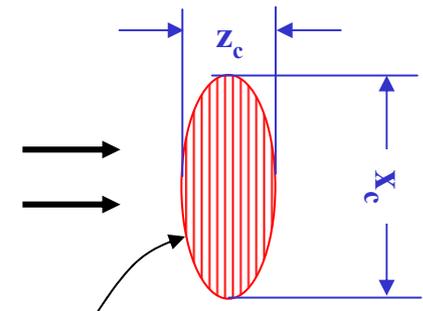
**Examples:**

**Diffraction:**  $x_c = y_c = 10 \text{ nm}$  for  $\lambda = 2 \text{ \AA}$  and  $\alpha \approx 4 \cdot 10^{-3}$ ;  
 $z_c = 10 \text{ nm}$  for  $\lambda = 2 \text{ \AA}$  and  $\Delta\lambda/\lambda \approx 6 \cdot 10^{-3}$ ;



make it spherical for equal resolution in all dimensions!

**SANS:**  $x_c = 10 \text{ (100) nm}$  for  $\lambda = 6 \text{ \AA}$  and  $\alpha = 10^{-2} \text{ (} 10^{-3}\text{)}$ ;  
 $z_c = 1 \text{ nm}$  for  $\lambda = 6 \text{ \AA}$  and  $\Delta\lambda/\lambda \approx 0.1$ ;



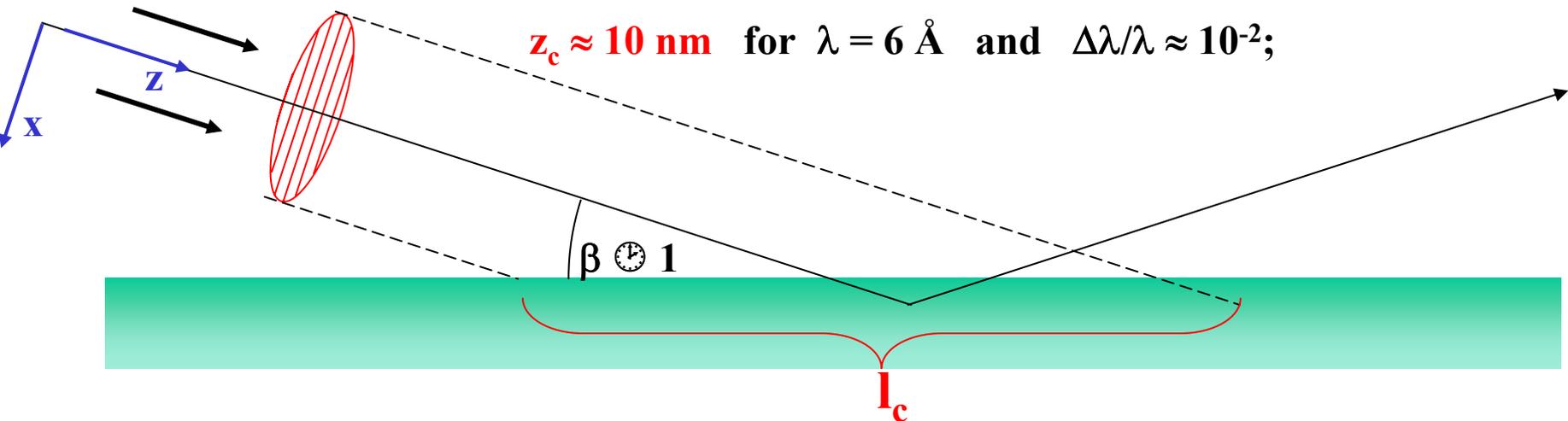
only lateral resolution counts!

## 3) Reflectometry:

$x_c \approx 100 \text{ nm}$  \* for  $\lambda = 6 \text{ \AA}$  and  $\alpha = 10^{-3}$ ; high resolution geometry

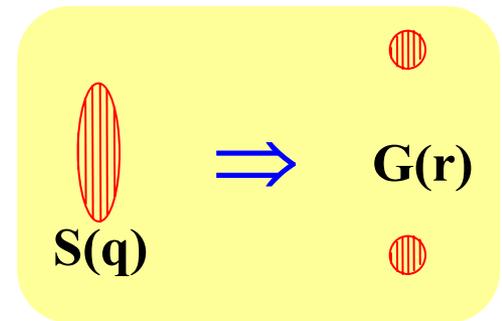
$y_c \approx 3 \text{ nm}$  for  $\lambda = 6 \text{ \AA}$  and  $\alpha = 3 \cdot 10^{-2}$ ;

$z_c \approx 10 \text{ nm}$  for  $\lambda = 6 \text{ \AA}$  and  $\Delta\lambda/\lambda \approx 10^{-2}$ ;



Along the beam direction, a length  $l_c \approx \beta \cdot x_c \approx 10000 \text{ nm}$  is probed! Time difference!  
 Normal to the surface, a length of  $\approx x_c$  is probed.

\* For more, split laterally the coherence volume!  
 => Sergis, NRSE, R. Pynn's magn. foils;



$$I \sim 1/V_c$$

Coherence times:

$$\tau = 1/(\mathbf{v} \cdot \Delta \mathbf{k})$$

Crystal Spectrometers ( $\Delta E = E_i - E_f = \hbar \omega$ )

$$\Delta E \geq 0.1 \text{ meV} \quad \tau \leq 6 \times 10^{-12} \text{ s}$$

$$\tau = t_0/(2\omega_0 T)$$

Time-Of-Flight Spectrometers

$$\Delta E \geq 10 \text{ } \mu\text{eV} \quad \tau \leq 6 \times 10^{-11} \text{ s}$$

$$\tau = 1/(\mathbf{v} \cdot \Delta \mathbf{k})$$

Backscattering Spectrometers

$$\Delta E \geq 1 \text{ } \mu\text{eV} \quad \tau \leq 6 \times 10^{-10} \text{ s}$$

$$\tau = \omega_L t_0/(2\omega_0)$$

Spin-Echo Spectrometers

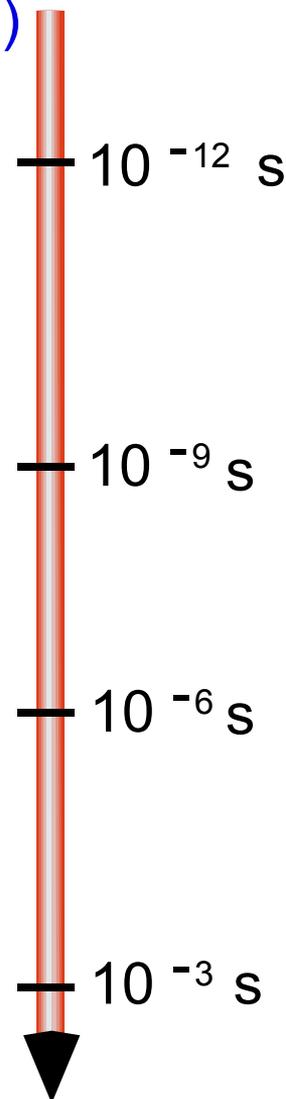
$$\tau \leq 10^{-7} \text{ s}$$

measuring the time modulation transfer function of a system

Time-Involved Small-Angle Neutron Experiments

Time-Slicing 'Snap Shots'

$$t \geq 10^{-1} \text{ s}$$



**Neutrons hardly ever do anything else than examining the nanoworld.**

**For magnetism on an atomic base, neutrons with their magnetic moment are the major tool.**

**Nanostructure of interfaces can be probed with high resolution; (new reflectometry method)**

**Fundamental properties of nano-fluids (in porous media) are explored with neutrons.**

**‘Going beyond the Bragg peak’ will be a major topic in n-diffraction.**

**The subtle electronic structure of nanoparticles is not disturbed by neutrons.**

**For biological samples, the controlled H-D exchange is the major tool for labeling.**

**On biological samples, neutrons only cause very low radiation damage.**

**Realistic environments for living matter can be realized.**

**Neutrons allow experiments at extreme sample environments.**

**Requested sample volumes may be reduced (1 – 3 orders of magnitude)**

**by  $4\pi$  analysis (this can only be done once)**

**by new techniques, using multi beams.**

**Using more correlation (spin echo) and modulation techniques will enhance resolution.**

**Using more correlation (spin echo) and modulation techniques will enhance resolution.**

**The time gap between 1ms and 1  $\mu$ s should be closed (for example: dynamics of mycelles).**

**The development of the coherence picture clearly defines the space/time range of computation.**

**Joint tomography with neutrons and X-rays. The software for joint evaluation is still missing.**

**Neutron tracer methods are very sensitive (absorption cross section Gd-157  $\approx$  1Mb @ 7 Å)**

**Neutrons and synchrotrons may share sample environment; (ESRF + ILL: 30-40T Magnet ?)**

## II Some scientific and experimental perspectives for nanoscience

**Assuming that we cannot increase brilliance, there may be only few possibilities:**

- **Uniting present techniques in a new way**
- **Multiplying instruments**
- **Introducing new techniques**

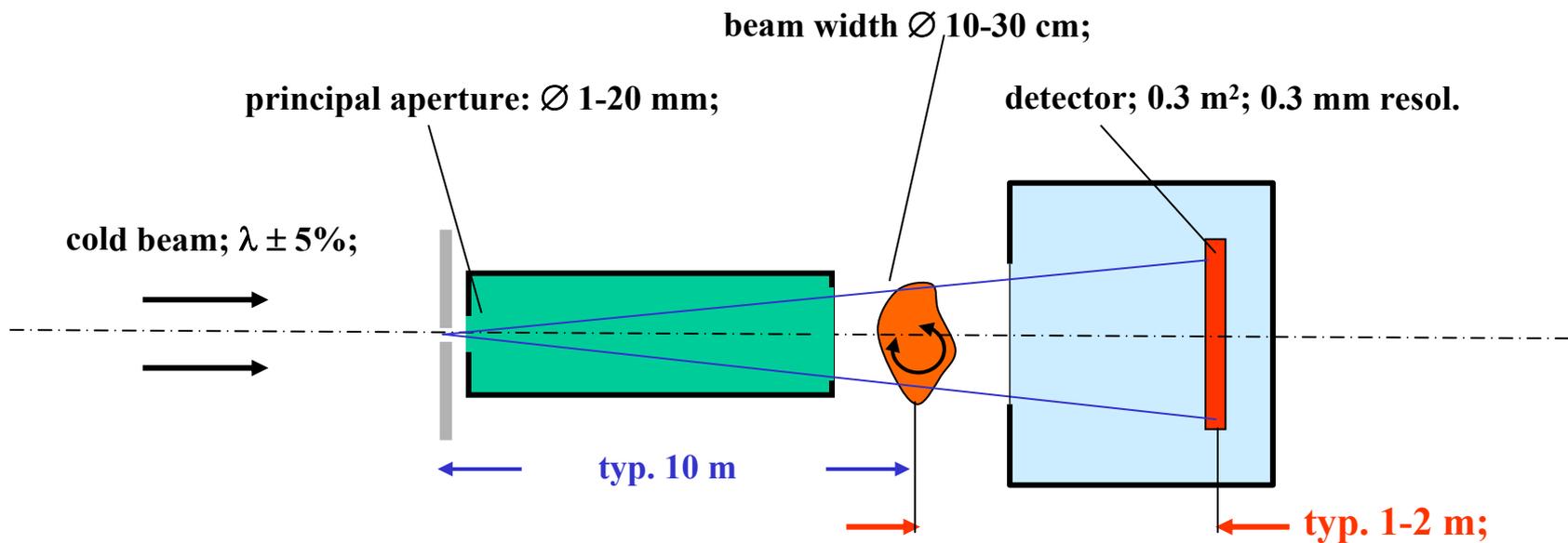
**1) 3D mapping of nano-structured materials: SANS-TOMOGRAPHY;**

**Standard Tomography uses absorption for contrast;  
SANTORIN uses SANS for contrast;  
Application: high tech materials;**

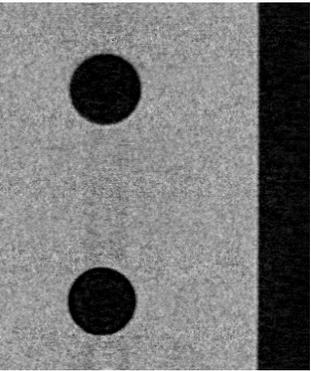
## II Some scientific and experimental perspectives for nanoscience

### SANTORIN:

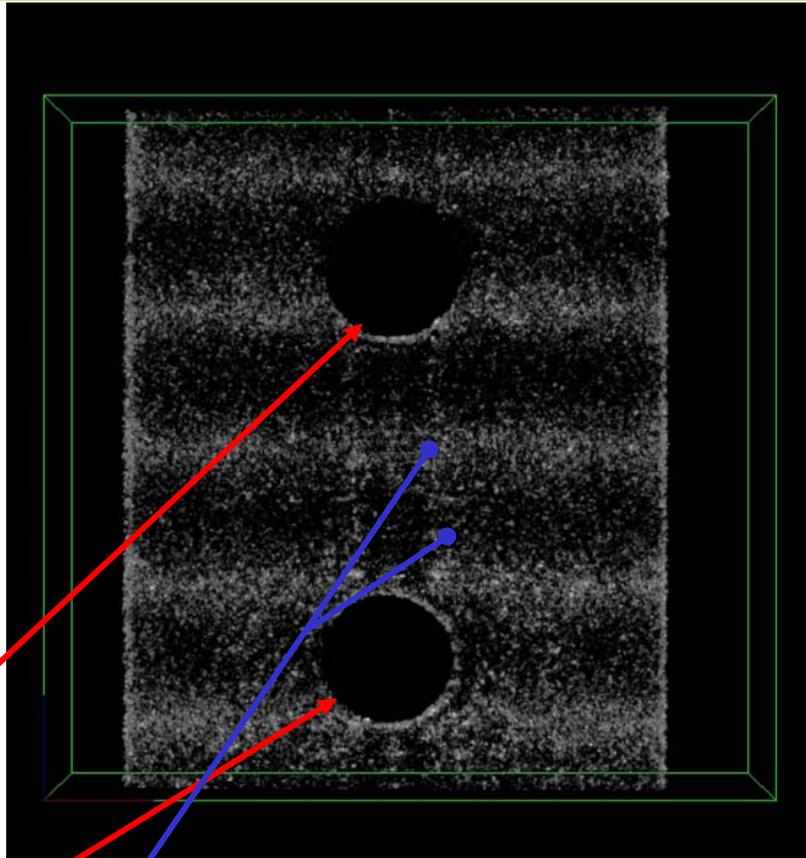
### Small ANGLE TOmographic and Radiographic Imaging with Neutrons



# SANTORIN: Example; Strength of aircraft components



Standard radiography



SANS radiography

Ordinary hole

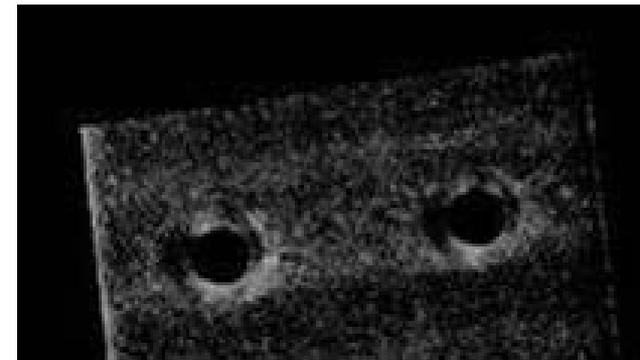
widened hole

Waves from rolling

Holes (in Al) widened with a thorn  
 ⇒ high-strength rims (texture!).  
 ⇒ Increased SANS  
 effect not visible at ordinary holes

**This will open a new field!**

SANS radiography of tapered holes



**No change in composition but in texture;**



2) Large scale structures, typ. size  $\approx 1 \mu\text{m}$  : USANS option; **SAMBA**

## **SAMBA: Small Angle Multi Beam Analysis**

**There is need to examine nano- and microstructured materials for larger correlation lengths!**

### **Examples:**

- **Nanotube-clustering in glue**
- **Micro-structure of tires**
- **Bubbles in Vicor glass**
- **Oil in Sediments**
- **Hardening of concrete**
- **Structure of marble**

**Aim: Extend beam correlation length  $l_C$  by factor 10 in 2 dimensions**

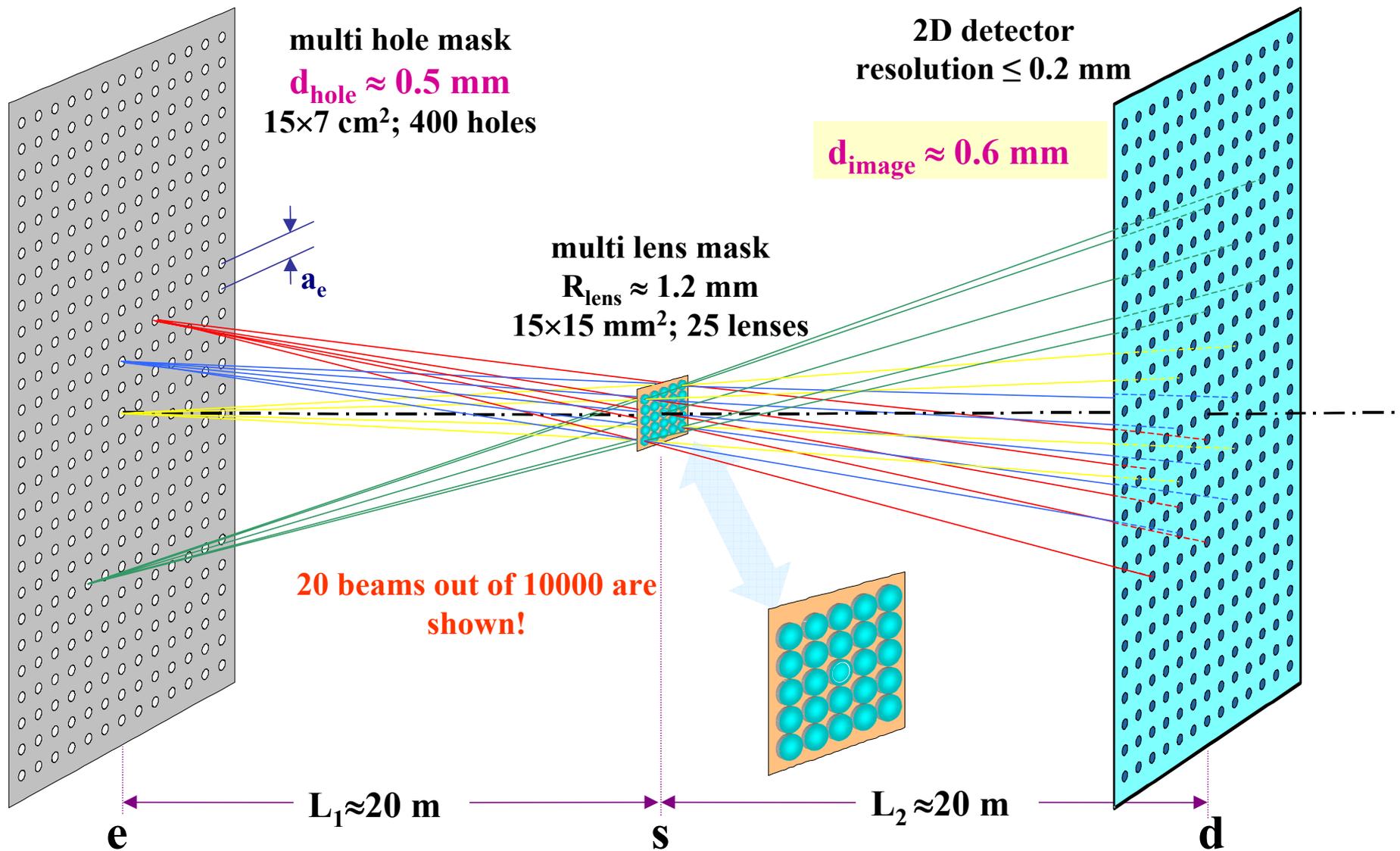
**at standard SANS machines:  $l_C = 1000 \text{ \AA} \Rightarrow l_C = 1 \mu\text{m}$**

**Consequence for standard SANS:  $I \Rightarrow 10^{-4} I_0$  (too low!)**

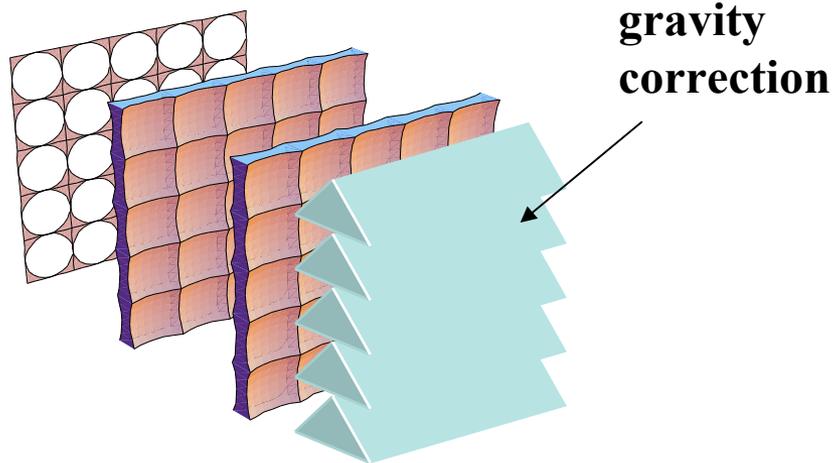
**SAMBA uses up to  $10^4$  narrow beams with  $l_C = 1 \mu\text{m}$**

**Only moderate loss in intensity but sacrifice in q-range**

# SAMBA in two dimensions at long base-line SANS machine:



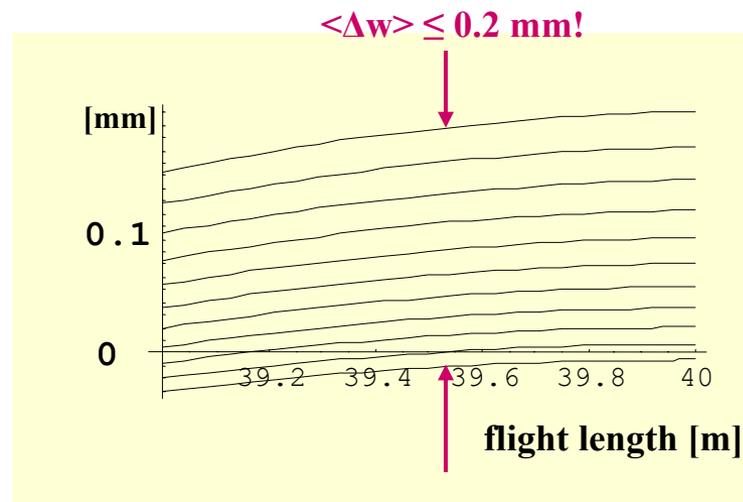
## Multi lens + prisms



2 lenses  $R = 2.28 \text{ mm}$

mean spherical aberration: 0.12 mm;

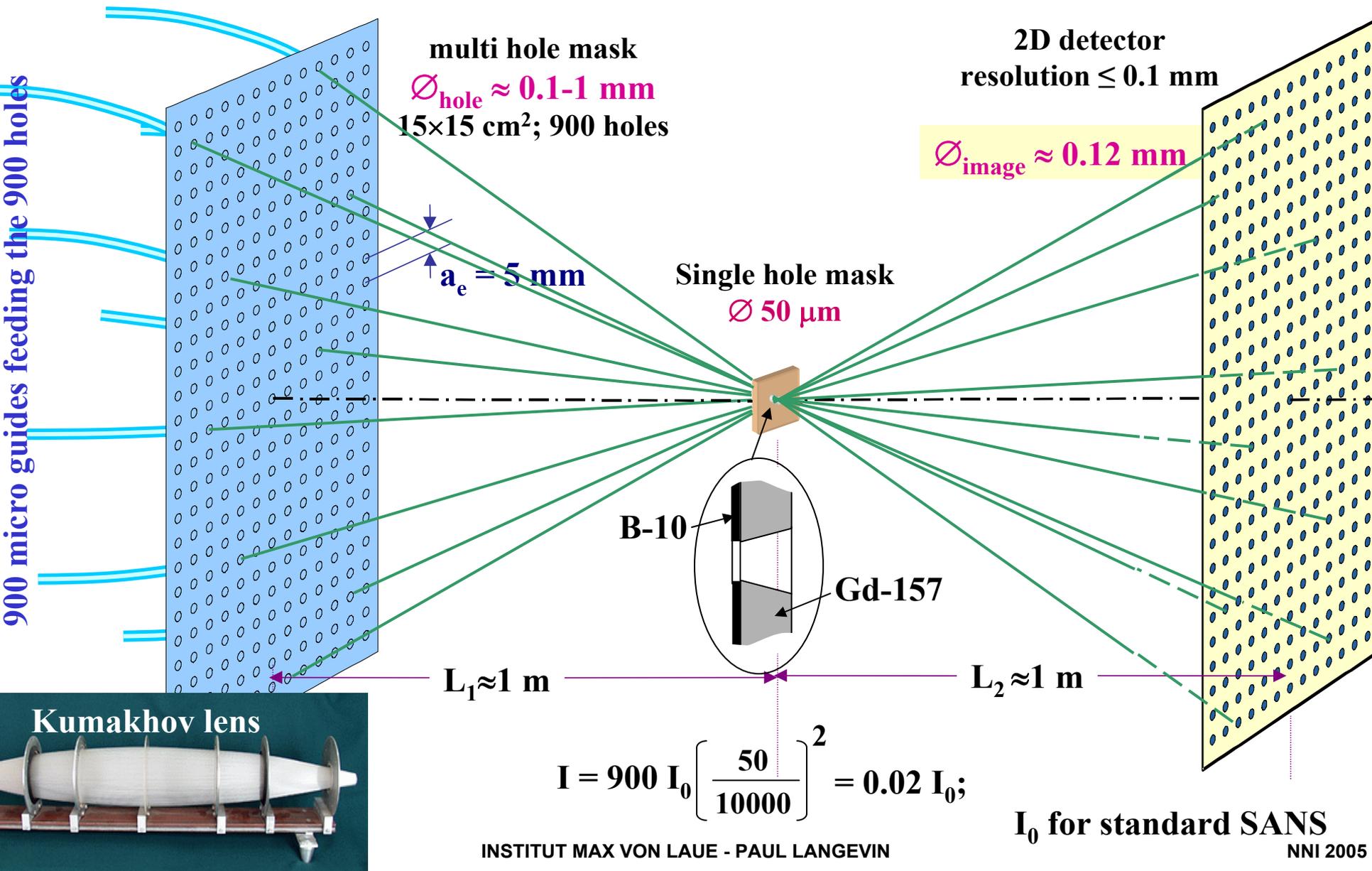
## Image quality



mean distortion: 0.2mm;

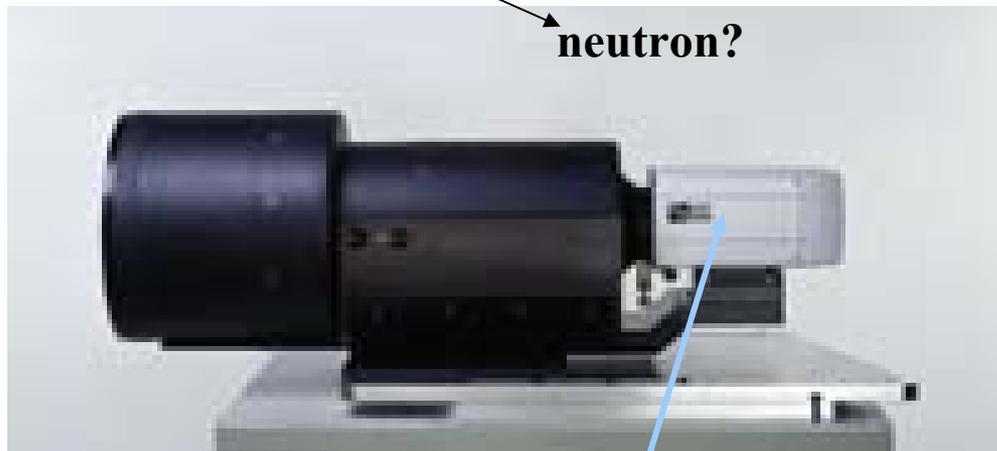
**Mean image width including all aberrations: 0.6 mm after 40 m flight path**

## 2) SANS (with standard q-resolution) for 50 $\mu\text{m}$ samples;

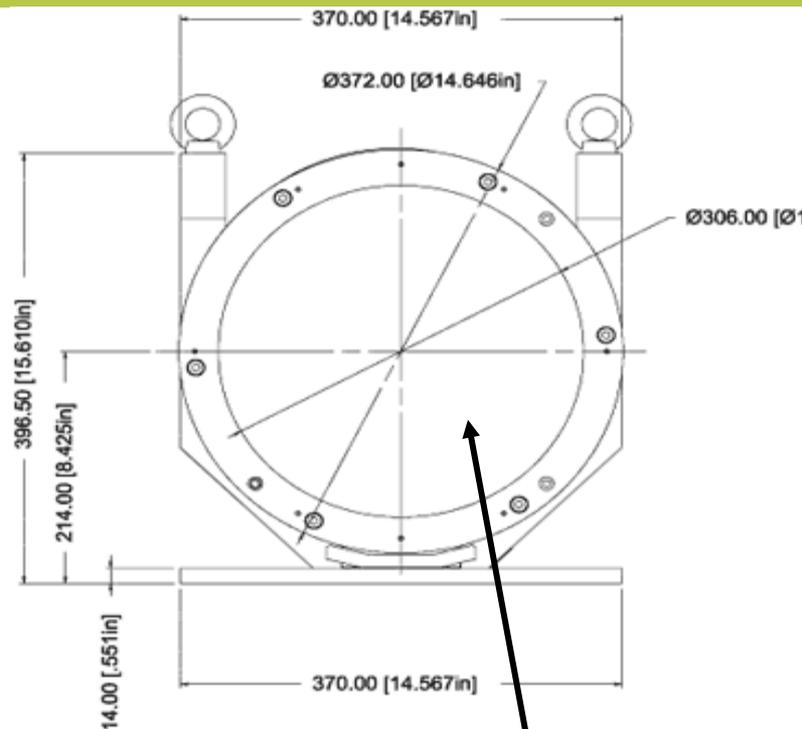


# off the shelf camera system [luxury]

BRUKER ADVANCED X-RAY SOLUTIONS

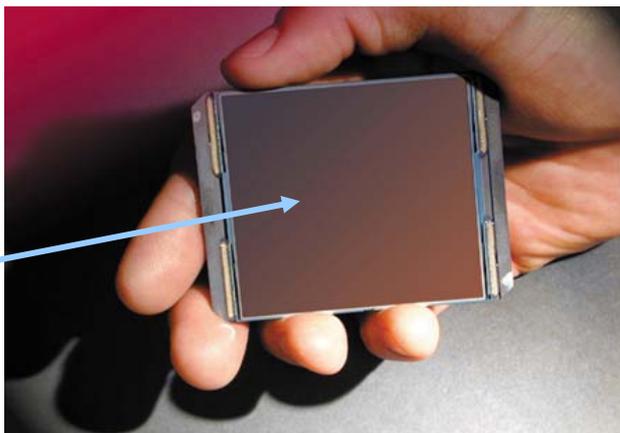


neutron?



resolution:  
73 $\mu$  on  $\varnothing$  300 mm

CCD: 62  $\times$  62 mm  
15 $\mu$ ; 4096 4096



**TISANE:**

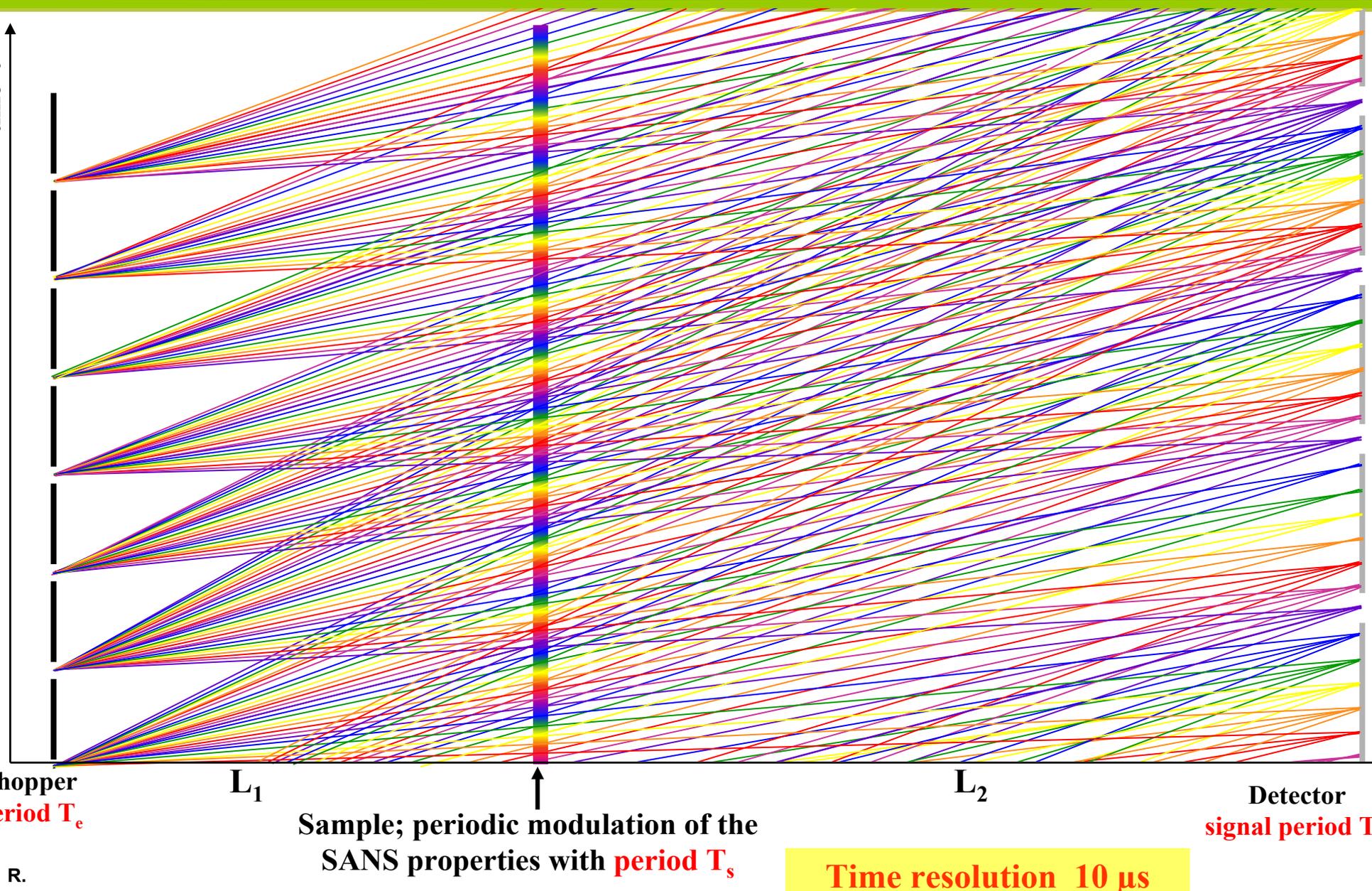
**T**ime-resolved **S**mall **A**ngle **N**eutron **E**xperiments;

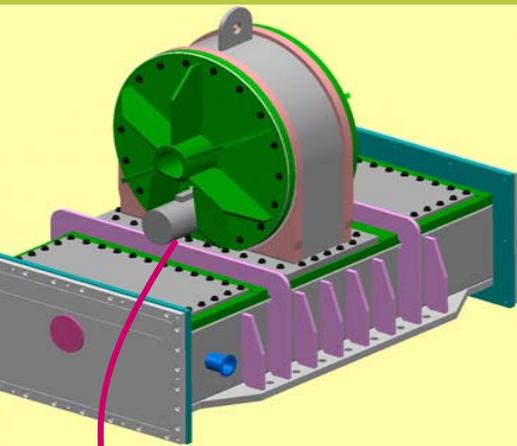
**TISANE** measures the time-modulation transfer function of a SANS sample for frequencies up to some hundred kHz, using a broad wavelength band;

**Examples:**

- Pseudo-crystalline ordering in ferrofluids induced by B-fields; (first tests)
- Conformational changes of photoactive membrane-proteins
- ion-driven conformational changes in model-membranes
- Ferro-electrics ?
- Spintronics ?

# TISANE - principle:



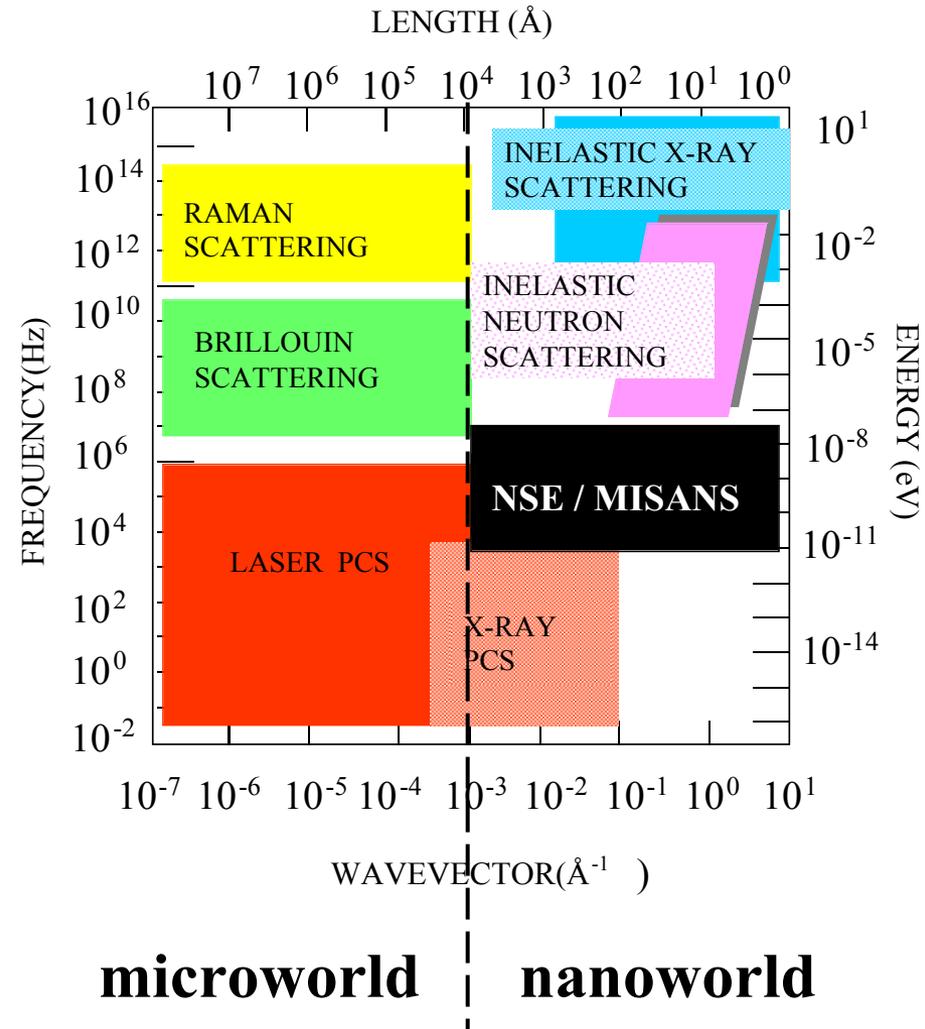


- structure in complex fluids induced by oscillatory shear (Bill Hamilton - ONRL, Lionel Porcar U. MD/NIST, Paul Butler NIST)
- biological processes, e.g. muscle contraction and membrane response to electrical fields (Ken Rubinson - CARB)
- double network polymer gels under compression loading (Wen-Li Wu – NIST Polymer)
- vortex structure as a function of oscillating driving current near the peak effect regime (Sean Ling – Brown University)
- T jump and P jump (Bill Hamilton - ORNL)

Access to time scales inaccessible by any other neutron technique

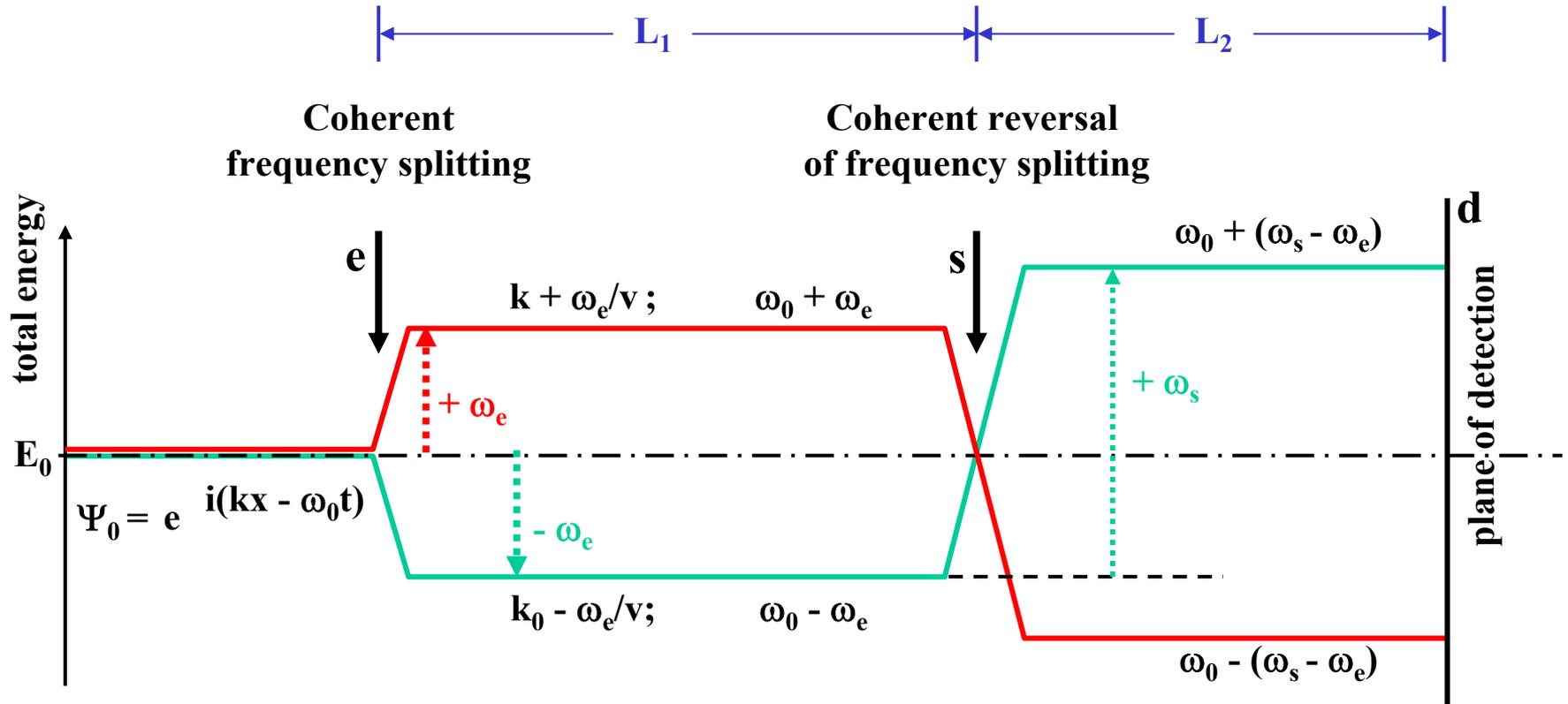
## D) High resolution spectrometry and SANS ; MIEZE (MISANS)

At small scattering angles, typical for SANS on large/medium nano-particles, the dynamics cannot be sensed by classical TOF methods. (time resolution!)



### Field of applications:

- macro-molecules (e.g. Mycelles);
- Polymers
- Biology;



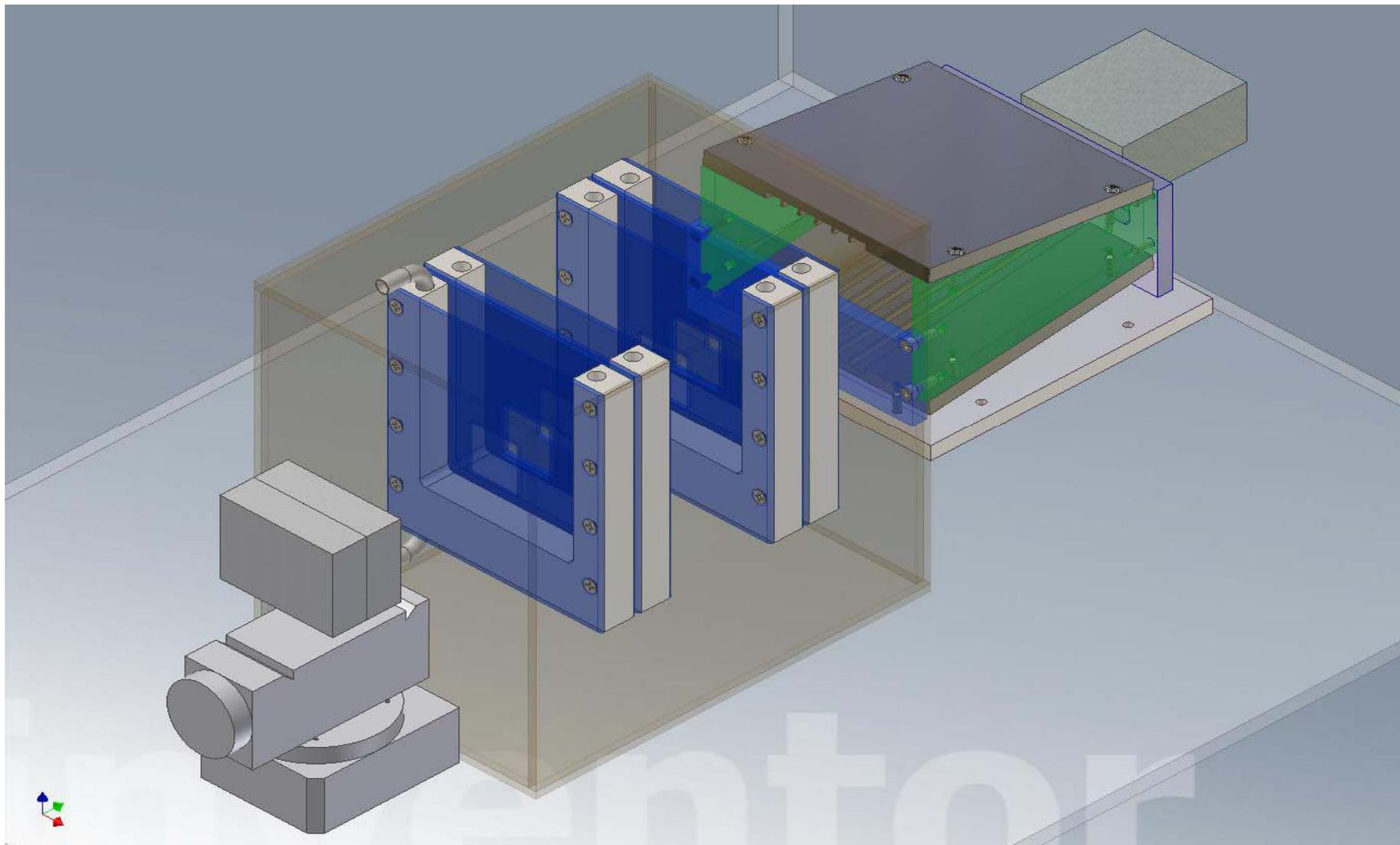
$$\Psi_{\text{detector}} = \begin{bmatrix} e^{+i(\Delta k_e L_1 - \Delta k_s L_2)} & e^{-i(\omega_s - \omega_e)t} \\ e^{-i(\Delta k_e L_1 - \Delta k_s L_2)} & e^{+i(\omega_s - \omega_e)t} \end{bmatrix} \Psi_0$$

$$\Delta k_e = \omega_e/v;$$

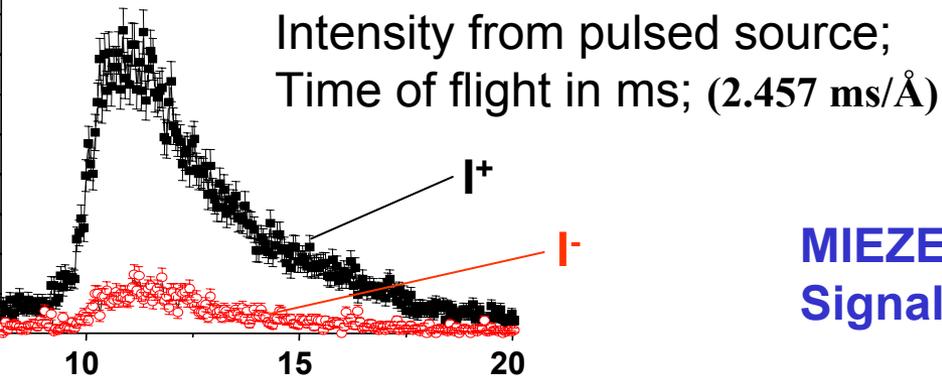
$$\Delta k_s = (\omega_s - \omega_e)/v;$$

For  $\omega_e L_1 = (\omega_s - \omega_e) L_2$ ,  $\Psi_{\text{detector}}$  gets independent from  $v$ .  $\Rightarrow$  beats in time with  $\omega_d = (\omega_s - \omega_e)$

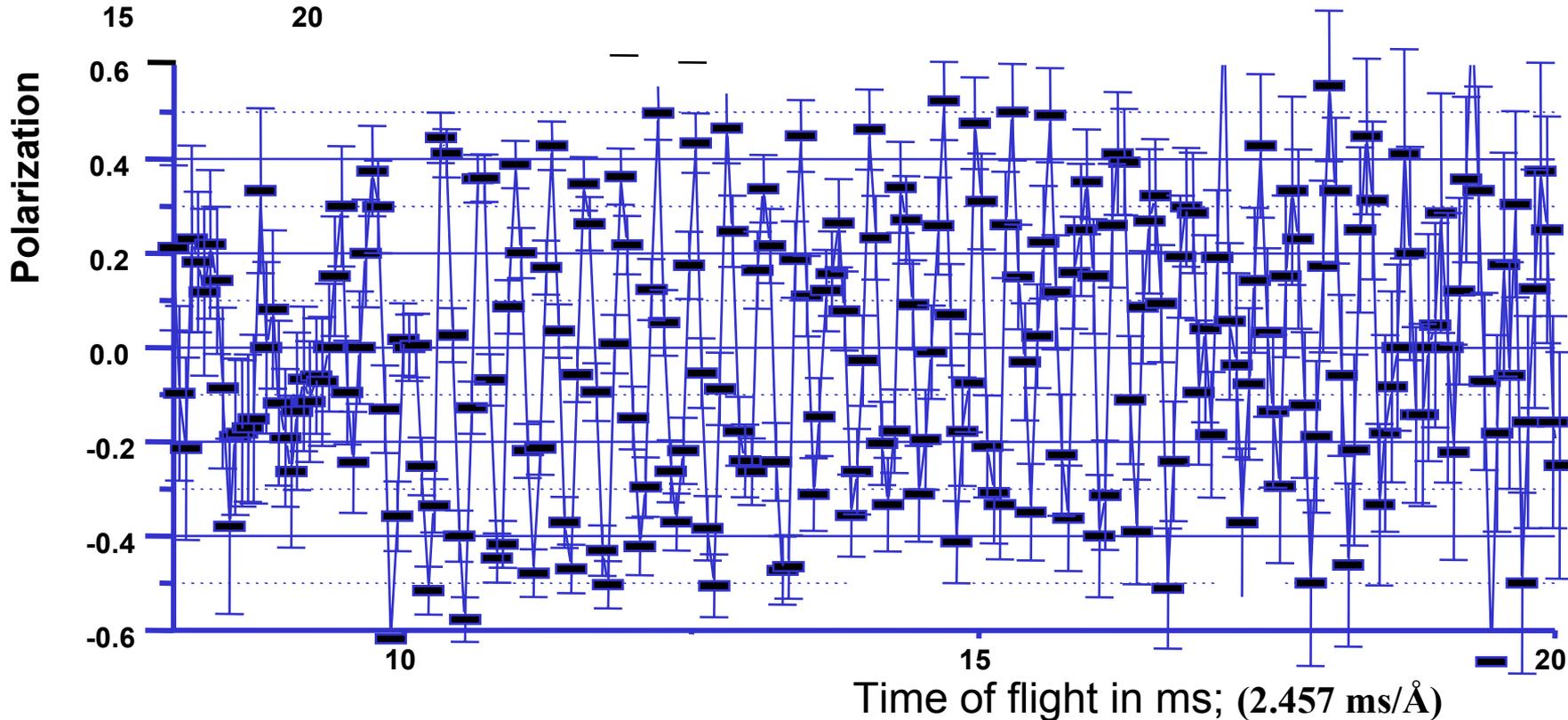
# MISANS – first tests at ANL (pulsed source)



# MISANS – first signals;



MIEZE signal at 2kHz (+ Larmor precession)  
Signal frequency limited by detector response;



- 1) **Cancer Therapy using nano technology**
- 2) **How to boost neutron brilliance at existing sources?  
for single shots in time-resolved reactions  
or for smaller samples**
- 3) **Beyond the SNS?**

## « Nanoparticles reveal tiny cancerous tumors »

pecially designed nanoparticles can reveal tiny cancerous tumors that are invisible by ordinary means of detection, according to a study by researchers at [Washington University School of Medicine in St. Louis](#).

Because nanoparticles can be engineered to carry a variety of substances, they also may be able to deliver cancer-fighting drugs to malignant tumors as effectively as they carry the imaging material that spotlights cancerous growth.

The spherical nanoparticles can carry about 100,000 molecules of the metal used to provide contrast in MRI images. This creates a high density of contrast agent, and when the particles bind to a specific area, that site glows brightly in MRI scans.

In this study, MRI scans picked up tumors that were only a couple of millimeters (about one twentieth of an inch) wide.

Small, rapidly growing tumors cause growth of new blood vessels, which feed the tumors. To get the nanoparticles to bind to tumors, the researchers equipped them with tiny "hooks" that link only to complementary "loops" found on cells in newly forming blood vessels. When the nanoparticles hooked the "loops" on the new vessels' cells, they revealed the location of the tumors.

**These Nanoparticles may not be poisonous and may be used as jumbo-carriers for B-10  
Revival of BNCT ?**

# How to boost the brilliance at existing sources?

It needs a higher phase space density in the source.  $\Rightarrow$  cooling

By cooling from 300 K to 4 K, the phase space density increases by 600!

**Solid D<sub>2</sub> at 4K  
produce UCN;  
Storage in bottle  
for 1000 s**



**Extraction  
and beam shaping  
by Wanderfeld**



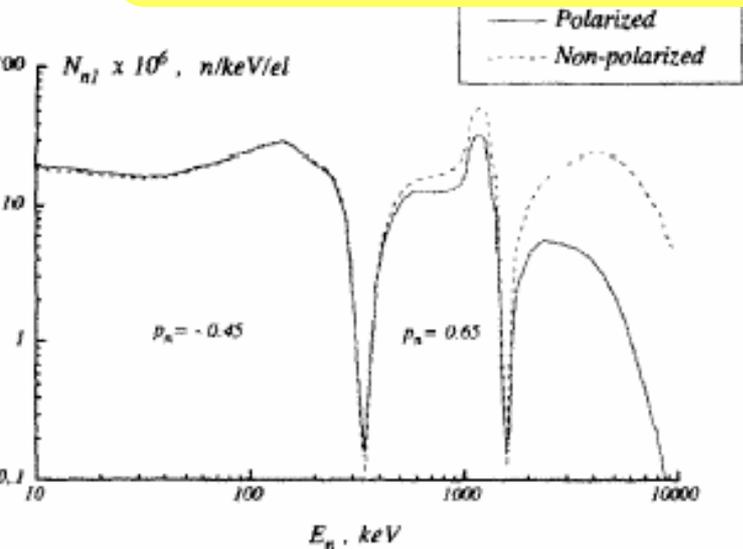
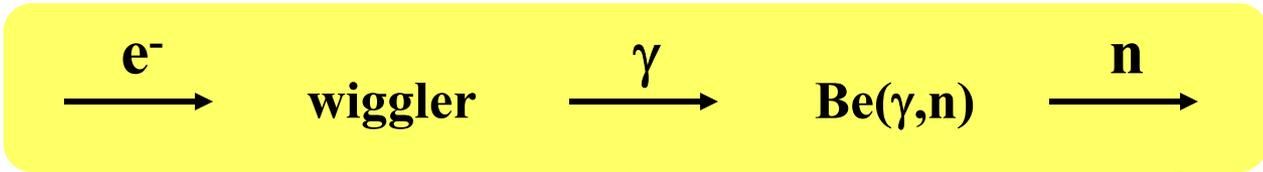
**Final  
acceleration by  
moving crystal  
to cold/thermal n;**

## A method for producing polarized neutrons by the magnetic bremsstrahlung $\gamma$ -radiation

I.P. Ereemeev<sup>a</sup>, A.L. Barabanov<sup>b</sup>

<sup>a</sup>International Business Nucleonic, Moscow, Russia

<sup>b</sup>Russian Research Centre "Kurchatov Institute", Moscow, Russia



MB polarization	Linear	Circular
$Q_\gamma$	0	0.90
$N_{\gamma 1}$ , q/el	35.4	16.6
$\Phi_{\gamma 1}$ , q/cm <sup>2</sup> el	435	175
$P_n$	0	0.45–0.65
$N_{n 1}$ , n/el	0.18	0.045
$\Phi_{n 1}$ , n/cm <sup>2</sup> s el	$3.7 \times 10^8$	$4.6 \times 10^7$
$N_n$ , n/bunch	$1.1 \times 10^{11}$	$2.8 \times 10^{10}$
$\Phi_n$ , n/cm <sup>2</sup> s	$2.3 \times 10^{20}$	$2.9 \times 10^{19}$
$\langle \dot{N}_n \rangle$ , n/s mA	$1.1 \times 10^{15}$	$2.8 \times 10^{14}$
$\langle \dot{\Phi}_n \rangle$ , n/cm <sup>2</sup> s mA	$1.2 \times 10^{15}$	$1.5 \times 10^{14}$

Fig. 1. The spectra of polarized (solid curve) and non-polarized (dashed curve) photoneutrons produced in the <sup>9</sup>Be target by circularly and linearly polarized MB  $\gamma$ -rays, respectively.