WP 20
« Advanced Neutron Tools for Soft and Bio Materials »

Six partners:

LLB (CEA) HZB JCNS ILL FRMII (TUM) STFC (ISIS)

Two topics:

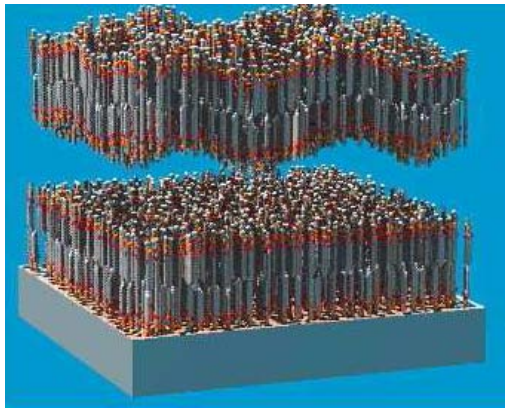
- **Platform for model biological membranes** Task 1
- **Specific sample environments for soft materials**
  - Kinetic & Dynamics experiments Task 2
  - Humidity chamber with sample changer Task 3
  - Cryogen free cryostat with sample changer Task 4

(Task 1) 91 MM
Platform for model biological membranes

ILL (task leader)- STFC, CEA (partners)

– HZB, TUM, JÜLICH (observers)

Develop methods to study biological membranes with neutron reflectometry



Artistic view of model Membrane
Lecuyer, Fragneto et al. 2006

✓ Preparation of model membrane (floating bilayer membrane) for further studies of interactions with numerous biomolecules

✓ Development of reliable protocols for reconstitution of membrane proteins into model membranes.

✓ Improvment of data analysis methods of reflectivity data

✓ Molecular dynamics simulations
-> structure
/ neutron data

✓ deuteration of lipid compounds (D_Lab)

(Task 2) 43MM
Kinetics, dynamics and in-situ devices

JULICH (task leader)- ILL, CEA (partners)

- STFC, HZB, TUM, Tübingen Univ. (Germany) (observers).

- **Develop kinetic & dynamics experiments (in situ) .**

  - Stopped-flow
  - Pressure cells
  - Electric field cells
  - Complementary spectroscopies : light scattering…

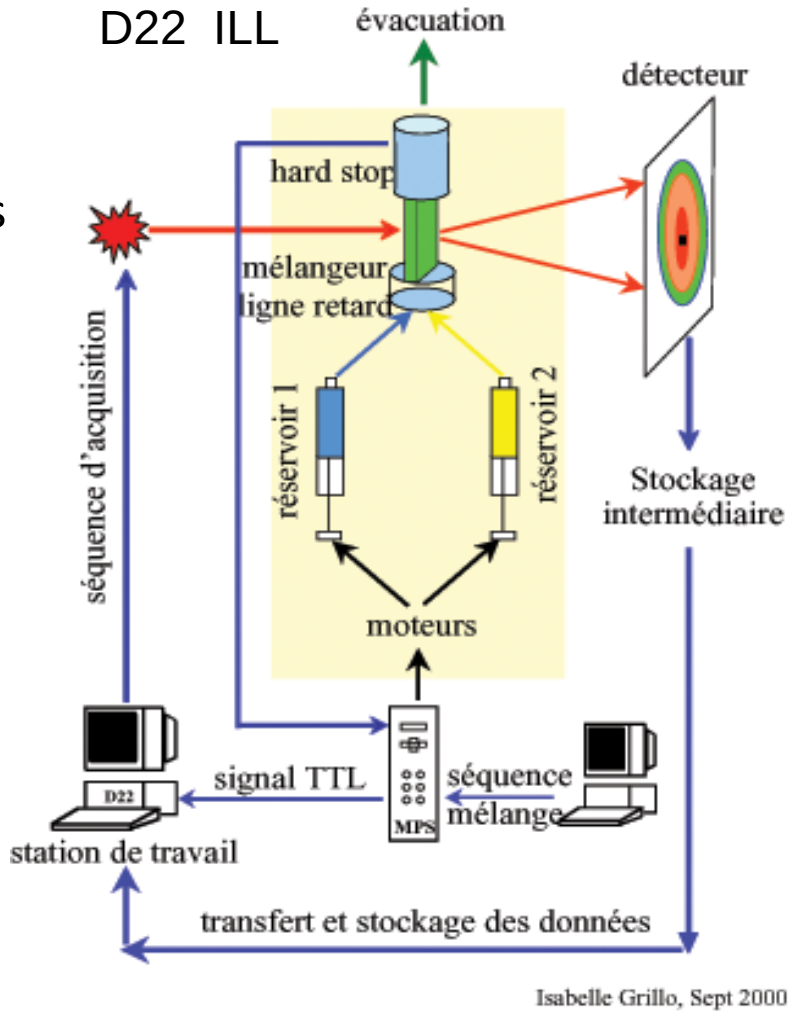
Stopped Flow

Kinetics of different phenomena after application of external stimuli (dilution, mixture 1 2 or 3 components , pH or T-jump…)

Formation of vesicles from micelles
Effect of salt on vesicles..
Growing of mesoporous materials from glycosyléic surfactants

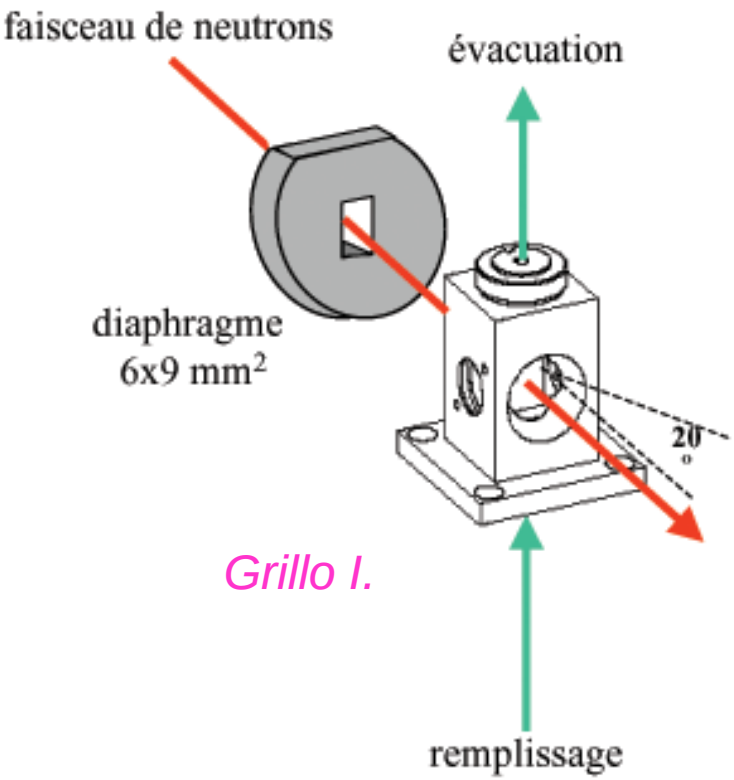
Grillo I.

D22 ILL



Stopped Flow

ILL



Grillo I.

Volume ~800µl

t_{min}~100ms

- ✓ Decrease the dead times (mixing time and filling up and emptying)
- ✓ Improve T control
- ✓ Different SF cells adapted to the available sample volumes
  - microcell
  - larger cells to decrease the repetition rate to obtain a good statistics

Kinetics, dynamics and in-situ devices

Pressure cell with sapphire windows and temperature control

✓ P up to 7kbars for SANS

Study unfolding of proteins

✓ Pressure cell for NSE : - larger samples 35*35 mm^2

- non magnetic elements to apply pressure

Electric field cell

Studies of charged colloids , polyelectrolytes or other biomolecules

✓ EF cell for SANS with T° control

✓ Design EF cell for TOF spectrometer (with larger samples, annular geometry)

Static LS /SANS

Complement the standard SANS Q-range to smaller Q range

$2x10^{-4}$ $Å^{-1}$ ≤ Q ≤ $3x10^{-3}$ $Å^{-1}$

Accurate monitoring of aggregation phenomena, approach to a phase separation.

✓ DLS for several scattering angles (measure S(Q,t) in the μs- to ms range)

(Task 3) 31MM
Humidity chamber with sample changer

HZB (task leader)- ILL, JÜLICH (partners)
- STFC, TUM, CEA, McMaster Univ. (Canada) (observers)

Control the hydration level of soft materials samples . Temperature control

Investigations - of the proton motion in Nafion membrane – of the dynamics of phospholipid membranes – of the structure and dynamics of clays,- for studies of the function/structure relationship of hydrated proteins.

✓ obtain faster and better controlled response in wider temperature and humidity ranges.
✓ different geometries for SANS, reflectometry, and NSE.
✓ Multi-position sample holder for SANS

(Task 4) 37MM

Cryogen free cryostat with sample changer

ILL (task leader) - STFC, TUM (partners)

– HZB, JÜLICH, CEA (observers).

ANSTO (Australia), ORNL (USA), JAEA (Japan)

Decrease dead times related to temperature and sample changes in cryostat

✓ Design a cryostat with a carousel of samples either placed at room temperature or thermalized at low temperature (for example at 80K by using a cold gas stream),

✓ Compact design with less cold mass (rapid cool-down) and sample changes by means of a robot.

✓ Different tails for different geometries (SANS, reflectometry in different facilities.

✓ Tail windows designed in order to apply in-situ light/UV or other external radiation.

Man Months distributions / Tasks & / Participants

		Total
Platform Biomembrane	Task 1	91
Kinetics/ Dynamics	Task 2	43
Humidity Chamber	Task 3	31
Cryostat MultiSamples	Task 4	37
	Total	**204**

	LLB	HZB	JCNS	ILL	FRMII	STFC	**Total**
	20	18	13	68	18	14	
Total	**28**	**25.2**	**18**	**91**	**22.4**	**19.6**	**204**