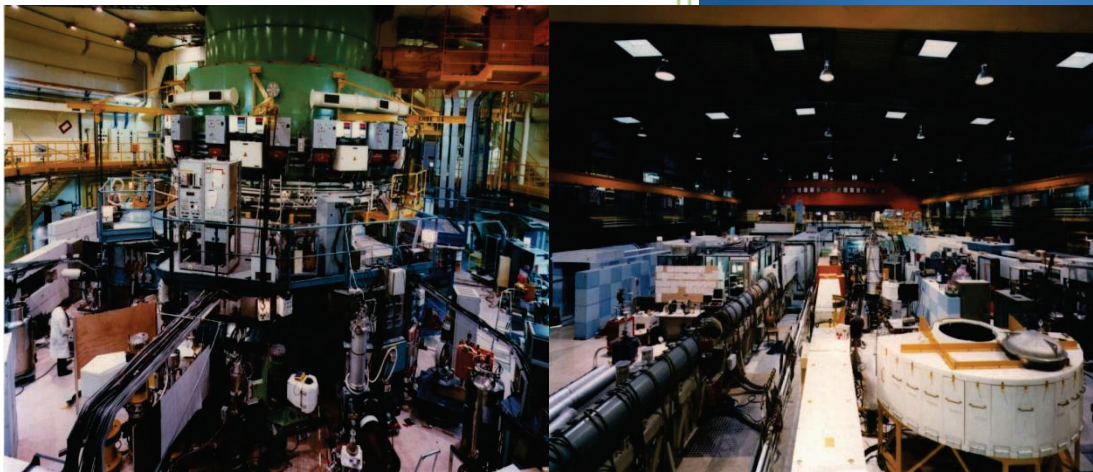




2008~2010

PART III : THE ACTIONS OF THE FACILITY, THE NATIONAL NEUTRON SOURCE



énergie atomique • énergies alternatives



2008-2010

➤ **SERVICE ACTIVITIES**

- User Program
- Beam time Statistics
- European collaborations: NMI3 and IAEA organization
- The CRG 1T
- Long term visitors
- LLB and SOLEIL
- LLB and Industry
- Bibliometric study: limits and tendencies
- Some scientific highlights

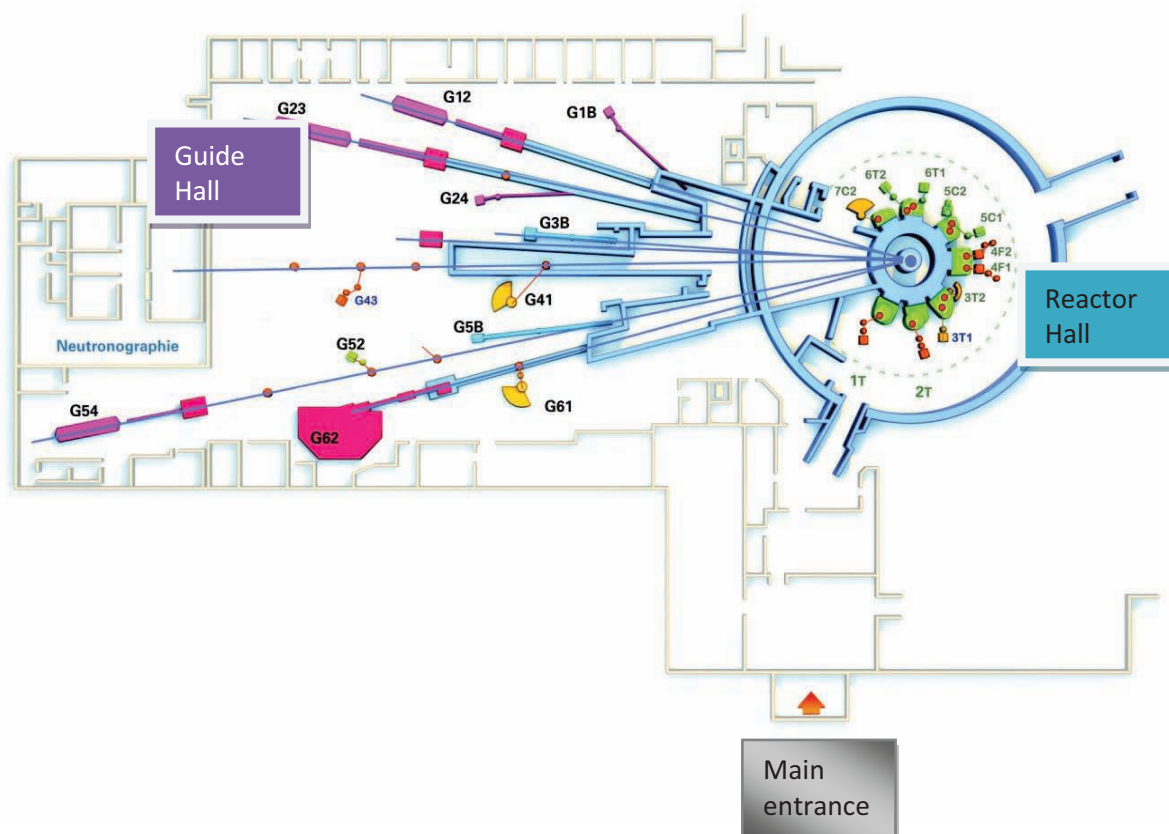
➤ **INSTRUMENTATION**

- Organization and expertise of the groups
- Current LLB instruments and platforms
- The Orphée Reactor
- Upgrade program of the instrumentation CAP2015 and projects
- The Instrumental Committee (November 2010)

The Laboratoire Léon Brillouin (LLB) is a French Research infrastructure supported jointly by the Commissariat à l'Energie Atomique et aux Energies Alternatives (CEA) and the Centre National de la Recherche Scientifique (CNRS). Its missions are defined in the French roadmap of large scale infrastructures. The TGIR LLB, attached to the 14MW Reactor Orphée, provides a fully-supported world-class suite of instruments dedicated to neutron scattering experiments to the French and European community, estimated to be 4500 people in 2005, with 1000-1500 French users. Academic and industrial use of neutron instruments encompasses a very broad range of science areas in physics, materials, soft matter sciences and biology, either from fundamental point of view or for applied research. As a national facility, its management of beam time is quite flexible, allowing more tests, thoughts and discussions between beginners and experts, the exploration of new areas or experiment preparation, and access to industrial partners. As mentioned already in the introduction of this report, it has an enduring and complementary role aside international centres such as the Institute Laue Langevin or the future European Spallation Source. Moreover, it belongs to a recently accepted Integrated Infrastructure Initiative (NMI3) in the EU Framework Programs, and accordingly, it develops and cultivates fruitful cooperation's with the other European centers. An important point for the future is certainly the recent French-Swedish cooperation agreement signed the 13th of December 2010 for neutron instrumentation: by enhancing the cooperation between neutron scattering communities of Sweden and France in the development of various technologies which will support the operation of their neutron user facilities, *i.e.*, the future European Spallation Source at Lund, this agreement proposes to participate in the construction of two types of instruments, a modern Time-of-Flight spectrometer and Small Angle Neutron Scattering instruments that will be built and operated at latest in 2016 at the TGI LLB/Orphée. Both types of instruments will provide the best performances on pulsed source such as the ESS; in the meanwhile it is therefore crucial to get staff expertise and prepare neutron user community to such an unprecedented performance. We are only in the preliminary stages of this cooperation agreement, which will be set up presumably at the end of 2011, thus no special attention will be devoted to it in this section.

The exceptional situation of the LLB in the southwest of Paris, in the scientific centre of Saclay, nearby faculties, engineering schools and other large scale facilities (TGIR), such the synchrotron Soleil, promotes external contacts and discussions, and stimulates new collaborations. Moreover it achieves its nationwide goals through several cooperation agreements with Regions, Universities (Rennes, Bordeaux, Marseille, ..) and by welcoming industrial users. The LLB operates 21 world-class spectrometers opened to the scientific community. The general lay out of the spectrometers is schematized in the figure below. The spectrometers are grouped by techniques: single crystal diffraction, powder diffraction and diffuse scattering, small angle scattering, texture and strain, reflectometry, triple axis and quasi elastic scattering.

In the first section, we present the overall service activities, user programs, beam time statistics and all aspects of the bilateral cooperations adopted by the LLB. In the Instrumentation section, a brief description of the scientific and technical expertise of the groups designated in the organisation chart is given, followed by the description of the current spectrometers open to users. The auxiliary services or platforms (chemistry and biological labs, Vacuum/Cryogenics, High Pressures, High Magnetic fields, Mechanics) available for users are also listed. More detailed information about the LLB facility can be found in the following web page: http://www-llb.cea.fr/fr-en/spectros_p.php. In the next section, the LLB policy for instrumentation improvements and upgrades is presented: the first step was done via the CAP2010 program ending last year, whose financing was mainly taken without extra funding. It was a modest phase before a more complete renewal with the CAP2015 program, presented with its ongoing projects. This program was recently well recognized by the Instrumental Committee made of international experts in the neutron scattering techniques; their report is given at the end of this Part II. Finally the status of the Reactor is considered.

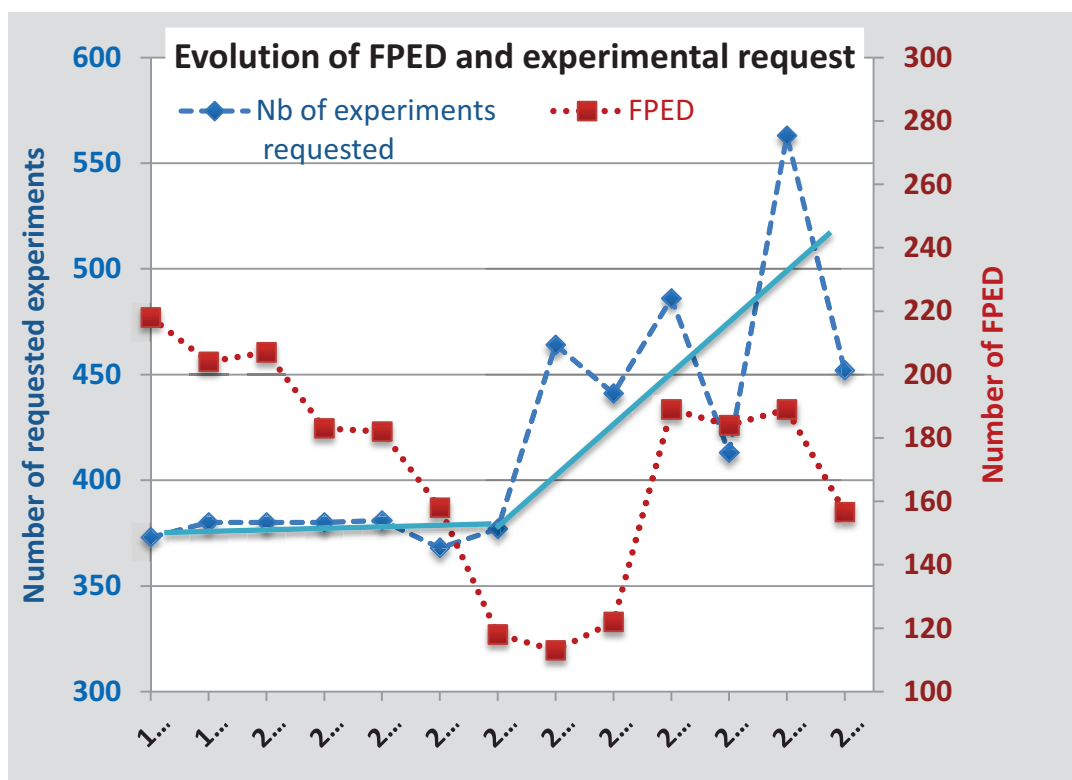


General lay out of the 21 spectrometers (+ 2 for tests) operated by the LLB and opened to the users program: 11 are in the reactor hall and 12 are installed in the guide hall
 (T= thermal, C= Hot, G for guide)

A- User Program

We present in this section the main facts and figures related to users activity of the LLB/Orphée facility followed by beam time statistics. The statistics about beam achievements are available for whole years, for the period 2006-2010.

The current CEA-CNRS Agreement (Convention), signed on January 2006, guaranties 180 operation days of beam time at 14MW per year. It represents a return to normal working conditions, after a period of reduced activity caused by severe budget cuts between 2003 and 2005. The Figure below summarizes the LLB-Orphée performance during the last years (2006-2010) in terms of Full Power Equivalent Days of the reactor (FPED). For 2006, the FPED was 123 instead of 180 because a technical breakdown occurred in the Orphée reactor after the long summer shutdown. In the following years, the number of FPED was slightly higher than the 180 days planned by the Agreement, in order to recover the days not delivered in 2006; unfortunately in 2010 another technical problem occurred in September and only 156 days were delivered. The figure below represents the most significant tendency over the last years, an increase of the number of submitted proposals by more than 50% since 2004.



Beam time Allocation and Selection Procedure

To perform an experiment, the researcher must submit a proposal on a special form where he specifies his scientific interest and describes the proposed experiment. Deadlines for submission are: May 1st and November 1st of each year.

Proposals for experiments are selected through a peer review. Selection Committees (SC) are composed of high level scientists from France and other

European Countries and meet twice a year, a typically month after the deadline for submission.

The Selection Committee ranks the proposals in three categories:

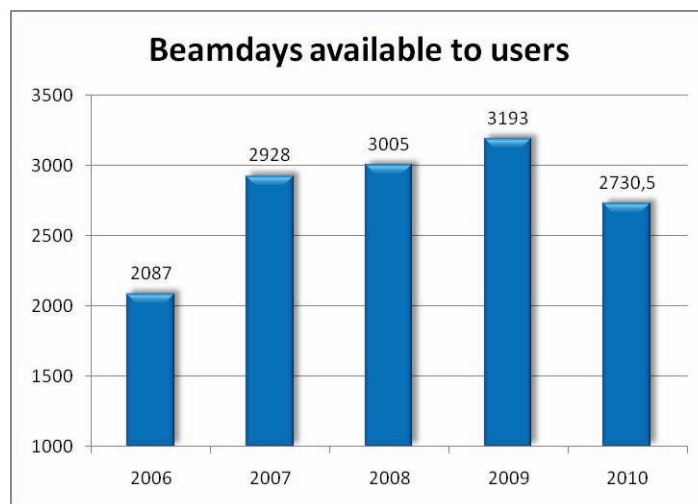
A = the proposal is accepted and is sure to be programmed.

B = the proposal will be programmed if additional time is available in the spectrometer scheduling.

C = the proposal is rejected because of insufficient scientific quality or because of lack of scheduling time or poor scientific level.

The scientist responsible for the proposal receives an official letter giving the SC grade. When a proposal is graded B or C, an explanation is included in the letter. Sometimes the SC revises the amount of beam time claimed in the proposal and then allocates more or fewer days.

The figure below displays the number of days of experiments performed on the LLB spectrometers during the last 5 years (2006-2010).



The number of "experiments days" employed by users is high; it is shared between about 70% of the "beam days" proposed for the category A, and the remaining 30% of the time for continuing or repeating experiments that encountered problems (technical or scientific), a possible transfer to A grade of beam time by the committees, industrial offers, training sessions and upgrade and maintenance.

Some considerations should be taken in account in order to compare this figure to that of other facilities. At the LLB, all the experimental proposals are judged by the SC. This means that:

- In-house beam time does not exist in the LLB. All the LLB scientists, post-docs and PhD students should apply for beam time to the selection committees for their internal research.
- Experiments to be taken in charge by the ACCESS NMI3 program are also selected by the SC and then included in this statistics.
- Beam time proposals concerning formalized collaborations (ANR projects, long term industrial collaborations, etc.) are also evaluated by the SC, to ensure the scientific relevance and its feasibility.
- The direct purchase of beam time by industrial companies (neutron irradiation, small angle scattering characterization, determination of residual strain, etc) it is not included in the statistics of beam request. These service deliveries do not go through the SC.
- The LLB offers two other ways to request beam time, which nevertheless remain exceptional. Their weight is negligible in the statistics.
- Submission of a proposal for an experiment to the laboratory management. This procedure shortens the time between submission and completion of the experiment. It should be only used in exceptional cases: hot topic, abnormality in the normal selection process, confidentiality. The president of the concerned reviewing panel is informed of the directors' decision.
- The procedure for quick access: this procedure makes possible, within the range of 1 to 2 months, an experience very short (typically 1 day). Preliminary

test, need of additional measurements to complete work, etc.. can be obtained very quickly.

- These kinds of proposals can be reviewed continuously throughout the year.

SELECTION COMMITTEES

In 2009, it was found necessary to reorganize and update the structure of the Selection Committees. The old thematic classification was the following:

- Theme A: CHEMICAL PHYSICS, BIOLOGICAL SYSTEMS
- Theme B: STRUCTURAL STUDIES, PHASE TRANSITIONS
- Theme C: MAGNETISM, SUPERCONDUCTIVITY
- Theme D: DISORDERED SYSTEMS, MATERIALS

The aim of this reorganisation was to make the selection process more efficient because theme C “Magnetism and Supraconductivity” had twice as many proposals as the other themes. We have merged the subthemes of committees B and C, and separated them into 3 committees. The other committees (A and D) remain unchanged. The new thematic classification is the following:

- Theme 1: CHEMICAL PHYSICS, BIOLOGICAL SYSTEMS
- Theme 2: CRYSTALLOGRAPHIC AND MAGNETIC STRUCTURE
- Theme 3: MAGNETISM/ SINGLE-CRYSTAL SYSTEMS AND THIN LAYERS
- Theme 4: DISORDERED SYSTEMS, NANOSTRUCTURED MATERIALS AND MATERIAL SCIENCE
- Theme 5: EXCITATIONS

The list of the themes can be found at this address:

http://www-llb.cea.fr/en/Web/hpr_web/HPRWEB10.php . The list of the actual members is given in the annexes.

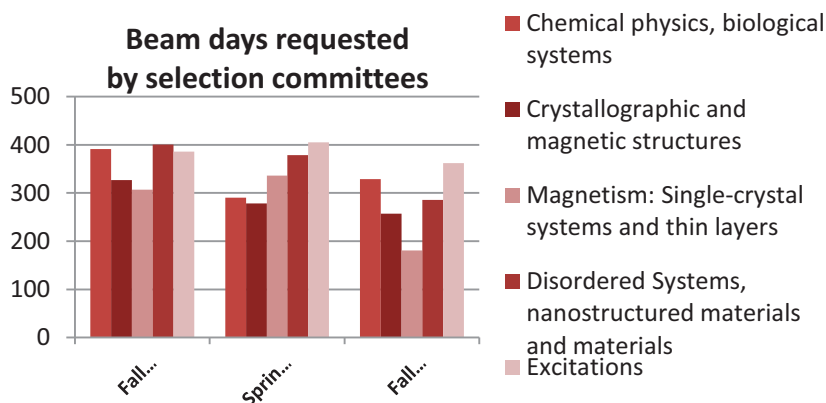
Information on applications for beam time and deadlines is given in real time on the LLB web site. <http://www-llb.cea.fr>

B- Beam time Statistics

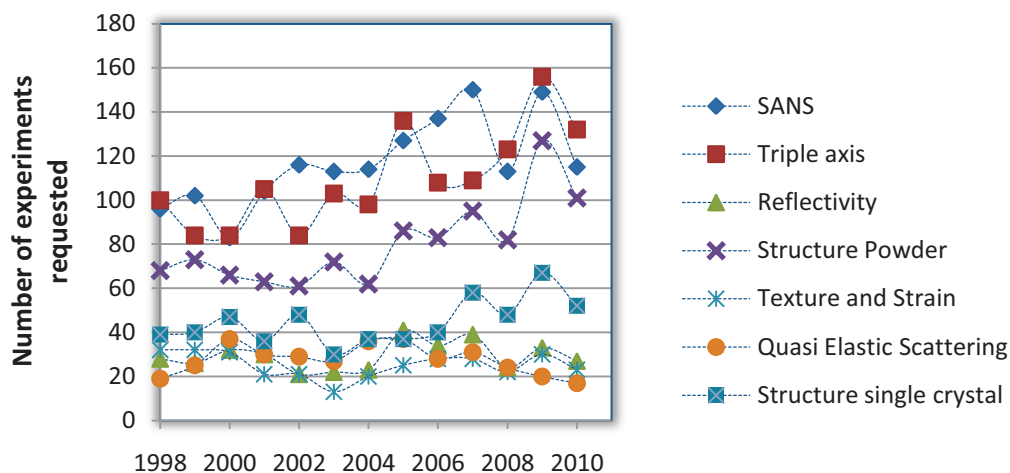
In this section we have analyzed the requests of users and allocation of beam time by the committees; then the distribution of beam time by committees, countries, French Institutions and scientific domains. We have extracted the main tendencies and showed where users have the largest needs in terms of instruments, which correspond to the upgrade instrumental program we propose in the ‘Instrumentation’ section.

Beam time and experiment requests

The figure below shows the distribution of the number of applications among the selection committees and their evolution; to equilibrate the number of proposals and consider the new tendencies, it was important to change into five committees, as the theme ‘excitations’ is still highly demanded.



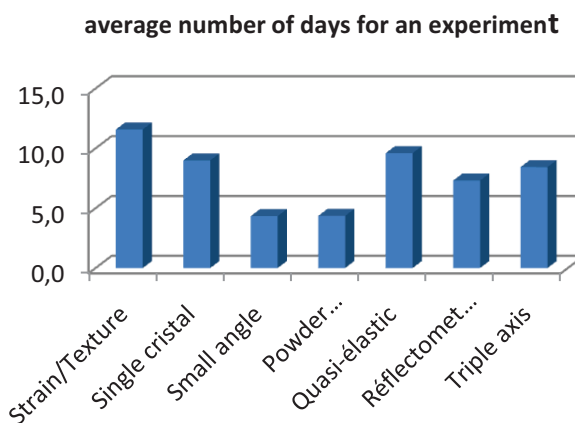
In the next figure, we have decomposed the demands in terms of neutron scattering techniques, as they will be presented in the second section : Small Angle Neutron Scattering, Triple-axis Spectrometers, Reflectometers, Two-axes Diffractometers: Powder and Liquids, Texture/strain Diffractometers, Quasi Elastic Neutron Scattering and Single Crystal Diffractometers.



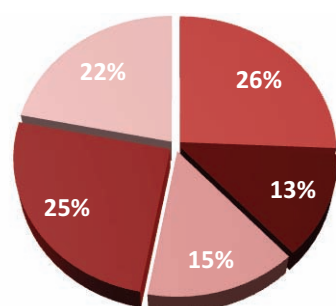
One can observe the important increases of the number of experiments demands over the last ten years :between 40 and 55% for Structure of Powders, for Tripe Axis, for SANS experiments, as well as for single crystal diffractometers; in all cases we have planned upgrades and new spectrometers in the CAP2010 and CAP2015 programs. For the three last methods, strong improvements of the instruments are required to convince the users to come back to the LLB: the upgrade of the Eros Reflectometer by decreasing the acquisition time and orienting its use to specific samples is under way, as well as for the texture/strain diffractometer super 6T1. For Quasi-Elastic Scattering, the Time Of Flight instrument Mibemol must be definitely replaced by a new one Fa#.

Beam time allocation and booking rate

The beam time is distributed along the themes of the selection committees; one committee might allocate time on most of the instruments if the topic of the proposal requires it. The figure displays the typical duration in days for an experiment using the different neutrons techniques. The experiments concerning strain/texture are the longest (12 days in average). Single crystal diffraction and quasi-elastic diffusion also need a high number of days per experiment. The shortest experiments are power diffraction and small angle scattering (4 days on average). The standard duration of a neutron experiment at the LLB is 6 days. The reduction of this number by optimizing the performances of the instruments is at the center of the upgrade program CAP2015.



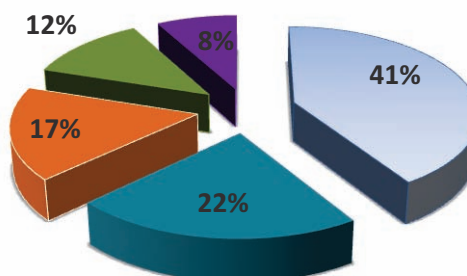
Thematic repartition of allocated beam days (2009-2010)



- Chemical physics, biological systems
- Crystallographic and magnetic structures
- Magnetism: Single-crystal systems and thin layers
- Disordered Systems, nanostructured materials and materials
- Excitations

The new distribution of themes leads to the above allocation of beam time according to the topics of the proposals selected; these ones are illustrated by the following balance between scientific domains: Material Science, Biology, Chemical Physics, Magnetism, structure of condensed Matter. Here again one can observe the strong contribution of magnetism studies, and the lowest one from Biology that needs to be supported and further developed.

Scientific Domains of beam time allocation 2008-2010



- magnetism
- superconductivity
- Material Science
- Chemical Physics
- Structure
- Biology

| Country | number of proposals 2008 - 2010 | number of experiments accepted 2008 - 2010 | beamtime requested (days) | beamtime allocated (days) | beam time requested (%) | beamtime allocated (%) |
|-----------------------|------------------------------------|--|------------------------------|------------------------------|----------------------------|---------------------------|
| France | 905.00 | 761.00 | 6 466.00 | 4 564.50 | 62.6% | 66.8% |
| Germany | 143.00 | 111 | 1035.5 | 693.5 | 10.0% | 10.2% |
| United Kingdom | 39 | 29 | 257 | 160.5 | 2.5% | 2.3% |
| Italy | 41 | 31 | 216 | 154 | 2.1% | 2.3% |
| Poland | 24 | 13 | 221 | 133 | 2.1% | 1.9% |
| Spain | 16 | 15 | 104 | 80 | 1.0% | 1.2% |
| Others (1) | 108.00 | 77 | 585 | 357 | 5.7% | 5.2% |
| EU countries | 371.00 | 276 | 2418.5 | 1578 | 23.4% | 23.1% |
| Switzerland | 4.00 | 4 | 27 | 25 | 0.3% | 0.4% |
| Others (2) | 6.00 | 3 | 41.5 | 11 | 0.4% | 0.2% |
| EU ass. States | 10 | 7 | 68.5 | 36 | 0.7% | 0.5% |
| United States | 55.00 | 39 | 608 | 339 | 5.9% | 5.0% |
| Russia | 32 | 18 | 264 | 124.5 | 2.6% | 1.8% |
| Algeria | 7 | 5 | 99 | 54 | 1.0% | 0.8% |
| India | 15 | 8 | 93 | 45 | 0.9% | 0.7% |
| Others (3) | 37.00 | 15 | 305 | 90.5 | 3.0% | 1.3% |
| Others | 146 | 85 | 1369 | 653 | 13.3% | 9.6% |
| TOTAL | 1432 | 1129 | 10322 | 6831.5 | 100% | 100% |

General balance sheet of the propositions of experiments 2008-2010 by country

(1) Czech Rep., Hungary, Sweden, Belgium, Greece, Austria, Slovakia, Ireland, Romania, Cyprus, Bulgaria, Portugal, Slovenia and The Netherlands

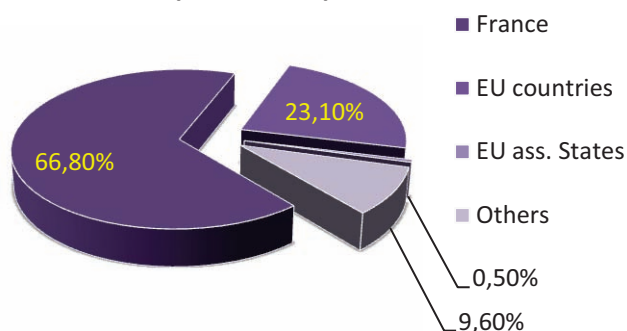
(2) Israel and Norway

(3) Ukania, Australia, Egypt, Japan, Morocco, Palestine, Singapore, Tunisia, Taiwan and South Africa

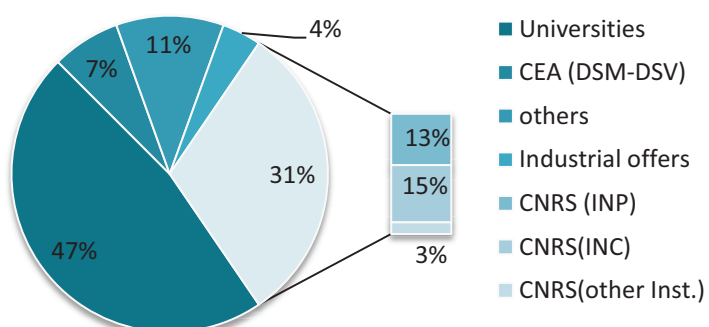
In the table we have analyzed the origin of the users sending proposals. As a whole it provides tall the details for an estimate of a booking rate or mean beam request overload: the ratio of beam time requested over the beam time allocated (10322/6831,5) of **1.5**.

Of course, the largest number of demands and consequently the largest number of beam days allocated come from France (67%) over the period of this report; Users from Europeans countries have received 23% of beam time, and their experiments were supported by the NMI3 access program.

Beamtime Allocation per Nationality (2008-2010)



Distribution of experiments along French Institutions for 2009



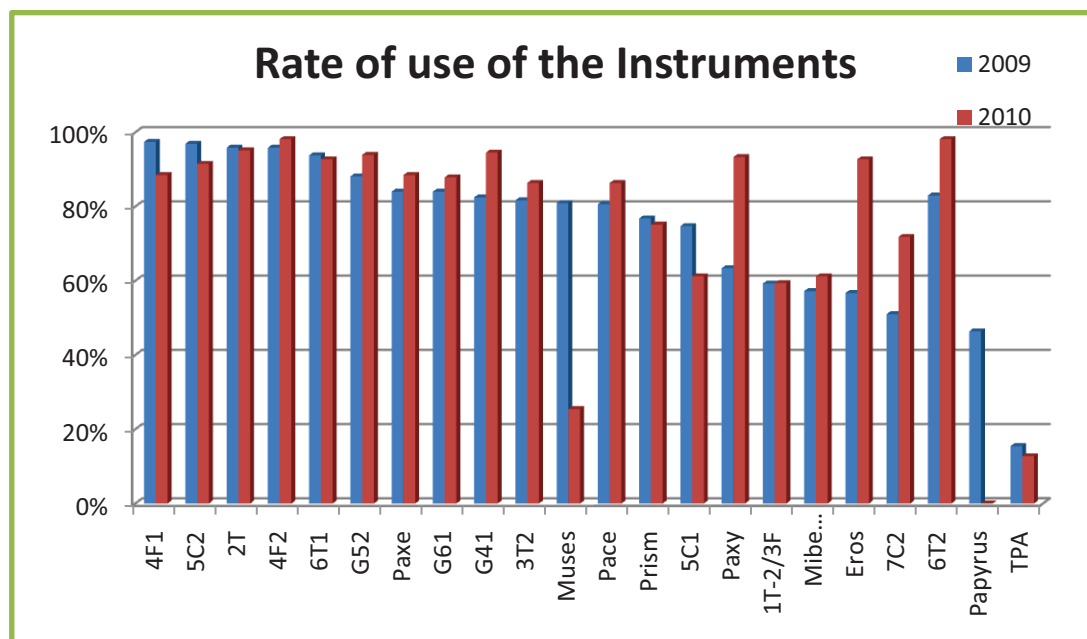
When focusing to the French users, and extracting their address, one can try to estimate how the various organisms: researchers and students from the universities are the most common visitors. The major contributing laboratories of the CNRS come from the Institute of Chemistry.

The rate of use of the instruments and experiments performed

The rate of use of the instruments is on average high: in addition to the 70% of experiments with rank A and according to the balance of the realizations in 2009 and 2010, we have estimated an additional 15% for 2009, and 14% for 2010, of the time for continuing or repeating experiments that encountered problems (technical or scientific), and transfer to A grade of beam time by the committees, corresponding to an average 13% of days (in 2009 and 9% in 2010).

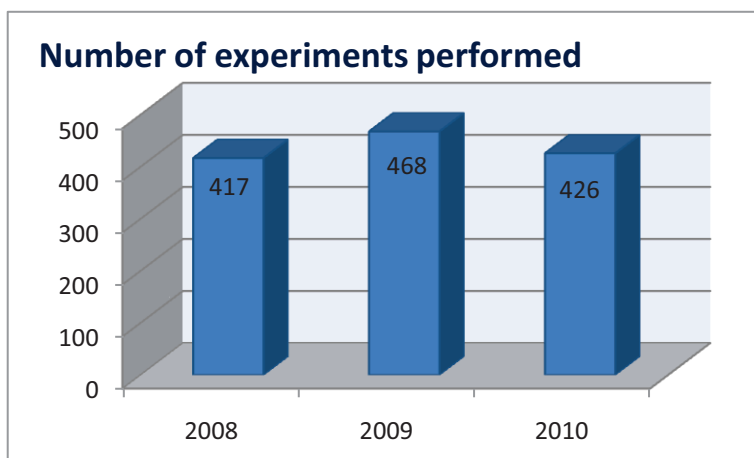
Only 10% of beam-time are devoted to upgrading and maintenance, the rest being for industrial use and training purposes. Of course this an average, it depends strongly on the instrument as detailed below, where the actions are considered; for instance the instrument Papyrus (SANS) was closed, the new TPA open to users (first friendly users), Muses (NSE) encountered a lot of technical problems in 2010, as well as Mibemol, an old ToF machine that needs to be renewed.

We would like to insist here again that there is *no in-house beam time for the LLB teams*. All the LLB scientists, Post-Docs and PhD students should apply for beam time to the Selection Committees for their internal research.



About the commitment of the members of the laboratory, it is important to specify that 90 % participate in the missions of local contacts at various levels (permanent researchers, post-docs and technicians); for each of them, we consider from 50 to 1 experiences supervised (15 on average) a year, representing 200 to 3 days of realization a year, with an average of 70 days per year and per person. To these numbers, one should add the time for finalizing the experiment (including writing a proposal) and the time for the data treatment and the help in finalising a publication.

Finally, we have considered the evolution of the number of experiments performed over these last years; this number fluctuates with the number of FPED available during the year, and it depends on the type of experiments performed. By very rough evaluation, one could estimate that a publication comes from 2 experiments performed.



C- European collaborations: NMI3 and AIEA organization

The LLB is a French Infrastructure, but has an intense European and International influence. We detail in this section the most significant formalised collaborations. They are basically of two types; on one hand, LLB is active and leading member of multi-partner projects as The Integrated Infrastructure Initiative for Neutron Scattering and Muon Spectroscopy (NMI3). On the other hand, LLB cultivate and develop various privileged bi-lateral partnerships.

In the EU Framework Programs, all of the different activities related to a common type of Research Infrastructure are combined into a single project - an Integrated Infrastructure Initiative (I3). The Integrated Infrastructure Initiative for Neutron Scattering and Muon Spectroscopy (NMI3) aims at the pan-European

coordination of neutron scattering and muon spectroscopy, maintaining these research infrastructures as an integral part of the European Research Area. NMI3 comprehensively includes all major facilities in the field, opening the way for a more concerted, and thus more efficient, use of the existing infrastructure. Co-ordination and networking within NMI3 will lead to a more strategic approach to future developments and thus reinforce European competitiveness in this area. The present NMI3-FP7 program is a consortium of 22 partners from 13 countries, including 11 research infrastructures (18 in the call of November 2010).

The objective of integration will be achieved by using several tools:

- Transnational ACCESS (TAA) will be provided by 10 partners offering more than 1400 days of beam time. This will give European users access to all of the relevant European research infrastructures and hence the possibility to use the best adapted infrastructure for their research.
- Joint Research Activities (JRA) focusing on specific R&D areas will develop techniques and methods for next generation instrumentation. They involve basically all those European facilities and academic institutions with major parts of the relevant know-how.
- Dissemination and training actions will help to enhance and to structure future generations of users.
- Networking and common management will help strategic decision-making from a truly European perspective

The Transnational ACCESS at the LLB

Transnational access allows researchers to choose the best-suited instrument/facility for pursuing their scientific questions. NMI3 includes access to all European neutron and muon facilities, (apart from the ILL). The EU provides free access to the facilities:

- by refund beam fees to the facility
- by providing support for travel and subsistence expenses for, typically, one or two scientist per experiment. Users affiliated to a host country institution are not eligible to this program, regardless their individual nationality. For example: A user from a German University could not apply for NMI3 financial support for beamtime at a German Neutron Source. But a German user working in France would be eligible to this program. The same is true for a Japanese user working in UK applying for beamtime in France. Note that the ILL (Institute Laue Langevin) is not eligible for the ACCESS program, because it is a Pan-European Facility.

LLB has been recognized as a "Large Scale Facility" by the European Union in the framework of the Human Capital and Mobility (1992), Training and Mobility of Researchers (1995), Improving Human Potential (1999), 6th and 7th (2003 and 2009 respectively). This has made it possible to receive a considerable number of individual European users (more than 450 since 1993). Up to now, more than 300 publications have come from ACCESS experiments.

The present LLB NMI3-FP7 Access program started on February 2nd 2009 for a period of two years; the LLB is required to provide 200 beam-days. 21 world-class spectrometers are opened to all scientists from European and Associated States. The travel and living expenses for usually two scientists per selected experiment are granted. However, the number of days the LLB is able to offer to European users is significantly higher. This is the reason why in this first 18 month-period, the LLB has actually provided 257 beam days. This is a voluntary effort to strengthen the European user community. In particular, this permits to groups from countries which don't have a national facility to come to the LLB for performing neutron experiments. Many user groups would be unable to travel without this kind of support.

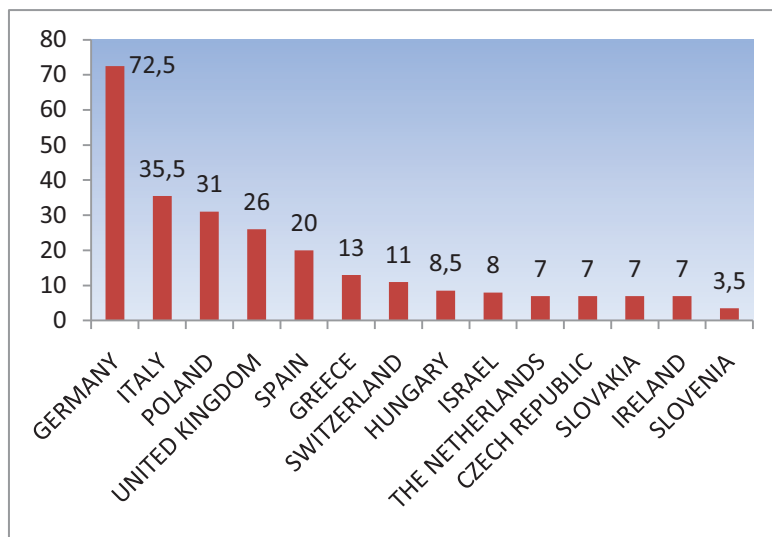
Experiments to be taken in charge by the ACCESS NMI3 program are selected by the SC on the basis of scientific merit. However, some additional criteria might be taken into account:

- new users
- Countries without neutron facilities.
- Experiments involving PhD thesis (or post-docs).

Some Statistics on the ACCESS FP7 Program at the LLB

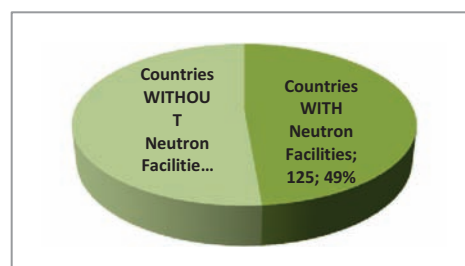
The access beam fee returns **722 k€** to the LLB for a period of two years. The most important part of the funding is mainly devoted to the improvement to the instrument infrastructure, in order to maintain the world-class of the neutron spectrometers opened to the ACCESS program. A part of this funding has been used for hiring two PostDocs and improving the user support.

The LLB delivered 257 days to the users within NMI3, which corresponds to 128 % of the total number of days (200) initially estimated for the 24-month period. This corresponds to 38 projects. 68 users from 14 different European countries were supported by T&S funds. In this graph, we show the number of beam days per country.



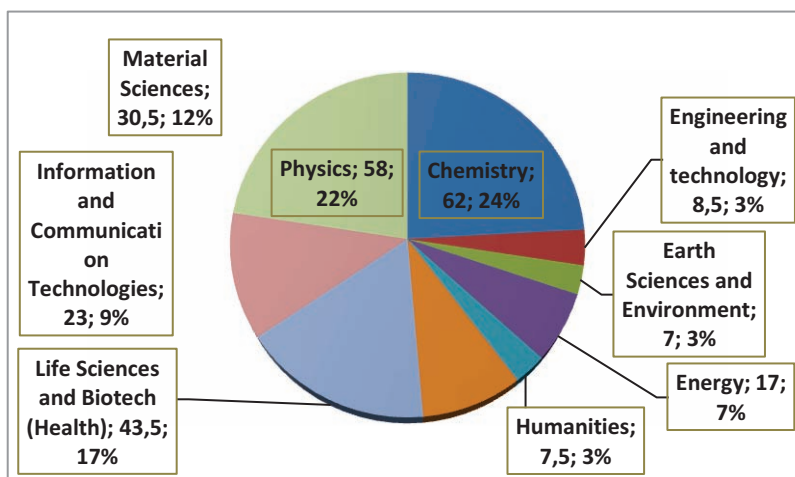
We note that Germany has got by far the largest number of beam-days. This is due to Germany's extensive involvement in neutron scattering and our long history of working together, mainly in the fields of strongly correlated systems and soft matter.

It is also interesting to show the number of beam days provided to Countries with and without national facilities. The LLB provided 125 and 132 beam days respectively, corresponding to 49% and 51% of total delivered beam time.



In the next graph, we show the share of the ACCESS beam days of each thematic field commonly defined for all the Neutron Centers:

The non-physics themes are allocated of 77% of the beam time. We observe that chemistry exhibits a quite high amount of ACCESS. This is certainly due to the worldwide reputation of the LLB in soft matter and solid state chemistry. We also note that the research concerning life sciences and health is quite significant, 17%. The percentage of the other topics (environment, life sciences and cultural heritage) is under 10%.



The Joint Research Activities (JRA) at the LLB

Joint Research Activities (JRA) are projects to develop instrumentation and techniques for neutron scattering and muon spectroscopy, with the long term aim of improving the scientific research possibilities for European users. Each JRA is a collaboration between a number of laboratories and research groups. Some JRA also have collaboration in the USA, Japan, Russia and Australia. Concerning the joint research activities, important break-throughs have been achieved in various areas.

During the FP6, the LLB was involved in research activities on polarized neutrons (PNT), neutron optics (NO) and detectors (MILAND).

In the PNT network, the LLB work was focused on the development of new techniques for polarized neutron diffraction on single crystals. This work led to the VIP concept for a new single crystal diffraction spectrometer which will be commissioned in autumn 2010. Work was also performed on magnetic wave-guide technology.

In the NO network, one of the challenges was to develop new techniques for Very Small Angle Neutron Scattering. The concept of multi-beam SANS was developed within this network and has eventually been implemented on the TPA spectrometer which was commissioned in spring 2010.

In the MILAND network, the objective was to develop a large area ($> 30 \times 30 \text{ cm}^2$) detector with sub-millimeter resolution. The LLB evaluated the possibilities of using small micro-strips modules. The objective proved to be hard to achieve with gas detector technology, especially in terms of spatial resolution. Our Prism reflectometer is now equipped with a detector issued from this development. The usefulness of such detectors was also not obvious for existing neutron spectrometers.

In the first call of the FP7 program the LLB has decided to get involved in the following research networks: Neutron Optics, Polarized Neutrons and Sample environment. For the new call currently under negotiation, the LLB will be involved in new detector development (jointly with CEA/DSM/IRFU), in Integrated User Access, in Structural and Magnetic Imaging and will lead Advanced Neutron Tools for Soft- and Bio-Materials (A. Brulet).

JRA “Neutron Optics” (coordinated by Frédéric Ott/LLB)

Neutron optics is revolutionizing the field of neutron scattering in the same way as telescopes changed astronomy observations compared to the naked eye. During the late 80' and early 90', tremendous improvements have been made in the fabrication of neutron mirrors. These new coatings allow building guide systems with an increased neutron flux of a factor 3 to 4. More recently these improved super-mirrors have been implemented into optical devices: trumpet guides, ballistic guides, polarizing benders etc. and have permitted to improve existing spectrometers. The challenge of the NO network is to go some steps further and to increase the luminosity of the neutron spectrometers even more. Neutron optics technology and components, which are presently available, enable to design new spectrometers which can be at least 10 times brighter than existing ones. The outcome will be a more efficient use of the existing neutron sources. This would benefit directly in the short term to neutron users.

This JRA is focused on 3 main objectives: (i) High flux reflectometry, (ii) High flux SANS and (iii) Focussing of thermal neutrons. This JRA gathers participants from almost all the neutron sources across Europe (ILL, JCNS, HZB, PSI, FRM2, LLB, BNC, NPI). The LLB is particularly involved in the two first tasks (F. Ott and S. Désert).

JRA “Polarized Neutrons”.

The objectives of this JRA are the following:

1. Develop and make available the wide-angle polarization analysis for neutron diffraction/spectroscopy

The realization of large solid angle neutron polarimetry will allow for the use of large solid angle detectors, which enable the simultaneous data acquisition over a wide range of the transferred momentum. This will result in an enormous gain in the efficiency of neutron polarimetric experiments and open new horizons for detailed understanding of the mechanisms involved in multiferroic compounds, photo induced and molecular magnets, magnetic nanostructures, spin electronic and new superconductors, which are at the forefront of condensed matter research.

Arsen Goukassov (LLB) is a leading expert in polarized neutrons. He is an active player in the development of large solid angle polarization analyzers.

To discuss the current state of the art in the field the workshop on "Wide Angle Polarization Analysis in Neutron Scattering" (WAPANS) was organized by the LLB on 22.2.2010. It was attended by JRA partners and observers, scientists from Australia and USA as well as representatives of commercial firms, producers of super mirror polarizers. It was reported about a number of wide-angle supermirror/³He analyzers that have been developed and manufactured.

Based upon the results of these discussions, the decision about the design of analyzers for the diffractometer Super 6T2 at LLB and spectrometer TOPAS at JCNS will be taken soon.

2. To extend possibilities of methods of Larmor labelling towards higher energy and momentum resolution.

The Larmor labelling of individual neutrons allows the development of "unusual" neutron scattering techniques. An extremely high energy (momentum) resolution that is not possible in conventional neutron spectroscopy (diffraction) because of intolerable intensity losses, becomes achievable.

S. Longeville and S. Klimko work on the development of a wide-angle neutron resonance spin-echo spectrometer at the LLB. A first exemplar of the primary spectrometer coils has been tested in May 2010 (radiofrequency part) and beginning of July (all coils) at the MUSES spectrometer of the LLB by measuring the resonance spin-flip. The development of the curved coils for the secondary spectrometer is under progress, the radiofrequency part of the shorter radius of curvature coil is under construction.

3. To broaden the user base of polarized neutron scattering by an extensive education and training program. Indeed, a great concern of the JRA "Polarized Neutrons" is education in this field they organize periodically schools on polarized neutron scattering.

JRA "Sample environment"

The *Sample Environment* JRA is a far-reaching collaboration, encompassing a large variety of innovative instrumentation and techniques. It is aimed at expanding the range of experimental conditions accessible to of neutron facilities. The new sample environments will open up new territories for hydrostatic pressure, temperature and advanced gas adsorption equipments, pushing at the boundaries of in-situ experimentation. One of the highlights is the very promising application of aerodynamic techniques to hold the sample in levitation in order to reach very high temperatures.

The three key areas of endeavor are

- high-pressure gas cells
- ultrahigh-temperature furnaces
- gas handling systems.

B. Annigöfer, F. Maignan and J.-M. Mignot take part in the first subtask, whose goal is to increase the range of available pressures to 1 GPa (10 kbar) for inert gases and 0.8 GPa for hydrogen. The pressure limit of existing helium pressure cells for neutron

scattering hardly exceeds 0.5 GPa. This project can thus be expected to have a significant impact on the feasibility of various scientific projects.

In this framework, a new top-loading cryogenerator has been implemented at LLB to cool down the new pressure cells in a more effective and reliable way. It was designed and constructed according to specifications by AS Scientific Products Ltd. Final delivery to Saclay took place in March 2010. Commissioning was completed and the equipment made available to users for the reactor re-start in May. Significant progress has been made in the design of the 0.8 GPa He-gas cell and a design plan review has been held. High-pressure prooftesting of several prototypes was performed in a securized “bunker” at ISIS, U.K.

The collaboration with the AIEA Organisation

LLB participates actively to the Coordinated Research Project Id 1575 on Development, Characterization and Testing of Materials of relevance to Nuclear Energy Sector using neutron Beams which is coordinated by International Atomic Energy Agency. The contribution of LLB is, essentially, to bring its experience and expertise to the study of Fe-Cr martensitic and ferritic steels considered for future generation reactors. The LLB is the leader of the SANS works group. The objective is to make a Round Robin measurement and to improve the data analysis. The laboratory will produce the studied materials (ODS steels) and organize the collaboration between the participants. We also participate to the workshop on the study of deformation mechanisms and crystallographic texture. We can share materials, data and software in order to enhance the using of the international neutron facilities, for the study of materials of nuclear interest

D- Collaboration Research Group between the LLB and the Forschungszentrum Karlsruhe for the operation of the instrument 1T

Since January 1980, the Forschungszentrum Karlsruhe (FZK) has started a collaboration with LLB. The status of collaboration is defined by a two-year contract. A CRG triple-axis spectrometer (TAS) was first installed on thermal beam line 2T1 until 1999, and later moved to the thermal neutron beam 1T1. The FZK has access to 1/3 of the beam time to develop its own scientific program. For the remaining 2/3 the instrument is made available for the LLB's scientific user program. The FZK annual funding for the neutron beam is 85 k€ plus 10-20 K€ of extra charge for liquid Helium.

In collaboration with the LLB-TAS group, a scientist (D. Lamago) and a technician (C. Meunier) from the FZK operate the instrument and are in charge of the developments of the spectrometer and the sample environment. The spectrometer 1T1 is a world-class high flux triple-axis spectrometer, equipped with double focusing monochromator and analyzer. In addition to a standard PG002 analyzer, three different monochromators are available: PG002, Cu111, Cu220. In particular, the Cu220 monochromator is rather unique allowing high resolution measurements of phonon and/or magnon dispersion curves.

Any sample environment of the TAS group (except the 9-Tesla magnet) can be installed on spectrometer 1T1. Important modifications have recently been carried out on the spectrometer: spectrometer 1T1 is now operating with the same electronics and the same command software as any other spectrometers of the TAS group. Furthermore, 1T1 has been recently equipped with a new top-loading displacer, operating from 3 K up to 800 K. In a close future, spectrometer 1T1 should be equipped with focusing super-mirrors (elliptic guides or trompette). This should allow one to focus the neutron beam on tiny single crystals or thin films and to significantly improve the signal/background ratio when using high cell (100 kbar). A feasibility study has been commissioned to Swiss Neutronics (5 KEuros) .

Highlights: *Nature* 455, E6-E7 (2008) - *Phys. Rev. Lett.* 101, 237002 (2008) - *Phys. Rev. Lett.* 102, 217001 (2009) - *Phys. Rev. Lett.* 102, 207201 (2009) - *Nature Materials* 8, 798 - 802 (2009)

E- Long term visitors

Over the period of this report we welcomed several long term visitors , whose financing support was obtained from the Institute of Physics of the CNRS, ANR contracts, local foundations or with the help of the “ Division des relations internationales “ of the CEA

- ✓ Dr Olga Makarova and Dr Sergei Kichanov (financial support from the CNRS and from the RTRA); they are collaborating with I. Mirebeau.

Olga Makarova (engineer at Kurchatov Institute, Moscow Russia) and Sergei Kichanov (post doctorate student at Frank Laboratory of Neutron Physics, JINR, Dubna Russia) spent between 1 and 3 months each year at LLB during the period 2008-10. They contributed to restart the pressure version of the G6-1 spectrometer, and performed several experiments on multiferroics compounds under pressure. They also took part in the training of the new CNRS engineer, Nicolas Rey and in the installation of the high pressure laboratory. Pressure experiments were performed up to 3.6 GPa and down to 1.5K. Among them, two important new results were observed: i) in BiMnO₃, a pressure induced the ferromagnetic to antiferromagnetic transition (Kozlenko PRB 2010); ii) in TbMnO₃ an incommensurate to commensurate transition (Makarova submitted in 2011). Other experiments such as the pressure study of the charge ordered LuFe₂O₄ multiferroic, subject of the thesis of Julie Bourgeois (LLB student), were also performed, and are currently being analyzed.

- ✓ Dr Youri Chumakov was long-term visitor from 2010/1/1 to 2010/10/31

Dr Chumakov is from Institute of Applied Physics of the Academy of Sciences of Moldova, Moldova. (supported by the ANR, CEDA project < < *Convergence of Electron charge, spin and momentum Densities analysis* > >); he collaborates with B. Gillon. Youri Chumakov worked on the realisation of a program for simultaneous refinement of charge and spin densities using the multipole model on the basis of Xray and Polarized Neutron Diffraction (PND) data. He performed PND experimental spin density studies at LLB on different organometallic complexes like a dinuclear Co(II) complex and a tetranuclear Ni(II) cluster which were also studied by Xray diffraction. At the same time, he developed a model for the analysis of momentum densities from Compton Xray scattering data that also permits to describe the charge and spin densities for the final joint refinement program.

A recent publication: Local magnetic moments in a dinuclear Co²⁺ complex as seen by polarized neutron diffraction: A step beyond the effective spin-(1/2)model, A. Borta et al., accepted in Phys. Rev B (2011)

- ✓ Professor Dr. Wolfgang Doster from Technical University Munich

Professor Doster came for the Habilitation of S. Longeville with whom he keep up a long collaboration since long time, and stayed several weeks at the LLB; their common project is about the influence of macromolecular crowding on protein diffusion and physiological implications. They have publications in common and chapters of books.

- ✓ Dr. Subhasish Mazumder , june 2011

Dr Mazumber is a physicist working at the main Indian research centre for Neutron Scattering: the Bhabha Atomic Research Centre (BARC), Trombay, Mumbai. Although member of the Solid State Division, he is the main responsible of the Small Angle facility. In this field he is the author of several seminal contributions, namely about the analysis of the effects of multiple scattering. S. Mazumder collaborates for long time with J Teixeira; their project is focused on problems of hydration of minerals, powders and cements, using contrast variation and an original analysis of the data. His team did experiments also with colloids, sprays and nano-objects.

For the year 2011 and after, we proposed our help to our Japanese colleagues from JPARC by welcoming and helping them in achieving their projects (especially for PhD students).

F- The LLB and the Synchrotron SOLEIL

The relations of this two national TGIR of the Plateau of Saclay became intensified these last years. It is a will clearly shown by the respective directions to meet periodically. Concerted actions in the perspective of the Plan Campus on the Plateau of Saclay been organized. They articulate on 3 axes: training, scientific diffusion and common offer towards the industrial customers.

- ✓ PhD program : with the co-supervision of the thesis of Anne Sophie Robbes (2008-2011):

« Nanocomposites magnétiques : contrôle de la dispersion par greffage et orientation des charges sous champ externe. » Supervisors : J. Jestin, F. Cousin (LLB) et F. Meneau (SOLEIL).



- ✓ The LLB and Soleil organize since the beginning of 2005 thematic meetings (Saint-Aubin meetings) around the use of the large scale facilities in the various domains for the study of the condensed matter:

- Diffusion aux petits angles 2011
- Confinement et nano-systèmes : mars 2009
- Matière Molle : mars 2008
- Diffraction sur monocristal : mars 2007
- Electrons fortement corrélés : juin 2006
- Diffraction de poudres : mars 2006
- Dynamique, fonction et cinétique des biopolymères Protéines : juin 2005
- Magnétisme et nanostructures : mai 2005

The theme of the future scientific meeting will be around the technique of small angles scattering. Indeed, it is a technique extremely asked by the scientific community (30%) , particularly suitable

for the characterization of nano-objects, and it turns out that both X-rays and neutrons are remarkably complementary. Consequently, the LLB and Soleil have common users, who for most part come from laboratories of the ' Plateau of Saclay ' and of the Region around Paris. Another topic is under reflection: WATER exploring the structure and the dynamics of this ' abnormal' liquid via its hydrogen network.

- ✓ About relations with industry :

A meeting took place on June 11th, 2009 with the aim of establishing links between the LLB (M.H. Mathon) and the persons in charge of the industrial evaluation and communication at Soleil. This meeting allowed to begin a common reflection on the envisaged tools to be promoted and the strategy to adopt in terms of prospecting and practices. It was decided to set up concerted actions towards the industrial customers (A common plaque Soleil / LLB-Orphée in the same style as that of the ILL and the ESRF ,...)

- ✓ The development of a common platform for very high pressure (above 10GPa), **LUCES**: " Laboratoire d'Utilisation des Conditions Extrêmes du Plateau de Saclay " supported by the Region and the RTRA, for the development of very high pressure cells for both neutrons and X-Rays. The LLB had long tradition in this field remarkably

developed by I Goncharenko in the past; recently a new engineer N. Rey was hired at the CNRS to ensure this activity at the LLB, and several long term visitors came to help him in that task.

G-The use of LLB by industrial companies

In parallel to the development of fundamental research project, the LLB attaches equal importance to develop and maintain studies in the context of contract research. These cover many fields of science and may take different forms detailed below. Neutron scattering has a great potential of application in applied research and industrial research, mainly in the fields covered by the chemical industry (polymers, green chemistry....), and by the metallurgical and mechanical industry. The materials for nuclear industry constitute a wide range of research topics. Occasionally, specific studies are undertaken about the development of new advanced materials (magnetic materials, ceramics, cements....). Finally, neutron radiography and the neutron irradiation, commonly used by some industrial customers to Orphée, can also be requested through collaborations with the LLB.

The interest of neutrons for industrial research

The structural information's obtained using neutron scattering techniques are of various types and quantitative because obtained on large volumes. They arise from specifics of the neutron-matter interaction; the most important are the high penetration depth, the sensitivity to light elements, especially hydrogen, and the magnetic scattering.

The neutron scattering techniques most used at the LLB, in industrial collaborations or in contract research are summarized below :

- *Diffraction Technique*: most of the industrial applications of the diffraction techniques concern the analysis of residual stress and crystallographic texture. Due to the high penetration of neutrons in the majority of studied materials, it is the unique method to determine complete tensors of **residual stresses** firstly, and to obtain cartography of the stresses in volume with a spatial resolution of the order of mm³. In general, the industrial need is to be able to describe the evolution of the cartographies of residual stresses in parts during the manufacturing process, after the service or mechanical loading. Various industrial parts were studied: track railway, train wheels, cylinder heads, brake rotors, crankshafts... The residual stresses have to be evaluated also after the steps of formatting and assembling. For example, the welded materials are an industrial concern.

Neutron diffraction allows the texture measurements on large volumes (cm³) and by transmission, giving them a quality and accuracy not equalized. The industrial problematic requiring this technique, relate to materials with a complex and heterogeneous microstructure (welding, several phases materials, large grains alloys...) or, to a studied contribution very weak as for example the effect of impurities on the recrystallization or the evolution of minority texture components.

The neutron diffraction also displays a wide range of industrial applications. One very important field is constituted by the possibility to localize the light atoms and in particular, to determine the hydrogen content in a structure. For example, the studies of the materials for hydrogen storage or molecules inserted in zeolites, present an industrial interest.

- *The Small Angle Neutron Scattering*:

The SANS is a very sensitive technique to characterize the microstructural heterogeneities of materials at the nanoscale (1 to 50 nm typically). Coupling of this kind of analysis with the advantages of the neutron beam makes this technique a powerful tool for many industrial applications.

In the metallurgy field, the SANS technique contributes to the development of new composite materials constituted of a metallic matrix reinforced with nanoparticles (carbides, oxides, intermetallic...). This technique allows characterizing the microstructure evolution (precipitation, porosity ...) under thermomechanical processing, aging and under loading (irradiation, milling) mainly for the nuclear industry.

In the physico-chemical field, the industrial needs are very numerous and various: we can cite the characterization of asphaltenes in crude oils, the study of gelation (for food industry), the development of nanocomposite materials (elastomers filled with inorganic particles), ...

- *The reflectivity*: The reflectivity is a surface analysis technique that allows to obtain unambiguous information on the composition, thickness and roughness (or distances of interdiffusion between layers). The main studies of industrial interest concerned the analysis of Supermirrors for neutron guides but also, the study of polymers at interfaces, grafting, and bonding.

- The neutron irradiation: The neutron beams may occasionally be used to irradiate the matter and study the induced damage.

An overview of the LLB' s industrial partnerships

The Laboratoire Léon Brillouin already displays much industrial collaborations in various sectors. The existing collaborations materialize in different forms:

- *ANR Program (Agence nationale de la recherche) and All Project (Agence Innovation Industrielle)*:

The LLB has several industrial collaborations through ANR projects, particularly in the field of Materials and Processes. The projects AMARAGE and aXtrem aim to develop new strengthened steels: (i) for the aviation industry, a steel having a double precipitation (NiAl and Mo₂C), which is a technological challenge (ANR led by Aubert and Duval); (ii) for the nuclear industry, ferritic steels 9Cr Fe reinforced by a nanodispersion of Y₂O₃. The size distribution of oxides is governed by the elaboration conditions (mechanical alloying and thermomechanical treatment) and is crucial for the creep properties (controlled by the CEA). These studies are based on SANS measurements.

The Laboratory is participating to a research program GENESYS (All initially, now OSEO), piloted by ARKEMA. The goal is the production of membranes made of aligned carbon nanotubes and impregnated with a polymer. A major potential application of this system is filtration. The nanostructure is studied by SANS.

The laboratory participates in industrial studies funded by ANR without being a partner. In this case, the beam time is charged to holders of the project. We can cite the example of the Nanohpcuivre project (development of new copper alloys by mechanical alloying) for which the SANS techniques brings a description of the nanostructure.

- *Contractual actions*:

This type of partnership leads generally by a co-financing of a PhD grant.

Currently, collaboration with INRA is underway on the development of green chemistry for applications in food processing. The aim is the valorization of hydroxylated fatty acids chains, purchased from renewable materials for agriculture resources, for the conception of stable foams and/or emulsions. A key point for the design of such materials is the accurate characterization of the fatty chains assemblies, both in bulk solution and at the air/water interface, which can only be achieved by SANS experiments for the bulk and by neutron reflectivity for the interface.

Furthermore, LLB and Michelin are working closely on model systems of Nanocomposites: a matrix of polybutadiene (PB) reinforced with nanoparticles of silica functionalized with small chains of PB. Thanks to the specific deuteration of the chains, SANS experiment will allow determining the conformation of chains in the composites which is, with the local structure of charges, connected to the macroscopic mechanical properties of materials.

- Service delivery

These specific actions, which are billed and confidential, concern mainly characterization of residual stresses, reflectivity and neutrons irradiations.

In this context, electronic components irradiations were performed for various companies. Boron which is contained in most of the electronics components captures thermal neutrons and the resulting nuclear reaction emits a high energy alpha particle. While losing its energy within the component, this particle creates damages that can lead to the failure of the device. In order to avoid this problem in specific high technology use like satellites, the electronic industry has developed boron free components. The testing of the hardening of these components to thermal neutron irradiation requires the use of pure neutron thermal beam containing no fast neutrons and as few gamma rays as possible. Thermal neutron beam ports available in the guide hall of Orphée are ideally suited for this very specific sake. Moreover, a study has been performed for the General Electric; the expertise of LLB in the field of residual stresses permitted to follow the development of residual stresses in gas turbine crankshafts with the objective to improve the manufacturing processes.

Conclusions

The Laboratoire Léon Brillouin displays a high potential of expertise, already exploited in a number of industrial collaborations. In the field of materials science, the laboratory has developed various recurrent collaborations. Indeed, in the metallurgy field, we have partnerships with the automotive and aerospace sectors (PSA, Renault, EADS, Dassault Aviation), generally to study residual stresses in industrial parts.

In the area of nuclear energy, the LLB is working with CEA, EDF, AREVA in order to define new materials and study their performance in service.

In the physical chemistry field, strong collaborations with Michelin, INRA, Arkema.. have been developed over the last decade.

These collaborations must be further strengthened and diversified particularly in industrial sectors which are yet poorly represented, as the cosmetics industry, the food industry (emulsions, foams...), the cements, ceramic materials, biocompatible materials, joining process

H- Bibliometric study: limits and tendencies

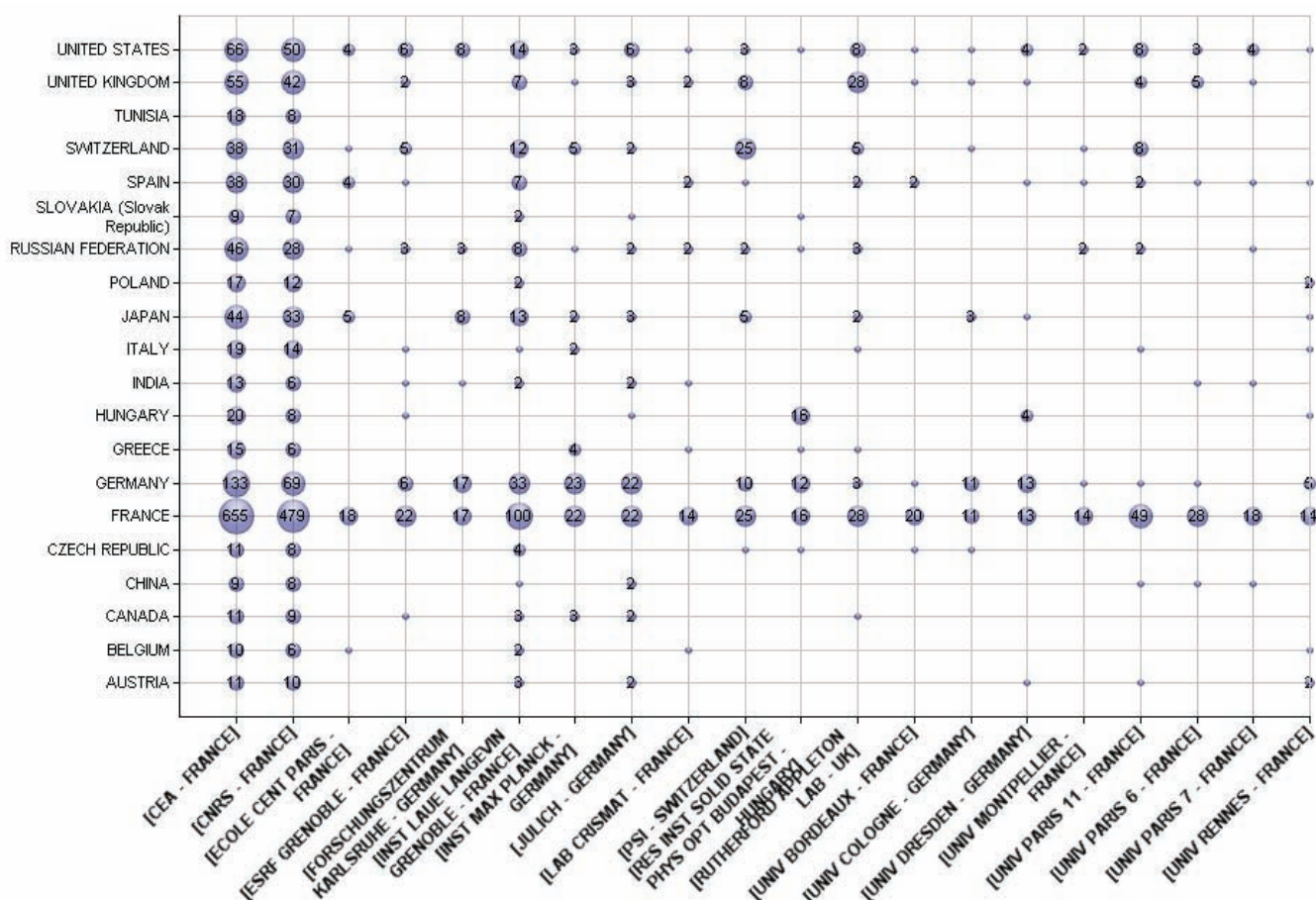
It is always tempting to make comparisons and to position some research in a national and international context in order to assess ' the performances ' of a center. We have presented in the Part I "Overall Report " the scientific production of the LLB in terms of publications (by distinguishing the proper research performed in close collaboration and the work of users out of the research axis even if it was done in collaboration); we have shown the national and international recognition of our teams by their successes in answering at various calls and the number of invitations at international conferences or seminars, in addition to patent registration. The number of publications (and an extensive use of the data basis ISI web of knowledge) is certainly one indicator for the comparison, but more than one would be required to assess the performance, as well as a relevant combination of all of them. It is thus important to put a frame for all these comparisons, as far as the LLB is at the same time, a research unit and a large-scale infrastructure. This dual activity, to which is added the more and more important teaching part, must be taken into account, and corresponding items can be taken either among the other research laboratories (UMR), or among other national facilities, or among the other centres of neutron scattering,

what can be made only at the international level. As a TGIR of national vocation, localized in one site, we opted for a comparison between centres of neutron scattering, as requested by the Steering Committee.

Next to the number of publications and the recognition of the scientific expertise of our researchers, we could introduce other indicators:

- The insertion of the LLB in the international community can be an illustrative one. In the following diagram, we have defined the main scientific partners: on the y-axis, are listed the 20 main countries with which we collaborate, and on the x- axis the 20 main institutions; in the circle, the number of publications with both affiliations is counted (publications can be counted several times depending on the number of partners, also in the first two lines, CEA and CNRS are the majority partners by definition, but as the name CEA appears clearly in the publications, as that of the CNRS is less used thus explaining the difference). The main collaborations or users come from French Universities (Bordeaux, Paris 6, Paris 7, Rennes, Montpellier) and German Universities or Institutes (Köln, Dresden, Karlsruhe..) ; moreover one can see from this graph the strong partnership with other facilities illustrating their complementarities (ILL, ESFR, Jülich, PSI, ISIS..)

Partnerships analysis (through publications) of the LLB according to countries and institutions



- The booking factor = the number of experiments requested/ the number accepted (1.5 on average at the LLB over the 21 spectrometers). It is shared between pretty high demands on some instrument and much less on others, depending on the instrument performances and the tendencies in various scientific fields (one should be ready for any new one appearing in the literature). These numbers are based on the evaluation of the selection committees; however here again there are various practices: a preselection made by the local contact asked in advance, well prepared proposals, request for test time.... However the beam time allocation must also consider the time required for training and education and industrial offers, and the special case of CRG' s.

- User satisfactory form. One can define user criteria reflecting their expectations: the scientific and technical support, the performances of a given instrument, the adaptation to specific requirement, the flexibility in choosing running time, the ability to start again in case of problems, the supervision of inexperienced users, and the help in interpretation... Such a form does not exist explicitly at the LLB thanks to of the strong implication of its members in the scientific community and the spontaneous interaction and discussions that exist. However, it could be done for the future.

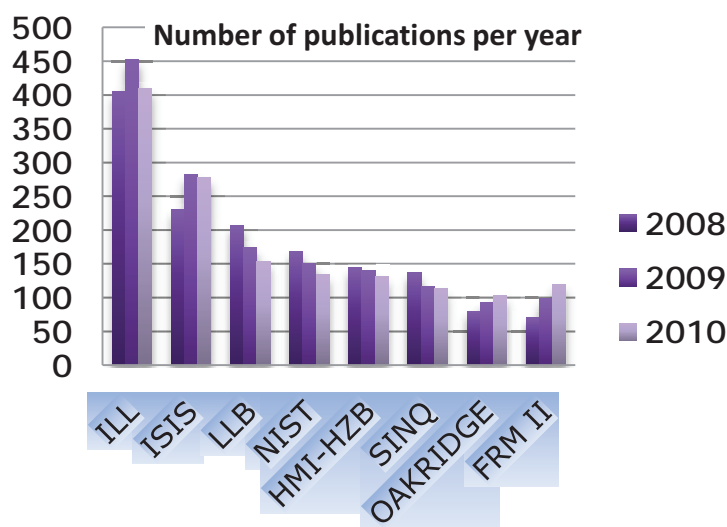
- As proposed by the ILL, one could introduce a 'proposer factor' reflecting how many teams are involved in the selected proposals (the same team can ask for many proposals), how many are new teams, and the occurrence of submitted proposals in time. It will require unfortunately additional manpower just for such statistics, and the LLB has other needs.

○ Finally, the numbers should be normalized by the following parameters illustrating the working conditions of the centers:

- The flux : number of neutrons / $\text{cm}^2 \cdot \text{s}$ (and reactor power)
- The number of days of functioning per year
- The number of instruments (in particular opened to ACCESS NMI3)
- The number of realized experiments per year
- The number of requested days / number of possible days
- The technical and scientific permanent staff (and the age pyramid)
- The global cost of a day of neutron scattering experiment

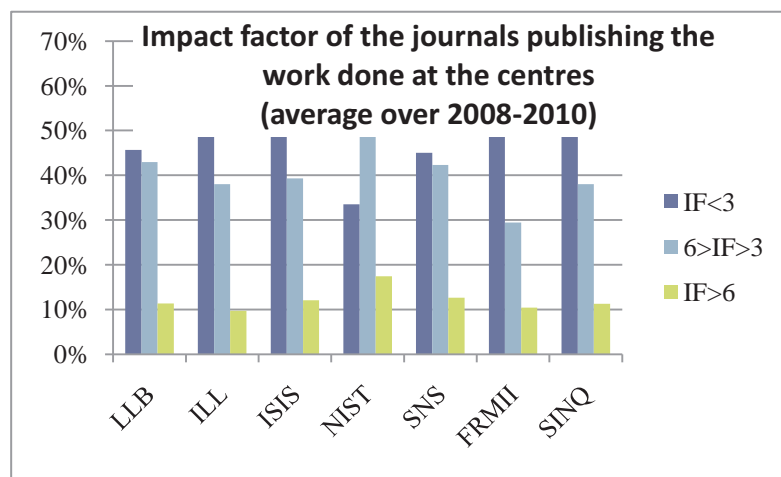
In an attempt to rationalize some of these parameters, we have added at the end of this section a table summarizing them.

More indicators can certainly be defined and adapted to each question addressed. Here we are restricting our analysis to data accessible by everybody, the number of publications as found in ISI Web of Knowledge, when the name of the institution is explicitly written in the address. As mentioned earlier, 10 to 20% of publications might be miscounted, but we consider that the error is valid for all the centers. A realistic list of publications is better done by the centers themselves and can be often found in their respective Annual Reports. We have selected 8 institutions: 2 in the United –States, NIST (Reactor at Washington) and SNS at Oak Ridge (the new American Spallation Source); 6 in Europe (including the LLB), ILL (the international center at Grenoble), FRMII (the German Reactor at Mü nich) ISIS (the British Spallation Source close to Oxford), HMI-HZB (the German reactor at Berlin,) PSI SINQ (the Swiss Spallation Source, at Villigen).

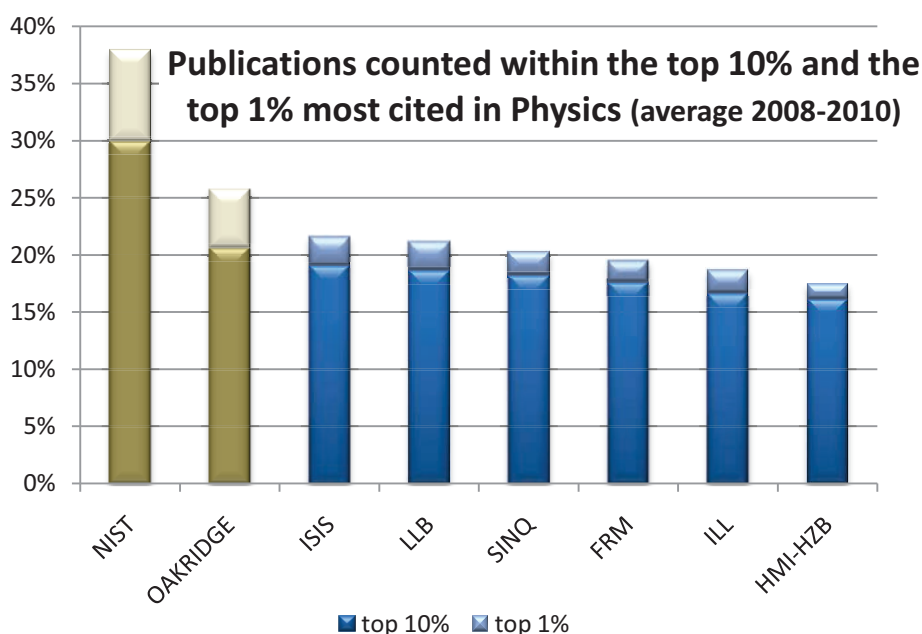


Over the period of this report, the LLB might be ranked as the third center in the world in publishing the results of experiments done (a number that must be considered within the set of parameters defined above).

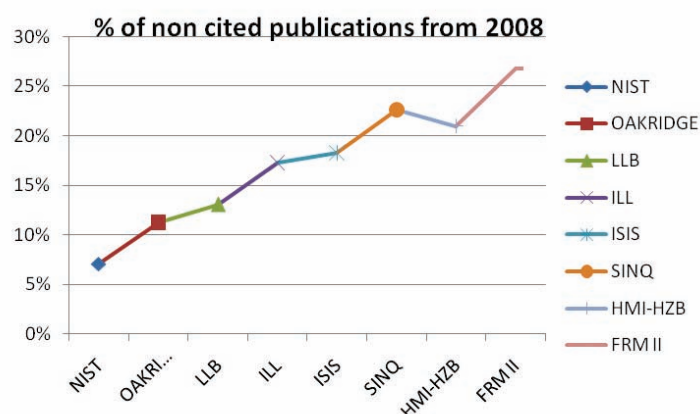
In terms of the impact factor of the journals where the results of these experiments are published: it is equally distributed along the centers for the journals having the highest IF, and depends on the fields for the others. (Note: It was not possible to perform this analysis for the HMI, because it changed his name in 2009).



It turns out that an analysis built on a citation index basis is more relevant for the evaluation of the technical and scientific expertise, than an expected impact factor of a given journal. However one must be aware of citation index basis, which might vary between fields and over time. The figure below illustrates two important points: i) the communication policy is rather different in the United States and in Europe since the most cited papers are from the two American sources; for this study one should consider the time over which the analysis is done: the European publications require apparently more time to be cited (or known), but their citation number is increasing with time, while the US publications reach faster a plateau value; ii) The position of the LLB is quite good, and one can see that the main countries having neutron sources, *i.e.*, UK, De (FRMII+ HMI), Fr, have the same percentage of publications in the top 10% and the top 1%.



The counterpart of the above observation is the number of non-cited publications; accordingly, the next figure shows the % of articles published in 2008 that are still non-cited in March 2011. Here again the American communication policy is different since the two American centers have the smallest number of non cited articles, and one envision the slowest European communication rate. Here again, the



LLB is in a good position; one can observe that it follows the large contribution to journals with an IF between 3 and 6 (above 40%) for NIST, SNS and LLB. (As a reference number, one should notice that in physics , it is considered that between 30-40% of publications are non cited).

In order to compare properly the centers we have considered in the publications study, we have recorded in the table their characteristics according to some criteria that we found appropriate; unfortunately we still need to complete this Table.

Main features of the different neutron sources

| Source | Power | History | Flux (n/cm ² .s) | Moderator | Operating days en 2008 | Nb of instruments | Permanent staff |
|----------------|--|------------------------------------|-----------------------------|-----------------------|---------------------------|----------------------|--------------------|
| ILL (RHF) | 58 MW | 1971 | $12 \cdot 10^{14}$ | Thermal, Hot, Cold | 182 | 37 | 453 |
| ISIS | 600MeV 1.5mA pulsed | Target 1 : 1985 Target 2 : 2009 | $0.56 \cdot 10^{14}$ | Thermal, Cold | 174 | 31 | 350 |
| FRM II | 20 MW | 2005 | $7 \cdot 10^{14}$ | Thermal, Hot, Cold | 241 | 23 | 230 |
| HMI-HZB | 10 MW | 1973, upgrade 1993 | $1.2 \cdot 10^{14}$ | Thermal, Cold | 224 | 23 | |
| SINQ | 590 MeV 1.8mA continuous 1MW on target | 1996 | $0.16 \cdot 10^{14}$ | Thermal, Cold | 162 | 17 | 160 |
| LLB-Orphée | 14 MW | 1980 | $3 \cdot 10^{14}$ | Thermal, Hot, Cold | 189 | 23 | 151 |
| NIST | 20 MW | 1969, upgrade 1994 | $3 \cdot 10^{14}$ | Thermal, Cold | 250 | 25 | 148 |
| SNS Oak-Ridge | 1 GeV 1.4 mA pulsed 2 MW on target | 2006 | $1 \cdot 10^{14}$ (at 1MW) | Thermal, Cold | | 17 | |
| HFIR Oak-Ridge | 85 MW | 1966, upgrade 2007 | $10 \cdot 10^{14}$ | Thermal, Cold | ~160 | 9 | |

I- Some scientific highlights

Until recently, serendipity and experimentation have been the most frequent design principles of formulations for either cleaning or consolidation of our Cultural Heritage. Accordingly, the past has witnessed a number of actively detrimental treatments, such as the application of acrylic and vinyl resins, whose ageing and degradation can irreversibly jeopardize the appearance (or even the continued existence) of irreplaceable works of art, as below illustrated for the copolymer film application to mural paintings in “Templo de los Nichos Pintados” in Mayapan (Yucatan, Mexico).



Figure. 1 – Damages caused by the inappropriate application of polymers to Mesoamerican mural paintings.

Often the degradation of these polymers makes them no more removable by organic solvents, whose use on painted layers is also not always advisable. The search for alternative, environmentally benign cleaning tools for the removal of polymeric films has therefore acquired an extraordinary relevance. In the last years we have designed, prepared and tested micellar and microemulsive formulations where solvents are dispersed in aqueous media, which are among the most effective systems available for the removal of several acrylic and vinyl resins.

A detailed characterization of structural features at the nanoscale is the key to achieve a predictive knowledge on their performances for a given application. As their structural complexity grows in response to many different requirements, scientists need more and more tailored tools to investigate them.

Illuminating examples are the systems obtained by adding to a SDS/1-pentanol (PeOH) aqueous dispersion either an immiscible oil (**a**) (xylene) or a mixture of partially water-miscible solvents (**b**) (ethyl acetate (EA) and propylene carbonate (PC)) [1, 2]. While the former is a classical microemulsion, the latter, was not yet defined, in

NANO-STRUCTURE OF AMPHIPHILES-BASED SYSTEMS USED IN CONSERVATION OF CULTURAL HERITAGE

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terms of structural features. The **b** system provides better results in the removal of acrylic/vinyl coatings (removal tests of an ethylmethacrylate/methylacrylate 70/30 copolymer, Paraloid B72 from glass slides showed that in 90 minutes it removed ~90% of the polymer, while the **a** system only ~60%) [2, 3]. Since Paraloid has similar affinities for xylene and PC (or EA) the reason for different performance should be related to the composition and to the microstructure of the systems.

For both systems, the interaction with a polymer film results in a “phase separation”, where an aqueous micellar or oil-in-water microemulsive phase coexists with a polymer solution, constituted by a clearly defined blend of solvents, particularly enriched in PeOH, which is, in itself, a non-solvent for Paraloid.

The purpose of the work was to understand how the microstructural details are related to the different effectiveness in polymer removal and which factors drive the composition of the polymer-rich phase.

Small Angle Neutron Scattering (SANS) is a unique tool in this respect, because it lends itself to H/D isotopic substitution, without changing the chemical composition and properties of the system, but allowing to get information on different regions or domains [4], while SAXS is not as informative, being insensitive to isotopic composition (Figure 2).

Using contrast variation series of samples, we have been able to precisely define and compare the

microstructure of both systems, which were

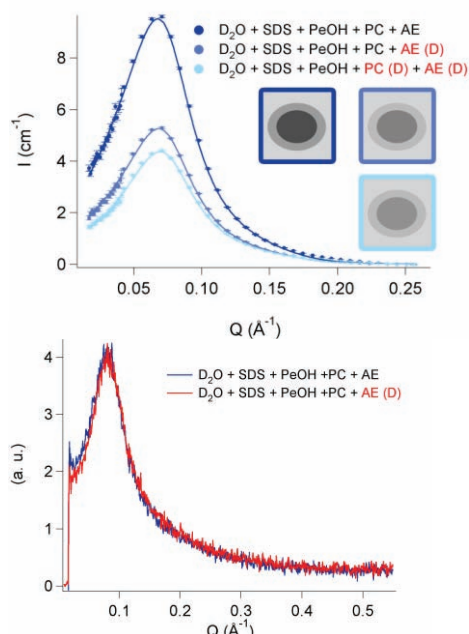


Figure. 2 – Top: a contrast series, recorded on the EA/PC system; the lines are the result of a global fitting analysis. Bottom: SAXS curves of two of the same samples.

modeled as composed of monodisperse core-shell prolate aggregates, with effective charge Z and interacting with each other according to a screened Coulomb potential. The neutron scattering length density of the core and of the shell and the geometrical parameters of the aggregates have been determined through global fitting of each contrast variation series, giving access to the composition of each micellar domain [5].

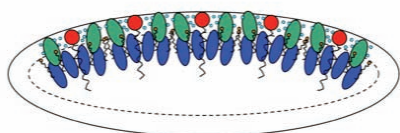
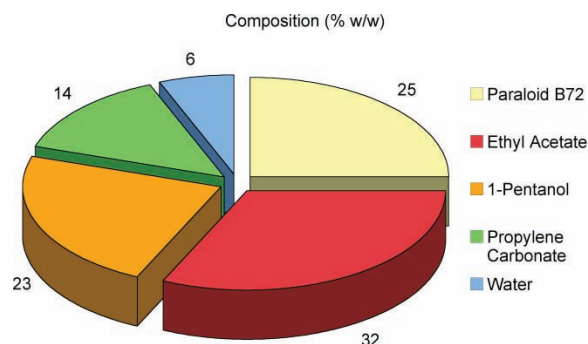


Figure 3 – Schematic structure of the EA/PC system aggregates.

Experiments were also performed letting the EA/PC micelles and the xylene-in-water microemulsion in contact with known amounts of Paraloid B72 films for a few hours. As anticipated, for both systems the formation of a droplet of swollen polymer is observed, which, for a wide range of initial Paraloid content, has the same composition [3].

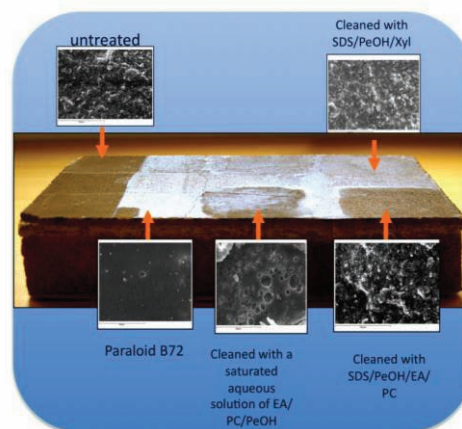
After the interaction with the polymer, the micellar aggregates lose about 30% of their initial volume, and, in particular, they are depleted of PeOH, which, as a neat solvent, does not solubilize Paraloid, but rather acts as a co-solvent for one of the two blocks constituting the copolymer.

Figure 4 – Composition of the polymer-rich phase obtained after the interaction of the EA/PC system with Paraloid B72.



We believe that the partition of PeOH, EA and PC between the aqueous and the micellar phase leads the initial swelling steps and determines the more efficient removal observed for the EA/PC micellar system.

Figure. 5 – Removal tests of Paraloid B72 from laboratory fresco model samples. Glazing light picture and SEM images.



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Note: no kinship exists among the authors

Liquid crystals LCs confined in porous materials exhibit exceptional structural and dynamical properties, resulting from an intricate balance between topological, interfacial, finite-size, and quenched disorder effects. They offer remarkable opportunities to address fundamental questions of current condensed matter physics.

During the recent years, we have conducted an extensive study of both structural and dynamical behaviors of a series of calamitic rod-like liquid-crystals LCs belonging to the family of cyanobiphenyls nCB, with $7 < n < 12$ confined in 10 nm cylindrical pores of porous silicon (pSi), porous silica, and aluminum oxide. Neutron diffraction, SANS, and quasielastic scattering experiments performed at LLB and ILL have been combined with a variety of in-lab experiments and molecular simulations.

1. Low Dimensionality Effects

LCs materials are elastically soft and may directly couple to the surface of the porous matrix, which acts as an external field. Hence they are unique prototypical systems to achieve experimental realizations of different theoretical cases by changing the nature of the porous morphology. Using macroscopically aligned straight silica nanochannels, we have provided the first quantitative test of a prediction derived from a Landau–de Gennes model in the case of unidirectional confinement [1]. It supports the existence of a critical threshold in the strength of uniaxial coupling of the nematic order parameter with the pore that separates discontinuous from continuous paranematic-to-nematic behavior.

2. Unidirectional Random Fields Effects

Another point of fundamental interest is the influence of random fields on phase transitions, which counts among the most debated topics since Imry and Ma (1975). Using the highly corrugated nature of the inner surface of porous silicon we induced anisotropic quenched disorder effects in terms of random orientational fields that couple to the nematic director and random positional fields

that couple to the smectic order [2]. Moreover, we tuned the strength of the coupling between

LIQUID-CRYSTALS CONFINED IN NANOCHANNELS

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the nematic and smectic order parameters by varying the chain length (from 8CB to 12CB). Thereby we have analyzed the critical behavior of the isotropic-to-smectic and the nematic-to-smectic transitions induced by anisotropic quenched disorder [2, 3] (see Fig. 1).

3. Metastability and Bridgman Growth

The formation of low-temperature metastable states is ubiquitous in nanoconfined systems, and a complex phase diagram including new lamellar phases has been characterized for nCB [4]. What is more spectacular is the possible thermal switching between two metastable configurations of the smectic phase. It has been attributed to a collective molecular reorientation during thermal cycling through the crystalline state, which is driven by a nanoscale analogous of the Bridgman growth [5].

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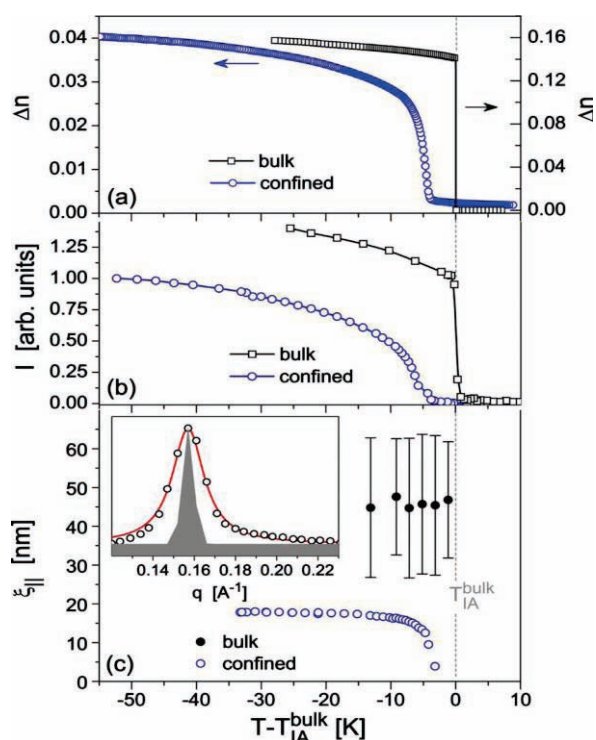


Figure 1: (a) Birefringence (Nematic order) and (b) integrated intensity of the smectic neutron diffraction peak (Smectic order) of bulk and nanoconfined 12CB. (c) Related smectic correlation lengths. After ref. [3].

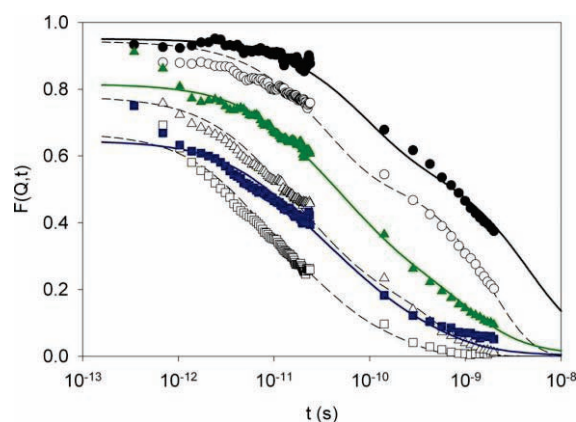


Figure 2: (a) Incoherent intermediate scattering functions of bulk (open symbols) and nanoconfined 8CB (filled symbols) for three values of the transfer of momentum. Solid lines are theoretical models based on homogeneous/heterogeneous distribution of simple modes in the bulk/confined states respectively. After ref. [8]

4. Dynamic Heterogeneities and their Structural Counterparts

Finally, we have emphasized a glass-like dynamics as an important feature of confined LCs (drastic molecular slowdown, non-Debye decays, and super-Arrhenius temperature

dependence) [6]. The concept of dynamic heterogeneity plays a key role in the current understanding of systems as diverse as polymers, supercooled liquids, colloidal suspensions, or granular media. Although it may not be ubiquitous to all glass-forming systems, the static nature of the observed heterogeneity is still debated. On the other hand LCs constitute archetype examples that can naturally develop static order parameters. Moreover, unlike supercooled liquids, the molecular dynamics of LCs is generally described by a finite set of correlation times and well-defined relaxation mechanisms [7] (see. Fig. 2).

Through independent static and dynamic measurements, we have shown that the temperature dependence of the dynamic correlation length ξ_{wall} that quantifies the distance over which a memory of the interfacial slowing down of the molecular dynamics persists, is closely related to the growth of the short-range static order ξ_{stat} arising from quenched random fields [8]. Models used to analyze neutron scattering experiments have been corroborated by the computation of spatially resolved quantities from molecular simulations [9, 10, 11].

Acknowledgements

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The rule of Meyer-Overton that establishes a correlation between lipophilicity and potency of anesthetics is generally accepted. Exceptions were first observed for *n*-alcohols, C_nOH : the anesthetic potency reaches a maximum for $C_{11}OH$ and the compounds with $n > 13$ are non-anesthetic [1]. This problem can be studied at the molecular level by dissolving long alcohols (C_8OH to $C_{18}OH$) in the lipid part of biomembranes [1]. In this work we analyse the structural changes of fluid PCPS bilayers, composed of dioleoylphosphatidylcholine (DOPC, 96 mol %) + dioleoylphosphatidylserine (DOPS, 4 mol %), in unilamellar vesicles (ULVs) prepared by extrusion. Indeed, unsaturated phospholipids are important constituents of biomembranes and due to their low gel-liquid crystal phase transition temperature they are currently accepted as models of fluid bilayers in biological membranes, and ULVs are topologically similar to cell membranes. The small amount of DOPS in DOPC charges the bilayer surface negatively and thus prevents ULV aggregation after extrusion. We measure the bilayer thickness, D , and the lateral area of the unit cell consisting of a phospholipid molecule and a particular fraction of the alcohol at the bilayer – aqueous phase interface, A_{UC} .

Solid DOPC+ DOPS+ C_nOH mixtures were dispersed in 100, 90, 80, 70, 60 and 50 % D_2O in H_2O mixtures (outer contrasts) at 10 mg/ml concentration and extruded through 50 nm pores in 2 stacked carbohydrate filters as described in [2]. SANS spectra were measured on PAXE (sample to detector distance 1.3 m and 5.05 m, $\lambda = 0.6$ nm) at 25 °C. It is supposed that extruded ULVs are polydisperse hollow spheres with a single bilayer separating the inside and outside aqueous compartments, and that the bilayer can be divided into three strips corresponding to two polar headgroup regions and the bilayer center spanning hydrocarbon region. The normalized SANS intensity $I_{exp}(q)$ as a function of the scattering vector modulus q can be then fitted by

HOW MUCH ANESTHETICS EFFECTS DEPEND ON THE LENGTH OF ALCOHOL CHAINS?

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$$I_{exp}(q) = N_P \int_{q'} T(q') \int_R G(R) I(R, q - q') dR dq'$$

where N_P is the number density of particles, $T(q)$ is the PAXE resolution function, $I(R, q)$ the structure factor of the ULV with radius R , and the ULVs polydispersity is described by the Schulz function $G(R)$. The scattering length densities of polar and hydrophobic regions were calculated using the known scattering lengths and component volumes of DOPC, DOPS and C_nOH measured in [3]. Details of the model and fitting procedure were described earlier [4].

Selected D results as a function of C_nOH :PCPS molar ratio (Fig. 1) and as a function of C_nOH chain length n at fixed C_nOH :PCPS = 0.4 molar ratio (Fig. 2) are shown and compared with control value of D (dashed line) obtained for the pure lipid. As expected, the thickness D decreases due to mismatch of the lengths of the two chains, the effect being smaller with longer alcohols. The lateral area A_{UC} increases due to C_nOH intercalation between lipid molecules (Fig. 1), particularly for large chain

alcohols. The resulting partial area at the interface, A_{C_nOH} , (Fig. 2) is anomalously small for anesthetically active alcohols ($n < 12$), even smaller than the area of the chain cross-section in solid rotator phases of *n*-alkanes, which is of the order of 20 Å² (dashed line). We suppose that this is due to the lipid head group: its interface area A_{PCPS} is equal or larger than the sum of the areas

of the hydrocarbon chains cross-sections, so that a small OH group of C_nOH is located underneath at the lipid glycerol fragment. Our experimental results are reproduced by molecular dynamics simulations of DOPC+ C_nOH bilayers carried out with the GROMACS molecular dynamics package, using the MARTINI coarse-grained force field (M. Bulacu and S.-J. Marrink, personal communication).

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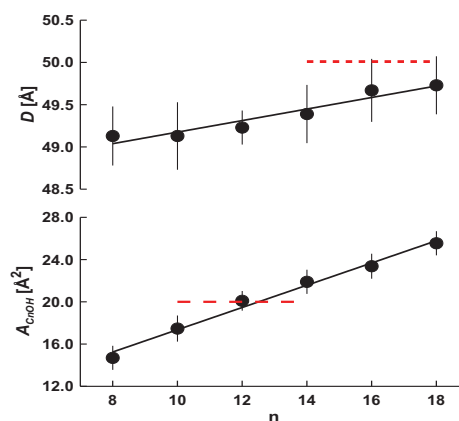


Figure 1. Bilayer structural parameters as a function of C_nOH :PCPS molar ratio.

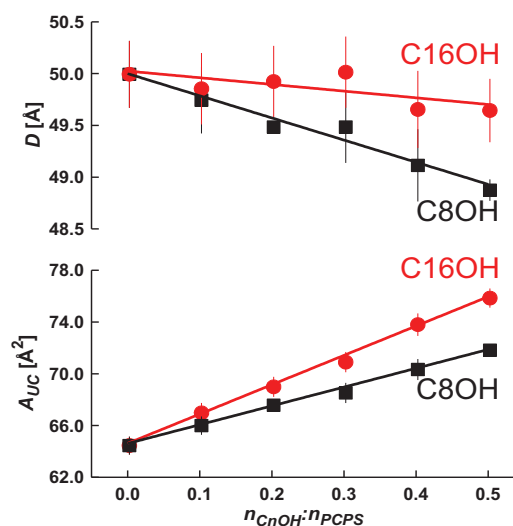


Figure 2. Bilayer structural parameters as a function of C_nOH chain length for C_nOH :PCPS=0.4 molar ratio.

An important aim of research on telluride glasses is the design of single mode fibers guiding infrared light until 20 μm . Due to their excellent glass forming ability, selenium based glasses are extensively used in the mid infrared region. However the cut off of these glasses is near 14 μm , making them inappropriate for novel far infrared applications. The most straightforward strategy of shifting the cut off to longer wavelengths is the replacement of selenium by a heavier element e.g. tellurium. Unfortunately, tellurides are usually poor glass formers. Indeed, a critical cooling rate of only ~ 1 K/sec is enough to vitrify Se, while an extremely fast quenching of 10^6 K/sec is necessary to obtain small chips of vitreous Te. In order to shape lenses or fibers for optical devices, one has to improve the glass forming ability of such glasses by preventing Te from crystallizing.

In the past, this has been achieved by adding halogens (Cl, Br or I) to pure Te. These materials (also known as TeX glasses) exhibit excellent optical properties, but their glass transition

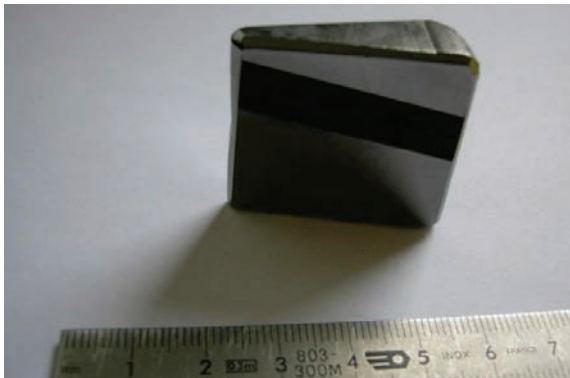


Figure 1. A prism made of TGG ($\text{Te}_{78}\text{Ge}_{11}\text{Ga}_{11}$)

temperature T_g is low and the resulting poor thermal stability prevents their optical applications. Glasses with higher T_g can be obtained in the binary $\text{Ge}_x\text{Te}_{100-x}$ system along a narrow compositional range at $x \approx 15-25$ [1], but these can only be vitrified using a cooling rate around 10^3 K/s, which restricts the sample size to about 0.05 mm thickness. Different strategies can be applied to improve the glass forming ability and thermal stability of binary Ge-Te glasses [2,3]. For example, by addition of Ga; compositions lying along the GeTe_4 - GaTe_3 tie line are characterized by T_g around 150 $^\circ\text{C}$ and T_x (crystallization temperature) close to 250 $^\circ\text{C}$. Besides having a better thermal stability, their shaping is also relatively simple allowing the preparation of long fibers, lenses or prisms

LOCAL ORDER IN Te-RICH Te-Ge-X (X=Ga, I, Se) IR OPTICAL GLASSES

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as demonstrated in Fig. 1. Doping with iodine also results in a better glass forming ability and thermal stability. For instance, in the case of $\text{Te}_{73}\text{Ge}_{20}\text{I}_7$ T_g is also 150 $^\circ\text{C}$ and T_x is 274 $^\circ\text{C}$ [3]. Terminal iodine atoms are believed to split the Te-Te chains preventing tellurium from crystallizing. More recently, special attention has also been paid to Te rich alloys of the GeSe_4 - GeTe_4 system. Among them, the $\text{Te}_{77}\text{Ge}_{20}\text{Se}_3$ composition appears to be the best compromise between thermal stability and optical transparency [4].

Table 1. Coordination numbers of Te obtained in various Te-Ge-X glasses (X= I, Se, Ga) [7].

| Alloy | N_{TeTe} | N_{TeGe} | N_{TeX} | N_{Te} |
|--------------------------------|-------------------|-------------------|------------------|-----------------|
| $\text{Te}_{85}\text{Ge}_{15}$ | 1.41 | 0.70 | – | 2.11 |
| TGI | 1.00 | 1.02 | 0.03 | 2.08 |
| TGS | 1.07 | 0.93 | 0.09 | 2.09 |
| TGG | 1.36 | 0.57 | 0.43 | 2.36 |

The aim of our study was to gain insight into the structure of bulk glass formers $\text{Te}_{78}\text{Ge}_{11}\text{Ga}_{11}$, $\text{Te}_{70}\text{Ge}_{20}\text{Se}_{10}$ and $\text{Te}_{73}\text{Ge}_{20}\text{I}_7$ (denoted with TGG, TGS and TGI, respectively) and understand how the third component builds in the host network. For this purpose, we have carried out neutron and X-ray diffraction measurements as well as extended X-ray absorption spectroscopy (EXAFS) experiments at Ga, Ge, Se, Te and I K-absorption edges. For each composition, the experimental datasets were fitted by the RMC

simulation technique [5,6]. In this method, large scale atomic models compatible with experiments and physical constraints (e.g. density, coordination constraints) are generated. Coordination numbers of Te obtained by the RMC technique are listed in Table 1. For comparison we also give the corresponding values of $\text{Te}_{85}\text{Ge}_{15}$ glass. N_{Te} , the average coordination number is close to 2 in TGI, TGS as well as in the binary glass while it is significantly higher in TGG. It can also be observed that in TGG $N_{\text{TeGe}} + N_{\text{TeTe}}$ is very close to 2 suggesting that Ga participates in the ‘third bond’ of Te atoms. Thus, unlike Se or I, Ga does not build into the Ge-Te covalent network. Instead, it forms a covalent bond with the non bonding p electrons of Te, which results in an increase of the average Te coordination number. This is consistent with the expected role of Ga in the initial composition: catching the Te lone electron pairs to prevent tellurium from crystallizing. Fig. 2 shows a schematic model of TGG based upon the above results.

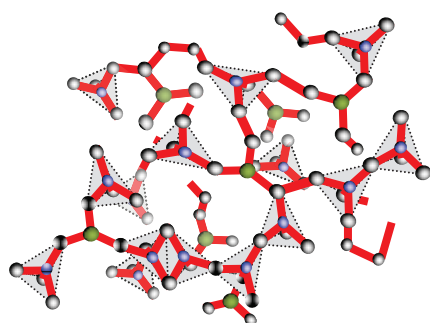


Figure 2. A model structure of TGG with threefold coordinated Te atoms (Ge: blue, Ga: green, Te: gray).

Bond lengths are summarized in Table 2. Our results clearly show that the third component has strong influence on the average Te-Te distance. While the Ge-Te distance is essentially the same in all alloys investigated (2.60 ± 0.02 Å), the Te-Te bond is significantly longer in TGG (2.80 ± 0.02 Å) than either in TGS (2.73 ± 0.02 Å) or in TGI (2.70 ± 0.02 Å). The Te-Te distance in $\text{Te}_{85}\text{Ge}_{15}$ (2.75 ± 0.02 Å) is just half way between the corresponding values of TGI and TGG.

Table 2. Comparison of the r_{ij} bond lengths (in Å) found in glassy $\text{Te}_{85}\text{Ge}_{15}$, TGI, TGS and TGG.

| Alloy | r_{TeTe} | r_{GeTe} | r_{XGe} | r_{XTe} |
|--------------------------------|-------------------|-------------------|------------------|------------------|
| $\text{Te}_{85}\text{Ge}_{15}$ | 2.75 | 2.60 | – | – |
| TGI | 2.70 | 2.60 | 2.58 | – |
| TGS | 2.73 | 2.60 | 2.35 | 2.60 |
| TGG | 2.80 | 2.60 | – | 2.60 |

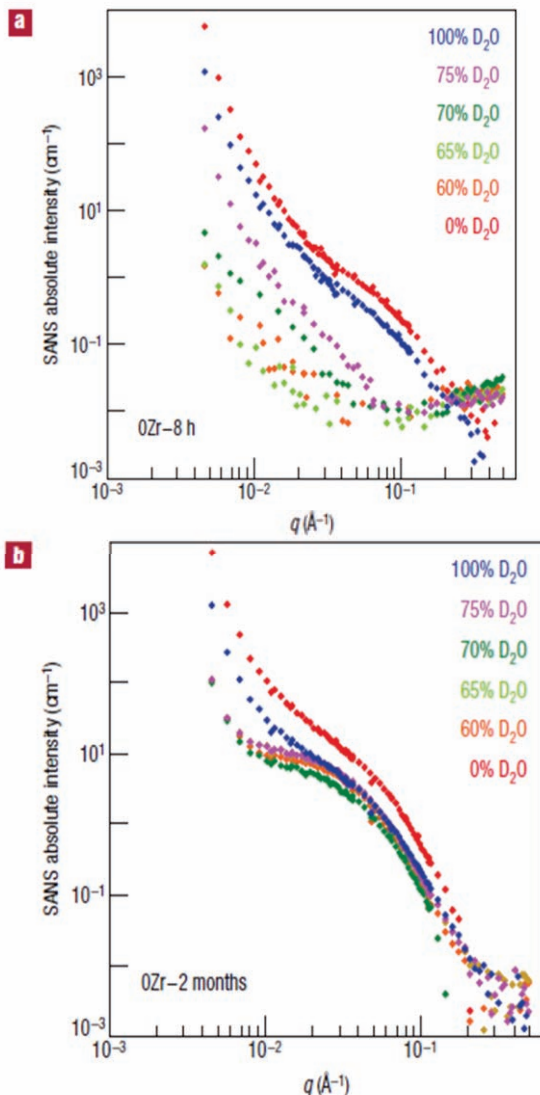
According to these observations, the strength of GeTe_4 (respectively GeTe_3I , GeTe_3Se) ‘units’ is very similar in $\text{Te}_{85}\text{Ge}_{15}$, TGG, TGI and TGS, but the connection between these units is different. Shorter Te-Te distances in TGS and TGI suggest that Te-Te bonding is stronger in these alloys than in TGG.

By combining different experimental techniques it was possible to determine short range order parameters in Te-Ge-based glasses. It was shown that the improvement of glass forming ability is achieved by entirely different strategies. While I and Se build in the covalent network making Te-Te bonding stronger, Ga increases the average coordination number of Te (and also network connectivity) but decreases Te-Te bond strength.

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This study investigates the long term behavior of glasses used for confinement of nuclear wastes. The results have been obtained from a fruitful collaboration between different CEA laboratories (LLB, LIONS, CEA Marcoule) and the Ecole Polytechnique. The corrosion process of the glasses by water creates at the glass surfaces, an altered porous layer, hydrated and amorphous, called “gel”. This gel, which is the result of the release of soluble elements, of hydrolyses and of silica network recondensation can in specific conditions strongly limit the exchange process between the glass and the solution. Our hypothesis to describe this phenomenon is the closure of the gel porosity.



INFLUENCE OF THE ALTERATION LAYER MORPHOLOGY ON THE SILICATE GLASS CORROSION MECHANISMS: ROLE OF THE CALCIUM AND OF THE ZIRCONIUM

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We present an original approach of the corrosion of silicate glasses, usually describe in term of chemical thermodynamic, and based on the influence of the morphological modifications of the gel on the slowing down of the kinetic of dissolution.

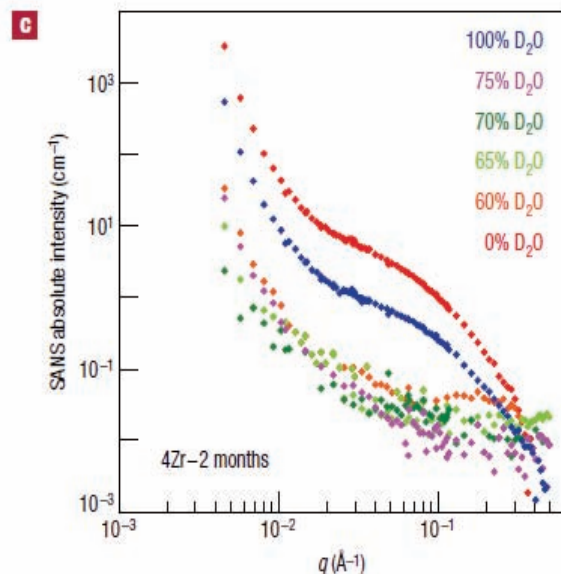
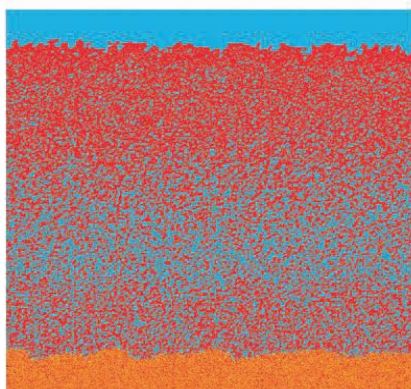


Figure 2: Scattered intensity (SANS) for different isotopic mixtures for the sample without Zircon (0Zr) after 8 hours of alteration (a), after two months (b), for the sample containing 4% of Zircon (4Zr) after leaching 2 months (c). The residual signal observed on figure (b) for the « matching » composition (70%D₂O) illustrates the existence of the closed porosity.

The studied glasses are of composition of $\text{SiO}_2\text{-B}_2\text{O}_3\text{-Na}_2\text{O-CaO-ZrO}_2$. These elements constitute the different species present in nuclear glasses which can be classed according to their reactivity with water: soluble (B, Na), partially soluble (Si, Ca) and less soluble (Zr). We have been interested in the specific effects of Calcium and of Zirconium on the kinetic of alteration. We have observed that substituted the Calcium by the sodium improves the reticulation of the glass network to finally gives a decrease of the alteration rate. Regarding Zirconium, the increase of Zr-content decreases strongly the initial dissolution rate, which was expected, but increases paradoxically the degree of glass corrosion. Conversely, the increase of pH increases the initial dissolution rate but



decrease the corrosion. To explain this

Figure 2: Monte Carlo simulation of the altered gel without Zirconium (0Zr). The silicon atoms are shown in red, other element in yellow, water in blue.

surprising effect, the morphology of gels has been probed by Small Angles X-ray Scattering (SAXS).

These experiments have highlighted the reorganization of the porous network of the gel during the alteration and show that this reorganization is limited by the increase of the Zr-content. This suggests that this is the restructuration of the gel which is at the origin of the blockage of the alteration observed with the glass containing low Zr-content. This hypothesis has been successfully confirmed by Small Angle Neutron Scattering (SANS) according to an original application of the contrast matching method. Measurements for various solvent compositions ($\text{H}_2\text{O-D}_2\text{O}$) have showed the porosity is closed for the glasses without Zircon (0Zr) and stay open for the glasses containing Zircon (figure 1).

These experiments of Neutrons Scattering, coupled with Monte Carlo (figure 2) simulations, permit to clearly establish a link between the gel morphology and the kinetic of alteration for a series of simplified glasses mimicking composition of nuclear glasses.

References:

- [1] C. Cailleteau, F. Angéli, F. Devreux, S. Gin, J. Jestin, P. Jollivet, O. Spalla, Insight into silicate glass corrosion mechanisms, *Nature Materials*, 7, 978-983, **2008**.

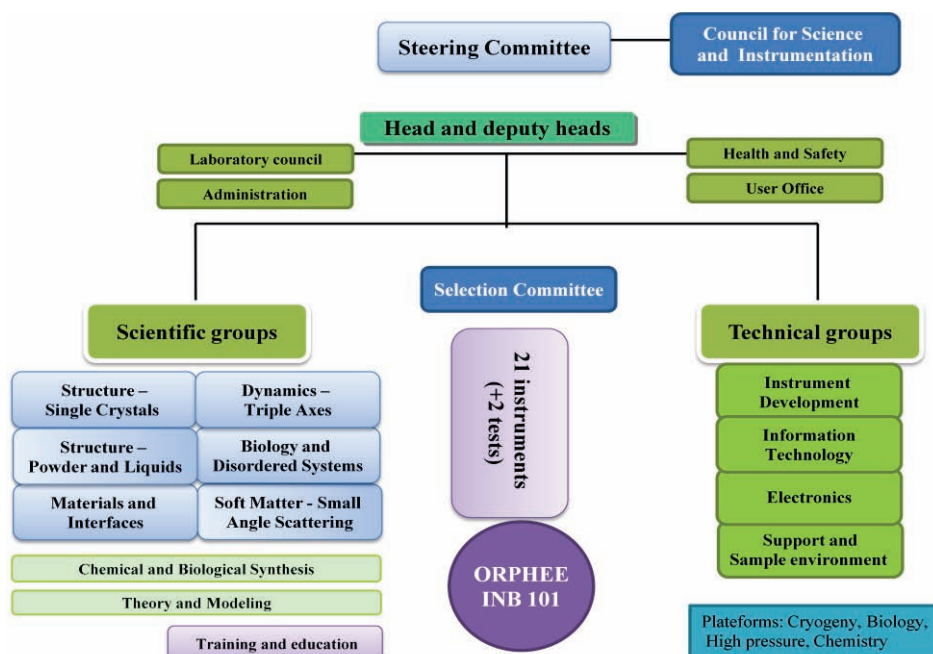
INSTRUMENTATION

This part of the document provides a description of the groups and the common platforms operating around the instruments, of the Orphée reactor, a list of the current neutron instruments available at the LLB and a presentation of the instrumentation program, CAP2015.

A- Organisation and expertise of the groups

As mentioned in Part I, the organization of the LLB is dictated by the use of the neutron scattering spectrometers. In order to provide users with special expertise that spans the broad spectrum of topics accessible and the multidisciplinary aspect of neutron methods, it comprises six groups of scientific and technical experts responsible of the spectrometers, and four groups of engineers and technicians for the maintenance and the development of the instrumentation. Additional common research activities and transverse actions are conducted and represented in the organization chart below. All the neutron scattering methods are installed and distributed along the 21 spectrometers (+ 2 for tests), supported by common platforms proposed to the visitors.

The groups are defined according to their scientific and technical expertise described below. The Scientific Group members are not only expert in a given neutron scattering method but they have developed their own scientific domain of expertise; they are able to establish a perfect link between inexperienced and professional users. Consequently they attract, help and guide new users from the early stage of writing a proposal to the data analysis and the interpretation of the experiments within numerous scientific domains. This scientific expertise is reinforced by transverse axis dedicated to i) chemical and biological synthesis and sample preparation, and ii) Theory and Modeling, helping the visitors.



◇ Scientific groups

The six LLB Science groups are Dynamics - Triple Axes; Structure - Powder and Liquids; Structure -Single Crystals; Materials and Interfaces; Biology and Disordered Systems; Soft Matter - Small Angle Scattering. They are responsible for the operation of 21 neutron instruments and 2 test instruments and for providing expertise in data analysis.

Structure - Single Crystals

Members: A. Goukassov (head, CEA), B. Gillon (CNRS), A. Bataille (CEA), A. Cousson (CEA), R. Papoular (CEA), J-L. Meuriot (CEA), Th. Robillard (CEA), A. Sazanov (post-doc CEA), M. Leroy (PhD Student), J-M. Kiat (collaborator, EC Paris)

Scientific Expertise in neutron scattering

The Single Crystal Group carries out personal and collaborative research programs using neutron diffraction in various fields of physics, like superconductivity and magnetism as well as in organic and inorganic chemistry. A. Goukassov covers the domains of magnetism, superconductivity and polarized neutrons. A. Cousson is specialized in crystallographic studies of complex structures. B Gillon is a specialist in chemistry and physics of molecular magnets and polarized neutrons. A. Bataille concentrates on studies of magnetic properties of epitaxially grown single crystals. A. Sazonov works on the crystal and magnetic structures of strongly correlated systems, in particular on the properties of frustrated magnets. R. Papoular is an expert of data treatment using Maximum Entropy Method. J. M Kiat brings his expertise in multiferroics and diffraction.

Instrument technicians J-L. Meuriot and Th. Robillard provide functioning of diffractometers, assure users support and participate in instrument developments.

Ph D student: MA Leroy. “ Tunnel coupling between antiferromagnetic thin films”

Technical Expertise in neutron scattering

The group operates three instruments **5C2**, **Super-6T2** and **VIP**.

5C2 (A. Cousson), hot neutron four-circle diffractometer focuses largely on the high resolution crystallographic studies of complex structures, in particular in hydrogen containing molecular compounds.

Super-6T2 (A. Goukassov, A. Bataille), highly polyvalent brand new diffractometer completed in 2007 offers rapid data collection, opening up the field of in situ photo-excitation experiments, high fields (< 7.5 T) and very low (50 mK) temperatures. Its high flux in combination with highly efficient PSD Detector allows routine measurements of sub millimetric crystals and epitaxial single crystals.

VIP (A. Goukassov, B. Gillon and A. Sazonov), the most recent instrument delivered in October 2010 is a new type of single crystal polarized single crystal diffractometer equipped with a large PSD covering 1 steradian on the diffraction sphere. It is still in commissioning stage but first experiments show that it boosts the data acquisition rate by an order of magnitude. After replacement of its Heussler monochromator in 2012 it is expected to be the most efficient polarized neutron diffractometer in the world.

The Single Crystal group is also heavily involved in developing instrumentation, experimental techniques and software for the full range of crystallographic work undertaken at LLB.

Structure – Powder and Liquids

Members : G. André (head, CEA), B. Beuneu (CEA), J. Bourgeois (PhD Student), F. Damay (CNRS), J. Darpentigny (CNRS), X. Guillou (CNRS), I. Mirebeau (CNRS), F. Porcher (CEA), N. Rey (CNRS), B. Rieu (CEA)

Scientific Expertise in neutron scattering

The Powder Diffraction Group develops numerous personal and collaboration research studies using neutron diffraction in various fields of physics and solid state chemistry. G. André works mainly on the determination of complex magnetic structures and on structural phase transitions. B. Beuneu is involved in short range order in materials, and structural properties of liquids and amorphous materials. F. Damay specialises in the resolution of the crystal and magnetic structures of complex metal transition oxides, such as frustrated antiferromagnets or multiferroic compounds. I. Mirebeau works on strongly correlated electron systems, geometrically frustrated magnets and multiferroics mostly, and studies the influence of extreme conditions (pressure, temperature...) on such systems. F. Porcher is an expert in zeolithes, microporous materials and high resolution crystal structure determination. N. Rey is a research engineer performing neutron studies at high pressures and involved in instrumental and pressure cells development. Instrument technician X. Guillou and engineer B. Rieu are responsible of user's support and actively participate in instrument developments. J. Darpentigny is responsible of the electronics of the two new tube detectors of G6.1 and 7C2.

Ph D student : J. Bourgeois, subject : Mixed valence ferrites RFe_2O_4 .

Technical Expertise in neutron scattering

The Powder Diffraction group manages four diffractometers, **3T2**, **G4.1**, **G6.1** and **7C2**, opened to LLB users and actively participates in developing sample environment, instrumentation, and new data acquisition and treatment.

3T2 (F. Porcher, F. Damay), upgraded in 2007 with a new 50 collimators/detectors block, is a generalist, high resolution, thermal diffractometer more particularly adapted to precise crystallographic determinations of compounds with cell volume $< 1200 \text{ \AA}^3$.

G4.1 (G. André) is a polyvalent, medium resolution instrument and high flux equipped with an 800 cells multidetector, optimized for magnetic structure determination and study of phase transitions in function of temperature.

G6.1 (N. Rey, I. Mirebeau) is a high wavelength ($\lambda = 4.8 \text{ \AA}$) and high flux powder diffractometer, devoted to the measurement of crystal and magnetic structures of very small samples under high pressure. In 2011 the implementation of a new tube detector with two sample-detector distances (one with very large solid angle) will boost its capabilities.

7C2 (B. Beuneu), located on the hot source of the reactor, performs structure factor measurements over a wide scattering vector range, necessary for the determination of the atomic correlations and the molecular interactions in glasses, amorphous materials, liquids and solutions. An in-depth transformation of the instrument will be achieved in 2011 by using an assembly of 256 position sensitive tubes increasing the counting rate by a factor 25.

Materials and Interfaces

Members: F. Ott (head, CEA), S. Gautrot (CNRS) G. Chaboussant (CNRS), F. Gibert (CEA), F. Cousin (CEA), V. Klosek (CEA), L.-T. Lee (CNRS), M.-H. Mathon (CEA), M. Dubois (PhD Student), W. Fang (PhD Student), C. Said, (PhD Student), S. Zhong (PhD Student), O. Castelnau (collaborator, CNRS), V. Ji (collaborator, U. Paris-Sud), A. Lodini (collaborator, Univ. Reims).

Scientific Expertise in neutron scattering

The Interfaces and Materials Sciences group has a transversal expertise in materials sciences in fields ranging from polymer sciences, to magnetism and metallurgy. F. Ott and G. Chaboussant have expertise in the field of magnetism and especially magnetic nanostructures (thin films, nanoparticles). F. Cousin and L.T. Lee are experts in polymer sciences (composites materials). V. Klosek and M.-H. Mathon are experts in metallurgy (strain and texture distributions). The different research activities benefit from various types of neutron scattering techniques (SANS, reflectometry, texture spectrometer, and strain scanner).

There are presently 4 Ph students working on rather different fields. M. Dubois is working on Shape Memory alloys; W. Fang is working on polymer/magnetic nanoparticles composites; C. Said is working on nanoparticles/Au films; S. Zhong is working on new metallurgical composites (ODS).

Technical Expertise in neutron scattering

The group operates 4 instruments:

EROS (F. Cousin, L.T. Lee), horizontal soft matter reflectometer optimized to be a high flux / low resolution instrument for the study of polymer samples and free liquid surfaces.

PRISM (F. Ott), polarized neutron reflectometer optimized for high flux / low resolution studies on small surface magnetic samples (1cm²)

6T1 (M.H. Mathon), texture spectrometer dedicated to the measurement of in-situ pole figures (high temperatures, under load). It is also used to measure the shape of the diffraction lines to measure stored energies in dislocations. This spectrometer is presently undergoing renovation within the CAP 2015 program.

DIANE (V. Klosek), strain scanner used to map strain in metallurgical pieces. The gauge volume goes down to 1mm³. It is used for some characterization with industrial partners (Dassault, SNCF, STMI..) and can accommodate pieces weighting up to 500kg.

F. Gibert and S. Gautrot are responsible for the technical support of these spectrometers.

The different researchers of the group are also regular users of the SANS spectrometers and are involved in the construction of the new **PA20** SANS (G. Chaboussant); PA20 will replace PAXE SANS spectrometer; it is a larger SANS spectrometer dedicated both to soft matter (including neutron lens focalization) and magnetic systems (with polarization analysis).

Dynamics – Triple-Axis

Members : P. Baroni (CNRS), Ph. Bourges (CEA), Ph. Boutrouille (CEA), M. Hatnean (Ph.D) D. Lamago (KIT Karlsruhe), F. Maignen (CNRS), C. Meunier (KIT Karlsruhe), J.-M. Mignot (head CNRS), H. Moudden (CNRS), S. Pailhès (CNRS), S. Petit (CEA), D. Petitgrand (CNRS), J. Robert (CNRS), Y. Sidis (CNRS).

Scientific Expertise in neutron scattering

The activity of the *Dynamics–Triple-Axis* Group covers a broad range of subjects, primarily related to the physics of strongly correlated electron systems. Major breakthroughs have been achieved in the understanding of superconductivity in high- T_c cuprates, and studies are now extended to novel Fe-based materials (Ph. Bourges, Y. Sidis, D. Petitgrand, S. Pailhès and D. Lamago). Complex interplays between magnetic, electronic, and lattice degrees of freedom are actively studied in the dynamical properties of multiferroic compounds (S. Petit, J. Robert, PhD thesis of M. Hatnean). Unconventional magnetic and multipole interactions produce a variety of challenging ordering phenomena in $4f$ electron systems, which are addressed by means of elastic and inelastic neutron experiments (J.-M. Mignot, J. Robert). Ab-initio structure and lattice dynamics calculations are carried out on various materials, in particular the recently discovered Fe-based superconductor FeSe (H. Moudden). It is especially noteworthy that a large part of this research involves long term collaborations between members of the group and external user teams.

Technical Expertise in neutron scattering

The group is in charge of six spectrometers, four of which are included in the LLB user program and two instruments tests.

1T (D. Lamago, Y. Sidis, C. Meunier) is a thermal-beam triple-axis spectrometer, operated as a CRG instrument by the KIT Karlsruhe. It is equipped with three remotely interchangeable, double-curvature monochromators (PG, Cu 111 and Cu 220). This is a versatile instrument, suitable for a wide range of magnetic and lattice dynamics studies.

2T (Ph. Bourges, P. Baroni) is a thermal-beam, triple-axis spectrometer, equipped with double-curved monochromators (PG 002 and Cu 111) and a PG analyzer. A polarized option is also available by replacing the monochromator and analyzer by Heusler crystals.

4F1 (S. Petit, F. Maignen) and **4F2** (D. Petitgrand, J. Robert, Ph. Boutrouille) are twin triple-axis spectrometers installed on the same cold neutron channel. 4F1 can be equipped with a powerful polarized option using a polarizing supermirror, Mezei-type flippers, and a Heusler polarizing analyzer. 4F2 has been partly rebuilt using amagnetic components to allow measurements to be performed at magnetic fields up to 10 T.

G43, the former Austrian CRG spectrometer, now hosts training courses of Master students from French universities, tests of monochromators or detectors, as well as experiments on liquids and polymers using the LLB-patented CCD-camera neutron detector (P. Baroni and L. Noirez). **3T1** is a two-axis diffractometer, used for sample characterization and alignment.

A comprehensive set of “sample environments” allows users to perform experiments under extreme conditions of temperature from 30 mK to 1400°C (Ph. Boutrouille, P. Baroni), magnetic fields up to 10T (Ph. Boutrouille) and hydrostatic pressure up to 0.65 GPa (F. Maignen).

Biology and Disordered Systems

Members: Lairez (head CEA), V. Arluison (Univ. Paris VII), F. Audonnet (Univ. Paris XI), M.-C. Bellissent-Funel (CNRS emeritus), D. Bhowmik (PhD student), B. Cayrol (CDD), S. Combet-Jeancenet (CNRS), G. Fadda (Univ. Paris XIII), B. Homatter (CEA), A. Koutsioumpas (post-doc), D. F. Legendre (CNRS), A. Lerbret (post-doc), S. Longeville (CEA), N. Malikova (CNRS), C. Martret (CDD), J. Teixeira (CNRS emeritus), C. Thibierge (post-doc), J.-M. Zanotti (CEA).

Scientific Expertise in neutron scattering

Our researches at the interface of physics and biology are based on three main topics: 1) Proteins in complex media viewed as model systems for living environments. Experiments concern macro- or supra-molecular scales and their analysis is strongly influenced by our background in polymer physics, statistical physics and phase transition physics (V. Arluison, M.-C. Bellissent-Funel, S. Combet-Jeancenet, G. Fadda, D. Lairez, S. Longeville); 2) Local dynamics of proteins and hydration water in relation with the dynamical transition of proteins and their enzymatic activity (M.-C. Bellissent-Funel, S. Combet-Jeancenet, S. Longeville, J.-M. Zanotti). Neutron scattering techniques, which are very sensitive to protons, are particularly suitable for these studies; 3) Water and its specific properties are fundamentally related to life and to the very peculiar properties of some biological molecules like proteins (N. Malikova, J. Teixeira, J.-M. Zanotti). Here, water properties are studied in relation with the dynamics of hydrogen bonds network, the notions of hydrophobicity and confinement (F. Audonnet, JM Zanotti, N. Malikova); 4) Finally the quasielastic scattering technique is particularly well suited for the study of dynamical processes in viscous liquids and polymers, and low frequency properties of amorphous systems such as glasses.

Keywords: Protein folding-unfolding, protein crowding and confinement, macromolecules dynamics, water properties, transport properties, diffusion, slow dynamics, confinement.

Technical expertise in neutron scattering

The group operates 3 instruments:

PACE (D. Lairez, S. Combet-Jeancenet), Small-angle neutron scattering: spectrometer dedicated to the study of isotropic samples. It is characterized by its annular detector allowing the direct measurement of $I(\theta)$ and thus improving the interactive experiment driving.

MUSES (N. Malikova, S. Longeville, F. Legendre), Neutron resonance spin-echo spectrometer dedicated to the study of slow motions at a molecular scale in condensed matter (the time range covered spans from 0.5 ps to 22 ns). It is a mixed conventional-resonance spin echo which has been specially designed for intermediate and high angle studies.

Mibemol (S. Longeville, J.-M. Zanotti, B. Homatter), Inelastic time-of-flight spectrometer. This disk-chopper spectrometer is designed to study soft non dispersive excitations in condensed matter by quasi-elastic and inelastic scattering between 0.01 and 100 meV. The corresponding time-scale ranges from 10^{-13} up to 10^{-10} seconds. Mibemol will be replaced by **Fa#** (scientific responsible J.-M. Zanotti) that will be a high-resolution, direct-geometry, inelastic crystal spectrometer designed to provide full flexibility in the choice of energy resolution and to perform best at low incident energies (2–150 meV) on an extended Q range from 0.05 to 10 \AA^{-1} , with an energy resolution between 10 and 500 μeV .

Soft Matter and SANS

Members: F. Boué (head, CNRS), A. Brûlet (CNRS), A. Lapp (CEA), L. Noirez (CNRS), G. Carrot (CEA), J. Jestin (CNRS), M. Detrez (CEA), F. Muller (Postdoc), V. Thévenot (CEA), A. Hélyary (CNRS), E. Buhler (Associated researcher, MSC Paris).

Scientific Expertise in neutron scattering

The Soft Matter and SANS group carries out personal and collaborative research programs using SANS (plus reflectivity and quasi-elastic scattering) in soft matter and bio-inspired physics and physicochemistry, involving polymers. F. Boué works on aqueous (proteins, polyelectrolytes, electrostatic complexes), and anisotropic systems: synthesis, deformation and mechanical properties of nanocomposites, in collaboration with J. Jestin (working also in other systems – asphaltenes, and operating PAXE). A. Brûlet works on instrumental development (TPA, PA20) and selfassembly (polymersome vesicles), as does A. Lapp (e.g. polyrotaxanes), who operates and develops PAXY (neutron lenses). G. Carrot synthesizes nanocomposites (recently for biology), and is responsible for the chemistry lab. L. Noirez is interested in liquid crystalline polymers and other liquids, under special conditions (shear at low gaps, pressure).

Instrument technicians: M. Detrez (PAXE), V. Thévenot (PAXY and TPA), and A. Hélyary (PACE and TPA) ensure functioning of spectrometers, user's support and participate in instrument developments. All researchers not responsible of spectrometers ensure more or less extended welcoming of users.

Ph D students: A.S. Robbes (with SOLEIL), A.L. Fameau (with INRA/BIA Nantes), Li Shi (with E. Buhler MSC Paris7), A. Bouty (CIFRE Michelin), Wei Qing Fang (with Matériaux group), Z. Guinnouni (with M. Goldmann, SOLEIL, Paris-5).

Technical Expertise in neutron scattering

PAXY (A Lapp) and **PAXE** (J. Jestin) are small-angle neutron scattering spectrometers allowing a scattering vector range from $1.10^{-3} \text{ \AA}^{-1}$ to 1 \AA^{-1} , enabling the studies of correlations over scales from 0.5 nm to 1000 nm. A third SANS spectrometer, **PACE**, is dedicated to the study of isotropic samples, its responsible is D. Lairez.

The corresponding structures belong to soft matter, biology and metallurgy principally, but also to magnetic systems and glasses. The use of isotopic labeling, mainly deuteration in the case of soft matter and biology (use of heavy water), enables to visualize one species among the others in complex systems made of several components. Labeling can also be obtained through field action in magnetic and metallurgic systems. We are also experts in data treatment and simple modelization of structures, for us as well as for users.

TPA (A. Brûlet) is a very small angle spectrometer; the lowest scattering vector attainable, around $3.10^{-4} \text{ \AA}^{-1}$ (and lower in the future) enables access to scales of a few microns for large objects. In project **PAXE** will be replaced soon by **PA20** (G. Chaboussant from the Interfaces and Material Sciences Group).

Theory and Modeling

Members : *P. Pfeuty (head, CNRS), F. Damay(CNRS), N. Malikova(CNRS), H. Moudden (CNRS), J. Robert(CNRS), S. Aubry(CEA), F. Onufrieva (CEA), S. Petit (CEA)*

Scientific Expertise

The theory and modelisation group is a transversal interdisciplinary group. Part of the group (Aubry, Onufrieva, Pfeuty) is developing a full time theoretical approach and in the rest of the group the physicists who belong to other groups develop a modelisation in relation to neutron experiments which they perform in LLB. All members of the group are led at one stage or the other to use numerical approaches.

S. Aubry is involved in non linear physics (wave packet diffusion in a non linear medium and Anderson localization).

F. Onufrieva and Pierre Pfeuty are concerned with the theoretical study of superconducting pairing of electrons in high T_c cuprates through spin fluctuations.

S. Petit together with Julien Robert is calculating spin excitation dynamics in multiferroic systems , taking into account the spin lattice coupling.

J. Robert in collaboration with theorists in Grenoble is studies, through numerical integration of equations of motion and classical Monte Carlo method, the dynamics of classical spins coupled antiferromagnetically on a two dimensional Kagomé lattice (dynamics of frustrated spin systems).

F. Damay with Sylvain Petit has determined the incommensurate structure in a quasi one dimensional compound CaCr₂O₄.

N. Malikova determines, through classical Monte Carlo method and molecular dynamics, the dynamical behavior of charged ions in solutions (electrolytes both in bulk and in confined geometry) in relation to neutron quasielastic experiments.

H. Moudden is mainly interested in the role of phonons for superconductivity in compounds such as MgB₂, FeAs, FeS₂, SnO. He is developing ab initio calculations of both electrons, phonons and electron-phonon coupling which are then used to study superconductivity in several compounds recently studied experimentally.

Chemical and Biological Synthesis

Members : V. Arluison (Université Paris Diderot), G. Carrot (CEA), S. Combet-Jeanceneel (CNRS), N. Linder (Université Cergy), C. Martret (CDD-ERC), A. Castanar (Master 2 Pro).

Scientific Expertise

Since its creation, the LLB has always included important chemistry activities. The recent development of this platform permits to greatly improve its impact, regarding the direct collaboration with other LLB researchers, or the support to external users, either through a simple sample preparation, or a more elaborate synthetic procedure. On the other side, a biology activity has also developed in the last ten years and it is now important enough to be shown as an independent expertise at the LLB. The biology laboratory provides an experimental support at LLB for research projects in biology/biophysics and/or neutron scattering experiments made on biological samples. These two entities are sharing technical supports, equipments and scientific knowledge to build up new projects with further interactions with neutron facilities of LLB.

The chemistry expertise present at LLB involves mainly organic/polymer chemistry and/or inorganic/mesoporous materials. G. Carrot operates mainly in the area of organic chemistry, particularly in the fonctionnalisation and characterization of nanoparticles by controlled *surface*-polymerization and click chemistry. N. Linder is an expert in the synthesis and characterization of inorganic materials including mesoporous inorganic silica and its coordination with metal ions. S. Combet-Jeanceneel has developed several procedures in the laboratory for protein purification and characterization. V. Arluison has recently developed the laboratory expertise in molecular biology and microbiology, especially in the field of protein/nucleic acids interaction. A recent development is the adaptation of *Escherichia coli* bacteria to produce deuterated macromolecules.

Technical Equipments

Three rooms are dedicated to the chemistry activity and are equipped with hoods containing vacuum/inert gases. A special room is reserved for stocking chemicals (H and D) with adequate ventilation. The biology lab is equipped to prepare biological samples, particularly for neutron scattering experiments in the presence of D₂O. Equipments are available for DNA analysis and production (thermocycler, gel migration and imaging) and protein preparation and characterization (bacterial cell culture, chromatography, SDS-PAGE, Western-blotting). Some advanced characterization equipments are also available: size-exclusion chromatography (SEC), differential scanning calorimeter (DSC), thermogravimetric analysis (TGA), UV-visible, infra-red ATR and fluorescence spectrometry, fluorescence imaging, N₂ and H₂O adsorption/desorption apparatus. A technical support through the hiring of a technician, is essential for a continuous contact with the neutron users, particularly for the maintenance of the chemistry lab in the " Hall des Guides" and of the different equipment (calibration).

Organization: Group meetings, creation and maintaining a budget (purchasing of equipment and chemical and biological products), management of the security in the laboratories, scientific interactions with other scientific groups.

◇ Technical groups

The technical support for running experiments and instrument developments is provided by four groups: Instrument Development; Sample Environment; Electronics and Information Technology.

Instrument Development

***Members:** S. Désert (head, CEA), S. Klimko (CEA), P. Lavie (CEA), P. Permingeat (CNRS), S. Rodrigues (CEA)*

Technical Expertise

The Instrument Development Group (IDG) was created in the middle of the year 2008 in order to bring together the engineers in charge of projects and the engineering and design department with the aim of improving the effectiveness and the visibility of the instrumental projects of the laboratory.

To fulfill its tasks, the IDG exhibits complementary capabilities among which S. Désert covers the management of project, neutron optics and simulations; S. Klimko is an expert in magnetism – from design and simulations to fabrication, polarization of neutron and particularly the neutron spin-echo technique; P. Permingeat is an expert in mechanics and computer-aided design, resistance of materials and an engineer with a wide knowledge; S. Rodrigues concentrates on the management of projects and contracts reporting; and finally P. Lavie is the technician specialist of computer-aided design with expertise in vacuum.

Instruments

The IDG is involved at every instrumental level: it has the technical responsibility and the follow-up of the large instrumental projects within the framework of CAP2015, the contribution or assumption of responsibility in projects known as average (update of an instrument, specific equipment), the work “in emergency” to repair or adjust experiments, the assistance to the technicians and engineers for drafting and dimensioning, writing specification reports and scheduling, and the reporting of the contracts.

The IDG members are involved in six instrument projects as technical responsables: S. Désert for **TPA** (Very Small Angle) and **PA20** (Small Angle 2x20 m), S. Klimko for **Multi-muses** (Spin echo with multi detectors), P. Permingeat for the new **EROS** detector tank and S. Rodrigues for **VIP** (Crystal diffractometer) and **FA#** (Quasielastic) whereas P. Lavie is a common denominator of all these projects.

Information Technology

Members: G. Exil (head, CNRS), R. Lautie (CEA), A. Laverdunt (CEA)

The Group provides computer support for the LLB neutron spectrometers.

This support includes maintenance and evolution of software developed by the service, the development of new command software for the future spectrometers LLB and a technical expertise on computer hardware, installation and configuration.

Technical Activities

R. Lautie manages the network administration and system of the LLB, A. Laverdunt is in charge of the development of the new command software for the spectrometers and G. Exil oversees the deployment of the new platform software control of LLB spectrometers and the maintenance of software developed in Visual Basic.

Technical Expertise in neutron scattering (instruments)

Developments in Visual Basic

The command software written in Visual Basic6 is deployed on PAXY (G23), PAXE (G54), 6T1, 6T2 and 5C2.

This program allows the control of all instruments present in the experimental area of these spectrometers like engines, furnace, coil magnetic field or wavelength selector. It also offers an acquisition and a 2D visualization for the multi-detectors on PAXY, PAXE and 6T2.

Developments in POOPS

The program POOPS is command software written in VisualC++ which has been developed by previous IT Team in LLB. This program is no longer maintained but the group still offers a technical support of this. It's deployed on EROS (G3B), G41, G61, G62, G52, and 7C2.

No acquisition module for 2D multi-detector has been developed for this program.

Developments in .NET/IronPython

The new command software, called Pingouin, actually developed by the group is written on .NET Microsoft Platform with IronPython for the scripts. This program has a capacity to control all existing LLB spectrometers, and should become the basis of all future instruments under development. Actually, the spectrometers equipped by Pingouin are VIP (5C1), TPA (G5B) and BAROTRON (G56).

Electronics

Members: G. Koskas (head, CEA), M. Antoniadès (CEA), F. Coneggo (CNRS), F. Prunes (CEA), P. Lambert (CNRS)

Technical Activities

The Electronics group priority is to ensure operational availability and reliability of the instruments electronics.

The EG develops and works out new devices in order to achieve better technical specifications of the spectrometers (new features, dead time minimization, safety etc.)

Its field is very large since it comprises motion control, detector equipment, and data acquisition, signal processing up to the design, programming and microprogramming of real time controllers.

EG programs numerous applications for test and checking in order to ease maintenance and tunings. G. Koskas is specialized in digital electronics, data acquisition, real time software, and test programming. M. Antoniadès and F. Prunes carry out maintenance, tuning and installing of mono, 1D and 2D detectors. F. Coneggo is in charge of setting up positioning systems and of designing its new modules. P. Lambert is the only one assembly technician of the LLB; he is responsible for all the wiring of the spectrometers and its environment devices.

EG engineers and technicians are present in all the instrumental projects of the laboratory; they bring their knowledge and experience when selecting technical solutions and subcontractors as well. Due to their additional knowledge in mechanics and computer science, they provide a link with other domains.

Leading Projects

PSD's acquisition systems have undergone a major renewal; from now on they allow for a much more specific time of flight or kinetics measurements. Deployment began in 2006 and is going on multiple experiments **MI-BEMOL**, **PAXE**, **PACE**, **TPA** etc.

VIP and **6T2** spectrometers are being equipped with a new detection equipment designed by the ILL but implemented by the EG. The EG is also involved in the prototyping and testing of new ILL detectors, using wire erosion process, to be eventually installed on **PAXY** and **PA20**.

At the moment, the EG is concentrating on control/command, mainly axis motion and master controllers thanks to 32 bits microcontrollers within the framework of a distributed architecture. The goal of this major development is to renew the positioning system of all the experiments. This will allow to drive wider range of motors, notably more powerful, and of more sensitive encoders. It will facilitate and speed up maintenance in easing settings and breakdown diagnostics thanks to the embedded software and communications features.

Development strategy

Even though EG focuses firstly on maintenance, it has to face with weakening or simply ageing of the hardware. Therefore common spectrometer features such as positioning, counting and data acquisition systems are addressed and renewed on a 5 year period while taking into account downward compatibility.

Support and Sample Environment

Members: B. Annighöfer (head, CEA), K. Jiguet (CEA), O. Tessier (CEA)

Technical Expertise

The Support and Sample Environments Group was established in 2008 with the restructuring of the Technical Support Group and the Office of General Studies. The creation of this group has aimed to create a unit that represents a clearly identified point of contact for external collaborators to ensure a smooth running of experiments. Historically support for experiments was always provided by the scientific group to which the device was attached. For the smooth conduct of experiments, the Support group includes the activities of the mechanical workshop, the service of fluids, gases and other consumables.

B. Annighöfer covers the development of various devices for sample environment in collaboration with the instrument responsible or technicians as well as the development and design of high pressure chambers up to 3 GPa. Furthermore he is supervising the production by sub-contracting.

K. Jiguet covers the supplying of expendable goods as cryogenic fluids, gases or others. He is monitoring the recovery of helium as well as the vacuum of the neutron guides. During structural alteration works he is also contributing to the alignment of neutron guides and crane operator.

O. Tessier is full-time mechanic and responsible for the workshop and the realization of devices for the experiments. He is also training the technicians on different machine tools.

Collaborations

Development of a high pressure cell, 8 kbar, for inert gases in the European Framework NMI 3 FP7 (WP21 Sample Environment)

Development of high pressure vessels and participating in experiments using high pressure in the French ANR Framework « BIOSTAB ».

Health and Safety

Members: A. Menelle (CEA), Y Fournier (CEA), G Carrot (CEA), B Mailleret (CNRS), F Legendre (CNRS)

Tasks

Every equipment and building of the LLB and of the Orphée reactor are grouped within a single entity called the INB101 (Installation Nucléaire de Base #101). The director of the Orphée reactor is the safety responsible within the whole entity, and the director of the LLB has in charge the safety of the LLB visitors, equipments and buildings.

Most of the periodic regulatory controls, such as electricity, lifting equipments, fire detectors, cryogenics systems, are taken into account by contracts at the CEA/Saclay level. Specific contracts are set for the maintenance of special devices like centrifuges.

At his arrival at the laboratory each individual worker elaborates and signs his risk analysis sheet with the safety engineer. This document describes all risks linked with the work performed at the LLB. Various CEA softwares are used to evaluate the level of classical and chemical risks in all offices and laboratories of the LLB. This analysis has been done during the summer 2010. It suggests some modifications which are currently underway in order to improve safety in our chemical laboratories.

In order to set the radiological safety the director of the Orphée reactor is helped by an independent radiation protection group advising him on how to put in application all the regulations within the entity INB101. The main features of these actions are the following ones:

- Every people working on the spectrometers have a B classification. They receive radiological safety trainings every 3 years, benefit of specific health survey and are equipped with passive and operational dosimeters,
- Every area of the entity INB101 has received a different radiological classification which reflects the level of radiation observed. This classification is clearly displayed. By this way, workers are aware of the risk level in each individual area of the entity,
- Following the same principle, each area of the entity has its own waste classification as a function of the activation risk. Depending of the waste classification, waste produced will follow different routes for their evacuation. This classification has been set in order to decrease the risk of radioactivity dissemination.

Different actions undertaken recently aim to the reduction of the exposure of workers to radiations, chemical and mechanical risks. They are briefly listed here:

- Use of a new film dosimeter with higher sensitivity for all workers,
- Improvement of radiological shielding between spectrometers (1T-2T, 4F1-4F2),
- Set of interlock on the access of high flux spectrometers (G43, G52, 2T and 6T1),
- Improvement of handlings on spectrometer with new gateways and scaffolds (3T2, Muses, 5C1),
- Upgrade of our cold room,
- Upgrade of the majority of our hoods in the chemistry laboratories,
- New distribution of research activities in the laboratories of the ground floor of blg.563.

The next short time projects in safety are more dedicated to the improvement of wellness of work. They mainly concern the modification of the access to the experimental hall with a shorter path to blg.563 and the realization of a new cloakroom for all workers of the hall of neutrons guides in blg.541.

Administration

Members : C. Alba-Simionesco (CNRS), J-P Visticot (CEA), A. Menelle (CEA), C. Doira (CEA), A. Mostéfaoui (CNRS), C. Rousse (CNRS), A. Verdier(CEA), M. Noiran (CDD CNRS).

Tasks

The administration group takes care of the management of the unit. It manages the budget, the contracts, human resources... These tasks are performed in close relationship with the corresponding services of the CEA (IRAMIS institute) and the CNRS (regional delegation DR4). It has also in charge communications actions (web site, reports, publications...).

The general secretariat is assumed by A. Verdier. Human resources administration, records relating to permanent staff and non-permanent (Ph.D., Postdocs, trainees) are centralized at the secretariat and are treated in relation with relevant departments at IRAMIS or regional delegation CNRS, depending on the employer. Two correspondents are in charge of the professional training, C. Doira for CEA staff and A. Brulet for CNRS staff.

Order requests are validated at the management level and prepared by the secretariat. C. Rousse is specifically in charge of following mission requests. A few specifics records are monitored at the administrative level: contracts by J.-P. Visticot, in relation with CEA and CNRS services; fluid consumption by K. Jiguet-Covex; purchase orders by A. Menelle... C. Rousse has the responsibility of the administrative management of the European contract for access to large facilities: reception and stay of visitors; producing financial and scientific evidence for the European Commission.

For the organization of the access to the facility, A. Mostefaoui and M. Noiran are responsible for providing access badges, dosimeters, some logistic, housing and reimbursement to visitors. Supervised by M.H. Mathon they are also in charge of the organization of the selection committees that distribute beam time to users.

Finally, the administrative group is also in charge of some communication tasks. C. Rousse and C. Doira are in charge of the edition of communication materials of the laboratory (brochures, posters). F. Porcher is responsible for the annual report and A. Menelle of the LLB web site. Organizations of visits are also managed by the administrative group as well as some schools, meetings and training sessions (i.e. Fan, NMI3 ..).

B- Current LLB instruments

Triple-axis Spectrometers

Two-axes Diffractometers: Powder and Liquids

Single Crystal Diffractometers

Materials (texture/strain) Diffractometers

Reflectometers

Small Angle Neutron Scattering

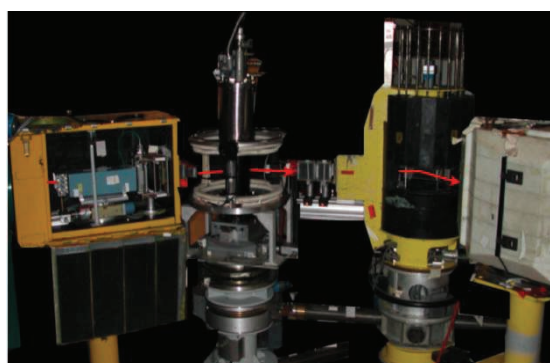
Quasi Elastic Neutron Scattering

TRIPLE-AXIS SPECTROMETERS

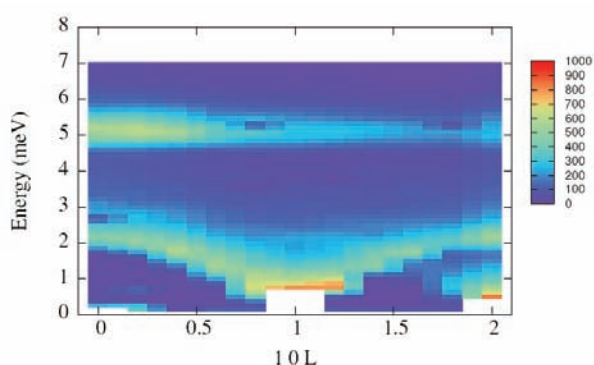
The triple-axis spectrometer (TAS) is considered the most versatile neutron instrument. It is basically designed to determine the neutron inelastic cross section, hence measuring the spectrum of excited states in condensed matter physics. It is primarily employed for studying single crystals, in which it provides access to microscopic quantities such as force constants, exchange couplings or anisotropies. The LLB's TAS are world-class instruments and should remain in the front line in the years to come, given the planned upgrades.

Four instruments are open to users at LLB: **1T** (Forschungszentrum Karlsruhe CRG) and **2T** are installed on thermal beams, while **4F1** and **4F2** are located on cold beams. All spectrometers are equipped with double-focusing pyrolytic graphite (PG) analyzers. PG and copper monochromators are available on both **1T** and **2T**. **4F1** and **4F2** benefit from a double PG monochromator system, allowing the incident energy to be changed without moving the sample table. This particular setup saves precious space within the reactor hall, while allowing the incident energy to be tuned up to 23 meV along with a reasonable flux (in contrast with usual cold source TAS installed on a guide).

On both **4F1** and **2T**, a polarized neutron setup can be implemented, with polarization being achieved by means of a polarizing mirror (**4F1**) or a vertical focusing Heussler alloy monochromator (**2T**). In both cases, the scattered neutron polarization is analyzed with a horizontally focusing Heussler crystal (a second bender is also available on **4F1**). A system of Helmholtz coils is used to rotate the neutron polarization vector along any arbitrary direction at the sample position.



Cold neutron triple axis spectrometer 4F1 in its polarized neutron setup.



Neutron intensity as a function of energy transfer and wave-vector taken along c^ in the multiferroic compound YMnO_3 .*

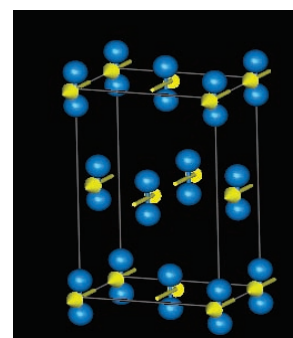
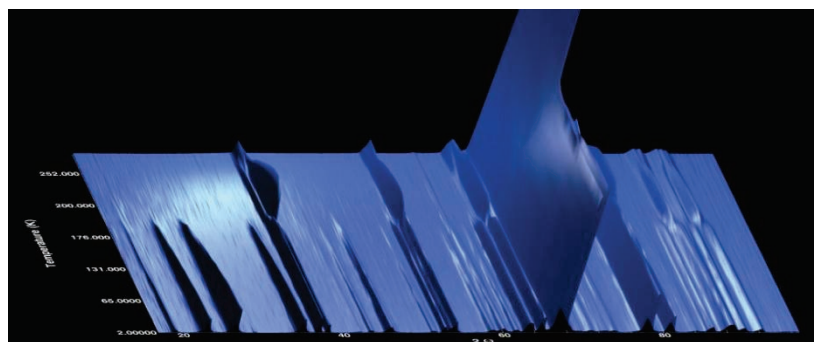
TAS are designed to carry out inelastic neutron scattering experiments and, therefore, to study lattice dynamics (phonons, soft modes ...) as well as spin dynamics. Magnon dispersions and crystal-field transitions are routinely measured, but interest often focuses on more exotic excitations such as spinons in low-dimensional systems or bound states in strongly correlated electron compounds. This technique is essential to shed light on the microscopic interactions responsible for the properties of novel materials such as superconductors, heavy-fermion systems, multiferroics, colossal magnetoresistance manganites, as well as low-dimensional and frustrated magnets. Elastic scattering experiments can also be performed, in which the analyzer provides attractive low-background conditions. The performance of TAS has improved steadily over the years, opening a wide range of possibilities in new areas, especially for the study of small samples. For instance, the static and dynamical magnetic properties of thin films grown for spintronic applications have now become accessible to neutron scattering experiments.

TWO-AXIS DIFFRACTOMETERS: POWDER AND LIQUIDS

Three powder diffractometers are opened to LLB users; 2 generalist instruments, 3T2 and G4.1, and a more unique specialized one G6.1, dedicated to studies under very high pressure. The 7C2 diffractometer is devoted to structure studies of disordered systems, liquid and amorphous during major evolution.

3T2 is a high-resolution thermal diffractometer more particularly adapted to precise crystallographic determinations of compounds with cell volumes $< 1200 \text{ \AA}^3$, D2B type at ILL or SPODI at FRMII.

G4.1 is optimized for magnetic structure determinations and the study of phase transitions as a function of temperature. It is a medium-resolution instrument that has high-flux capability and an 800 cell multidetector. It is comparable to D1B (slightly better resolution, lower flux but in a ratio less than the power reactor ratio).



Manganite $\text{Pr}_{0.5}\text{Sr}_{0.41}\text{CaMnO}_3$ $1.5 \text{ K} < T < 300 \text{ K}$ Diffractograms from G4.1 Molecular oxygen: $\delta\text{-O}_2$ phase exhibiting a succession of structural and magnetic transitions PRL 93 (2004) 055502

G6.1 is a high wavelength ($\lambda = 4.8 \text{ \AA}$) and high flux powder diffractometer, optimized for the measurement of crystal and magnetic structures of very small samples under high pressure.

7C2 is located on the hot source of the reactor. This allows performing measurements of the structure factor over a widely scattered vector range, which is necessary for determining the atomic correlations and the molecular interactions in glasses, amorphous materials, liquids and solutions. **7C2** is to be compared with D4 at ILL which, like ORPHEE, is one of the few reactors to have a hot source. Its renovation will make it a completely competitive instrument.

These instruments are complementary and comprehensively cover a great part of the needs in the classical domains of solid chemistry, crystallography, solid physics, and material science; and in new domains such as energy environment, pharmacology, geophysics.

The main scientific themes studied at present concern: metallic hydrides, oxides, multiferroics, ionic conductors, studies under very high pressure, frustrated magnetism, nanomaterials, geophysical compounds, microstructures, *in situ* kinetic studies, archeology, biological compounds, photomagnetism, and zeolithes.

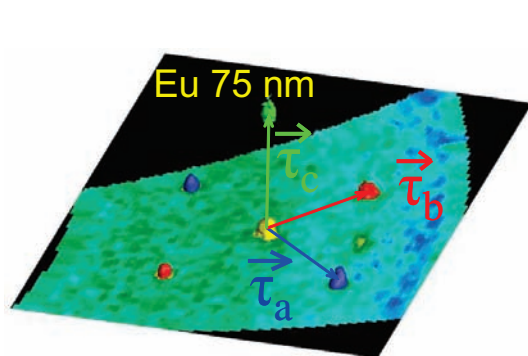
At present, studies of liquids and amorphous materials focus on the structure at middle range distance of oxide glasses, covalent alloys for data storage applications, confined liquids, and the solvent-solution interaction.

SINGLE CRYSTAL DIFFRACTOMETERS

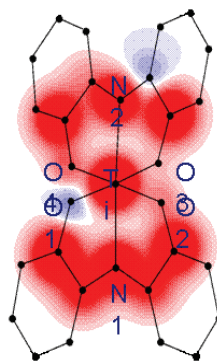
The three single crystal diffractometers available to LLB users are subjected to sustained and versatile demand. This is due to a significant gain in their efficiency achieved recently through the use of position sensitive detectors (PSD) and modern supermirror polarizers. The recently upgraded diffractometer, Super-6T2, now allows now interatomic or intermolecular magnetic interactions on sub-millimetric samples to be investigated. A large variety of sample environments which cover very low temperature (50 mK), in combination with high fields (8 T) and high pressures, provides numerous options in the study of multiferroics, heavy fermion systems and superconductors.

Super-6T2 is the most versatile of the single crystal diffractometers at LLB. Three wavelengths are available ($\lambda = 0.9, 1.5, 2.35$), with the beam at 1.5 \AA being highly polarized. The instrument is well adapted for crystal and magnetic structure determination of compounds having cell volumes $< 4000 \text{ \AA}^3$. The instrument also benefits from a large set of sample environment devices: superconducting magnet, Cu-Be and sapphire pressure cells, and a dilution refrigerator, which allow samples to be studied under extreme conditions.

6T2 was upgraded in 2007 within the CAP2010 program, in particular, by installing a 2D detector. It then became competitive with the best neutron diffractometers in the world, such as D19 and D10 in the ILL. It is widely used for diffraction studies of magnetic ordering in nanometric epitaxial layers. The polarized neutron option, realized with a supermirror bender, is extremely efficient in the spin density studies of complex molecular compounds.



Magnetic and nuclear neutron diffraction signal obtained from a 75 nm Eu thin film



Spin density of a molecular compound

The **5C2** hot neutron 4-circle diffractometer ($\lambda = 0.84 \text{ \AA}$) is optimized for high resolution crystal structure studies of compounds having a unit cell $< 2000 \text{ \AA}^3$. It is widely used in crystallographic studies of new molecular crystals containing hydrogen as well as in the phase transition investigation of complex modern magnetic materials, such as oxides with colossal magnetic resistance, and high T_c superconductors. **5C2** belongs to the first generation of the instruments built in the LLB in collaboration with Karlsruhe. Therefore, all vital parts of the diffractometer, such as the monochromator, sample unit, 4-circles, and displex, were replaced in 2009-2010. At present, **5C2** is a quite modern single-counter neutron diffractometer, and would become a world-class instrument if a large area PSD were to be installed.

MATERIALS (TEXTURE/STRAIN) DIFFRACTOMETERS

The diffractometers associated with "Materials Science" activities are DIANE (G52), located in the guide hall, and 6T1, in the reactor hall. They are respectively dedicated to the analysis of residual strains and to the determination of crystallographic textures.

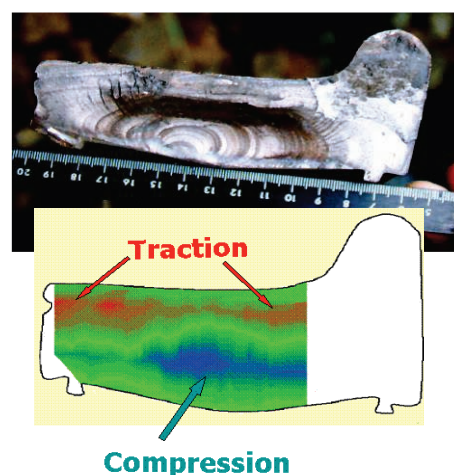
The strong penetrating power of neutrons is used to analyze in-depth metallurgical samples or industrial objects. The instruments are used for both academic and industrial research.

In recent years, neutron diffraction has become the technique of choice for the study of micro-deformations and the heterogeneities between phases (e.g. crystallographic, crystalline orientation, etc...). In a view of understanding and modelling the elasto-plastic deformation mechanisms, neutron diffraction provides a mesoscopic characterization which permits theoretical models to be validated or improved.

These fine studies require complementary acquisitions on both instruments texture spectrometer **6T1** and strain diffractometer **G5.2**, in order to obtain a description as complete as possible of the elasto-plastic deformation in the volume at each crystallographic orientation. Usually, these measurements are performed *in situ* under load.



DIANE (G5.2) : Residual strain spectrometer



Correlation between a rupture profile and a deformation map determined by neutron diffraction

G5.2 is optimized for the study of deformations and residual strain tensors. Its geometry allows a perfect definition of small ($\sim 1\text{mm}^3$) cubic gauge volume which is used to perform 3D maps describing the repartition of residual strains in bulk elements. The limitations are defined by the range of available wavelengths in the cold neutron guides, which limits the number of accessible diffraction lines. The measuring time is also rather long, so that detailed mapping of the strains is difficult in pieces having complex geometrical shapes.

6T1 is dedicated to the study of crystallographic textures. *In situ* ancillary equipment allows the evolution or the preferential orientation to be followed under thermal annealing (during phase transformations, determination of kinetics...) or under mechanical load. The instrument resolution allows micro-deformation to be analyzed by crystallographic orientations in the elastic and plastic regimes. The instrument is presently equipped with a point detector and a flat monochromator, so that the measurement of pole figures and peak profiles is very long. The penalty is especially large for *in situ* measurements, which can presently be only partially exploited.

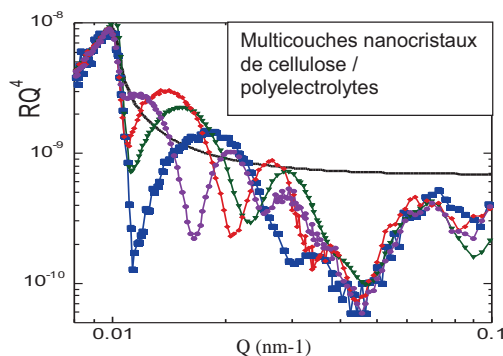
To remain attractive, the LLB is developing a new instrument (**SUPER 6T1**) that will have high flux, which will allow both texture and strain to be measured on a thermal neutron beam.

REFLECTOMETERS

As a pioneer in reflectometry techniques, the LLB operates 2 reflectometers: the horizontal time-of-flight reflectometer, EROS, dedicated to the study of soft matter (polymers - liquids); and the reflectometer, PRISM, with polarization analysis dedicated to the study of magnetic systems. The present technological developments in neutron optics allow us to foresee important evolutions in the future.

Experiments on **EROS** deal mostly with liquid/air, solid/liquid, solid/air interfaces as well as the organization at these interfaces for nano-objects; such as micelles, proteins, polymers, nanoparticles, and hybrid systems formed by association of such objects. A wide range of ancillary equipment is made available for users: e.g. furnace, rheometer, Langmuir trough, humidity cell, etc...

PRISM is dedicated to the study of magnetic surfaces; thin films and super-lattices of metals; semi-conductors; and oxides. The scientific problems are usually related to the field of spin-electronics, such as the coupling or the exchange bias fields at interfaces, or multi-functional magnetic sensors having multi-ferroic materials. Standard ancillary equipment is made available to users (cryomagnets 4K - 7T).



Typical reflectivity curves



Short collimator (1.5m) providing a x4 gain in flux by working with a broader angular resolution.

The majority of the measurements are restricted to the specular component which allows obtaining in-depth scattering length density profiles. Off-specular measurements can be performed to obtain in-plane information (both spectrometers are equipped with position sensitive detectors). These studies remain qualitative at the moment because of difficulties in data processing.

The trend towards the study of thinner and thinner systems (a few nm thick) has driven an evolution of the spectrometers in order to increase the flux on the samples by loosening the resolution. The PRISM spectrometer has switched from a graphite monochromator ($\Delta\lambda = 0.6\%$) to a multilayer monochromator whose resolution is $\Delta\lambda = 7\%$. The spectrometer EROS has evolved by using a multi-disk chopper ($\Delta\lambda = 7\%$) and by shortening the collimation length. These evolutions have allowed making significant gains in flux ($\sim \times 20$).

The next major improvement which can be done is to move the **EROS** spectrometer from the deviator G3bis to the guide end of G6 once **Mibémol** is closed. The move would increase the flux by a factor of 4.

SMALL ANGLE NEUTRON SCATTERING

Small-Angle Neutron Scattering (SANS) probes materials on the nanometer (10^{-9} m) to micrometer (10^{-6} m) scale. Structure on this length scale is critical to the performance of advanced engineering materials. For example, the toughness of high-impact plastics depends on the addition of stiff and flexible segments of polymer molecules. Nanometer/micrometer structure is also crucial in biological processes in cells, in the storage of information on magnetic disks, in the hardness of steels and superalloys, in the conduction of current in superconductors, and for many other materials properties.

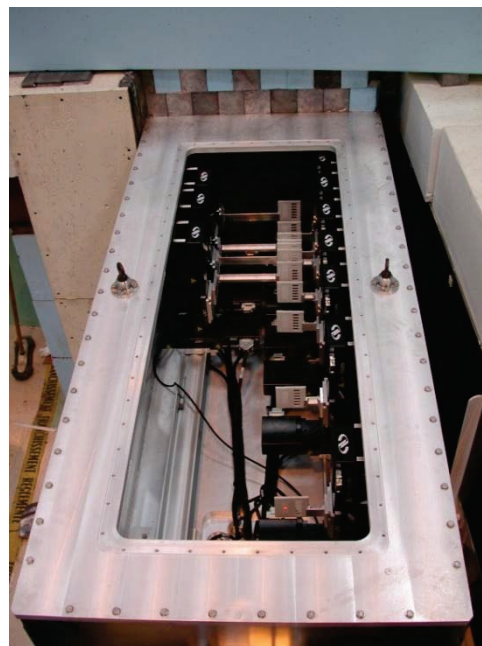
Themes studied at the LLB are: polymers, polymer blends, nano-objects of soft matter (micelles, vesicles), proteins, hybrid nano-objects biology/polymers/polyelectrolytes, chemical demixion or precipitates, magnetic particles of ferrofluids, spinodal decomposition or long range arrangement, cavities or structural porosity, magnetic fluctuations, and vortex lattice in superconductors.

LLB now offers the user community 3 conventional SANS spectrometers covering a Q range from $2 \cdot 10^{-2} < Q \text{ (nm}^{-1}\text{)} < 0.6$, and an original and unique Very Small Angle Neutron Scattering spectrometer, which allows reaching scattering wave-vector values Q down to $2 \cdot 10^{-3} \text{ nm}^{-1}$.

LLB has inherited the knowledge in SANS and in soft matter from pioneers who built the first SANS instrument, developed the contrast variation technique in SANS, and applied it to numerous studies of polymeric systems. **PACE**, **PAXY**, and **PAXE** are conventional (rather short, from 2* 5 to 7m) spectrometers located at the end of guides the first curved elements of which are $2\theta_c$ super-mirror guides. All the instruments are equipped with a BF3 gas multi detector $128 \times 128 \times (0.5 \times 0.5 \text{ cm}^2)$, $64 \times 64 \times 1 \text{ cm}^2$ and 30 concentric rings of 1cm width. **PAXY**, **PAXE** allow anisotropic scattering studies, while only isotropic scattering can be measured on **PACE**. All three are now equipped with the latest generation of high transmission neutron velocity selectors (95% transmission). By using three different configurations (wavelength, collimation and detector distances), users may access a large Q range, $2 \cdot 10^{-2} < Q \text{ (nm}^{-1}\text{)} < 6$ in one experiment.

To access very low Q scattering vectors, we have just completed the construction of a Very Small Angle Neutron Scattering spectrometer (VSANS), **TPA** («Très Petits Angles»). Its original design includes a high resolution Image Plate detector ($2300 \times 2300 \times 0.15 \text{ mm}$ pixel size), a double super-mirrors monochromator, allowing selection of wavelengths between 0.5 and 1.5 nm (FWHM= 14%). The most innovative element of this spectrometer is its multi-beam pinhole collimator, which converges onto the detector located 7 m away from the sample. By combining tiny collimation (diaphragms of 1.6 and 1 mm in diameter) with the small pixel size of the detector ($0.15 \times 0.15 \text{ mm}$), very high resolution measurements can be achieved without increasing the sample volume required for measurements.

TPA benefited from the CAP2010 program and financial support (200 k€) from Aquitaine region. It was opened for users at the autumn session of 2009's Selection Committees.



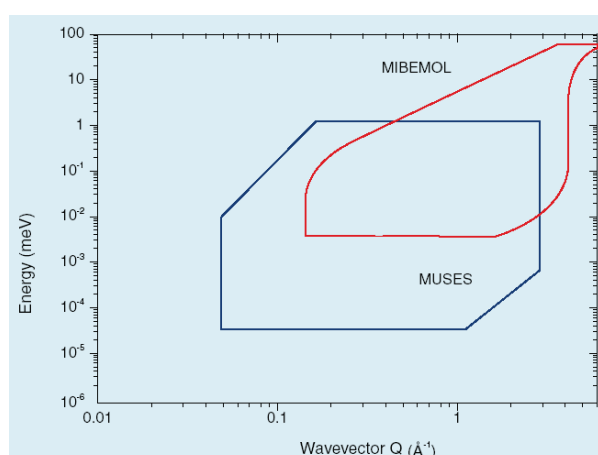
Top view of the interior of the collimator of TPA spectrometer.

QUASI ELASTIC NEUTRON SCATTERING

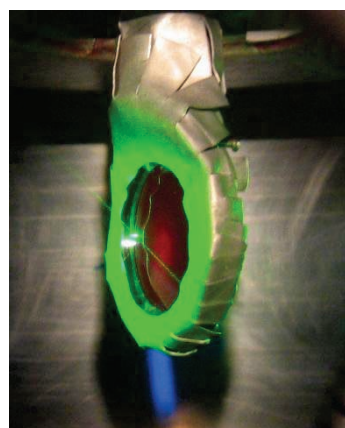
Inelastic and Quasi-elastic neutron spectroscopies are unique tools for the study of the dynamics of materials. Cold neutrons show associated wavelength and energy of few Å and meV. These quantities are both in tune with the atomic distances and the energies of the dynamical modes at play in condensed matter. Kinetic energy exchange resulting from an inelastic scattering process within a sample induces a significant change in the neutron's momentum, making this technique extremely sensitive to spatio-temporal changes. Time-of flight neutron scattering is therefore a perfect spectroscopic probe to reveal simultaneously the structural and dynamical phenomena (vibrational, diffusional and magnetic excitations..) in a vast variety of complex systems: atomic and molecular liquids, polymer, proteins, and glasses. On top of that, isotopic effects and/or polarisation of the neutron beam make it also possible to discriminate between collective or individual phenomena.

LLB operates two very complementary neutron spectrometers: **Mibémol**, a Time-of-Flight (ToF) instrument, and **Muses**, a non resonant spin echo machine.

Mibémol is designed to study loosely dispersive excitations in condensed matter by quasi-elastic and inelastic scattering between 0.01 and 100 meV ($1 \text{ meV} = 8 \text{ cm}^{-1} = 0.25 \text{ THz}$). The corresponding time-scale ranges from 10^{-13} up to 10^{-10} seconds. **Muses** takes over for **Mibémol** for measurements of longer correlation times up to 10 ns.



(Q,w) ranges covered by the LLB quasi-elastic spectrometer suite: Mibémol and Muses.



Sample environment used on Mibémol for an experiment of Biological relevance where a light harvesting protein (blue shadow) was illuminated by a laser beam (green color) triggered by the choppers of the spectrometer.

Experiments taking advantage of the performances of these two spectrometers make it possible to assess the broad (Q, ω) range shown on the figure above. Typical studies performed on **Mibémol** and **Muses**, used either alone or together, cover fields as diverse as spin dynamics in high T_c superconductors, tunneling, dynamics of quantum liquids, dynamics of soft matter, glass transition, confinement, biology, as well as local and long range diffusion in disordered systems. LLB has the project to replace **Mibémol** with a brand new ToF spectrometer. This is the **Fa#** project. Also, the detection area of **Muses** is being turned to a large solid-angle multi-tubes detector. This is the **Multi-Muse** project. Both projects are detailed later in the present document.

COMMON PLATFORMS PROPOSED TO USERS

Common platforms have been implemented to ensure and support specific research activities.

Biology Laboratory (contact: S. Combet-Jeanceneel)

The mission of the biology laboratory is to provide: (i) a technical and scientific support to users in Biophysics to prepare their experiments on neutron spectrometers, and (ii) the equipments used in the research projects of LLB scientists in the field of molecular biology, microbiology, and biochemistry.

The biology laboratory is equipped to prepare biological materials for neutron scattering experiments, *i.e.* in large protein and DNA quantities and exchanged in D₂O:

- DNA analytic and production techniques (thermocycler, gel migration, gel imaging),
- recombinant protein preparation (microbiology equipment, autoclave, sonicator, centrifuges) for bacterial culture and lysis,
- protein production and/or separation (centrifuges, FPLC chromatography) and characterization (SDS-PAGE, Western-blotting),
- protein and DNA determination (UV-visible and fluorescence spectroscopy),
- cold room: critical to use FPLC chromatography without denaturing the proteins and to dialyze at low temperature biological samples in D₂O (H-D exchange),
- ultra-pure water production, pH meter, vortex, magnetic stirrers, etc.,
- -20° C and -80° C freezers to store DNA and proteins.

A perspective is to update the microbiology equipment for cyanobacteria which have the ability to grow in D₂O media and, so, can be used to produce deuterated proteins, such as C-phycocyanin (a light-harvested protein present in cyanobacteria in large quantity). The objective is then to adapt more conventional bacteria (*Escherichia coli*) to produce any recombinant proteins in deuterated media.

Cryogenic Platform (contact: P. Boutrouille, B. Baroni)

Following a great increase in the use of cryogenic sample environments, the LLB has developed a cryogenic platform whose missions are to provide technical skills especially in the field of ultra low temperatures (0.01 K), intense magnetic fields or high temperatures (2000 K). This platform also provides LLB teams with local equipment (bench pumping, leak detector, temperature measurement equipment ...) needed for small repairs (leakages, thermometry ...).

A dedicated room was built for the development of new hardware and to give the necessary space to manage all the different tasks.

The most recent realizations are the development of a dilution without liquid helium and its programmable automat, the complex in-house repairing of Orange cryostats and development of a 4K cryogenerator with sample well.

High Pressure Platform (contact: N.Rey, B. Annighöfer)

The high-pressure research is one of the specialties of the LLB. There is a specially optimized powder diffractometer G6.1 (Micro) in the guide hall dedicated to this research. The instrument was optimized to find the best compromise between resolution, intensity and available scattering range to study magnetic superstructures or mesoscopic structures (such as nanomaterials). Therefore an independent sample focusing system in the vertical and the horizontal plane were installed. The increase of intensity was determined by a factor of 7. By applying cadmium screens inside the cryostat background scattering from the cryostat walls was avoided. These preparations give us the possibilities to study among others microsamples under very high pressure (up to 50 GPa). High pressure could also be combined with low temperatures (down to 0.1 K) and applied magnetic fields (up to 7.5 T). For the different sample volumes, different Kurchatov-LLB pressure cells with sapphire or diamond anvils are in use.

Dedicated to other instruments we also own a Paris-Edinburgh cell for bigger sample volumes.

Beside this very high pressure equipment, the LLB possesses different other types of high pressure material. Especially modified Orange cryostats using liquid helium (like the others) with heavy cool down power for the big masses of high pressure cells.

For the use up to 1 GPa (10 kbar) we have one high pressure gas generator, a two stage system. The first stage up to 0.3 GPa and the second stage up to 1 GPa. The two liquid pressure generators are hand driven commercial systems which work up to 0.7 GPa.

The different existing pressure cells are covering a huge field of investigation. There are cells for SANS experiments equipped with different windows depending on maximum required pressure. These are made from aluminium alloys or niobium. Then we have several high pressure cells made from a copper beryllium alloy (CuBe₂, alloy 25) with different sizes and maximum working pressures. Beside of this other cells made from aluminium alloys (7049A T6 or 2017A T4) or the titanium- zirconium zero-scattering alloy are also available. For the pressure range up to 2.5 GPa we possess a Mc-Whan type pressure cell with sample volumes up to 200 mm³.

To intensify the collaboration and experience exchange with the other neutron centers, the LLB is participating in the European NMI3 FP7 JRA Framework especially Sample Environment with the development of a high pressure gas cell for inert gases up to 0.8 and 1 GPa and the procurement of an automated gas handling system up to 1GPa. Over and above that the LLB participate in collaboration with SOLEIL to create a common laboratory to use extreme conditions.

Chemistry Platform (contact: G. Carrot)

Since its creation, the LLB has always included important chemistry activities. The recent development of this platform allows to greatly improve its impact on the support to our external users or research within the LLB, either through a simple sample preparation, or a more elaborate synthetic procedure. The chemistry expertise present at LLB, involves mainly organic/polymer chemistry and/or inorganic/mesoporous materials synthesis.

Some hoods are presents in the 3 rooms dedicated to chemistry and the construction of new ones, are scheduled before the end of 2010. A special room is reserved for stocking chemicals (H and D) with adequate ventilation. Regarding equipment, some hoods are equipped with vacuum/ inert gases ramps. Fridges, freezers and precision balances are also present. Some advanced characterization equipments are also available: size-exclusion chromatography (SEC), DSC, TGA, UV and infra-red spectroscopy.

Various improvements are planned in the near future, for better working and security conditions:

- A technical support through the hiring of a technician, essential for a continuous contact with the users and for the maintenance of the different equipments.
- The construction of an adequate place for the setting of our gases containers,
- The purchase of an equipment to measure the sizes in the range of those attainable with small-angle neutron scattering. A « Nanosizer » (light back-scattering).
- The improvement of the chemistry place in the Guide Hall.

LIST OF INSTRUMENT RESPONSIBLES

TRIPLE AXIS INSTRUMENTS

| | | |
|-----|---|--|
| 1T | Thermal triple axis with focusing | D. LAMAGO / Y. SIDIS/C. MEUNIER |
| 2T | Thermal triple axis with polarized neutrons | P. BOURGES / Y. SIDIS/P. BARONI |
| 4F1 | Cold triple axis with polarized neutrons | S. PETIT / J-M. MIGNOT / F. MAIGNEN |
| 4F2 | Cold triple axis | D. PETITGRAND / J. ROBERT / P. BOUTROUILLE |

TWO-AXES DIFFRACTOMETERS: POWDER AND LIQUIDS

| | | |
|------|--|-----------------------------------|
| 3T2 | High resolution powder diffractometer | F. PORCHER / F. DAMAY / B. RIEU |
| G4.1 | 2 axis with cold neutrons | G. ANDRE / B. RIEU |
| G6.1 | 2 axis with cold neutrons for high pressures | N. REY / I. MIREBEAU / X. GUILLOU |
| 7C2 | hot neutrons 2 axis | B. BEUNEU / B. HOMATTER |

SINGLE CRYSTAL DIFFRACTOMETERS

| | | |
|-----|--|--|
| 5C1 | 2 axis with polarized hot neutrons | B. GILLON / A. GOUKASSOV / T. ROBILLARD |
| 5C2 | 4 circles with hot neutrons | A. MENELLE / F. COUSSON / A. GOUKASSOV / J-L MEURIOT |
| 6T2 | 4 circles with thermal neutron and lifting arm | A. GOUKASSOV / A. BATAILLE / J-L MEURIOT |

MATERIALS DIFFRACTOMETERS

| | | |
|------|---|--------------------------------------|
| 6T1 | 4 circles with thermal neutrons for texture | M-H. MATHON / V. KLOSEK / S. GAUTROT |
| G5.2 | Strain scanner | V. KLOSEK/M-H. MATHON/S. GAUTROT |

REFLECTOMETERS

| | | |
|-------|--|------------------------------------|
| G3bis | Time of Flight reflectometer | F. COUSIN / A. MENELLE / F. GIBERT |
| G2.4 | Reflectometer with polarization analysis | F. OTT/F. COUSIN/F. GIBERT |

SMALL ANGLE NEUTRON SCATTERING

| | | |
|-------|--|-------------------------------------|
| G1.2 | Small angle with isotropic detector PACE | D. LAIREZ / S. COMBET / A. HELARY |
| G2.3 | Small angle with focusing PAXY | A. LAPP / J. JESTIN / V. THEVENOT |
| G5.4 | Small angle PAXE | J. JESTIN / G. FADA / M. DETREZ |
| G5bis | Very small angle | A. BRULET / S. DESERT / V. THEVENOT |

QUASI-ELASTIC INSTRUMENTS

| | | |
|-------|-------------------------------------|--|
| G1bis | Resonant spin-echo MUSES | N. MALIKOVA / S. LONGEVILLE / F. LEGENDRE |
| G6.2 | Time of flight spectrometer Mibemol | S. LONGEVILLE / J-M. ZANOTTI / B. HOMATTER |

TEST INSTRUMENTS

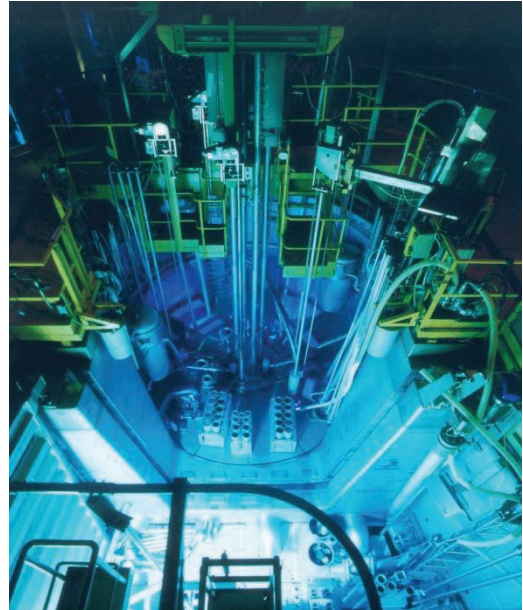
| | |
|-----|----------------|
| 3T1 | P. BOUTROUILLE |
| G43 | P. BARONI |

C- The Orphée Reactor

A- General presentation and historical background

The Basic Nuclear Installation n°101 located at CEA Saclay Centre, comprises the experimental 14 MW thermal power ORPHEE reactor and the buildings used the Léon Brillouin Laboratory (LLB).

After the creation of LLB in 1974, the ORPHEE reactor was built between 1976 and 1980 as a, national-based, sister facility of the High Flux Reactor (RHF) of the Laue Langevin Institute (ILL) in Grenoble. The decision to build the reactor stemmed from the continuous expansion of European and international neutronic research in the 70s. The ORPHEE design directly benefited from the safety, construction and operation feedback of previous generation reactors like RHF and was contemporary to the development of the PWR equipment program in France. The reactor first went critical on December 19th 1980. The designers' projections purposely resulted into a moderate investment cost - moderate operation cost facility, ensuring both reliable operation, good safety record and high performances.



Though the first five years of operation were perturbed by technical problems of youth rapidly solved, the compact design of the reactor enables the construction of very high performances spectrometers. User access on an open basis was already set up in 1983 with the organisation of the first "Tables Rondes". The construction of the LLB building (563) in 1986 and the first participation to the European programs in early 1993 finalized the way of operation of the LLB-Orphée entity.

During the long shutdown of the RHF-ILL in 1990-1993, Orphée operates up to 250 days a year. Up to now, since its first divergence, the reactor has been operated circa 5500 days.

B- Reactor technical characteristics

ORPHEE is a « pool » type reactor. The 14-MWth compact, light-water moderated, core provides up to $3 \cdot 10^{14}$ n/cm²/s thermal flux in the surrounding heavy water reflector tank. Core life cycle duration is 100 days. The core and the heavy water tank are immersed in a pool filled with demineralised light water. This ensures radiological shielding and facilitates handling from above the pool. The reactor hosts 9 horizontal channels (feeding 20 neutron beams) and 9 vertical channels (comprising 4 pneumatic channels for activation analysis and 5 irradiation pits for radio-isotope and other industrial productions). The heavy water tank is equipped with three local moderators: two cold sources (liquid hydrogen at 20K) and one hot source (graphite at 1400 K) which provide neutrons of respectively lower and higher energy

ORPHEE neutrons are currently supplied to 27 experimental areas. The experimental areas are located around the reactor, either in the reactor building (11 of them) or along the neutron guides of the guides hall (16 of them). One experimental area with specific radiological shielding has been designed for industrial neutronography (mostly used by the aeronautical or space industry). The ORPHEE reactor is operated by the Nuclear Energy Division of CEA (CEA/DEN) and is run by a 60 people team, about half of which work on a shift basis. This facility benefits from the support of the radiological protection teams and security teams of CEA Saclay Centre

C- Reactor safety

The safety design of the reactor enables to ensure permanent control of the three main safety functions: reactivity control, residual heat removal and containment of radioactive material. The design includes the following elements:

- Permanent reactor monitoring by a safety system using 3 completely independent channels. If necessary, 2 channels out of 3 will automatically trigger the reactor emergency shutdown.
- Once the reactor has been stopped, the residual power is removable by purely passive natural convection between the core and the reactor pool.
- The core and the core cooling circuit are located in the reactor building made of reinforced concrete.

Three barriers are placed between dangerous products and the environment. These barriers are: the reactor fuel cladding, the reactor main cooling circuit plus the reactor pool, and the reactor building. The reactor building has also been designed to sustain any accident which could occur to the reactor.

The supervision of the impact of the installation onto the environment is included in the Saclay Centre environmental monitoring program.

D- 2010 safety reassessment

The reactor safety case was reassessed twice since 1980. 2008 and 2009 had seen the preparation of the second safety reassessment. To this aim, a major non-destructive inspection programme was carried out. In parallel, substantial safety study work was carried out with notable support of, the CEA specialists from the Nuclear Energy Division technical departments of the Saclay Centre. The resulting work underwent CEA internal review and control beginning of the year 2009. Results of these actions confirmed the very satisfactory technical and safety condition of the reactor after 29 years of operation. The reassessment file was submitted to the French regulatory body on March 31st 2009. Some additional clarifications were then given to the IRSN (Institut de Radioprotection et de Sûreté Nucléaire) that did submit a technical report by July 2010 to the “Groupe Permanent” (GP), the group in charge of the final evaluation. After two final meetings with the CEA in September, the GP issued its final report to the French safety authorities on October 23rd. Though some improvement of safety were asked, the report points out that the initial reactor safety features remain in good adequation with up-to-date safety practices.

E- Future operations

This good report on the safety of the reactor opens up a future of at least ten years of operations. The main works to be performed are the replacement of the various thimbles of the beams that becomes fragile after 30 years of irradiation. This work has already been started in 2008 by the replacement of the 4F thimble that took place as scheduled. It will be continued during the next years doing roughly one thimble each year. When all completed, this type of replacements should not occur again before 2035. On the same line, cold sources have also to be replaced each 15 years. This will be done during the summer 2011.

All these maintenance operations will enable us to keep the Orphée reactor in a very well state. With that point and with the amount of fuel that we already have, we are prepared to reach the next safety reassessment in 2020 in good conditions.

D- Upgrade program of the instrumentation CAP2015 and projects

The main objectives of the **CAP2015** instrumental program are to provide a modern set of neutron instruments to the French neutron scattering community and to prepare and train a new generation of neutron users and scientists, especially in view of the future European spallation source. This is an extremely difficult challenge following the construction of second-generation neutron spallation sources in the United States (SNS), and in Japan (J-Parc). Moreover, after the closing of several older neutron sources in Europe and the USA (Studvisk, Julich, Argonne), other European neutron sources are entering important extension or renovation phases: the Millenium program at the European neutron source (Institut Laue Langevin); the second target station at ISIS (UK); the extension of the instrument suite at FRMII (Germany); the construction of a new guide hall at BENSC (Germany); and the development of new spallation targets at SINQ (Switzerland). In this context, the TGIR LLB/Orphee has the duty to remain competitive in this rapidly changing scientific environment and to join the European efforts to provide complementary equipment to the scientific community.

In 2005, after more than a decade of successful operation of the first-generation instruments at ORPHEE, LLB started its first instrument refurbishment program, CAP2010. The program was established in January 2005 on the basis of internal instrumentation project proposals, which emerged after a profound analysis of performance of existing instruments within each instrument group of the LLB. Among all the proposals, 7 projects were selected to launch the modernization; **3T2**, **MICRO**, **7C2**, **TPA**, **Fa#**, **EROS** and **VIP**. It was estimated that program realization would require an annual investment of about 1 MEUR per year during a 5 year period. Since no such funding was available at that time, the priority was given to low cost projects which could rapidly produce scientific output. Thus, the first instruments delivered in 2007, **3T2** and **6T2**, were essentially due to the financial support of Aquitaine and Rennes Metropole Regions and to the subventions from the European Neutron-Muon Integrated Infrastructure Initiative NMI-3. More costly projects, such as **Fa#**, **7C2** and **VIP**, remained on the "waiting list" separate from the part concerning the simulation of future instrument performances.

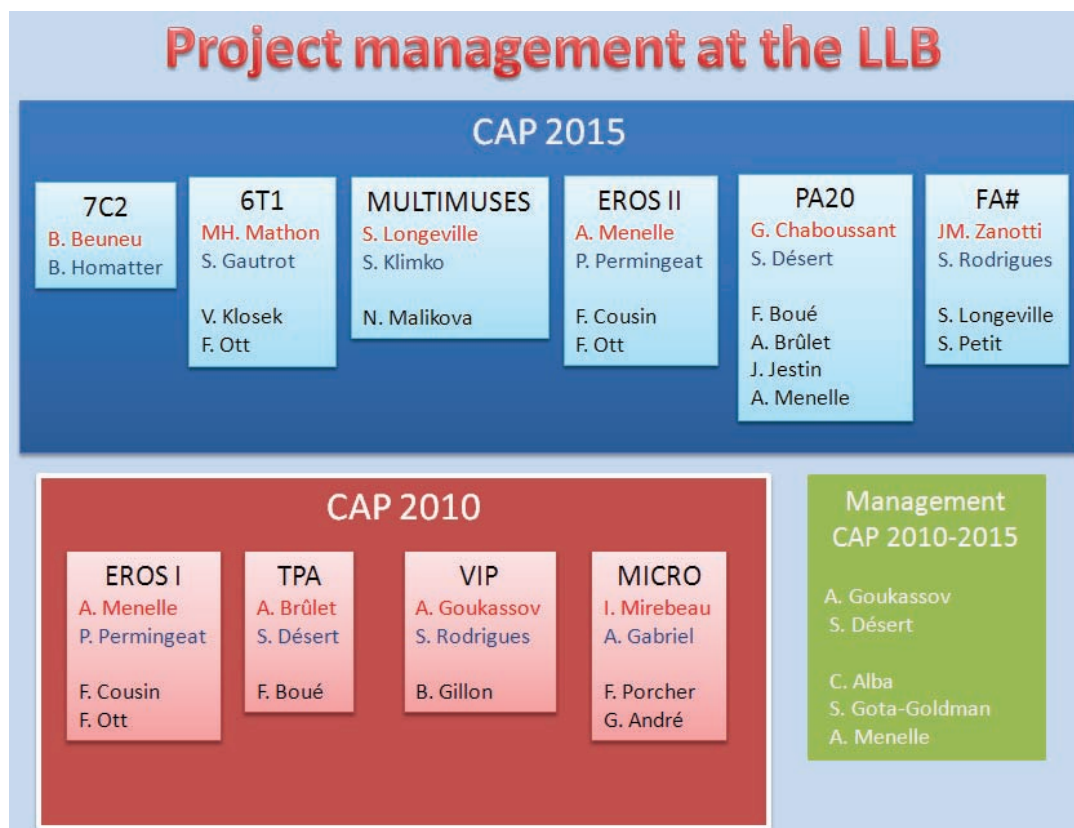
In November 2007, the first external evaluation of CAP2010 took place in Saclay. The International Instrument Committee (Table 1), consisting of neutron experts and representatives of the user community examined the existing instrumentation park of LLB, evaluated the instruments under construction, and gave several recommendations concerning the priority of projects and their management.

The Committee recognized the very high quality of the majority of the existing neutron instruments and in particular of **3T2** and **Super-6T2**, which became highly competitive instruments after their refurbishment. It also encouraged the efforts to complete other CAP 2010 instruments under construction: **VIP** (polarized neutrons), **MICRO** (High Pressure), **TPA** (Very SANS), and **7C2** (liquid). It further advised that sample environments be improved, polarization be developed on the instruments; and that some instruments be closed in order to focus on the new projects. Finally, five new instrument proposals were reviewed and recommended for realization: **PA20** (small angle scattering), **6T1** (strain and texture), **Fa#** (TOF), **Multimuses** (Resonant spin-echo), and **EROS-2** (reflectometer).

These recommendations have served as a basis for instrument development plan for the LLB. Indeed, **VIP**, **MICRO** and **TPA** are finalized and have entered the qualification stage; while **7C2** joined the **CAP 2015** road map. LLB also put effort into the development of polarization by hiring an expert in polarized neutrons, Sergey Klimko; ordering a new Heussler; adding the polarization option to **PA20**, and set the **NEPTUNE** project. Concerning the sample environment, LLB created the **Support Group for Experiments and Sample Environment** and the **Cryogenic Platform**. Finally, **PAPYRUS** and **G5.6** have been closed to create space for **PA20**.

More than half of our instruments (12 out of 21) should benefit from the completion of the **CAP 2015** road map. Realization of such an ambitious program, on time and within a constrained budget and limited manpower, without interrupting scientific activities represents a difficult challenge. To address the challenges and to coordinate these diverse efforts and activities, the

Instrument Development Group was created in 2008 and a project management structure was set.



Instrument development and management teams at LLB

Since 2009, projects have been executed following the “ Rules of project conduct in LLB” which were been established based on the experience of other neutron centers such as ILL. This includes the nomination of project leaders and project managers, as well as the creation of the piloting team (Instrument Development Team, IDT) presented in Figure above. Accepted projects usually contain four clearly identified stages, as well as milestones and deliverables. In the first, pre-design stage, the scientific orientation of the instrument and its expected characteristics are defined. After validation of the project by IDT and **CAP 2015** managers, the project passes to the design stage, which is followed by the realization and qualification stages. The passage from one stage to another, as well as the acceptance of deliverables and milestones, are validated by IDT and **CAP 2015** managers.

Time schedules of CAP2010-2015 instruments are summarized in Figure YYY. It shows that three instruments of CAP2010 are finished (**3T2**, **EROS** and **Super 6T2**) and that two have entered into the qualification phase (**TPA** and **VIP**). **MICRO** is close to qualification and five instruments are in realization stages at different levels. The state of these projects will be described in detail in Chapter **CAP 2015**. An open question remains concerning the realization of **Fa#**, which suffers from uncertainty in the financial capability of LLB to support its realization.

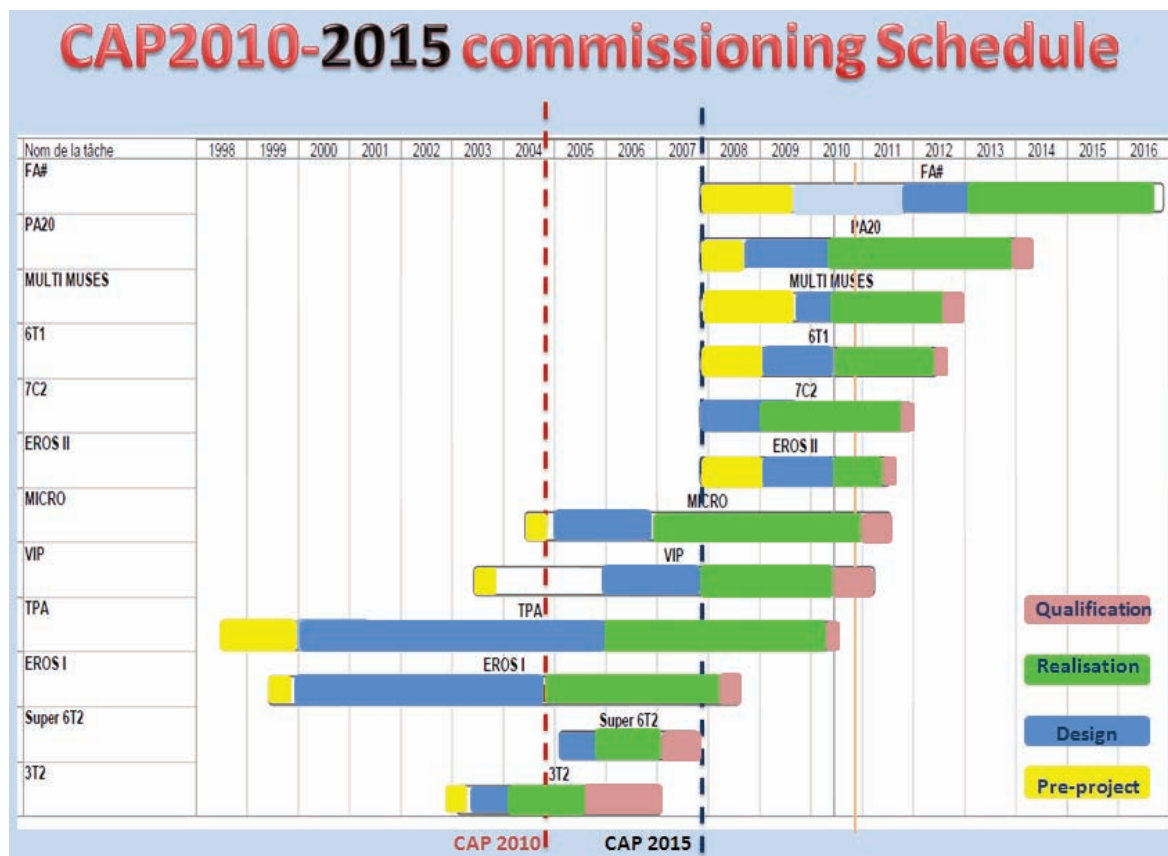


Figure CAP 2010-2015 projects schedule

However, Figure above shows that despite extremely limited instrumentation budgets and manpower, a total of 12 upgraded or new apparati should be on line by 2015. At LLB, the ratio of the number of permanent staff to the number of instruments is 5, which is abnormally low compared to the other similar facilities (13). These state-of-the-art spectrometers should assure the future of LLB for another decade to come. The realization of CAP2015 became possible largely thanks to the financial support of the Aquitaine Region in the **TPA** (250k€) and **VIP** (100 k€) projects. **PA20** benefits from the regional programs “ C NANO d’ Ile de France” (300 k€) and Triangle de la Physique (250 k€).

Triple-Axis Spectrometers

In 1999, the size of the **2T** thermal beam tube was enlarged, resulting in a gain in flux by a factor of three. **2T** is now fully equipped with a polarized neutron option.

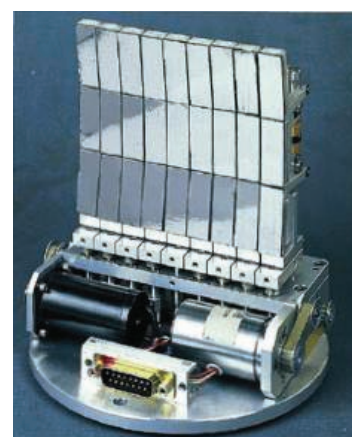
During the summer of 2006, a 30 \circ supermirror coating was installed inside the beam tube of **4F1** and **4F2**, thereby multiplying the flux by a factor of up to 1.8 depending on the neutron energy. The polarized neutron setup was also improved with a new bender on **4F1**. On **4F2**, the secondary spectrometer was rebuilt using non-magnetic materials to allow the superconducting cryomagnet to be energized up to 10T.

The renewal of the contract with the Karlsruher Institut für Technologie was accompanied by a refurbishment of **1T**, including the installation of new goniometers, and the replacement of all coders and electronics. **1T** now shares the same standards for electronics and software control as all other TAS at LLB.

Finally, new sample environments for very low temperatures (≥ 30 mK) and high magnetic field (≤ 10 T), as well as a new generation of more powerful cryogenerators (3 K – 800 K) have been commissioned and are open to users. Further improvements are foreseen, especially regarding intermediate-pressure equipment.

The upgrades initiated on each instrument must continue with the highest priority placed on further increasing the flux. **2T** should be equipped with a Cu200 focusing monochromator, optimizing the flux/resolution trade-off. A new focusing analyzer (silicon or graphite) is planned for **1T**. The sizes of monochromators and analyzers should also be increased on **4F1** and **4F2**

We also plan to improve the polarized neutron setup which requires better Heussler crystals for both the monochromator and the analyzer on **2T**. High magnetic field studies on both thermal and cold TAS will also require the secondary spectrometers on **2T** and **4F1** to be rebuilt using non-magnetic materials. This will allow the asymmetric 10 T cryomagnet to be used also on these two instruments, first for unpolarized neutrons, then for polarized neutrons.



Focusing mechanism of a PG analyzer with double curvature.

Finally, it is necessary to maintain and develop a large number of different sample environments, especially for very low temperatures and intermediate pressures.

Financing

| | 2009 | 2010 | 2011 | 2012 | 2013 | 2014 | 2015 |
|----------------------------------|------|------|------|------|------|------|------|
| <i>Monochromators</i> | | 125 | | 100 | | | 150 |
| <i>Non magnetic spectrometer</i> | 140 | | | | | 220 | 70 |

Two-Axis Diffractometers: Powder and Liquids

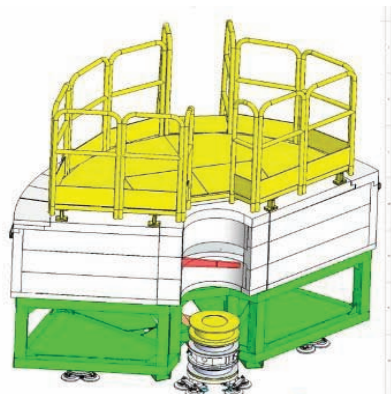
The CAP2010 project foresaw the recasting of 3 spectrometers: **3T2** recasting has been finalized, and **G6.1** and **7C2** are in progress at present and will be finished in 2011.

G6.1: This instrument favors a high flux and a high signal/background ratio at the expense of resolution. This spectrometer works with a supermirror guide and a focusing monochromator. Two focusing devices are installed before the sample in the high pressure version. The next improvement (planned in 2011) is the implementation of a new multidetector with two sample–detector distances (one with very large solid angle). This detector is at present tested on the G4-2 position and should be moved at G6.1 in spring 2011.

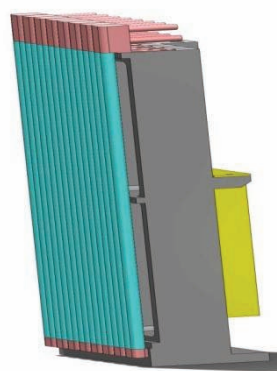
7C2: Equipped with a multidetector with efficiency 17% (for the wavelength 0.7 Å), **7C2** is strongly penalized with regard to his direct competitors, in particular D4 at ILL. An in-depth transformation of the instrument is in progress. The 640 cells multidetector will be replaced by an assembly of 256 position sensitive tubes 50cm high with an efficiency higher than 75 % (for 0.7 Å). It will increase the counting rate by a factor 25 and will make of **7C2** a competitive instrument in the scientific domain covered by very few instruments. It will present with regard to D4 the advantage to cover the whole angular range in a single measurement, which is indispensable during measurements of evolutionary samples.

The new **7C2** should be operational in the middle of 2011.

A later replacement of the monochromator could result in gaining another factor of 2.



7C2 – Detector design



7C2 - 16 detector modules (developed at LLB) associating 16 position sensitive tubes

3T2: With the secondary spectrometer reconstructed and its equipment of a new 50 collimators/detectors block, which has allowed dividing by 2 the diffractogram acquisition time, the **3T2** instrument is in a new operational phase. **CAP 2015** forecasts a possible channel replacement which would improve the counting statistics in multiplying the flux by 3.

Financing

| | 2009 | 2010 | 2011 | 2012 | 2013 | 2014 | 2015 |
|--------------------------|------|------|------|------|------|------|------|
| <i>G6.1 MICRO</i> | | 60 | 15 | | | | |
| <i>7C2</i> | 320 | 200 | 100 | | | | |
| <i>3T2 (pre-project)</i> | | | | | | | 550 |

Single Crystal Diffractometers

5C1 is a polarized neutron diffraction diffractometer mounted on the hot source of the ORPHEE Reactor. Polarised neutron diffraction (PND) is rather unique technique in magnetism as it takes full advantage of the neutron magnetic moment and gives a direct access to the spin density distribution in the unit cell. In contrast to electron density, usually determined from high precision X-ray diffraction techniques, the spin density distribution is directly related to the unpaired electrons. Thus, by comparing spin and electron densities, one can get an insight into magnetic interactions. The PND has been extensively used in the LLB for many years and has been successively applied recently to the studies of: anomalous spin densities in ruthenates, bilayer manganites, photoinduced molecular switching compound. PND is also traditionally of particular interest for the community of chemists working in the field of molecular magnetism.

5C1 refurbishment was included in CAP2010 instrumentation program and it will be replaced by **VIP** (Very Intense Polarized neutron diffractometer) this year. In summer 2010 all its mechanicals part, radial collimators and 64 position sensitive detectors have been delivered to the LLB and tested in the guide hall. Recently the new instrument was transported to its permanent place in the reactor hall. Now **VIP** enters in its qualification phase. It is planned that it will be open for users in the beginning of 2011. Compared to the current **5C1**, **VIP** will present a large detection area covering about one steradian angular range, which will increase the efficiency of the instrument by nearly two orders of magnitude.

The instrument is expected to be open for users after a one month qualification stage in December 2010. **VIP** benefitted from financial support (50 k€) of Aquitaine region.

In 2011 a replacement of focusing polarizing Heussler monochromator is envisaged.



VIP (5C1) diffractometer

Financing

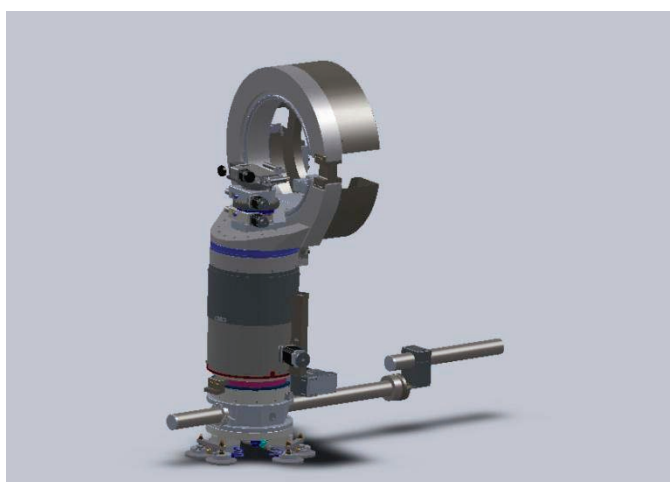
| | 2009 | 2010 | 2011 | 2012 | 2013 | 2014 | 2015 |
|-------------------------|------|------|------|------|------|------|------|
| <i>VIP New Heussler</i> | | 47 | 55 | | | | |
| <i>5C2 PSD</i> | | | | 150 | | | |

Materials (Texture/Strain) Diffractometers

SUPER 6T1: A new high flux texture and strain instrument

The optimal structural information is obtained by the simultaneous measurement of the texture and the strain state of the samples. This requires the measurements of the diffraction peaks (shape and position) for a maximum number of sample orientations. Counting must be performed as fast as possible with a flux as large as possible and with an optimized detection system.

The new instrument will be installed in the reactor hall on a thermal canal. It will be equipped with several monochromators compatible with strain measurements in a $2\theta = 90^\circ$ configuration, an Euler cradle equipped with translations stages and a position sensitive detector.



This instrument will be optimized for academic research and for the characterization of "small" industrial elements (30kg max). It will not be usable with large industrial pieces (> 100kg) which require handling and space not available in the reactor hall. Thus the instrument **DIANE** will remain operational for specific studies on large industrial pieces.

- 2009 : definition of the **SUPER 6T1** configuration
- 2010 : design and fabrication of the new sample stage
- 2011 : commissioning of the new sample stage
- 2012 : installation of a 2D position Sensitive detector (DENEX)
- 2013 : installation of new focussing monochromators (Cu and graphite)

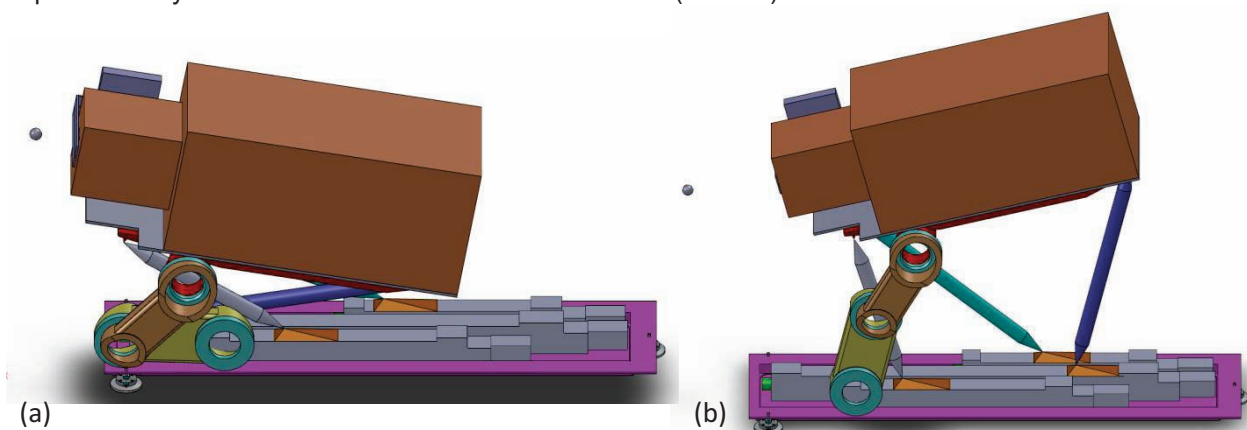
Financing

| | 2009 | 2010 | 2011 | 2012 | 2013 | 2014 | 2015 |
|-----|------|------|------|------|------|------|------|
| 6T1 | | 150 | 150 | 150 | | | |

Reflectometers

The users demand is oriented towards the in-situ characterization of the systems: evolution as a function of the temperature, the pressure, the strain, the UV illumination... This evolution is partly due to the availability of more and more complex sample environments for the users. However, systematic studies as a function of numerous external parameters are presently rather difficult to perform because of the long acquisition times (a few hours per sample and per external condition).

Our present strategy consists in trying to breach into new regions so that specular reflectivity measurements can be performed in a matter of a few minutes rather than a few hours. Our objective is not to be able to measure very low reflectivities nor to perform off-specular scattering measurements as in practice, these type of measurements (reflectivities $R < 10^{-6}$) represent only a small fraction of the user's demand ($< 10\%$).



New detector tank at two extreme configurations: (a) angle = 10° , sample height = 1265 mm, sample to detector distance = 200 mm, (b) angle = 15° , sample height = 1365 mm, sample to detector distance = 500 mm.

We propose to upgrade the spectrometer **EROS** in order to make it a very high flux instrument for specular reflectivity measurements. The propose program is the following:

- 2008: installation of a high count rate multi-tube detector ($320 \times 320 \text{ mm}^2$)
- 2011 : installation of a new vacuum tube and mechanics for the 2D PSD
- 2011 : test of a new optics for energy analysis
- 2012: implementation of the energy analysis option
- 2013: design of a new chopper (allowing a coarse resolution, up to $\sim 20\%$)
- 2014 : move on guide G6; set-up of a new casemate
- 2015 : commissioning of the new spectrometer

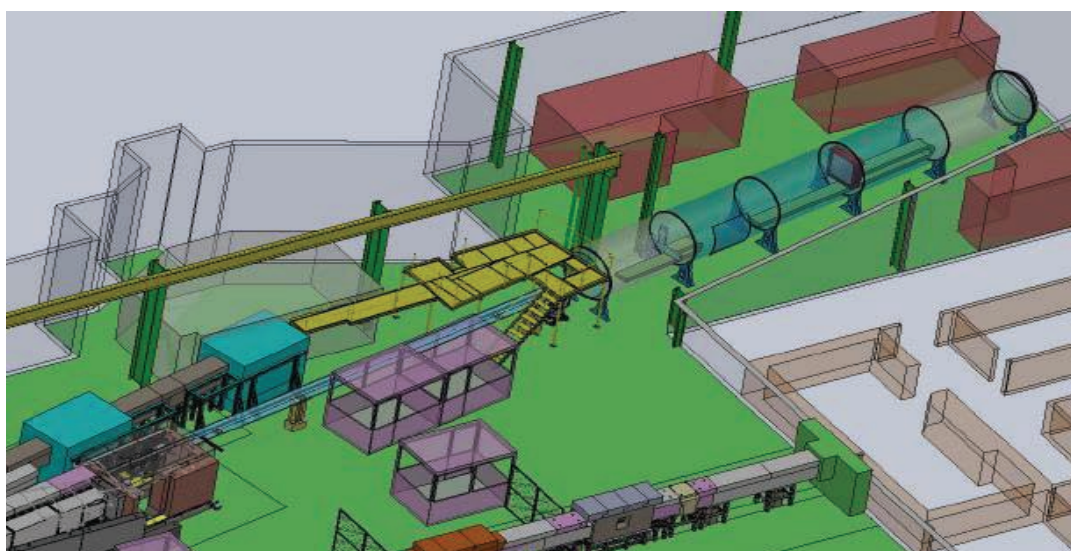
Financing

| | 2009 | 2010 | 2011 | 2012 | 2013 | 2014 | 2015 |
|------------------------------|------|------|------|------|------|------|------|
| Very high flux reflectometer | 100 | - | - | 100 | 100 | 300 | 350 |

Small Angle Neutron Scattering

In the instrumental program of LLB, CAP2015, we have planned a **new SANS spectrometer, PA20**, in replacement of one old SANS instrument (**PAXE**), located at the end of one neutron guide (G5 at ORPHEE). Owing to the G5 guide dimensions ($80 \times 25 \text{ mm}^2$), we can envisage to develop various focusing devices studied in the Neutron Optics program of NMI3. **PA20** will be a spectrometer of last generation equipped with the most recent technology in neutron scattering. We aim at increasing both the neutron flux going through the sample, by implementing **recent techniques of focusing** (super-mirrors guides of various geometries) and **focusing MgF_2 lenses**, which have just been successfully installed on PAXY. Important gain in the efficiency of the measurement of the scattering intensity can be achieved by **using new very efficient multi-detectors of new generation** covering in only one measurement a solid angle range of almost 2 orders of magnitude. The length of the instrument, approximately $2 \times 20 \text{ m}$, will make it possible to exploit both the flux and the resolution, and also to reach very small scattering vectors, at least 10^{-2} nm^{-1} (@ 8 \AA , 20 m). **PA20** will also provide a polarized neutron beam for magnetic studies with high polarization ($> 98\%$) between 4 and 20 \AA .

The global increase, up to a factor 10, will be particularly appreciable to study the nanometer scale objects, but also the larger objects (15 - 100 nm), which are observable only at small scattering vectors, where the scattering intensity is generally weak. The technical performances which are possible to obtain by using last generation neutron devices will place the new instrument **PA20** among the best in the world, very close to those of ILL (Grenoble).



Scheme of the project PA20 implemented in the guide hall

The replacement of the old **PAXY** multi detector is also scheduled. A contract with ILL has been signed in 2009 in order to build two new, high resolution ($5 \times 5 \text{ mm}^2$ pixel size), and efficient (up to 80% at 0.5 nm) multi detectors, one for **PAXY** and the second one for rear detector of **PA20**. Their delivery is scheduled for the end of 2012.

PA20 is financially supported within regional programs “C nano d’ Ile de France” (300 k€), Triangle de la Physique, Saclay (250 k€) and the Aquitaine Region (200 k€).

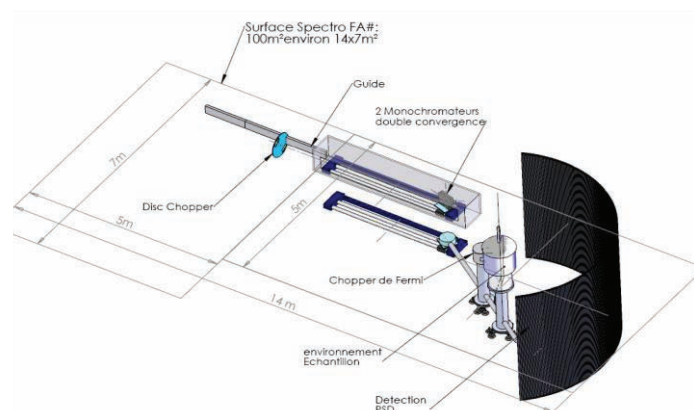
Financing

| | 2009 | 2010 | 2011 | 2012 | 2013 | 2014 | 2015 |
|----------------------|------|------|------|------|------|------|------|
| <i>PA20</i> | 400 | 500 | 400 | 200 | 100 | | |
| <i>Detector PAXY</i> | 400 | | | | | | |

Quasi Elastic Neutron Scattering

Fa#

After almost 30 years of good and efficient operation, the performances of **Mibémol**, the LLB-Orphée Time-of-Flight machine, are now challenged by the new generation of instruments, already in service or scheduled to come on-line in the next few years. In order to maintain a world-class scientific production, LLB has undertaken the design of a new ToF machine: this is the **Fa#** project.



Schematic view of the FA# spectrometer. A brand new "large m" neutron guide will shed the incident neutron beam onto a doubling focusing monochromator (Pyrolytic graphite and/or MICA).

Variable Guide/Monochromator and Monochromator/Sample distances will make it possible to switch from time to monochromatic focusing modes. A set ^3He detectors at high pressure (10 bars) will ensure high Q resolution under extended solid angle coverage

In the long run, **Fa#** will be the only ToF spectrometer at LLB. This machine must therefore show competitive performances in both quasi-elastic and inelastic measurements, for disordered systems (liquids, glasses, biology, chemistry, soft matter) but also crystalline samples (magnetism and solid state physics). **Fa#** will have to achieve high flexibility to reliably map energy resolution in the 15 to 500 μeV range on an extended Q domain from 0.05 to 5 \AA^{-1} . The spectrometer should meet these criteria with the highest flux achievable.

Among the different possible ToF technologies, a direct geometry so-called "hybrid" set-up seems to be able to meet all the criteria above. The design of **Fa#** is based on the FOCUS machine in operation at the Paul Scherrer Institute, Switzerland and also operated by Saarland University, Germany.

The performances of **Fa#** will come from use of the state of the art following key elements:

- a large surface super mirror, possibly with an elliptical shape, fully dedicated to the instrument,
- a set of doubly focusing (both vertical and horizontal) monochromators,
- a short flight path from sample to detector to maximize the detection solid angle (1.7 st),
- ^3He detectors at high pressure (10 bars) to maximise the detection efficiency of neutron scattered with high energy (routine detection up to 150 meV).

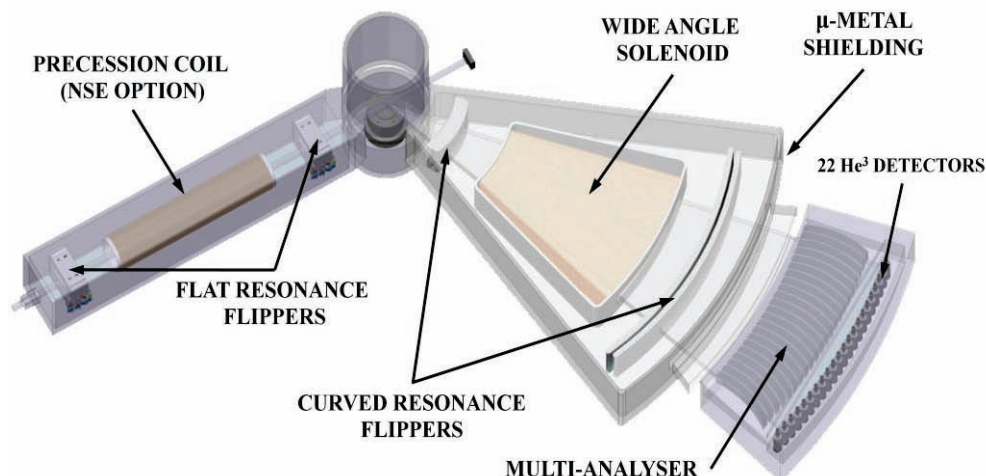
Variable Guide/Monochromator and Monochromator/Sample distances will make it possible to switch from *time* to *monochromatic focusing* modes. This will be a key feature to reach the best flux vs. resolution balance, while accommodating the Bose population factor in experimental situations as different as fundamental magnetism related studies in the mK range and material oriented research conducted at temperatures up to a thousand Kelvins.

Financing

| | 2009 | 2010 | 2011 | 2012 | 2013 | 2014 | 2015 | 2016 |
|------------|------|------|------|------|------|------|------|------|
| Fa# | | | 850 | 1300 | 1400 | 1100 | 900 | 350 |

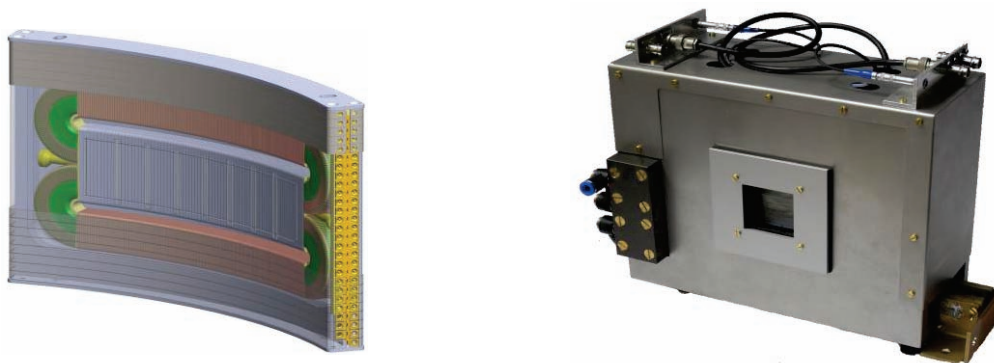
MULTI-MUSES

The aim of the **MULTI-MUSES** project is to design and construct Large Solid Angle (LSA) resonance coils for the implementation of a multi detector system on the Neutron Resonance Spin-Echo (NRSE) **MUSES** instrument and gain 2 orders in solid angle detection. The curved resonance coils are the critical difficulty we have to overcome to realize the project. The coils are made of a vertical static of the order of few hundred Gauss in which are inserted a radiofrequency coils used in the frequency range between 50 kHz and 1 MHz. In order to produce an echo two coils are necessary per arm.



General design of the Multi-detector NRSE spectrometer

We started the design of the first curved coil which corresponds to the shorter radius of curvature and thus the most difficult to realize with a good field homogeneity. We also designed and constructed new flat coils that should be located in the first arm. New principles were developed in order to improve the field homogeneity (better resolution quality) and the maximum reachable frequency (maximum spin echo time). These coils are going to be tested within the next weeks and if the quality is satisfactory then we will start the construction of similar curved coils within the 6 next months.



Design of the first curved coil of MULTI-MUSE and view of the flat flipper.

Financing

| | 2009 | 2010 | 2011 | 2012 | 2013 | 2014 | 2015 |
|--------------------|------|------|------|------|------|------|------|
| <i>MULTI-MUSES</i> | 20 | 120 | 75 | 110 | 105 | | |

Changes of the neutron spin state in scattering provide quite unique information about the scattering media. Spin dependence of neutron cross sections is known to be a powerful probe in magnetic structures and excitations studies. Polarized neutrons allow separation of coherent and incoherent contributions in spectra, as well as separation of magnetic and nuclear contributions. They are used in Larmor time labelling and in spin-echo techniques. In recent years the use of polarised neutrons was rising very rapidly and all modern facilities possess a variety of polarized neutron scattering instruments. Growth of interest to polarized neutrons is due to a drastic improvement of modern polarization devices both based on the polarization of Helium 3, which can be achieved via spin-exchange optical pumping (SEOP), high quality modern supermirror devices and Heussler crystals. An advantage of the SEOP technique is that it can be easily adapted to several families of spectrometers:

1 - Small angle scattering and reflectometry, almost unique methods to study the structure of nanomaterials, complex systems, polymeric organic compounds and biological systems, where the isotope labelling is a major advantage of neutron scattering and polarization (PA20 Project, ESS, NanoInnovation).

2 - Quasi-elastic spin echo and time of flight, enabling studies of the dynamics at different time scales in complex systems, in particular discrimination between local movements and collective modes. In some cases, the effectiveness of these instruments could be increased by a factor of 50 due to the use of multi-detectors with polarization analysis. Investigation of mesoscopic dynamics is expected to be greatly expanded. At present, only one instrument in the world, MAF at ILL, is adapted for this problem.

3 - 4 circles diffractometers, where polarization analysis will open a way for detail studies of small single-crystal samples (used, for example in spin electronics), powder diffractometers for the study of complex magnetic structures and 3-axis spectrometers, where the separation of magnetic and nuclear contributions provided by polarized neutrons is of extreme importance.

The **NEPTUNE** project which is at present in the phase of prospective development, addresses the possibilities of creation of such polarized instruments cluster at LLB.

The funding required for the realization of NEPTUNE program is estimated as 3.5 M€

NEPTUNE upgrade program of LLB/Orphée instrument suite based on the SEOP in combination with other modern polarizing techniques should allow to maintain the TGE LLB/Orphée among the best international facilities, keeping or improving its current rank (at present LLB occupies the place of the third neutron facility in the world regarding the publication number in highly recognized international journals).

D- Instrumental Committee (November 2010)

Minutes and recommendations of the instrument evaluation at the Laboratoire Léon Brillouin on November 8th, 2010

Introduction

After a first evaluation of the instrument suite of the Laboratoire Léon Brillouin and its further development in the year 2007 the direction of the LLB has invited for a second meeting of the Instrument Committee (IC) on November 8th, 2010. Most of the members of the committee are involved in the instrumentation of the six neutron sources in Europe with an international user community. The members of the committee¹ are

- Laurent CHAPON ISIS (excused)
- Daniel CLEMENS Helmholtz-Zentrum Berlin, HZB
- Jean-François LEGRAND* Université de Strasbourg
- Thierry STRAESSLE Paul Scherrer Institut
- Andreas MEYER German Aerospace Center, Cologne
- Winfried PETRY* Technische Universität München, FRM II (Chairman)
- Helmut SCHÖBER* Institute Laue Langevin
- Charles SIMON* CNRS
- Françoise Leclercq* Hugueux, SFN (observer)

The direction of the LLB has asked the IC for advice on the following aspects:

- ⇒ Are the measures and actions taken within the renovation program CAP 2010² (after the advice of the 1st IC in 2007) adequate?
- ⇒ Evaluation of the instrument upgrade and renovation within CAP 2015³.
- ⇒ Classification of the program CAP 2010 and CAP 2015 with respect to the needs of the french neutron community and within a wider perspective of the European landscape of six decent neutron sources with international user programs and in particular in view of the project of the future long pulsed European Spallation Source (ESS) at Lund.

The following personal from the LLB participated mainly by oral presentations in the evaluation

- Christiane ALBA-SIMIONESCO (Directrice LLB)
- Brigitte BEUNEU
- Annie BRULET
- Sylvain DESERT
- Grégory CHABOUSSANT
- Arsen GOUKASSOV
- Stéphane LONGEVILLE
- Marie-Hélène MATHON
- Alain MENELLE
- Jean-Marc ZANOTTI

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¹ Persons which have also been members of the 1st IC are marked with an *.

² CAP 2010 comprises the instrument renovation and upgrade in the period of 2005 to 2010.

³ CAP 2015 comprises the proposal for the continuation of CAP 2010, i.e. the instrument renovation and upgrade for a period ending in 2015.

The instrument suite of LLB

The instrument suite at LLB is perfectly adapted to the particular interest and strength of the French neutron community. Almost⁴ all instruments are competitive with those at the neutron sources of Table 1. Some of them are among the very best - like triple axis spectrometers and small angle cameras.

Triple axis spectrometry

- Thermal 1T, 2T,
- Cold 4F1, 4F2,

Quasielastic spectroscopy

- MIBEMOL, MUSES

Wide angle diffraction

- Thermal, powder 3T2, single crystal 6T2, materials 6T1
- Cold, powder G4.1 G6.1 (high pressure), materials G5.2
- Hot, liquids 7C2, single crystal 5C1,5C2

Large scale structures

- Reflectometers PRISM, EROS
- Small angle cameras PACE, PAXY, PAXE
- Very small angle camera TPA

Conditions for a healthy instrument development and renewal programme

The capital costs to build a new scattering instrument at a decent neutron source like LLB amounts to about 3 - 4 M€ The scientific life time of an instrument extends to a maximum of 20 years. As today the LLB operates a suite of 21 instruments in its general user programme. This results in an annual investment need of 3 - 4 M€ for the renewal and upgrade of its instrumentation. This has already been stated in the minutes of the instrument evaluation from November 2007. The current budget for instrumentation is far away from that. On medium term this discrepancy will have severe consequences with respect to the actual outstanding scientific output and strong international reputation of the LLB. The IC therefore strongly reminds the stake holders CEA and CNRS to do their best to close this gap in due time. The IC also asks the direction and the scientists at LLB to be imaginative in finding additional funds like regional funds, support by the European Framework Program. This has been done successfully in the past with regional funds from Aquitaine, Bretagne, Framework Program 5 & 6 & 7 of the EC. Recent evolution of funding for science in France opens the way for new opportunities which will replace historical funding which are decreasing: EQUIPEX of "grand emprunt national", ANR in instrumentation, Swedish contract for future ESS.

Further the minimum personnel needed to operate the scientific instruments of a neutron source with an extended user program amounts to 5 persons per instrument (2 scientists + 1 technician directly attached to the instrument, 2 persons per instrument for general services like sample environment, IT, directors, secretaries, electronics, detectors, neutron optics ...). With 21 instruments for the general user service this number should be around 105 persons; however the current personnel (77 permanent researchers and technicians plus 25 post-docs and PhD students) is quite low to fit with the minimum needs.

The LLB in the landscape of the European neutron sources

Although being a national source dominantly serving the needs of the French science community LLB is an important part of the European landscape of five national neutron sources, all with a considerable international user community and international impact. These five national sources are the indispensable condition for the effective use of the European Institute Laue Langevin at Grenoble

- and with a longer perspective for the successful taking into operation of the European Spallation Source at Lund. By means of this suite of national and international neutron sources the Neutron Community in Europe is by far the leading community - and will remain when compared to the American and Pacific regions. The share of these centres in the education of future specialists in the different fields of neutron scattering is unmatched, and relies on modern instrumentation. Table 1 displays the key figures of the European neutron sources and Figs. 1 & 2 give an impression of the wide spread usage of the LLB. France, Germany, Great Britain and Switzerland, each having a decent national neutron source are also the countries contributing most to and having the biggest feed back from the international source HFR at ILL.

With respect to the complementarities of the instrumentation at LLB and at a future ESS the IC view is as follows:

- ⇒ The predominant task of the instrumentation of LLB is to serve the needs of the French neutron community, its particular interests and fields of expertise.
- ⇒ As a consequence, there will be instruments at LLB and at a future ESS of similar momentum, energy (Q,co) range, resolution ... This competition is an absolute prerequisite of a healthy development of the French utilisation of ESS: i) French scientist will be better prepared to use those instruments at ESS, ii) also instrumentation needs competition to become excellent.
- ⇒ In fields like hot neutrons, strain measurements, radiography and tomography, production of (radio)isotopes, particular sample environment or ultra cold neutrons strong continuous neutron sources like ORPHEE might stay ahead of a long pulse spallation source.

Table: Neutron Sources in Europe with an international impact. Numbers relate to 2009 or 2010. By its nature some of the figures are rough estimates and not directly comparable. This holds in particular for the personnel. While all the institutions are open to European and even international access, the national facilities are funded by national and even regional resources.

| Source | Operational since | Thermal power, | Nominal integrated flux [m-V] | Nominal peak flux [m-V] | Nominal operation time/a | No. of user instruments | Scientific users/a ¹ | Personnel Operation + scientific usage ² | Estimated overall budget p.a. ³ |
|--------------------------|-----------------------------|-----------------------------|-------------------------------|-------------------------|--------------------------|---|---------------------------------|---|--|
| HFR, ILL | 1971 | Nominal 58 MW, actual 51 MW | $1,3 \cdot 10^{19}$ | | 200 d/a | 27+ 10 CRG | 1400 | 490 ind. 30 thesis students full time equ. | 83 M€ stand alone budget |
| FRM II, TUM & JCNSS GKSS | 2005 | 20 MW | $8 \cdot 10^{18}$ | | 240 d/a | 23 operational 7 under construction + positrons + irradiations facilities | 1000 | 230 actual 320 future | actual 33 M€ future 55 M€ stand alone budget |
| ORPHEE, LLB, CEAS CNRS | 1981 | 14 MW | $3 \cdot 10^{14}$ | | 180-200d/a | 21 external use 3 internal use | 600 | 59 reactor 77 scientific use permanent 25 students + post doc | 10.8+ 5 M€ reactor 10 M€ LLB |
| BER II, HZB | 1973 1993 upgrade | 10 MW | $1,2 \cdot 10^{10}$ | | 220 d/a | 16 operational 3 restricted access | 400 | | > 25 M€ |
| SINQ, PSI | 1996 | 1 MW at target | $1,5 \cdot 10^{10}$ | | 210d/a | 13 external use 4 internal/ restricted 4 x Muons | 945 visits by 465 persons | 120 ind. postdocs excl. PhD, muons, p-accelerator) | 30-40 M€ realistic estimate |
| ISIS, STFC Rutherford | 1985 Target 1 2009 Target 2 | 200 MA- | | $4,5 \cdot 10^{19}$ | 180 d/a | 27 | 1500 | 340 | 55 M€ stand alone budget |

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¹ No. of scientific users comprises the no of scientist visits to perform an experiment. If the same person comes two times a year for two different experiments it is counted twice.

² The no. of personnel for the operation of the facility and its scientific service is particular difficult to compare. For instant the figure for ILL includes the security personnel, but ISIS and FRM II do not. The operation of Orphee heavily relies on services from CEA-Saclay. Here only the personnel for the operation of Orphee is quoted.

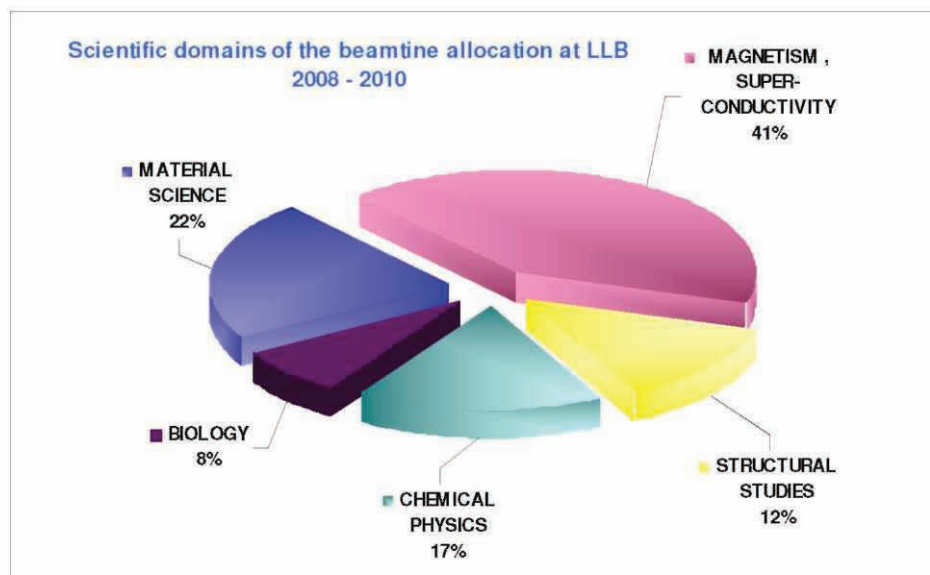


Fig. 1: Allocated beam times at LLB for the years 2008 – 2010, according to science fields.

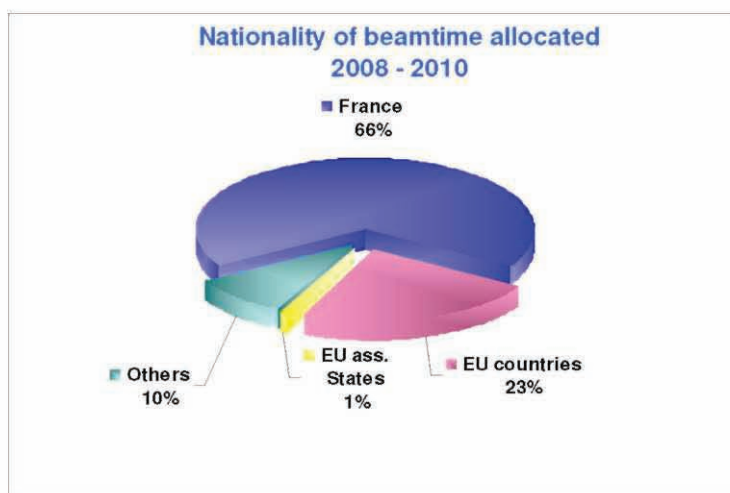


Fig. 2: Allocated beam time at LLB according to countries over the years 2008 -2010

Achievements by CAP 2010

The structural and organisational measure, namely to create groups of personal dedicated to the upgrade of existing and the construction of new instruments has been very successful. Time schedules and budget plans with precisely allocated budgets and aims have been established and are closely followed by both, the direction and the staff. Further the institute has focused on a well defined number of projects and has started to shut down less performing instruments.

The instruments PAPYRUS and G5.6 have been closed in order to create the space for PA20

MICRO (G6.1)

Construction finished, its main achievement is the detector made out of 16 position sensitive tubes with 12 bar ^3He , high pressure guarantees for high counting efficiency also at small wavelength, detector tubes about 1 m long are horizontally oriented, now in commissioning phase, first measurements show perfect separation of Debye-Scherrer cones, routine operation around March 2011. This instrument will be dedicated to the very high pressure program LLB is widely renowned for (The LLB keeps the record for highest pressures for neutron scattering).

VIP (very intense polarized powder diffractometer)

Vertically oriented position sensitive detector tubes, completely new construction almost finished. A new type of single crystal polarized diffractometer equipped with a large PSD covering 1 steradian on the diffraction sphere. It is in commissioning stage but first experiments show that it boosts the data acquisition rate by an order of magnitude. After replacement of its Heussler monochromator in 2012 it is expected to be the most efficient polarized neutron diffractometer in the world

TPA (ultra small angle scattering)

This is a multi pin hole instrument. The commissioning is on the way to be finished and routine operation has been started. This instrument completes the small angle capacities of LLB to very small scattering vectors - i.e. large structures up to the μm range. This instrument is judged as the best possible compromise between intensity and access to very small scattering vectors in the range of 10^{-4} - 10^{-3} \AA^{-1} . Further it stands out with its inovative concept of multi pin holes, its exceptionally small length and last not least its relatively low investment budget.

7C2 (liquid diffractometer at hot neutron source)

Following the advice of the previous IC the multi-strip-detector project has been abandoned. Instead a multi detector composed of 256 position sensitive tubes with 30 bar ^3He pressure has been purchased. The 30 bar pressure guarantees for excellent neutron detection at wavelength as short as 0.5 \AA . Despite the shortage of ^3He for neutron detectors the 256 detectors have been delivered in December 2009 and the missing 2nd half was expected towards the end of 2010. The instrument will be commissioned beginning 2012.

In view of the limited resources in capital and personnel available for the renewal of the instrument the IC considers the achievements of CAP 2010 as excellent.

Considerable progress in design, purchasing orders or prototype construction has been achieved for the instruments

- PA20 (small angle)
- 6T1 (strain and texture)
- FA# (cold hybrid-TOF)
- EROS-II (reflectometer)
- MULTIMUSES (resonant spin echo)

They all are at the heart of CAP 2015 and will be reported in the following section.

Evaluation of CAP 2015

A detailed multi annual budget and time schedule for the CAP 2015 instrument suite has been presented. The IC judges this as a very realistic and feasible base for the realisation for CAP 2015, provided the announced investments are available in due time.

PA20, PAXY (small angle)

Traditionally the LLB operates flag ship instrumentation for the detection of large structures by small angle scattering and reflectometry. Partly this has been initiated by the French community in material science, solid state physics, soft matter and biophysics/biochemistry, all of which are very competitive on the international scale. To a certain extent this instrumentation has also re-enforced that community. The progress achieved in the modernisation of the suite of small angle instruments at LLB is impressive. The very small angle scattering camera TPA received its first users, two multitube detectors of an active area of $64 \times 64 \text{ cm}^2$ have been ordered at ILL, one foreseen for the new PA20 and one to upgrade PAXY. Delivery is foreseen for 2012. Impressive progress in the design of the new $2 \times 20 \text{ m}$ SANS PA20 has been presented. It will benefit from new focussing lenses, optimised polarisation, greater detector area with higher resolution and greater versatility in Q-range. With the completion of CAP 2015 the LLB will certainly maintain and probably even strengthen its competitiveness in the field of small angle scattering.

EROS-II (reflectometer)

Two reflectometers are in service at LLB. PRISM serving the magnetic community with its polarization analysis and EROS the soft matter community. The closure of MIBEMOL and installation of FA# at a new dedicated neutron guide opens the possibility to move EROS II to the former MIBEMOL position giving access to significantly larger primary neutron intensity. The IC strongly endorses this planning, also considering a timely closure of MIBEMOL (before accomplishment of FA#).

Super 6T1 (strain and texture)

Stress and texture are properties of prime importance for material sciences. Its measurement with neutrons will be combined in the new Super 6T1, replacing 6T1 and keeping G5.2 for only very large pieces. Central for the upgraded 6T1 is a DENEX 2 dim. detector making possible the combined measurement of strains (stresses) and textures on the same instrument and same sample. Gain factors in intensity exceeding 10 are expected. Both, the 2-dim. multidetector and the combination of strain/stress measurements with those of texture will give to the French materials science community an instrument which is fully competitive with the present upgrades of similar instruments at ILL, FRM II and ISIS.

FA# (cold hybrid-TOF)

Together with IN5 from ILL MIBEMOL has been the leading cold time-of-flight spectrometer in the

80ths and 90ths. New cold time-of-flight instruments like IN5new at ILL and TOFTOF at FRM II have made MIBEMOL obsolete to a large extent. *The French magnetic excitation, soft matter and biophysics community urgently needs a competitive instrument for (polarized) quasielastic and inelastic scattering up to 15 meV over a large Q-range with very low background.* To that purpose an instrument project based on a focussing monochromator, Fermi-chopper and time-of-flight analysis in the secondary spectrometer - a so-called hybrid-tof

- has been launched in the course of CAP 2010. To enhance the intensity at the sample and/or detector position the instrument combines time focussing with optical focussing elements. A first version of this concept has been realized with FOCUS at PSI. FA# - as this project is called at LLB - has the potential to conquer the market of comparable instrumentation and to be world leading in intensity, background and versatility. In view of the importance and uniqueness of FA# for the French community - together with MULTIMUSES it will be the only instrument for quasielastic scattering at LLB - the IC strongly recommends accelerating the design phase. Otherwise the ambitious time schedule with an FA# operational in 2016 will be in danger. A basic decision (i) whether, (ii) how and (iii) for whom, the instrument shall provide polarization analysis should be taken now within the design phase. The growing trend for the study of single-crystalline samples on TOF spectrometers should also be taken into account in the design. The presented budget plan is judged as being tight, but still feasible. There remains a financial risk related to the ^3He shortage.

MULTIMUSES (resonant spin echo with multidetector)

MUSES is the existing spin echo spectrometer at LLB for quasielastic scattering mainly applied for soft matter including biomaterials. It measures in the time frame (intermediate scattering function), is of the resonance spin echo type and has a time resolution in the range of 1 ps - 20 ns. MUSES in its present configuration has a single detector and is therefore intensity limited in its applications. To remain competitive with conventional spin echo spectrometers like those installed at ILL and FRM II MUSES *has to be equipped* with a multi detector secondary spectrometer, i. e. MULTIMUSES. Such a wide angle multi detector for NRSE does not yet exist and its development is a real technical challenge. First very promising design options have been presented. However none of the technical challenges is so far really solved. FRM II operates with RESEDA an instrument very similar to MUSES. Also FRM II is in the course of developing a multi detector design. The IC strongly urges the MULTIMUSES working group for an intense exchange with the Munich group (and vice versa!). MULTIMUSES has a clear chance to become unique and leading in its field, this in particular due to the very intense cold neutron guide and its excellent primary polarisation. Spin manipulation will be one of the innovative techniques used for ESS instrumentation. MULTIMUSES is an excellent training field for this technology.

Both, time of flight techniques and spin coding are techniques which will be used extensively for the advanced instrumentation of the ESS. So, the realisation of FA# and MULTIMUSES is the ideal playground to considerably strengthening the French ability to compete for instrumentations projects at the ESS.

7C2 (liquid diffractometer at hot neutron source)

This diffractometer for the structure analysis of liquids and amorphous materials will largely profit from the excellent detector renewal within CAP 2010. The IC recommends including an

enlargement of the monochromator in the program of CAP 2015. This would increase the intensity measurable in the detectors once again, probably without compromising on the resolution of the diffractometer.

NEPTUNE (neutron polarisation for all instruments)

Polarisation of incident neutrons and subsequent analysis of the scattered neutrons is an absolute necessity to tackle the questions of modern solid states physics. A few examples: correlated electron systems, high T_c-superconductors, quantum phase transitions, multiferroics, ... But also soft matter physics needs polarisation analysis, i.e. to properly separate coherent from incoherent scattering. Some of the instruments at LLB are already equipped with polarizing supermirrors. However at LLB Heusler monochromators and broad band polarisers on the base of polarized ³He are missing. Heusler single crystals are the best choice for polarizing the incident beam of triple axis spectrometers. The suite of triple axis spectrometers would considerably profit from such an investment. Only ³He absorption filter types of polarizer or analyzer makes full polarisation analysis available for time-of-flight instruments and small angle scattering. This is why ³He polarization filters are important for LLB. They can be operated in two alternative ways, either by MEOP or SEOP. MEOP has the advantage that the technology is completely available for polarisation degrees of 75% and key ready facilities can be purchased for 1 - 2 Mill. € Its inherent disadvantage is the decay of the polarisation over some 100 hours. SEOP has the advantage that the polarisation of the spin filter is constant over time, the disadvantage that the technology for reliable and reproducible 75% polarisation is not yet available and each instrument needs its own polarisation equipment. Whereas the ³He polarisation for a single instrument might be cheaper with SEOP, both methods need about the same investment in case a suite of instrumentation is considered. And in particular both methods need additional personnel - 1 scientist, 1 technician - dedicated solely to the task of ³He polarisation. LLB opts for the SEOP technology. In view of the urgent scientific need for polarization analysis the IC strongly recommends to realize NEPTUNE (SEOP + Heusler). Given the limited capital as well as manpower resources at LLB external funding should be asked for.

Only the above mentioned instruments and project have been evaluated during the meeting. It is well understood, that CAP 2010 & 2015 comprise also the modernisation of further instrumentation as for instance the triple axis spectrometers and in particular the extension of the support for experiments like sample environment.

Executive Summary

⇒ The IC considers the structural and organisational measures for CAP 2010 & 2015, namely to create groups of personal dedicated to the upgrade of existing and the construction of new instruments as appropriate and very successful.

⇒ In view of the limited resources in capital and personnel available for the renewal of the instrument the IC considers the achievements of CAP 2010 as excellent.

⇒ The instruments considered for CAP 2015 perfectly match with the urgent needs of the French neutron research community.

⇒ The projects for small angle scattering, reflectometry and materials science are in good progress and essential all technological challenges have been solved.

⇒ The projects MULTIMUES and especially FA# urgently need additional resources for finishing the design phase and for the required accompanying feasibility studies. The main technological tasks are not yet solved. This is in contrast to the importance of these instruments for the LLB. The LLB risks losing its expertise in the study of the dynamics of magnetic fluctuations, soft matter and biological materials.

⇒ The IC judges the multi annual budget and time schedule for the CAP 2015 instrument as a realistic and feasible base for the realisation for CAP 2015, provided the announced investments and allocated personnel are available in due time.

⇒ In view of both, the limited capital as well as men power resources at LLB and the urgent scientific need for polarisation analysis the IC strongly recommends to realize NEPTUNE (SEOP + Heusler). It is an ideal project, for which external funding should be asked for.

⇒ From a more general point of view the IC wants to stress that in order to keep the LLB at its present level of world renowned excellence, to fully meet the needs of the French user community and to be prepared for the scientific and technological adventure of the European Spallation Source a continuous high level of re-investment and a minimum of five persons per instrument are required.

Agreed upon by all members of the committee, in January 2011

Winfried Petry
(Chairman)