# REPORT ON
# WORKSHOP ON
# DISORDERED MATERIALS
# LONG WAVELENGTH TARGET STATION
# SPALLATION NEUTRON SOURCE
University of Delaware – April 28-29, 2000

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## PREAMBLE

Below is a report on the Workshop on “Liquids, Glasses and Disordered Materials” held at the University of Delaware, April 28-29, 2000. The workshop was one of four topical workshops held prior to the Spallation Neutron Source (SNS) Users Meeting held in Washington, DC May 22-24, 2000. The workshop was organized jointly by Henry R. Glyde, University of Delaware and Chun Loong, Argonne National Laboratory.

The purpose of the topical workshop was to identify the scientific challenges in the field of Disordered Materials and the opportunities to address these challenges opened by the Long Wavelength Target Station (LWTS) and its associated neutron scattering instruments. A second purpose was to introduce the LWTS and instruments to several major players in the field who do not normally use neutron scattering.

The report consists of (1) The Workshop Program, (2) A list of participants, (3) The Scientific Case for the LWTS, i.e. for structure determination at long wavelength and for determination of low energy excitations in the field of disordered materials and (4) A first cut at translating the scientific case into specific instrumentation needs.

## 1. PROGRAM

**WORKSHOP ON**
**DISORDERED MATERIALS**
**LONG WAVELENGTH TARGET STATION**
**SPALLATION NEUTRON SOURCE**
**University of Delaware — April 28-29, 2000**

***Friday, April 28, 2000***

| | | |
|---|---|---|
| 8:15 | | BREAKFAST, Rm. 206 Trabant Center |
| 9:00 | Henry Glyde | Welcome, Introduction and Purpose of Workshop |
| 9:10 | Lee Magid | SNS-LWTS – Developing the LWTS science case and the full proposal |
| 9:25 | Guebre Tessema | LWTS – Role of National Science Foundation |
| 9:40 | Javier Bermejo | Dynamics of structurally disordered matter: Challenges for next-generation cold neutron instrumentation. |
| 10:10 | Don Kearley | Cold neutrons and numerical methods. |
| 10:40 | | COFFEE |
| 11:00 | Austen Angell | The amorphous state equivalent of crystallization: new glass types by first order transition from liquids and crystals. |
| 11:30 | Dennis Klug | Neutron scattering studies of the structure and dynamics of amorphous ice and related materials. |
| 12:00 | | LUNCH – Rm. 206 Trabant Center |
| 1:30 | Jack Carpenter<br>Ken Herwig | The LWTS and Instrument Selection and Design |
| 2:30 | Herbert Strauss | Neutron spectroscopy of hydrogen gas dissolved in ice. |
| 3:00 | Susan Kauzlarich | Synthesis and Characterization of Group IV Semiconductor Nanoclusters |
| 3:30 | Shenda Baker | Examination of polymer dynamics under shear flow by neutron reflectivity. |
| 4:30 | | Discussion – New Netherland Rm/ Embassy Suites Hotel (Jack Carpenter, Ken Herwig, Chun Loong, Paul Sokol, Herbert Strauss) |

| | | |
|---|---|---|
| 5:45 | | RECEPTION – Atrium/Embassy Suites Hotel |
| 7:00 | | DINNER – Fort Casmir Rm/Embassy Suites Hotel |

***Saturday, April 29, 2000***

| | | |
|---|---|---|
| 8:15 | | BREAKFAST – Rm. 206 Trabant Center |
| 9:00 | Marie-Louise Saboungi | Neutrons and soft matter: Lithium conducting polymers. |
| 9:30 | Lennox Iton | Molecules in zeolites. |
| 10:00 | Henry Glyde | Disordered quantum systems. |
| 10:30 | | COFFEE |
| 11:00 | | Discussion and Wrap-up (David Price, Michael Klein, Chun Loong, Ken Herwig and Henry Glyde) |
| 12:30 | | LUNCH and CLOSING REMARKS |

## 2. LWTS WORKSHOP PARTICIPANTS


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## 3. THE SCIENCE CASE: SCIENTIFIC OPPORTUNITIES OPENED BY LWTS

Below we list scientific opportunities and challenges identified at the workshop that can be addressed at the LWTS and the associated neutron scattering instruments. These are listed under six topics. The topics have no specific role or meaning and are simply convenient categories under which the points made at the workshop can be collected.

### A. Liquids and Glasses

**i)** A broad challenge is to reveal the nature of liquids and glasses by determining their excitation energies with high precision over a wide energy ($\omega$) range. This demands high energy resolution

$\delta\omega \leq 5\text{-}10\ \mu\text{eV}$ over a range $0 \leq \omega \leq 10$ meV

The goal is to understand the dynamics and thermodynamics of these systems based on precise knowledge of excitation energies. Systematic studies as function of bulk variables such as temperature, pressure and composition are needed. This requires regular access to a dedicated instrument with high energy resolution and high beam intensity. Some specific issues are: understanding "Boson" peaks in $C_V$, shear modulus in liquids at higher Q values, transitions from free rotation to glassy regime.

**ii)** It was found important to explore dynamics to higher Q values ($Q \geq 2.2$ Å$^{-1}$). Aim is to cover continuously the Q region in which collective excitations are observed ($Q \leq 2$ Å$^{-1}$ typically) to higher Q values (up to $Q \cong 5\text{-}10$ Å$^{-1}$) where single atom (molecule) excitations are observed. Most existing "time of flight" instruments go up to $Q \cong 2$ Å$^{-1}$ only. Essentially, want to cover a wide Q range of the dynamics. Also seek good Q resolution (ÅQ $\leq 0.03$ Å$^{-1}$ mentioned).

**iii)** It would be a great advantage to separate coherent from incoherent scattering. Essentially, in many materials (systems) there is large incoherent scattering which masks the coherent structure and dynamics. The classic example is liquid $H_2$. Need spin-polarized beam and polarization-analysis capability for opportunities noted above in i) and ii) above as for magnetic systems.

**iv)** Annealing of glasses: Goal is to do "real time" studies on structure and dynamics of glasses as they anneal and age. Essentially, need high beam intensity, rapid data collection for this.

## B. Chemical Reactions, Catalysis

**i)** One aim is to study diffusion and tunneling directly as a means of investigating chemical reactions.

**ii)** Other topics are real time studies of composition change (reactions in progress) as a function of environment and impurities, surfaces and other agents.

**iii)** Investigate structure and dynamics of molecules, defects, and impurities on surfaces.

**iv)** Ability to study small samples and small changes in composition is a great advantage here.

**vi)** A flexible and versatile sample environment is essential to these studies. The neutron instrument should provide the capability of in-situ measurements under conditions simulating those within a chemical reactor.

## C. Membranes, Proteins

This topic overlaps with the "soft materials and polymers" group but is of clear interest to several people at the present workshop. Topics identified were:

**i)** Structure of proteins, membranes and macromolecules.

**ii)** Issue of concentration of constituents, currently need to push this up to 10% to get a signal.

**iii)** Isotopic substitution of H/D to reveal role of specific components of large molecules.

**iv)** Study "things" on membranes, e.g. head group changes, impurities, water.

**v)** Dynamics of lipids and proteins, time scales of motion.

These topics need:

— diffractometer for large length scale structures, high intensity and low background
— high energy resolution spectrometers for measurements of low-energy motions

— high beam intensity for small samples, high sensitivity for small changes reflectometry.

**D. Nanostructures**

The important role of neutrons in characterizing the structure, composition, dimensionality and size of nanostructured materials was discussed. This Included replicated materials, powders, structure of porous (especially nanoporous) media and other absorbing and disordering media. Needed here is high resolution SANS at low Q. Given the perceived importance of nanostrcutures, this could be an important user field.

**E. Systems in Porous Media**

The properties of liquids, classical and quantum liquids, in porous media is a field of great current interest. Of special interest is the impact of disorder and confinement on the characteristic excitations and phases of liquid or crystalline systems. For example are there “Bose Glass” phases or new excitations at low energy that destroy order (e.g. superfluidity) in the presence of disorder? Accurate measurement of the change in the structure and of the excitations from the bulk/uniform case to the confined/ disordered case is needed.

Needed here is high Q resolution SANS and high energy resolution spectrometers. High beam intensity to get high statistical precision is also a great advantage when searching for small, subtle changes introduced by disorder.

**F. Films and Substrates**

A goal is to measure surface roughness and characterize other properties of surfaces. The properties of impurities and films on these surfaces is a topic of much interest. Properties include structure and phases of films, growth and aging action on surfaces, excitations in the films (3D and 2D), role of impurities in structure and dynamics, surface diffusion, mechanical and other properties.

The same instrumentation as needed for (E) applies here. Of special interest is low Q (L = 40, 60 m) SANS with large Q range and low energy, high energy resolution spectrometers. Capability to study smaller samples and lower impurity concentration is important (requires high intensity).

## 4. INSTRUMENTATION REQUIREMENTS

Some specific comments on instruments by the scientific speakers and participants were:

**i)** Desire for polarized neutrons and polarization analysis routinely to do liquid dynamics separating coherent from incoherent components.

**ii)** Reflectivity for study of surfaces is most important – also with polarized neutrons.

**iii)** A goal is to measure low energy excitations of large systems (e.g. collective excitations in membranes). Need high energy resolution over a wide energy range. Need intensity at low Q.

**iv)** In addition to iii) above, want to determine excitations over a wide Q range, in the range $2 \leq Q \leq 4$ Å$^{-1}$ as well as lower Q as can do on MARI. However, want $\delta\omega \leq 10$ μeV. Measure dispersion beyond first Brillouuin zone, density of states $g(\omega)$ at higher Q to average out incoherent effects, to separate different motions.

**v)** Quasi elastic scattering is important – diffusion, tunneling.

**vi)** Want to go to smaller samples, observe impact of small changes in composition in samples. This requires high beam intensity, high statistical precision.

**vii)** Real time studies of systems.

## 5. THE CASE FOR THE LWTS: GENERAL COMMENTS

— ***based on discussions following the workshop and visits to ISIS.***

**A)** In the "Blue Book" (RL-77-064/C) "A pulsed neutron facility for Condensed Matter" edited by L.W.C. Hobbs, G.H. Rees and G.C. Sterling, (June 1977), there is no mention of low energy neutrons. The "Blue Book" is the scientific case document for ISIS but it does not include any discussion of low energy neutrons to study low energy excitations or large structures. That was not foreseen at the time but low energy neutrons have become a major part if not the major part of the program (e.g. IRIS, OSIRIS). Similarly, for the LWTS it is very difficult to look ahead 20 years and articulate precisely the scientific opportunities opened by the LWTS. However, there are clear opportunities now (five years ahead of the LWTS) and the trend is rapidly and clearly in that direction — both in science and in source and instrument capability. A case for the LWTS can be made on the broad trend.

**B)** A case for the LWTS can be made on the total number and variety of instruments. That is, SNS will be the major neutron facility in the USA for some time. A major facility, such as ILL, has approximately 45 instruments. The second target makes this number of instruments possible. The second target particularly makes it possible to build a wide spectrum of instruments covering a wide energy range that can be optimized to take advantage of each target. The HPTS and LWTS together enormously improve the instrument capability of the whole facility in variety and performance of each instrument.

**C)** A case for the LWTS can be made on "ownership" of instruments by the scientific community. That is, the NSF funded portion could be regarded as "owned" by the University community. They would have to and want to be directly involved in developing this suite of instruments to its optimum level and take responsibility for its performance. This would be a major step in getting the community directly involved in instrument development and "ownership" in the neutron field as has been achieved in a stepwise way at synchrotron sources.

**D)** Affiliate Institutions. There could be a set of affiliate universities who are affiliated with JINS (UT) and in this way supportive of the LWTS proposal. That is, the proposal comes from JINS or UT but there are "affiliated" universities to JINS that endorse the proposal and add some national representation to the proposal.

**E)** There could be a large number of "mini" biosketches of scientists across the nation who support the SNS attached to the proposal. Each "bio" could in a line or two be connected to a field or instrument. This would demonstrate support in the scientific community and show that it comes from the community.

**F)** The LWTS proposal does not compete with awards to individuals.

- it is a major facility in Materials Science like a telescope or particle physics facility.
- NSF seeks new funds for this CMMS facility as it does for other major facilities. Funds do not come out of existing programs.
- These new funds provide instruments. If the LWTS were not funded as a single new major facility, groups would seek funds for individual instruments. Funded in this way, the instruments would come out of existing programs.

**G)** Corporations — would some presence in the proposal improve funding prospects?