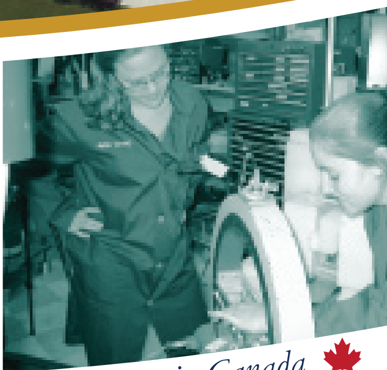
CINS

Canadian Institute for Neutron Scattering

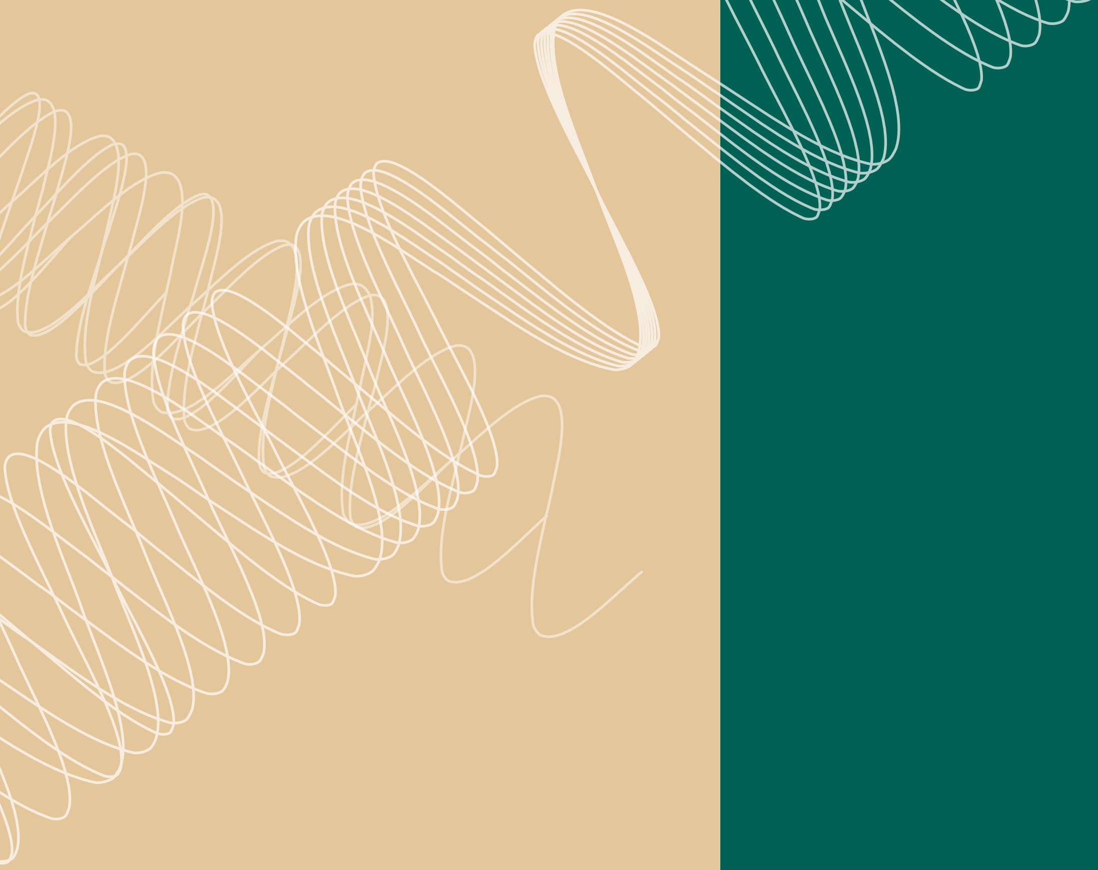
*Plan to 2050*

# CINS

## CANADIAN INSTITUTE FOR NEUTRON SCATTERING



*Planning to 2050 for Materials Research with Neutron Beams in Canada*



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CINS

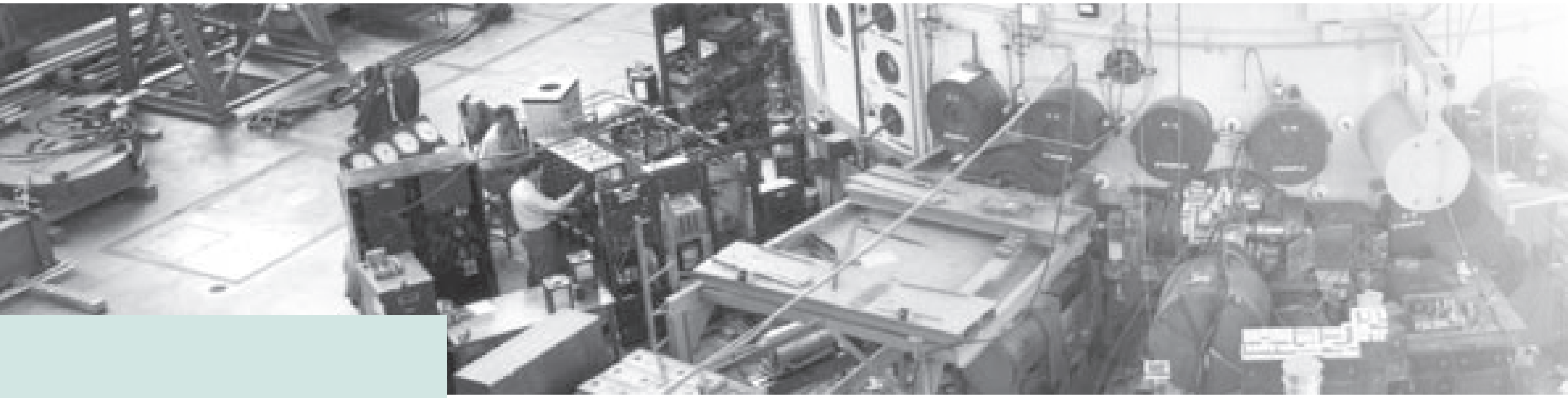
CANADIAN INSTITUTE FOR
NEUTRON SCATTERING

# Planning to 2050 for Materials Research with Neutron Beams in Canada

Canadian scientists describe the importance of neutron beam
research and recommend how to maximize future impact

# CONTENTS

The NRX reactor (pictured here) was the most powerful neutron source in the world when it was constructed in the 1940s. It enabled Canadian scientists to pioneer the field of neutron scattering, and launched the modern nuclear medicine industry, making isotopes: two fields in which Canada has enjoyed over 50 years of excellence.



## THE CANADIAN INSTITUTE FOR NEUTRON SCATTERING

The Canadian scientific community of neutron beam users is organized within the Canadian Institute for Neutron Scattering (CINS). This organization, incorporated in 1989, now has more than 400 members, including about 300 Canadian academics with other members from industry, government laboratories and foreign institutions. Canadian neutron scattering researchers and students are found in over 50 university departments, distributed in more than 20 universities, which are spread across every province of the nation. There are currently 15 institutional members who pay fees that are applied to encourage scientific research using neutron beams, and to ensure access of the Canadian neutron scattering community to competitive research facilities.

## CINS CONTRIBUTORS TO THIS PLAN

At the 2006 Annual General Meeting of CINS (October 13-15, at The University of Western Ontario), a workshop was included to consider long-range planning for neutron beam research requirements to a time horizon of 2050. The workshop anticipated a possible proposal for a new Canadian Neutron Centre, and recognized that this was an appropriate occasion to define the needs of the Canadian community of neutron beam users. A subcommittee was appointed to lead the first draft of the following Plan.

At the 2007 Annual General Meeting (October 26-27, at Queen's University), the draft was presented. Working groups reviewed the text for their respective communities of interest, and then recommended priorities for neutron beam instruments that would best serve their requirements. A subcommittee was established to finalize the Plan.

## CINS Subcommittee for the First Draft

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|---|---|
| John Greedan (Chair) | CINS VP, McMaster University, Chemistry |
| Carl Adams | St. Francis Xavier University, Physics |
| Lynann Clapham | Queen's University, Materials Science |
| Thad Harroun | Brock University, Biophysics |
| John Root | NRC, Canadian Neutron Beam Centre |

## CINS Subcommittee to Finalize the Plan

| | |
|---|---|
| Dominic Ryan (Chair) | CINS President, McGill University, Physics |
| Mark Daymond | CINS VP, Queen's, Materials Engineering |
| John Root | NRC, Canadian Neutron Beam Centre |

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October 13-15, 2006

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October 26-27, 2007

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Scientists employ a great number of probes to aid them in understanding, characterizing and improving materials. However neutron beams are a particularly important and irreplaceable part of the 'scientific toolkit'. The importance of neutron scattering methods for materials research is a consequence of the special way that neutrons interact with matter.

# 1. OVERVIEW

## 1.1 The importance of materials research

By improving our understanding of the way that materials work, we can generate positive impacts on every aspect of our lives, for one simple reason. Everything is made of materials: people, food, energy technologies, the Earth and our environment, infrastructures to transport water and goods, buildings, computers, airplanes, cars, and devices for medicine, communication, entertainment and everything else.

Materials are pervasive and we may be unaware of their presence, let alone their evolution. However, when a fundamental discovery is made about materials, technologies are revolutionized, and the effects are felt across society. A little thought provides examples to illustrate how the advancement of materials has changed our human experience of the world.

The advent of the steam-engine made possible the rapid expansion of North America, and enabled people to travel so quickly across longitudes that 'local time' could no longer be measured practically with reference to 'noon' as the local solar zenith. Canadian Sir Sandford Fleming defined time zones to enable orderly scheduling of the trains, and 'jet lag' was born! Today, we take this concept completely for granted, but it would never have arisen if materials and manufacturing methods had not been developed to withstand the temperatures and pressures for steam-powered locomotion, or to support trains on thousands of kilometres of steel rails. Materials development was fundamental to this, profound change in the human experience.

Prior to the advent of the transistor, vacuum tubes were required to control large currents from small electrical signals - the basis of electronic amplification, and electronic logic components. As marvellous as the idea of an electronic computing machine might have been in the mid-20th century, with vacuum tubes providing the fundamental logical unit, the vision of that time was towards vast computers. However, a fundamental shift occurred with the development of the transistor. This solid-state device provided the same logical function, electronically, as did the vacuum tube, but in a package that could be made exquisitely small. Mastery of the production of high-purity silicon, the controlled addition of specific atoms, and an underlying knowledge of electronics in the solid state (all 'materials research') were necessary steps towards the new technology. The human experience of computers today is not some imposing structure of glass, metal and electrical power, but a handheld package that contains thousands of songs, a personalized movie system in the seatback in front of you aboard a plane, a global-positioning, speaking, adaptive navigation system in your car, or an automatic cash dispenser that gives you access to your own bank account from many places in the world. We hardly realize it, but our human experience has shifted tremendously from the results of materials research and development, which started with the transistor and led to computers in our homes and access to a worldwide web of information exchange. People around the world are affected. Doors are opened for greater understanding, sharing of cultures, and engaging in a global marketplace.

In this document, references to 'materials' should be understood to include structural materials (metals, alloys, ceramics, or composites, which are used to build machines and infrastructures), functional materials (nanostructures that store gases, help chemical reactions to occur with less energy, or filter toxins from air and water; and crystal structures that change shape or magnetic alignments, which can be exploited in batteries, information storage or other useful applications), and 'soft' materials (plastics, membranes, proteins, gels, or complex fluids like milk or blood).
Similarly, references to 'Materials research' should be understood to encompass a full range of scientific disciplines, a few illustrations being:

- Condensed-matter physicists are trying to track down some of the challenging phenomena at the frontiers of knowledge, and which could introduce a new technological revolution, such as high-temperature superconductivity and other highly correlated electronic systems.
- Structural chemists are tuning the performance of materials for energy management, such as hydrogen-storage or lithium-ion batteries.
- Earth scientists acquire a firm understanding of the temperature and pressure responses of minerals, from which conclusions can be made about geological history and the condition of planet Earth.
- Materials engineers seek to understand what is really happening when we manufacture components at high or low temperatures, the reasons why some materials fail prematurely and how to make stronger, tougher, more reliable materials, cost effectively.
- Polymer chemists develop thin film coatings that make medical implants safe and reliable, new organic electronics, membranes for fuel cells, and much more.
- Biophysicists investigate the nanostructures that occur naturally in cells and tissues, to provide fundamental clues that may provide more accurate directions for research on life processes, diseases and therapies, than is possible from large-scale clinical studies alone.

The importance of materials research is that materials underpin every aspect of the human experience, and that discoveries of new materials, or refinements of existing materials constitute the essential building blocks of advancement in technology, industry and society.

## 1.2 The importance of neutron scattering for materials research

Scientists employ a great number of probes to aid them in understanding, characterizing and improving materials. But neutron beams are a particularly important and irreplaceable part of the ‘scientific toolkit’. The importance of neutron scattering methods for materials research is a consequence of the special way that neutrons interact with matter.

All matter is made of atoms, which can be arranged in orderly (crystalline) solid structures, or in random (amorphous) structures in the solid, liquid or gaseous states. Neutrons are sub-atomic particles that interact (a) with the nuclei of atoms and (b) with atomic magnetic fields.

The unique aspects of atom-neutron interactions open up scientific possibilities that are simply not accessible by other probes such as NMR, microscopy, ultrasonics, muon spin resonance or scattered electromagnetic radiation, such as laser light, X-rays or gamma rays. This is not to diminish the importance of all these other techniques, but to highlight that neutron beams provide another window for investigating materials that sometimes reveals complementary information that is essential for the final understanding of how materials behave. The way neutrons scatter from atoms (changing their direction, energy and magnetic polarization) provides direct knowledge of the structures and dynamics of materials at the level of atoms, molecules and nanostructures. Neutron scattering techniques include diffraction, spectroscopy, reflectometry and small-angle scattering. These techniques enable research in all kinds of materials, such as metals, minerals, ceramics, composites, polymers, lipid membranes, and peptides; in all kinds of states, such as crystals, powders, liquids, gels, and colloids; and for all kinds of applications, such as aerospace, automotive, energy, environment, medicine, communications, manufacturing, fundamental scientific exploration and education.

### *Neutrons are penetrating but non-destructive*

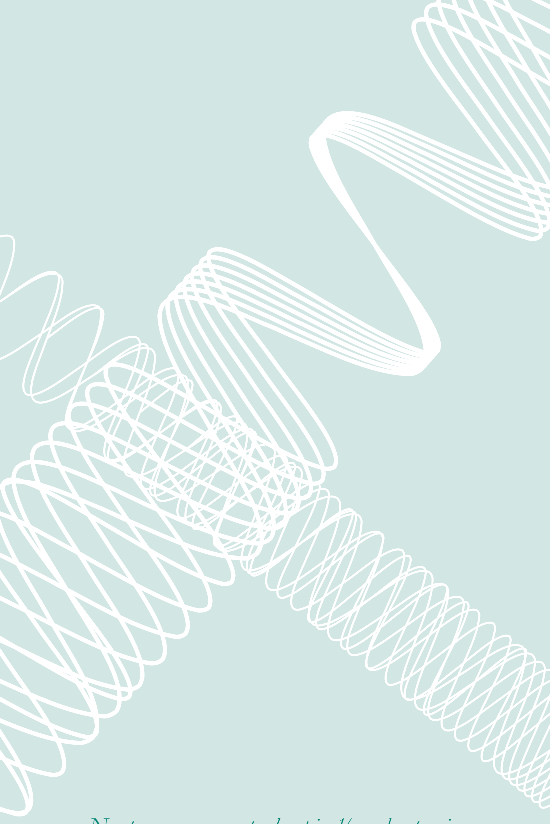
The typical energies of thermal neutrons are measured in the meV range, a million times less than X-rays of corresponding wavelengths in the range of 1 - 10 Å. Although these neutron energies are so low, neutrons penetrate easily through many centimetres of most materials, so that truly representative sampling of bulk materials is possible, completely non-destructively.

### *Neutrons are magnetic*

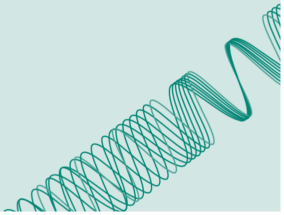
Neutrons have a magnetic moment that interacts with the magnetic electrons in atoms. The interaction is simple and well-known, making neutron beams the absolute reference technique for determining the structure and dynamics of magnetic materials.

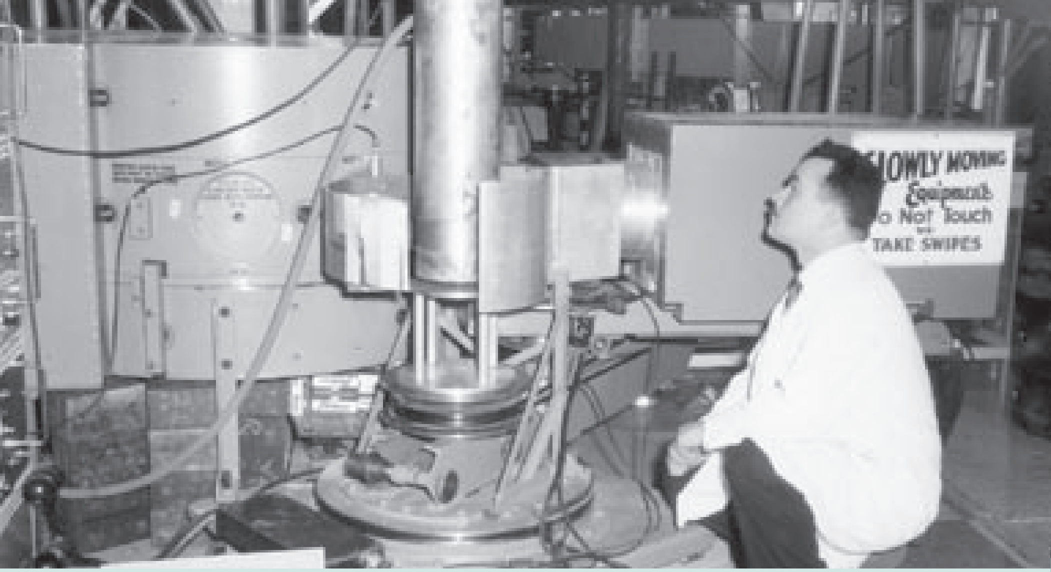
### *Neutrons are sensitive to isotopes*

Neutrons interact directly with the nucleus of the atom, and so determine the centre of mass of an atom free of electronic influences. The strength of the interaction varies from one nucleus to another but is similar in magnitude, making it as easy to see light atoms (e.g. hydrogen, lithium) as heavy atoms (e.g. manganese, uranium). Most notable is the huge difference between light hydrogen and heavy hydrogen (deuterium), a property that can be exploited to unravel the complex structures of biological materials and polymers, where hydrogen is a major constituent. By substituting varying amounts of deuterium for hydrogen, the 'contrast' of particular features of a molecular structure can be adjusted to make them readily observable, or to eliminate them from the signal through 'contrast-matching' of the particular feature with the surrounding solvent, for example.



*Neutrons are neutral, spin-½ sub-atomic particles that interact with the nuclei of atoms through the short-ranged strong interaction, and with the magnetic fields associated with unpaired electrons in atoms. Neutrons propagate as waves, being so small that their quantum-mechanical, wave-particle duality is strongly evident. The typical wavelengths of neutrons are of the order of the atomic radius, 10,000 times the size of any atomic nucleus. Therefore, from the viewpoint of the neutron, the atomic nucleus is a truly tiny target, a so-called "point scatterer".*





Because Canada constructed the world's most powerful neutron sources in the 1940s and 50s there were opportunities for imaginative young scientists to make significant impacts in various fields. That was the period in which Canada launched the modern field of nuclear medicine. It was also the time when Bert Brockhouse developed new methods and instrumentation for studying materials with neutron beams. In recognition of that pioneering contribution to world science Brockhouse and Shull were awarded the Nobel Prize in Physics in 1994. By that time, materials research using neutron beams had been recognized as an essential scientific tool internationally with national facilities operating around the world.

## 1.3 Canadian neutron beam research - stature and status

In 1994, Canadian scientist Prof. Bertram Brockhouse shared the Nobel Prize in Physics for pioneering the method of neutron scattering to reveal the internal energy states of solid materials. His triple-axis spectrometer, developed at Chalk River in the 1960's, has been replicated at neutron beam research centres worldwide, and continues to serve as a primary instrument for exploring the frontiers of condensed-matter physics. In the mid-1980's Canadian researchers developed the neutron stress scanner, which again has been replicated at neutron beam research centres worldwide because it has been recognized as the most effective method to probe stresses non-destructively within industrial components. The information arising from neutron stress scanning has direct consequences for public safety, regulatory practices and industry competitiveness.

Today, our national centre for neutron beam research is situated at Chalk River laboratories and operated by the National Research Council's Canadian Neutron Beam Centre (CNBC). The CNBC was recognized, in a recent study by the Council of Canadian Academies, as a valuable advantage in Canada's infrastructure for science and industry (82% of international respondents' opinions – the highest rating of any element of the federal S&T infrastructure) [1]. As a piece of our national science infrastructure, NRC-CNBC is open and accessible for all members of the community that is represented by CINS: established neutron beam researchers as well as students and first-time users. It is a national centre that is used by scientists from every province.

Users are granted access to the CNBC facility based on the scientific merit of their proposals for beam time (as judged by external peers); therefore, in general, users' programs are positioned at the leading edge of whatever science or technology they are addressing. For example, the importance of neutron beam research on YBCO superconductors was recognized by NSERC's Brockhouse Prize to Hardy, Bonn and Liang [2]. Research on peptide / membrane structures may shed light on the mechanism of diseases such as Alzheimer's, HIV, or antibiotic resistance of certain bacteria. The quality of research on cholesterol in membranes was recognized by designation as a 'Hot Article' for 2006, in the journal 'Biochemistry'. [3] Neutron diffraction is being applied to build a fundamental understanding of magnetic Barkhausen noise, which is important as a non-destructive, high-speed indicator of defects in buried gas pipelines to evaluate fitness-for-service and help avoid catastrophic accidents. Neutron reflectometry has provided a novel method to explore photo-mechanical polymers, which are potential candidates as light-activated mechanical nano-switches.

The scientific productivity of Canadian neutron scatterers is very competitive. An illustrative snapshot is that the 5 thermal-neutron instruments at the NRC's facility in Chalk River, and their 22 continuing staff supported the production of 135 publications in 2003-2005, plus 18 proprietary reports for industrial users. The papers appeared in high-quality journals appropriate to the relevant scientific disciplines of the participants, for example: 11 in Phys Rev Lett, 27 in Phys Rev B, 21 in Langmuir, 16 in Rev Sci Inst, 10 in Phys Rev E, 9 in J. Sol. Stat. Chem., 7 in J. Appl. Phys., 5 in Mat.Sci. and Eng., etc. Citations of papers published in 2001-2005, arising from collaborative work at the CNBC facility have been analyzed in terms of impact factor: number of citations per paper per year since publication. The average value was found to be 4.5, substantially higher than most physical-science journals.

Canadian researchers maintain an international reputation for innovation in neutron beam instruments and methods. A good example is the world-first demonstration of molecular holographic imaging by thermal-neutron incoherent scattering from hydrogen atoms, which led to articles in Nature [4] and Phys Rev Lett [5], as well as the cover of Physical Review Letters, followed by extensive further exploration to the present day. One important application of neutron holography may be to enable molecular structure determinations to high resolution in the class of membrane-associated proteins (about 1/3 of known proteins) that are difficult to fully crystallize and therefore have defied detailed characterization in all but a few examples. Such a capability would have a major impact on the understanding of structure and function for the life sciences.

The Canadian world-first demonstration of neutron holography was prominently published in leading scientific journals. This new technique may unlock new areas of knowledge on the materials of life: membrane-associated proteins.

There is an awareness and interest amoung Canadian researchers to apply the knowledge from neutron scattering to realize an impact in technology. A recent example was the neutron diffraction investigation of stress annealing to improve the performance of magnetostrictive Fe-Ga alloys for energy-harvesting applications by Defence Research and Development Canada and the US Office of Naval Research. In-situ neutron diffraction experiments demonstrated that, at most, a 20-30% increase in performance could be achieved by optimizing the stress-annealing process, rather than the ten-fold increase that was hoped for. As a result, R&D resources were redirected to other avenues for improving performance. Another example was an ongoing program to investigate residual stresses in feeders for CANDU™ nuclear reactors, to optimize manufacturing practices for reliable service over prolonged lifetimes. An outage due to a cracked feeder could cost millions of dollars, and the safe life extension of nuclear power stations is an important part of plans in Ontario and New Brunswick for electricity in the coming decades.

Although recognized for its excellence in some areas of science and technology, Canada's neutron beam facility has fallen behind laboratories in other nations who have acquired decades of experience with cold neutron beams that are especially powerful for research in soft materials, life sciences and nanotechnologies. Canada's existing NRU reactor does not include a cold neutron source, and there is relatively little experience with techniques such as small-angle neutron scattering, neutron reflectometry, high-resolution neutron spectroscopy, spin-echo spectrometry, etc. Some Canadian researchers avail themselves of cold-neutron beam methods in foreign neutron beam laboratories; however, it is very challenging to foster a national capacity to exploit these advanced techniques without a domestic centre that maintains a strong presence in the relevant scientific fields, for example, the structures and dynamics of proteins and other polymers in solution.

> *"The Canadian science community has lived up to the expectations of the federal government, who invested in the NRU reactor in 1950. We have exploited the NRU's full potential for materials research, ranging from exploratory science and education to problem-solving for industry. Now, a new neutron facility is needed so that our new generation of scientists can continue to deliver benefits across Canada's innovation system in the coming decades."*
>
> *- Prof. B.D. Gaulin (McMaster),*
> *Past-president of CINS*

## 1.4 The need for a domestic facility - international context

The demand for neutron beam facilities is growing. Most developed countries already have neutron beam facilities. There are 6 facilities in North America, 12 in Europe, 5 in Australasia and a few others. There have been some recent closures of aging plants, for example in Denmark (Risø), Germany (Jülich), the US (Brookhaven) and Sweden (Studsvik). To expand capacity for neutron beam experiments and to meet growing demands, new facilities are currently under construction or have recently been completed, for example in Japan ($2.4B), Australia ($300M), the USA ($2.2B), Germany ($750M), and the UK ($250M). This activity demonstrates a widespread recognition of the social and economic benefits arising from materials research using neutron beams.

A domestic neutron facility connects Canadian scientists from dozens of universities and laboratories to a global network of neutron laboratories for advanced materials research, and attracts international scientific collaboration at Canada's centre for neutron beam research. In the last five years, NRC's Canadian Neutron Beam Centre has attracted scientific collaborations with over a hundred institutions in nineteen countries, connecting the Canadian science community with scientists in developed and emerging economies. Providing access for foreign researchers to Canada's neutron facility ensures that Canadians are welcome at complementary facilities in other countries.

Canada is an active member in the North American network of six neutron laboratories engaged in materials research. It is possible to evaluate the potential for increased scientific activity in the field, by examining other labs across the continent. Currently, the busiest neutron laboratory in the USA is located at the National Institute of Standards and Technology (NIST). With 18 neutron instruments and a staff of 100, the NIST Centre for Neutron Research has 2,000 scientific users each year and is oversubscribed to a level over 170%. [6] As a result of the 2006 American Competitiveness Initiative, [7] the NIST Centre for Neutron Research is undergoing a substantial expansion, adding a new building and five new instruments, to allow them to accommodate experiments from an additional 500 scientists each year.

It is sometimes pointed out that Canadian astronomers and nuclear particle physicists are accustomed to remote access or travelling to foreign facilities, in lieu of access to a state-of-the-art domestic research facility. The possibility might be considered that we likewise send Canadians to foreign neutron beam facilities, instead of building a new national centre. 'Canadian Participation at the Spallation Neutron Source' was a capital project enabled by the Canada Foundation for Innovation to install a 'Canadian' beam line at the new SNS at Oak Ridge, TN. This $15M investment does, indeed, provide a Canadian presence at the leading neutron source in North America, but the sporadic access to the SNS or other foreign neutron facilities by experienced Canadian neutron researchers cannot substitute for our current situation, with an established national neutron user program. International experience in attempting to maintain 'virtual neutron beam centres', where the real sources are elsewhere, has uniformly resulted in loss of neutron beam expertise. In all cases, highly qualified staff migrated to facilities in other locations, instead of remaining as a local centre of activity, and the national / regional user communities were diminished. If Canada loses its domestic neutron source, the expertise will either leave the country or the field, and there will be no national 'hub' fostering innovation in neutron scattering that might respond to the specific research interests of the Canadian user community.

*Neutron beams can also be applied to the most practical of questions making an aircraft safer or a steel manufacturer more competitive.*

It must be understood that, unlike the situation for condensed matter research with neutron beams, astronomy and particle physics are strongly influenced by the facility that can see the farthest or achieve the highest energy. Internationally, science in these domains has reached the point where facilities must be on the scale of enormous, multinational undertakings to be at the leading edge. This is the realm of 'big science', where Canada has few opportunities, on its own, to build telescopes or particle accelerators of world class. Surprising for many, a neutron facility is not 'big science' – where a massive investment is needed to answer a relatively small number of fundamental questions. A neutron laboratory is a major facility with expert staff, constituting an infrastructure that enables tens of thousands of individual scientific projects for a large user community. It is well within the grasp of a single nation like Canada to build a world-class neutron beam laboratory; as already demonstrated with the NRX and NRU reactors. Any neutron facility beyond a certain level of flux makes an important contribution to global S&T, by adding capacity for worldwide access and supporting specific fields of scientific focus, appropriate to the strategic needs of the host country.

While a neutron beam facility can, like particle-physics and astronomy facilities, help to answer fundamental questions about the nature of matter, energy and the universe, neutron beams can also be applied to the most practical of questions making an aircraft safer or a steel manufacturer more competitive. Neutron beam facilities were specifically linked to economically significant innovation, in the U.S. President's 2006 State of the Union address, announcing an 'American Competitiveness Initiative.' [7] For practical impacts, a Canadian neutron facility can be operated and evolve in response to strategic goals of Canada. Obviously, Canadian priorities would exert little influence over developments and policies at foreign-owned neutron facilities. Our current Canadian framework allows us to apply neutron beam methods in direct support of industry development (paid by clients). Conduct of proprietary neutron beam research by Canadians at foreign facilities is currently difficult, and could not be sustained for the long-term as a Canada-based service to industry, in the absence of a domestic facility.

# GROWING Highly QUALIFIED *people*

Engineering graduates Stephanie Stafford (Kinectrics Inc.) and Paula Mosbrucker (Queen's University) using neutrons to investigate a material for nuclear power stations.

I came to the Canadian Neutron Beam Centre for the first time with my professor to do a class project where we used neutrons to measure residual stress. Now I am back again, using the neutron beam to get information about a zirconium / niobium alloy I am studying as part of my job. It's always a great learning experience; the staff are very knowledgeable and I've learned how to set up and run this experiment myself, to get the information I need. I'll keep coming back as often as I can.

Stephanie Stafford
*Engineer, fuel channel integrity, Kinectrics*

Neutron facilities are national science centres that act as a focus for a community. About 20 countries operate such centres which support the education and training of new scientists, the interaction of multidisciplinary research groups and the achievement of national goals through materials research for energy, health or the environment. CINS members come from across Canada to use our current national facility, which fosters those goals and connects Canadian scientists with the wider international community.

## 1.5 The need for a domestic centre - developing highly qualified people

A national neutron scattering centre, operated as an accessible resource for academic research and education, provides an exceptional learning opportunity for students and young researchers. In this regard, the track record of NRC-Canadian Neutron Beam Centre has been outstanding. In the five years 2001-2006 there were 284 visits of young, highly qualified people to the laboratory, including 12 post-doctoral fellows, 106 graduate students (78 Canadians) and 51 other students (48 Canadians), many of whom visited more than once. The Canadian students came from 23 universities in six provinces. Many more young, highly qualified people attended workshops and biennial summer schools in addition to those already counted, who were engaged with hands-on research measurements at the CNBC.

When students visit the national facility for an experiment, their education is enhanced in several ways:

- Training is provided to enable them to work safely, including industrial safety training and radiological self-protection training, specifically to work around neutron beam instruments close to the research reactor.
- Experimental set-up provides the experience of working with technical staff, trouble shooting, designing and producing sample mounts, per forming alignments and gaining the full hands-on experience of real, experimental science.
- Supervision by full-time facility scientists augments the learning that has already occurred at the students' home institution, and provides a deeper understanding of techniques, their applications and limitations.

- Once adequately trained, students are able to operate neutron spectrometers by themselves, and (depending on technical complexity) often change specimens and conditions of specimen environments, such as applied load, temperature, magnetic field, etc. to achieve a higher degree of scientific self-reliance.

- Training from CNBC staff scientists in data analysis and interpretation of results, often with follow-up discussion when the student returns to his or her home institution, is a further enhancement of the student's learning.

- Opportunities to join researchers and other visitors in informal settings, such as coffee breaks, lunches, etc. provide the student with networking opportunities that can help in later career development – science essentially being a human activity with exchange of ideas, and collaborative effort.

Through access to the domestic neutron scattering centre, students gain insight, into a multidisciplinary scientific and engineering environment quite different from the academic situation in their home institution. They gain in-depth exposure to a powerful and versatile experimental method for materials research at a world-class facility, one of 20 in the world. Through access to the national centre, students may be inspired to persist towards careers in advanced materials research, confident that they will find opportunities, in Canada, to apply their knowledge and express their creativity for positive contributions to their communities in the future. While, at present, there are about 40 to 50 graduate students per year whose access to the NRU-based neutron laboratory is a part of their thesis work, in a future, expanded Canadian Neutron Centre, this number will triple or quadruple. Over its lifetime, a new Canadian Neutron Centre will support the development of at least 2000 new, highly qualified materials researchers, whose careers will continue to be supported by access to a competitive domestic facility.

## 1.6 Prospect of a new Canadian Neutron Centre (CNC)

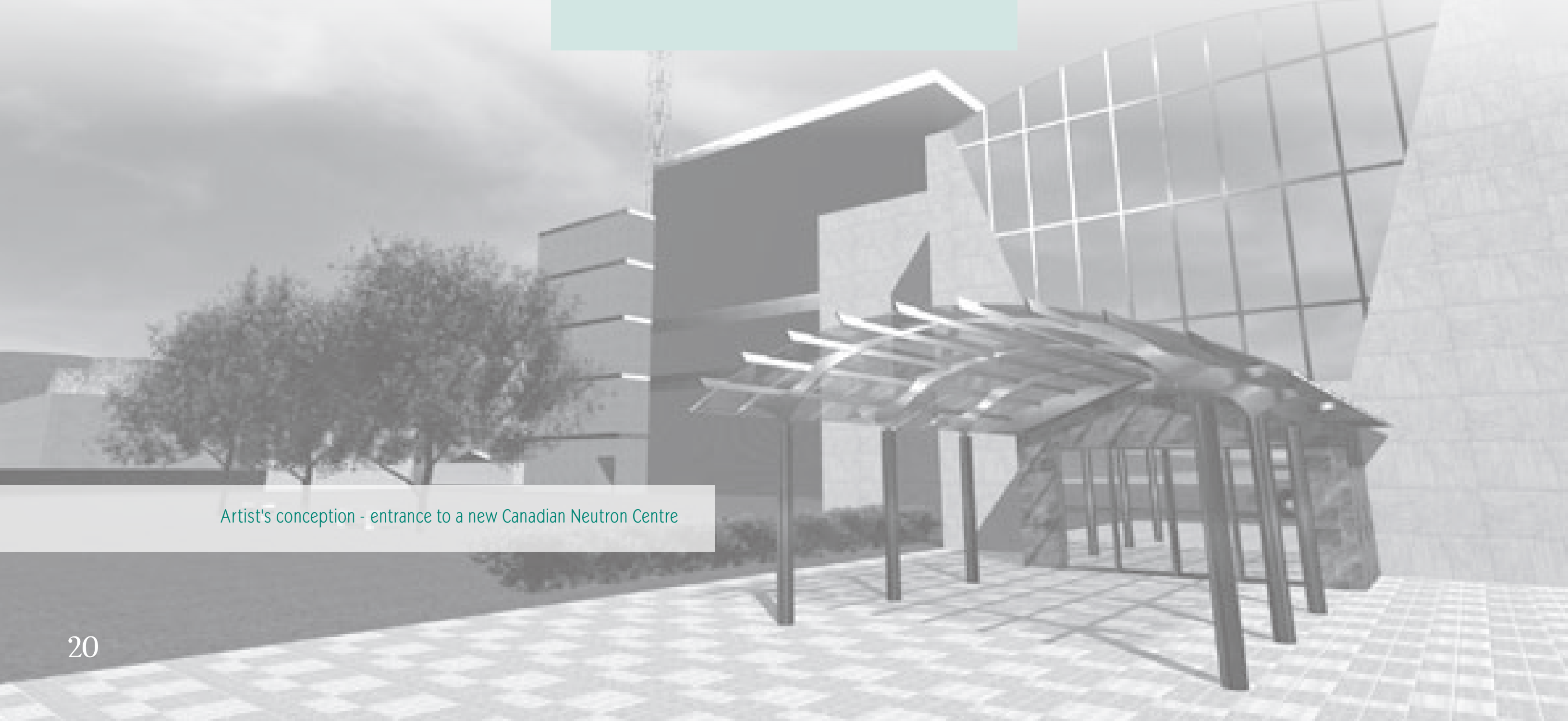
The need to replace and augment the NRU reactor's capabilities has long been recognized by academics, industry, committees and the authors of various studies, both national and international. [8] - [14] The NRU reactor has been operating for over 50 years, delivering excellence in neutron-based science and technology to Canada in several sectors, of which advanced materials research with neutron beams is one. It is now an urgent matter to complete the analyses of scientific and industrial requirements, impacts on Canadian society and the economy, risks, full costs of capital, operation and decommissioning, mandate and governance of new facilities for neutron-based S&T, and to prepare recommendations for government consideration of a major science investment as soon as possible.

This is the appropriate time to consider what capabilities should be designed for a new, world class Canadian Neutron Centre (CNC), which could maintain and expand the current missions of the NRU reactor to a time horizon of about 2050. Having learned from over 50 years of experience with the NRX and NRU reactors at Chalk River, and from their experience with foreign neutron sources, Canada's neutron beam users are well positioned to state their requirements for a facility that enhances Canada's position of excellence and leadership in the global network of neutron beam laboratories. It is certain that a new Canadian Neutron Centre must include at least one cold neutron source as well as a suite of cold-neutron instruments that will enable research on soft materials or nanotechnology as never before possible in Canada. It is also clear that Canada already maintains a leading presence in certain areas of neutron-beam research, a foundation upon which the next generation of instruments and methods can be built.

## 1.7 Industrial Impact of the CNC Project

The industrial impacts of knowledge arising from materials research with neutron beams will be illustrated in the later sections of this document – from the viewpoints of the Canadian scientific communities that need neutron scattering. However, a few words should be said about the industrial impacts that would arise from a major capital investment to provide Canada with a new Canadian Neutron Centre. In the spring of 2004, NRC commissioned a study [15] to compare costs of three different approaches for constructing a new neutron source in Canada. Part of that study quantified the economic impact arising from the construction of a new multipurpose facility that could serve the neutron beam scientific community as well as the isotope industry and the nuclear R&D community. The economic impact from such a project was recognized in two distinct forms:

> *'We applaud the government of Canada's S&T strategy, Mobilizing Science and Technology to Canada's Advantage, and propose that a new investment in neutron scattering infrastructure could be an excellent realization of "..ensuring that higher-education institutions have the leading-edge research equipment and facilities required to compete with the best in the world." Universities from every province use Canada's current neutron source, and, given a world-class replacement facility, will continue to excel in this field.'*
>
> *- Prof. D.H. Ryan (McGill),*
> *President of CINS*

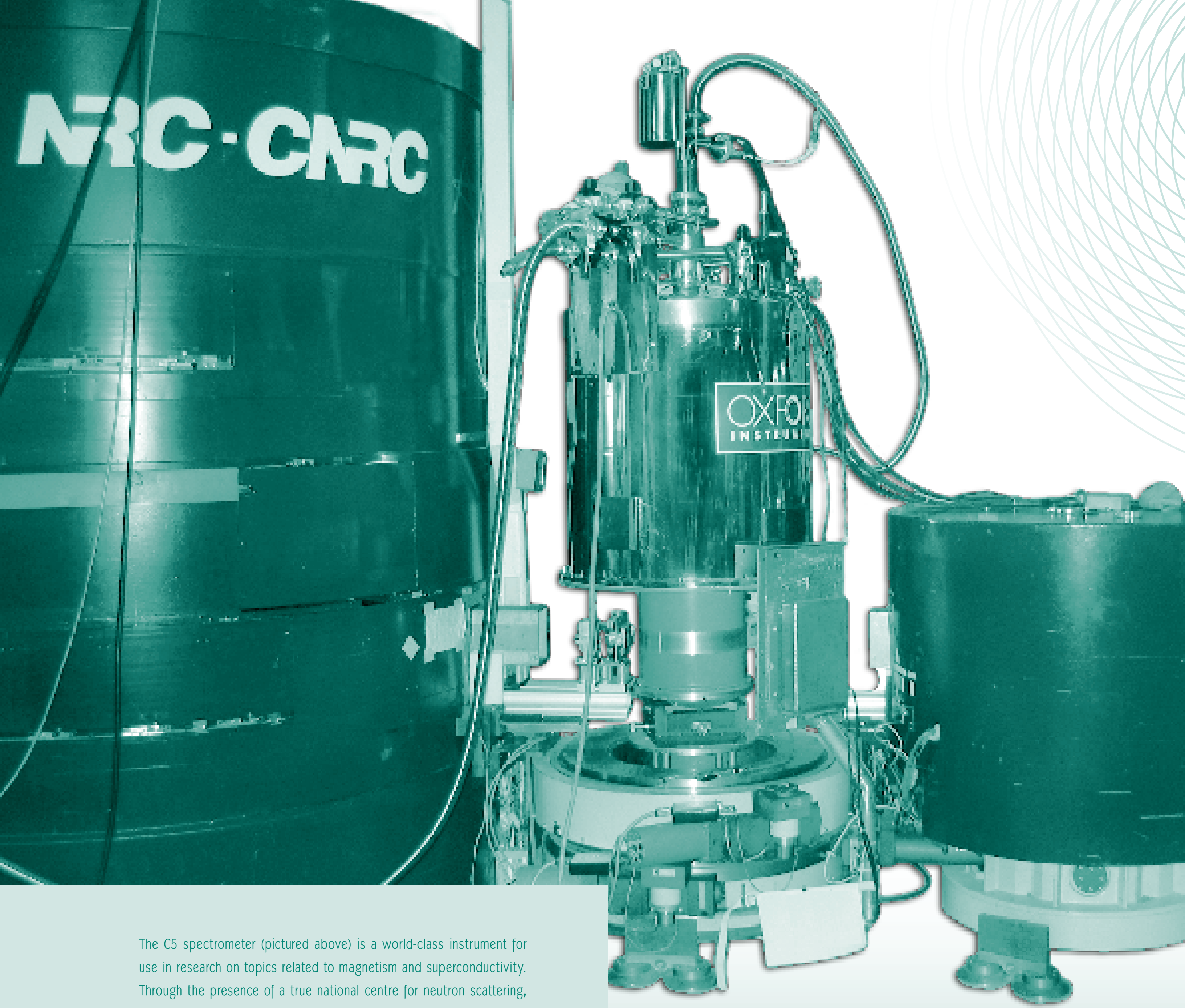

Artist's conception - entrance to a new Canadian Neutron Centre

1 *Industrial Impact from the Construction Project* - The 2004 study found that design and construction of a new Canadian Neutron Centre will generate approximately 9,000 person years of employment, 2,500 person years of which involve highly qualified people. Approximately $190M of equipment and materials will be required for a new facility. The study found that a majority of that supply would come from Canadian Small and Medium-sized Enterprises (SMEs): a similar, recent project sourced 85% of its equipment and materials from 109 Canadian SMEs. The study indicated that construction of a nuclear research facility is suited to SME activity, in contrast to very large nuclear power station projects, which are typically undertaken by large companies. SME involvement is also described as a route for these enterprises to grow and improve as they face technical challenges to produce the specialist equipment required. The facility with between 10 and 25 beamlines, addressing many areas of materials research, must evolve over its lifetime, in response to the inevitable advances of science and technology. There will be a continuous need for capital upgrades over the 50-year lifetime of the facility, and an ongoing requirement for companies to keep pace with advances in the laboratory infrastructure.

2 *Industrial Impact from Facility Operation* - Today, the NRU reactor supports a community of neutron beam users who research materials of all kinds. Examples of academic and industrial research are detailed in Section 2 of this document. Some of this research is carried out directly for companies who pay full cost recovery for access to the special knowledge about materials that is uniquely obtained by neutron scattering methods. With such proprietary knowledge, companies have improved their products or processes, to build competitiveness and to expand their markets. Those science facilities, such as neutron laboratories, which generate knowledge about materials are thus set apart from other major science facilities in that the arising knowledge is often of direct practical and economic relevance. [7] Beyond such direct transfer of materials knowledge to industry, the materials research that appears in the public domain, and the highly qualified people whose education includes experience with powerful neutron-scattering methods, are also the resources upon which companies can build new businesses in key sectors, such as transportation, manufacturing, energy and health. A new Canadian Neutron Centre, including between 10 and 25 beamlines will help to educate over 2000 new highly qualified people for jobs at the forefront of knowledge-intensive industries.

Because NRU is a multipurpose science facility, there have been even more economic impacts arising from its operation, beyond the results of materials research with neutron beams. NRU supports the world's largest isotope business: MDS Nordion and Best Medical Canada Inc., both based in Ottawa. With a revenue of approximately $300M [16], MDSN obtains the majority of their isotopes from NRU. The two companies use isotopes for the treatment or diagnosis of over 20 million patients in 80 countries annually. NRU also provides a test bed for the nuclear electricity generation industry. The current fleet of CANDU reactors, that generate a sixth of Canada's electricity, could not have been designed and built without the essential knowledge gained in NRU. According to the Canadian Nuclear Association [17], that industry today represents $5B of annual economic activity employing 21,000 people in 150 companies.

CINS is proud of the benefits that thousands of neutron beam experiments have brought to Canada over the years, measured in terms of the education of highly qualified people, the advances in scientific understanding of the world around us, as well as supporting industrial competitiveness. These achievements, when added to those in the fields of isotopes and nuclear power development, make NRU one of Canada's most successful investments in any science facility. To anticipate a renewal of Canada's neutron source is to foresee another 50 years of excellence in neutron-based science and industry.



The C5 spectrometer (pictured above) is a world-class instrument for use in research on topics related to magnetism and superconductivity. Through the presence of a true national centre for neutron scattering, scientists in universities and industries across Canada have access to the very best scientific tools.

# 2. SCIENTIFIC COMMUNITIES

The CINS system of peer-reviewed access to neutron beam instruments is organized by subject area rather than the practice adopted at many other neutron facilities, where proposals are addressed to specific beam lines. Neutron scattering projects at Chalk River therefore tend to be associated with one of five scientific communities of interest. Each community has distinctive characteristics, such as the distribution of scientific disciplines, the degree to which members are full-time neutron scatterers or casual users, the degree to which the community is established and internationally recognized, and so on. Representatives of these scientific communities drafted the following sub-sections. Each subsection includes an overview of the community's current activities and impacts, as well as their thoughts about world trends and how a new Canadian facility should be configured to respond to the emerging future.

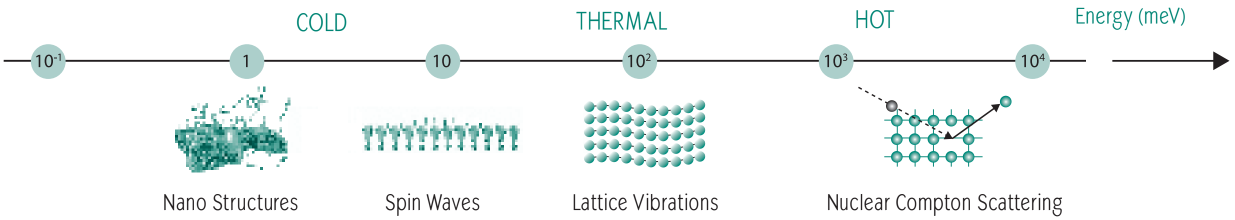
## 2.1 Excitations in Condensed Matter

The research community that studies excitations in condensed matter includes some of Canada's most experienced neutron scattering scientists, for whom access to neutron beam facilities is central to their programs of research and education. Canada's scientific presence in this area of materials research can be traced back to the pioneering work of Nobel prize-winning Prof. Bertram Brockhouse in the 1960s, and continues with experimental programs that challenge fundamental theories of condensed-matter physics.

### *Overview*

All properties of materials ultimately depend on what atoms they are made of, how these atoms are arranged, and how they are moving or vibrating. Here, we focus on the movements of atoms, commonly referred to as 'dynamics' or 'excitations', pertaining to energy states of condensed matter as opposed to structures. One of the neutron's most important properties is that, by virtue of its mass, neutrons with de Broglie wavelengths appropriate for determining the structure of materials (1-4 Ångstroms), possess energies typical of the low energy excitations of condensed matter [5 - 80 milli-electron-Volts (meV)]. This energy scale is usually referred to as the 'thermal' range, which corresponds to the spectrum of kinetic energies of atoms in equilibrium with materials spanning temperature ranges from about 20K to about 2000K. Speaking of energy in terms of temperature, neutrons with lower energies are referred to as 'cold' and with higher energies 'hot'. The following figure shows what type of phenomena can be measured by neutron scattering and a comparison of the temperature and meV energy scales.

Figure 2.1.1 - Energy scales of neutrons and materials [European Spallation Source Project Report, 2002]



Understanding low-energy excitations (up to 100 or so meV) lies at the heart of contemporary materials physics and chemistry. Quantum mechanics, our most accurate fundamental physical theory, makes very specific, testable predictions about these excitations. The everyday properties of materials are an average of the ground state (the lowest energy state) and low-lying excited states (on temperature scales below room temperature), very well matched to the typical energies of neutrons. Therefore, when a neutron creates or absorbs an excitation it loses or gains enough energy that the change is easy to detect. Neutron scattering from excitations is denoted as inelastic scattering because the energy of the scattered neutron is changed from the initial energy (elastic would imply no change in the neutron's energy). Inelastic neutron scattering (INS) is the most versatile technique available for mapping out the excitation spectrum of condensed matter (i.e. solids and liquids) from very low energies to approximately 10 times room temperature. The fact that the technique is entirely general and applicable to most materials makes it a universal tool – one that materials scientists and condensed matter physicists could not do without. According to Brockhouse, the Canadian scientist who shared the 1994 Nobel prize with American Clifford Shull on neutron scattering for his pioneering contribution in the development of inelastic neutron scattering, "If the neutron had not been discovered by Chadwick in 1932, it would have been invented." [18].

The magnetic moment of the neutron allows for the probing of magnetic excitations. A large fraction of the Canadian inelastic neutron scattering community works in the general field of magnetic materials. Neutrons are the primary scientific technique for studying magnetic excitations in magnetic materials and, historically, there has been a lot of emphasis on this area. Especially powerful is the fact that neutron beams can be prepared with an initial polarization (i.e. the magnetic moments of the neutrons are all pointing the same direction), and by measuring the change of polarization on scattering, magnetic excitations can be distinguished from non-magnetic ones.

INS has its own challenges, distinct from those associated with elastic neutron scattering or diffraction. Chiefly, the likelihood of a neutron scattering inelastically is 100 to 1000 times less than it being scattered elastically. As a consequence, contemporary INS is carried out with an eye to being as efficient as possible with the available neutrons. These efficiencies are gained by using samples that are as large as possible, by directing as many incident neutrons as

Senior scientist Bill Buyers is well-recognized in the field of condensed matter physics, with neutron scattering as his primary tool. Among many scientific contributions, he made the first observation of the "Haldane Gap". This discovery confirmed a highly controversial speculation by theorist D.M. Haldane, overturned the wisdom of the day, and ushered in a host of experimental and theoretical studies worldwide that still continue. Here Bill is pictured at a Summer School in Chalk River, explaining neutron spectroscopy to a group of graduate students.

possible to the sample, and through detection systems that can simultaneously measure neutrons scattered over a range of angles and with a range of energy transfers.

Some of the most topical research areas in modern materials physics and chemistry are particularly demanding, as they are carried out on new materials for which large samples may not yet be available, and they may focus on 'quantum materials' where the magnitude of the magnetism in the material is inherently small, and therefore the signal is inherently low. Nonetheless, in many of these very topical research areas, particularly in the study of magnetic excitations in materials, neutron scattering is by far the most important experimental probe available to materials physicists and chemists. Such experiments have, and will continue to have an enormous impact in fundamental materials research. Canadian scientists have strong programs in these areas, and it is very important that cutting edge neutron scattering instrumentation be developed to allow us to maintain this international strength and build upon it.

### *Impacts on S&T, economy and society*

The invention of the triple-axis spectrometer (TAS) by Brockhouse opened up the possibility of measuring excitations that influence everyday properties of materials. Entirely general and applicable to most materials, the technique was enthusiastically applied first to simple crystalline solids, and then to more complicated systems such as alloys, chemical compounds, magnetic materials, and even to liquids. In the 1980's the use of INS to study much bigger molecules (polymers) grew rapidly. In all cases the general trend has been that INS experiments generate new knowledge that becomes the essential component of condensed matter theory, to confirm or disprove the theories proposed based on other experimental techniques.

Thousands of materials have been studied with INS. Among them are many materials that have already found important industrial applications, prior to understanding why they work. A good example is the role INS has played in the research and development of shape-memory alloys (SMAs). Discovered by accident in 1961, SMAs return to their original shape if heated above a critical temperature. Diffraction experiments soon after the discovery indicated that a collective movement of one type of atom against the rest of the crystalline structure causes the shape restoration. This in turn led to the idea that the sudden release of the atoms, frozen in at a particular excitation (like energy stored in a compressed spring), is the driving force for the transition. The direct confirmation of this theory came from INS [19], and the theory has enabled intelligent design of other SMA materials. The first commercial application for the material was as a shape memory coupling for piping, e.g. oil line pipes for industrial applications, water pipes and similar types of piping for consumer applications. The late 1980's saw the introduction of Nitinol as an enabling technology for endovascular medical applications. While more costly than stainless steel, the self-expanding properties of Nitinol alloys manufactured to 'body-temperature response', have provided an attractive alternative to balloon-expandable devices. On average, 50% of all peripheral vascular stents currently available are manufactured with Nitinol.

Canadian expertise in INS for magnetism and quantum materials is applied to subtopics such as those listed here:

**High-temperature superconductivity (HTSC):** The discovery of HTSC in 1986 sparked a new interest in the field of superconductivity. Despite a large number of studies on HTSC, there is still no consensus on the mechanism responsible for superconductivity so that these materials still remain one of the most challenging problems facing condensed-matter physicists today. It is believed that an understanding of the normal state of these superconductors is a prerequisite to elucidating a microscopic theory for HTSC. Of particular interest is the nature of any spin and/or charge ordering in these materials as a function of doping. Neutron scattering has played a vital role in exploring the fundamental properties of the charge carriers and testing current theories of HTSC in both superconducting and normal states. There are several reviews on this topic, featuring Canadian authors and research. [20]-[22].

The 'special' property of superconductors is that they have zero resistance to electric current (absolutely none, while in normal conductors such as copper wire the atoms of the wire impede the free flow of electrons, depleting the current's energy and wasting it as heat). What is so exciting about the new materials is that their superconducting transition temperature ( $T_c$) is much higher than the classical, low-temperature superconductors. (The record $T_c$ for HTSC is now about 165 K (-108°C) at high pressures, more than half way to room temperature.) So their discovery not only sparked hope that room temperature superconductivity is around the corner but also allowed more technical applications of superconductors to come to life at temperatures only as low as liquid nitrogen compared to liquid helium (much more expensive and not practical in most cases). People now envision future applications of superconductivity such as:

- Replacing electrical transmission lines with super conducting wires to eliminate losses between power plants and consumers, boost utilities' efficiencies, and eventually help in reducing greenhouse gas emissions and pollution. [23]

- Enabling large amounts of energy to be stored for peak demand times and greatly enhancing the usefulness of energy sources which are not available on-demand 24-7 (like wind power and solar energy). [24]

- Enabling magnetically-levitated transportation, where research and development is strong in the United States, Japan, China, and Germany [25].

- Making possible a 'table-top' MRI (magnetic resonance imaging) machine as a routine medical diagnostic tool. [26].

- Implementing a superconducting electronic device, known as a Josephson junction, which could serve as the basis of the next generation of supercomputers. [27]

Worldwide, the current market for HTSC wire is estimated to be US$30 billion and is expected to grow rapidly. However, more research is needed to understand the underlying phenomenon and to allow progress in obtaining superconductors with even higher $T_c$, which can be integrated cost-effectively into technological applications that affect our daily lives. Maintaining the ability for neutron beam research on superconductors will help to ensure that Canadians can lead and benefit from developments in these materials.

**Heavy fermion superconductors and itinerant magnets:** All materials contain electrons, which belong to a group of particles known as fermions. The electrons in most metals flow like a liquid; that is electrical conduction. In certain materials, electrons are strongly correlated by the presence of magnetic rare-earth ions (e.g. Ce or U). These 'correlated' electrons do not simply move through the background that all of the other electrons provide, but have an extra, interaction where they can still flow as in a metal but they seem up to 1000 times heavier. They are called 'heavy fermions'. One puzzling aspect of their complex behaviour is the presence of superconductivity, [28] which coexists and couples with static magnetism. This fact is surprising, since magnetism is very effective at destroying conventional superconductivity; therefore, these materials may be revealing a new and unconventional type of superconductivity and nobody can predict where this discovery could lead. However, neutron scattering is the key method to investigate the peculiar magnetic properties of these systems, and could therefore help to answer many questions.

In a related branch of inquiry, there is a longstanding Canadian strength in studying 'itinerant' magnetism, where the magnetic structure resides in the liquid of fermions rather than being associated with the ions of the crystal lattice. Also known as spin density wave (SDW) magnetism, itinerant magnetism is considered in the same sector of condensed-matter physics research as are HTSC and heavy fermion systems. Classic examples are elemental chromium, and low-dimensionality $FeGe_2$. [29] There are also examples of materials that are neither HTSC nor heavy fermion systems but are correlated and show SDW magnetism, for example $V_{1.973}O_3$. [30]. It is believed that an understanding of these systems, which should be easier to describe from a theoretical viewpoint, will lead to better descriptions of HTSC and heavy fermions.

**Low Dimensional and Singlet Ground State Magnetic Materials:** Several different families of materials have been of intense recent interest as they exhibit an extreme form of quantum behaviour at low temperatures. These materials exhibit collective singlet ground states, in which S=½ magnetic moments within the crystalline structure pair off into a quantum 'singlet'. In this singlet state you cannot observe the S=½ moments separately (it is this disappearance of the magnetic degrees of freedom that is the quantum effect). As the ground state of these materials in non-magnetic, they display no elastic magnetic neutron scattering at all. However, INS can induce transitions from the singlet ground state to the triplet excited states, and has thus become the principal probe of these quantum systems. INS data is essential for developing a detailed understanding of these unique magnetic systems and their quantum excitations.

Materials can reach this non-magnetic singlet ground state in several ways depending on the effective number of dimensions. Quasi-one dimensional materials can be composed of either chains of S=½ magnetic moments, which undergo a spin-Peierls phase transition to a distorted structure composed of a one dimensional assembly of dimers (pairs of magnetic ions). This occurs in $CuGeO_3$ and TiOCl, for example. $KCuF_3$ is another example, which shows evidence of a crossover between one and two dimensional behaviour in the magnetic excitation spectrum. [31] In contrast, chains of S=1 (not ½) magnetic moments can display what is known as a Haldane state at low temperatures but never form the dimer state. This is a unique quantum state first observed in Canada with neutron scattering. [32] Finally, quasi-two-dimensional materials, such as $SrCu_2(BO_3)_2$ are composed of orthogonal Cu S=½ dimers arranged on a square lattice, and are known to exhibit a Shastry-Sutherland ground state at low temperatures [33].

Broadly speaking these materials exhibit novel electric and magnetic properties, many of which are not well understood. Although the main focus of this research is fundamental science, new technologies will emerge for novel applications, as a natural result of this research. In fact, understanding the physics behind low dimensional and quantum systems is a prerequisite for future development of successful applications of sub-micron materials systems and nanotechnologies. Hence, such fundamental research will have a crucial role in developing new solutions in different areas: electronics, optics, medicine and so on. As an example one could consider electronics, where the ever growing complexity in microprocessor and memory chips over the past few years has lead to a large chip density and hence to very small dimensions of individual electronic components (about 100 nm or smaller), bringing them into the quantum and low-dimensional regime. As a result, in addition to its role in training highly qualified personnel in fundamental science, such research will help Canadian scientists to be among the leading researchers in nanotechnology.

**Geometrically Frustrated Magnetic Materials:** Many magnetic materials are composed of arrangements of interconnected triangles or tetrahedra. In the presence of antiferromagnetism (which makes magnetic moments that are close to each other line up in opposite directions), the

A large fraction of research on excitations and magnetism requires ancillary equipment to hold specimens at low temperatures while neutron inelastic scattering reveals the characteristic energy states. Here, a closed - cycle helium refrigerator provides a range from room temperature to -266°C.

magnetic moments cannot find a simple low-energy configuration, and the resulting arrangement of atoms is referred to as geometric frustration. Only within the last decade has a rich landscape of new phenomena been recognized in the physics of geometrically frustrated antiferromagnetic systems.

Magnetic cubic pyrochlore materials, such as $Tb_2Ti_2O_7$ and $Ho_2Ti_2O_7$, for example, have magnetic rare earth ions arranged on networks of corner-sharing tetrahedra. At low temperatures, neither material finds a conventional long-range ordered state, but rather each finds a distinct exotic disordered state, a 'spin liquid' state for $Tb_2Ti_2O_7$, a 'spin ice' state for $Ho_2Ti_2O_7$. On the application of an appropriate magnetic field, the spin liquid state in $Tb_2Ti_2O_7$ can be caused to order, complete with well-defined spin excitations, characterized and ultimately understood through INS. [34]

Frustrated magnets have attracted attention recently, because they have a high potential for new technological applications, such as magnetic refrigerants. A magnetocaloric effect arises from the presence of strong magnetic interactions, high densities of spins and suppressed ordering temperatures. On decreasing the magnetic field, heat is drawn into the material. Cooling is faster with demagnetization than with more conventional technologies (dilute paramagnets). There is great potential to achieve low temperatures in space-limited situations, and to develop a new generation of environmentally friendly refrigerators.

**Colossal magnetoresistance (CMR):** is a phenomenon of greatly reduced electrical resistance in the presence of a magnetic field, which was discovered in 1993. Chemically, CMR materials are similar to high temperature superconductors except that the copper is replaced by manganese, which is more magnetically active. Unlike superconductors, many CMR materials display the maximum effect near room temperature, and there is already a microscopic model (double exchange) that provides a basic description of the effect. However, double exchange fails to explain several observations. Canadians have studied the magnetic excitations, lattice excitations, and lattice distortions using neutron scattering during the ferromagnetic transition associated with the CMR effect [35], to see how it varies across a family of CMR materials with a range of compositions. CMR materials hold promise to be used as sensitive magnetic detectors, possibly in computer hard drive read heads where 'giant' magnetoresistance sensors are currently applied. The 2007 Nobel Prize in Physics was awarded to Albert Fert (Université Paris-Sud, Orsay, France) and Peter Grünberg (Forschungszentrum Jülich, Germany) for the discovery of giant magnetoresistance.

**Ferroelectrics:** These materials exhibit exceptionally high dielectric constants, meaning they have enormous ability to develop bound surface charges when placed in an electric field. They find application as the medium for electrical energy storage devices or capacitors. Since virtually every household electronic gadget contains at least a few to tens of capacitors, this application alone represents a huge technological and economic impact. Ceramic disk capacitors made of a ferroelectric material $BaTiO_3$ are simple to manufacture and have captured more than 50% of the ceramic capacitor market. Transparent ferroelectric crystals are used commonly for doubling, tripling and quadrupling of laser frequencies, and as electro-optic modulators, Q-switches, Pockels cells, and so on.


Courtesy of Raytheon Commercial Electronics

Figure 2.1.2 Pyroelectric Imaging. Lighter colors correspond to warmer temperatures.

Ferroelectric materials also exhibit two other important properties: piezoelectricity (generation of voltage when compressed); and pyroelectricity (generation of voltage when heated). These properties have led to many more applications. For example, the 'pendulum' in all electronic clocks and watches is a small piezoelectric crystal vibrating at many MHz. Piezoelectrics are also used for medical imaging and treatments (ultrasound), underwater navigation and detection (sonar and hydrophone arrays), and nano-precision motion (actuators), just to name a few important applications. Pyroelectrics are at the heart of infrared detectors and thermal imaging devices (e.g. Fig. 2.1.2) used for fire fighting, law enforcement and border patrol, land mine detection, building surveillance, process control, vision testing, facial recognition, and traffic control.

Ferroelectricity was originally discovered in 1918 in Rochelle salt. [36] Since then, many materials, existing or newly synthesized, have been found to be ferroelectric. The first theory of the phenomenon was proposed in 1940; however, this theory was specifically for KDP, a relatively simple material. A more fundamental and generally applicable theory emerged nearly twenty years later, predicting how the dielectric constant would vary as the frequency of the lowest energy atomic vibration changes with temperature. The direct confirmation of this theory came from INS. Indeed, Canada played the pivotal role in this endeavour as the key INS measurements were carried out at the NRU Reactor, Chalk River. [37]

**Polymers:** INS has provided insights into the excitations of polymers, such as the 'plasticizing effect' when an additive dioctylphthalate (DOP) is added to polyvinylchloride

(PVC). [38] The amount and type of plasticizer is used to control the strength and rigidity of the final product but may also contribute to its brittleness. The neutron spin-echo technique was needed to investigate the effects of DOP addition at the microscopic level. Thin films of polystyrene and its excitations as a function of temperature and film thickness have also been studied by a chopper spectrometer technique. [39] Polymer thin films play an important role in industry for their use in dewetting, lubrication, and photolithography. The advanced chemical techniques that are used to tailor the properties of polymer systems can also be used to provide important prototype cases to study magnetism. In one particular study [40] magnetic copper ions were combined with quinoxaline bromide (complete chemical formula $Cu(C_8H_6N_2)Br_2$) to form a spin ladder, which is formed from two spin chains that interact more strongly with each other than the surrounding chains. INS measurements of the excitations confirmed the predictions of a model Hamiltonian.

**Liquids/Non-ideal Solutions:** In a non-ideal solution the interactions between molecules are not negligible. They depend on the molecules themselves and how they are oriented with respect to each other. A common example is soap, where one end of the molecule is hydrophilic and the other end is hydrophobic. Quasi-elastic neutron scattering is needed to obtain quantitative values for diffusion rates. In an example of such a study [41] the authors investigated how dimethyl sulfoxide, a common organic solvent used in biological studies and also as a drug carrier across membranes, affected water molecule interactions at different concentrations.

**Biological Materials:** INS studies of proteins and peptides date back to the 1960s. Much of this early work was exploratory and often involved comparison of spectra from simple polypeptides in different conformational states. [42] The emergence of supercomputers has enabled realistic molecular dynamics calculations of biologically relevant systems. Since the mid-1980s there has been an ongoing ‘match’ between INS, molecular dynamics and Raman spectroscopy where one technique would observe or predict the existence of a vibration mode with a particular energy and the others are used to confirm or reject it. Through this multifaceted approach the understanding of how these complex molecules work is steadily increasing. For instance, INS on an enzyme revealed a vibration mode that is likely to be responsible for how the enzyme holds down a hydrocarbon chain and shears it off very much like a pair of scissors. [43]

For research on biological systems, a key strength of neutron scattering is the ability to exploit selective deuteration to enhance the sensitivity of INS to the dynamics of a particular part of a complex molecule. The technique takes advantage of the uniquely strong incoherent scattering of neutrons by hydrogen (but not by deuterium), was proposed in 1986 by Smith et al., and was applied immediately to a number of proteins, notably myoglobin and hemoglobin, with continuing applications today. [44]

Unlike inorganic compounds, proteins, peptides and other polymers do not naturally exist in crystalline form. This lack of order leads to yet another type of ‘excitation’ or energy transfer, which arises due to relatively slow large-scale diffusion of atoms and is measured with quasi-elastic neutron scattering. The study of diffusion requires neutron back-scattering or spin-echo spectrometers that Canada does not have at this time. Consequently, there are few Canadian examples in this field of research, which is currently dominated by US and European scientists. Part of the motivation in this document is the hope that a new Canadian neutron research centre would be better able to provide the facilities needed for research of relevance to life sciences.

### *Advances in Inelastic Neutron Scattering*

One way to follow the development of INS internationally is to review how the measurable excitation energies have been extended beyond its initial range. With early triple-axis spectrometers (TAS) (e.g. Brockhouse's machine and those not much different from his), excitations with energies in the range 5-30 meV have been accessible – i.e. probing the 'thermal' energy range mentioned earlier. Neutrons naturally match this range of energies because they are in thermal equilibrium with a moderator (e.g. water in a nuclear reactor) that is maintained close to room temperature.

Currently the energy range of a TAS has been expanded to 0.1 – 120 meV. In stating the lower limit of this energy range, the key point is not the minimum energy transfer available but a statement about the resolution. Any instrument can be set to '0' meV but only a high-resolution instrument can distinguish inelastic scattering at 0.1 meV from the strong elastic scattering at 0 meV. Most of this improvement in range and resolution has come by introducing 'cold' moderators, which collapse the thermal-energy spectrum of the emitted neutrons to much lower energies than 'room temperature'. The cold-neutron source is basically a vessel of liquid hydrogen (temperature ~20 K), which is located inside the reactor vessel, close to the core, where the neutron flux is very high. Neutrons lose energy through collisions with atoms in the cold liquid and then travel towards the scattering instruments. With the availability of 'cold neutrons', spectrometers based on totally different principles have been developed e.g. chopper/time-of-flight, backscattering, or spin-echo spectrometers. The table below compares the energy windows for these machines to that of a modern thermal TAS.

In combination, a number of these spectrometers can probe excitations spanning over 7 orders of magnitude (up to 2000 meV for a chopper spectrometer, and down below 2 x $10^{-4}$ meV for spin-echo ) making inelastic neutron scattering a very powerful and flexible tool for materials research.

### *Canadian perspective*

Canada has three TAS instruments including the DUALSPEC instrument at the C5 beamline, which was half-funded by NSERC, and is one of the best thermal instruments in the world and is certainly the best polarized neutron spectrometer in North America. However, Canada has no cold source and no specialized instruments such as chopper/time-of-flight, backscattering, or spin-echo spectrometers.

The fact that Canada has no cold neutron source or other types of spectrometers limits Canadian scientists' participation in tackling the current problems – they can do only part of their experiments at home and have to travel to other laboratories to complete their research. With C5, numerous Canadian research groups are making important contributions to most of the topics described earlier: high-temperature superconductivity, heavy fermion systems, frustrated

## TABLE 1 - Comparison of energy ranges for various spectrometers

| Instrument Type (Name, Location) | Max. *Energy* Transfer (meV) | Best Resolution (meV) |
|---|---|---|
| Modern thermal TAS (C5, CNBC) | 100 | 0.2 |
| Cold TAS (SPINS, NCNR) | 10 | 0.06 |
| Chopper spectrometer (MAPS, ISIS) | 2000 | 0.3 |
| Chopper spectrometer (DCS, NCNR) | 7 | 0.04 |
| Backscattering (HFBS, NCNR) | 0.036 | 0.001 |
| Spin echo (NG-5 NSE, NCNR) | 0.041 (0.1 ns) | 0.0002 (20 ns) |

When the DUALSPEC instrument was installed in the early 1990s some modifications were made to the main concrete shielding of the NRU reactor.

magnets, and low-dimensional and quantum magnetism. Problems at today's leading edge often require access to lower energy excitations, such as low energy excitations in superconductors, or slow and sluggish movement of large polymer molecules. Types of spectrometers are needed to access different ranges of momentum and energy transfer, spanning 7 or 8 orders of magnitude.

Canadian scientists currently have to rely on foreign labs for cold neutron spectroscopy. This need is likely to increase as more and more problems in materials science require a probe of low energy excitations (diffusion of polymers, low lying excitations causing electron – lattice vibration coupling). A future Canadian neutron facility should include a cold neutron source and the cold neutron spectrometers that will enable Canada to sustain an active national competence to participate at the leading edge of materials research in such areas. These instruments are described in Section 3.

## 2.2 Crystallographic Analyses

The research community that exploits neutron beam methods to study crystal structures includes highly experienced neutron scattering scientists, for whom access to neutron beam facilities is central to their programs of research and education. On the other hand, a large fraction this community can be described as 'casual users'. These 'casual users' may be experienced practitioners of X-ray diffraction who need occasional access to the complementary information that can only be obtained by neutron diffraction. They may also be researchers whose primary characterization techniques are not diffraction based, and who need expert help to plan and execute a neutron diffraction experiment to complete a plan of research or education. Our ability to carry out crystallographic studies of materials was greatly enhanced in 1992, when the powerful C2 powder diffractometer was commissioned.

### *Overview, key applications and challenges*

The determination of structure is the first step towards understanding phenomena in condensed matter. Diffraction methods, in general, constitute the most powerful probes of structure at the scale of atoms, molecules and nanostructures. Diffraction is applicable across several scientific disciplines (e.g. materials physics, structural chemistry, materials science and earth science) for the study of battery materials, fuel cell components, superconductors and magnetic materials among many others. As a result, diffraction instruments like C2 are the most heavily used spectrometers at any neutron facility, and they are consistently oversubscribed.

Traditional diffraction methods determine what is known as the average structure, i.e., the long-range order integrated over an infinite length scale. Structural details of very great accuracy and precision concerning interatomic distances and angles can be obtained routinely from either polycrystalline or single crystal samples. Developments in software for the analysis of powder data over the past few years have made full *ab initio* structure determination from powder neutron data quite feasible. As well, diffraction measurements provide information on local order, which may extend only over nanometre length scales, using the technique of 'full pattern' analysis in which the real space pair distribution function is derived from the diffraction data. Neutron diffraction has a number of special advantages, as described generally above, but the two most important for crystallographic purposes are its sensitivity to magnetic structures, i.e., the arrangement of magnetic moments in materials, and its relative insensitivity to the atomic number of the elements involved in the scattering.

### *Current Canadian Use of Neutron Diffraction*

Powder neutron diffraction is by far the most widely used technique by Canadian scientists, which is also the situation internationally. The C2 diffractometer at the CNBC is the most efficient and most easily accessed powder diffractometer at any reactor-based neutron source in North America. The user assistance is outstanding as is the availability of ancillary equipment which makes possible measurements over a wide range of temperature from mK to ~ 2000°C. Currently, C2 is used by several research groups for the following experiments: refinement of crystal structures – especially those based on light atoms such as lithium or oxygen but also to distinguish elements of similar atomic number, *ab initio* solution of crystal structures, study of crystallographic phase transitions as a function of temperature and the study of magnetic structures and phase transitions. Users come from several academic disciplines in universities such as chemistry, condensed matter physics and materials science as well as from multi-disciplinary groups in national laboratories. There is no dedicated single crystal diffractometer at the CNBC, so these experiments cannot be done in Canada. In addition to C2, Canadian scientists make use of instruments at international neutron sources in both North America and Europe, such as the Neutron Scattering Centre at Los Alamos National Labs and the various diffractometers at the Institute Laue Langevin in Grenoble, France.

The following is a brief outline of recent and current research involving neutron diffraction by Canadian scientists using mainly the existing CNBC facilities, i.e., the C2 diffractometer. The disciplines represented are inorganic/solid state chemistry, condensed matter physics and materials science, primarily. Research areas range from more or less pure science topics to applications-oriented fields such as thermoelectric, magneto-caloric, non-linear optical, lithium battery and dielelectric/ferroelectric/relaxor materials. A significant number of undergraduate and graduate students as well as postdoctoral fellows have been trained in the use of neutron diffraction. The existing infrastructure has been essential in the success of these projects and in the training of highly qualified personnel; however, in order to remain internationally competitive, significant new investment in instrumentation is needed and will be described in later sections.

Refinement of crystal structures - In solid-state chemistry, it is often not possible to obtain single crystal samples for use in conventional laboratory X-ray structure determinations. If the materials contain light elements or elements with similar atomic number, X-ray powder diffraction is often not adequate to determine the structure. When a basic structure model is available, the structural details can be determined from a refinement of neutron data. For example the structure of the highly defective perovskite materials, $Ln_{1/3}NbO_3$ (Ln is a lanthanide ion) had been investigated using X-ray powder diffraction and the structural model of Figure 2.2.1 became widely accepted.[45] The X-ray data are dominated by scattering from the heavy elements and there is little information about oxygen. Subsequent neutron diffraction experiments, Figure 2.2.2, from a McMaster University group showed several reflections, which could not be explained by the X-ray model, and which arose from subtle shifts in positions of the oxide ions.[46] In an example from the organic solid state, the long-standing puzzle concerning the true structure of ammonium cyanate, $NH_4CNO$, which transforms to urea upon heating, was solved by neutron powder diffraction.[47] In this case the choice was between two hydrogen-bonding schemes in the solid state, N – H --- O or N – H --- N where the dashed line represents the hydrogen bond. Synchrotron X-ray data of the highest quality could not resolve this issue but a powder neutron experiment at C2 using a deuterated sample showed clearly

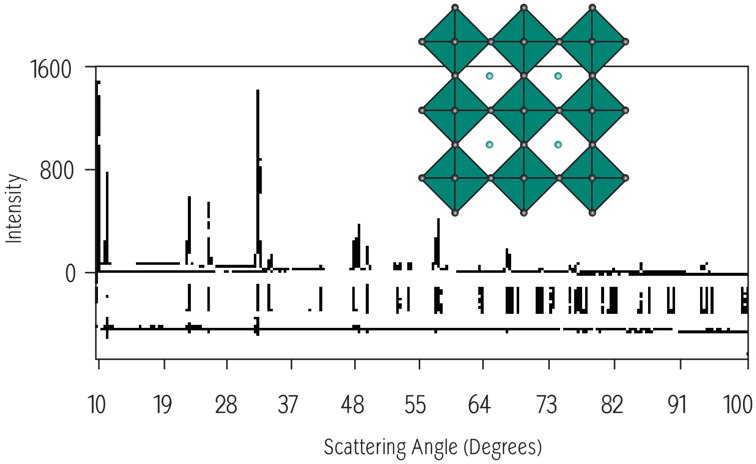


Figure 2.2.1 - The powder x-ray diffraction pattern of $La_{0.33}NbO_3$ and the derived structure.

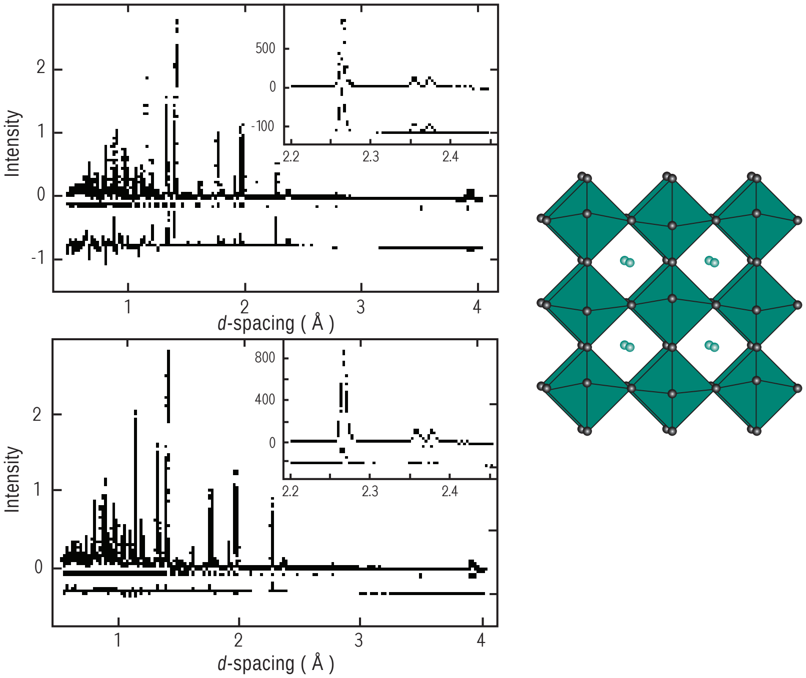


Figure 2.2.2 (Top Left) Neutron data refined on the x-ray model showing a poor fit. (Bottom Left) Neutron data refined on a model, which allows octahedral tilting (Right)

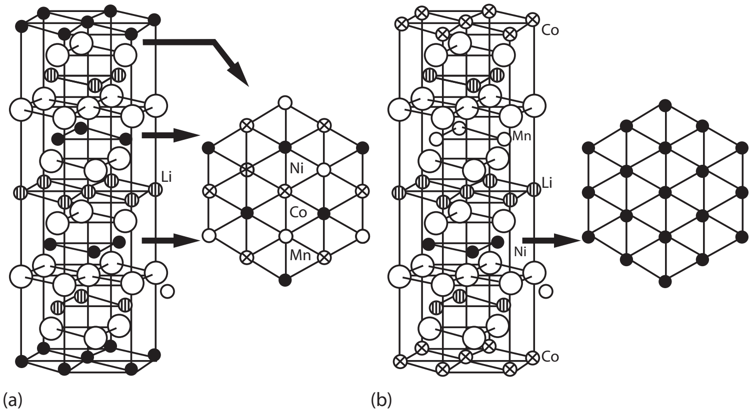


Figure 2.2.3 - Cation ordering models proposed for $Li(Mn_{1/3}Co_{1/3}Ni_{1/3})O_2$

that the N – H --- N model was correct. Here both the sensitivity of neutrons to H (or D) atoms and the ability to distinguish between N and O provided the key to the solution. Detailed studies of hydrogen bonding have also been carried out on inorganic materials, notably hydrated minerals with extensive H-bonding networks, such as $ZnSO_4 \cdot 7H_2O$ and $CaCO_3 \cdot 6H_2O$.[48], [49] In the case of the zinc sulphate, a combined refinement of single crystal X-ray data and neutron powder data was needed to elucidate fully the H-bonding scheme. For the calcium carbonate a new H-bond, undetected in a previous X-ray single crystal study was observed and much more accurate H – O distances were determined.

In an example from lithium battery research, the correct average structure of the candidate cathode material, $Li(Ni_{1/3}Mn_{1/3}Co_{1/3})O_2$, was determined by a group at NRC.

[50] Theorists had proposed two possible cation ordering models for the transition metal ions, Figure 2.2.3. Neutron diffraction is ideally suited to this problem as the scattering 'lengths' of Ni(10.3 fm), Mn(-3.73 fm) and Co(2.50) are very different. It was thus easy to determine, Figure 2.2.4, that there was no long range order of the transition metal ions in this structure. Groups from the University of Waterloo and Dalhousie University are also active in lithium battery research and are users of neutron powder diffraction.

The search for new thermoelectric materials is also an active area in Canada with a strong, established program at Waterloo and a developing program at McMaster. Such materials are usually small band gap semiconductors or semimetals comprised of heavy p-block elements, recent examples being Re$_3$Ge$_x$As$_{7-x}$ [51], and Ti$_{11-x}$Sb$_{8-y}$ [52]. In the former case, Ge and As are adjacent elements in the periodic table and, while difficult to distinguish with X-rays, the use of neutrons can handle this task quite well as scattering powers of Ge and As differ by more than 20%. In the latter case, a combined X-ray and neutron diffraction study was needed to refine the occupation of a defect site in the structure.

**Crystallographic Phase Transitions -** Powder methods are ideally suited to the study of crystallographic phase transitions as these induce twinning and often more severe problems in single crystals. When the materials of interest involve light atoms such as hydrogen or oxygen in the presence of heavy elements, neutrons are essential. For example WO$_3$, an important electrochromic material undergoes a number of phase transitions upon heating from room temperature.

A detailed analysis of one of the high temperature transitions, Pnma to P4/nmm, was based on high resolution neutron diffraction data. [53] A study of the orientational order-disorder phase transition in CaCO$_3$ was made possible using a special sample cell which takes advantage of the high penetrating ability of neutrons vis a vis X-rays. The transition which takes place at ~1260°C can only be studied under a

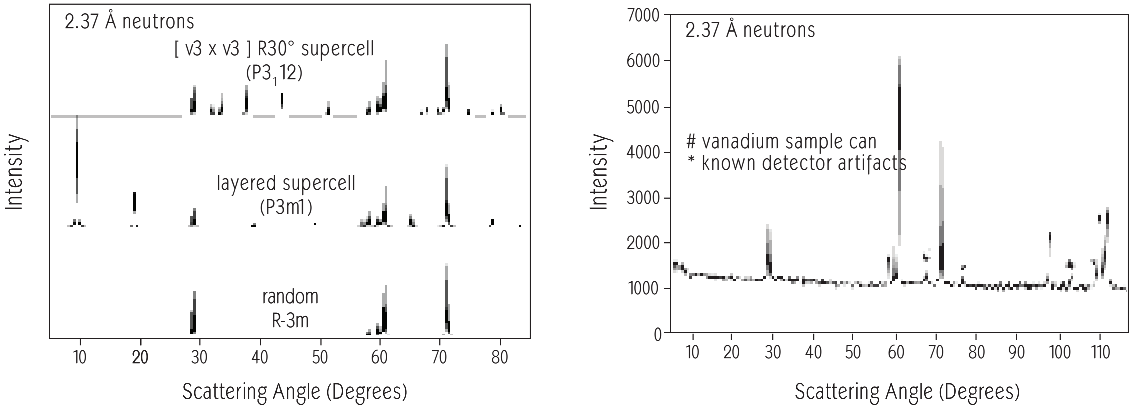


Figure 2.2.4 - Calculated neutron diffraction patterns for the two cation ordering models and a random model for Li(Mn$_{1/3}$Co$_{1/3}$Ni$_{1/3}$)O$_2$. The actual data show evidence for the random model (Right).

high $CO_2$ overpressure to prevent sample decomposition. A vanadium cell was constructed which could withstand both the required high pressure and resist the corrosiveness of $CO_2$ under those conditions. The nature of the phase transition could then be characterized as being due to rotations of the triangular $CO_3^{3-}$ ions.

When the perovskite is also an organic/inorganic hybrid compound, such as $CH_3NH_3PbBr_3$, the orientational order of the non-spherical cation can exhibit phase transitions. A study of this material in deuterated form using powder neutron diffraction showed that the sequence of phase transitions from low temperature is Pnma – I4/mcm – Pm3m. The Pnma space group of the lowest temperature phase was shown to be determined largely by the need to accommodate both the non-spherical cation and its H-bonding requirements into the cavity formed by the $PbBr_3$ framework. [54] Such a study could only be done with neutrons. Other perovskites of great current interest are the dielectric/ ferroelectric/ relaxor oxides with compositions such as $Pb(Zn_{1/3}Nb_{2/3})O_3$, $PbTiO_3$ and a variety of solid solutions between these and related phases. Here phase transitions can be introduced by variation of temperature and the application of high pressure and electric fields. An internationally leading program is well established at Simon Fraser University.

**Ab initio structure solution -** Developments in software for the determination of crystal structures ab initio from powder data have made this approach quite feasible if not yet routine. There are two basic approaches, one treats the powder dataset as a limited single crystal dataset and phasing is done using standard direct methods, which are applied to as many independent reflections as can be isolated. SIRPOW is such a software package. The second is a radical departure in which the structure is modeled in direct space using Monte Carlo methods exemplified by TOPAZ and FOX. A McMaster-based group has succeeded in solving fairly complex structures of non-linear optical materials using the latter approach with X-ray and neutron powder data. In one case the structure of $Bi_2ZnB_2O_7$ was solved ab intio using FOX. Here, a trial structure was obtained from X-ray data and the final refinement was carried out using C2 neutron data to locate the B and O atoms. More interestingly, the crystal structure of the non-linear optical material, $SrBi_2O(BO_3)_2$ was solved *ab initio* using only neutron powder data. This was a highly challenging problem as the structure is non-centrosymmetric, P63, and there was ambiguity whether the borate group was present as a pyroborate, $B_2O_7$, or orthoborate, $BO_4$. In addition, the use of neutron data disclosed a weak superstructure due to displacements of O atoms, which would have been invisible to X-rays. This activity will only increase in the future.

**Magnetic structures and phase transitions -** Neutron diffraction is the ultimate probe of magnetic structures. Several Canadian groups focus on magnetic materials, especially transition metal oxides, pnictides and intermetallic compounds. Strong programs exist at McGill, McMaster, Manitoba and Alberta. Some highlights include the discovery of a new itinerant electron ferromagnet, $LaCrSb_3$, $T_c$ = 125K with a Cr moment of ~ 1.0 $_B$. [55] Many studies of either low dimensional or geometrically frustrated materials have been carried out including the very rare ferromagnetic insulator $PbMnBO_4$ [56], the frustrated spinel $Li_2Mn_2O_4$ in which the magnetic correlations are two dimensional while the $Mn^{3+}$ lattice is three dimensional [57] and the unique layered ferrimagnets $La_5Re_3MO_{16}$, where M = Mn, Fe, Co and Ni. [58] The use of the high resolution mode at C2 permitted the unambiguous determination of the magnetic structure of a distorted perovskite, $NdTiO_3$, for the first time from powder data. [59] Ordered moments as small as 0.3 $_B$ were refined for $Ti^{3+}$. As well, it was also possible to show that long range antiferromagnetic order vanishes well before the onset of true metallic behaviour in hole doped $Nd_{1-x}TiO_3$, correcting an earlier report which claimed that antiferromagnetic order persisted well into the metallic regime. A variety of intermetallic magnetic structures

Graduate students, who visit the neutron facility, benefit from hands-on experience under the joint supervision of their professor and a facility scientist.

have been determined for several materials with the $Ln_5Si_4$ structure type which is the basis for a new generation of magneto-caloric materials, including $Er_5Si_4$ and $Nd_5Si(Ge)_4$. [60] A very complex non-collinear magnetic structure was detected for $TbFe_{10}V_2$ resolving a controversy concerning the interpretation of its bulk magnetic properties. [61]

One important and rapidly growing area in which Canadian scientists are in a leadership position internationally with strong programs at Waterloo, UBC and McMaster, is that of highly frustrated magnetic materials. Such materials often adopt so-called "exotic" ground states which lack long range order such as spin glass, spin liquid or spin ice states. Neutron diffraction is the ultimate tool for establishing or ruling out long range order. This has been the case for iconic compounds such as the pyrochlore lattice phases $Tb_2Ti_2O_7$, $Li_2Mn_2O_4$ or the ordered double perovskites $Sr_2CaReO_6$ or $Sr_2MgReO_6$. [62],[63],[64]

## *New Directions in Neutron Diffraction at a New Neutron Source*

Qualitatively new experiments will be possible at an advanced neutron source. Currently, it is possible to study the thermodynamics of phase transitions and chemical transformations in the solid state within certain limitations as discussed below. One can envisage moving to studies of the kinetics, involving time as a critical variable, of solid state transformations which can take place in situ – for example in the operation of lithium batteries or fuel cells under realistic conditions. Currently, we can determine the so-called 'average structure' of materials. As the study of so-called nano-materials expands, there will be increasing demands for structural information on more local length scales, which may range from nearest neighbours to several 10's of nanometres. Neutron pair distribution function analysis (NPDF) will become invaluable as information can be obtained on essentially all possible length scales from infinite (the average structure) to nearest neighbours and nearly every intermediate regime from the same experiment. The anticipated order of magnitude increases in flux on sample and companion developments in counting efficiency will make small (< 1g) samples routine. This will open the door to experiments using separated isotopes, thus greatly expanding elemental contrast situations and most importantly, enabling magnetic scattering studies of compounds containing the notorious neutron absorbers Sm, Gd and Eu.

The most significant advances will take place in single crystal neutron diffraction, because single crystal facilities are not currently available at the CNBC. Exploiting new technologies in the focusing of neutron beams and improvements in detector efficiency, the size of a 'neutron sample' can be shrunk to the dimensions used in conventional X-ray diffraction studies – opening the neutron technique to a new class of users. In particular, we expect to include pressure as a variable in the study of solid-solid transformations where small sample sizes cannot be avoided. It should be possible to study hydrogen bonding for example in complex biomacromolecules using neutrons for the first time in Canada.

In addition to new areas, our capabilities in the more traditional applications of neutron diffraction will be greatly enhanced, placing us on a truly competitive footing, internationally. The existing powder diffractometer, C2, while still performing admirably, was designed and constructed in the early 1990's and has some limitations. For example the upper range for scattering angle is less than 120° (2 ), whereas 160° is desirable for most applications, and the 800-element detector is no longer state of the art. Focusing monochromators are not used, so the potential flux on sample falls well short of that available on the best instruments internationally. Basically, C2 must satisfy contradictory demands of high efficiency and high resolution and it is no longer able to do either at internationally competitive levels.

## 2.3 Materials Science and Engineering

The materials engineering community includes some highly experienced scientists, many of whom work closely with industry. They tend to view neutron beam methods as an innovative complement to other experimental tools. Therefore, the majority of community members are 'casual users'. These casual users may have some experience with X-ray diffraction but need occasional access to the complementary information that can only be obtained by neutron diffraction. More frequently, they are researchers whose primary characterization techniques are not diffraction based, and who need expert help to plan and execute a neutron diffraction experiment to complete a plan of research or education. Canada's contribution of neutron beam methods to fundamental materials science and engineering developed synergistically with the emergence of the program 'Applied Neutron Diffraction for Industry', beginning in the mid 1980s.

### *Overview – how neutrons support materials science and engineering*

Materials Science and Engineering (MSE) deals with the development, design, processing, characterization, and qualification of materials used in structures, devices, products, and systems. Thus, MSE is concerned mainly with the materials that will become part of a device or structure or product made by man.

The applications of neutrons in MSE have tended to focus on practical problems related to material performance and reliability, public safety, and fitness-for-service. Most of the neutron beam research is performed in partnership with university researchers, with the results made available in published literature. By collaborating with universities, companies can explore new directions that could revolutionize their products or businesses, with little economic exposure. On the other hand, neutron beam methods can also be used to solve immediate problems of industrial importance. This has led to consistent fee-for-service work by NRC staff at the Canadian Neutron Beam Centre, since the mid 1980's, under the Applied Neutron Diffraction for Industry (ANDI) program. The ANDI program was designed to put neutrons to work for industry and society by enhancing industry competitiveness and stability, ensuring reliable services (rail, aerospace, automotive, power generation and distribution) to the public, and ensuring public safety. Over 200 proprietary reports have been provided to industry clients, such as: Pratt & Whitney Canada, Alcan International, Sydney Steel Corp., Syncrude, Welding Institute of Canada, Atomic Energy of Canada Ltd., Defence R&D Canada (Atlantic), Ontario Power Generation, IPSCO, IVACO, Dynetek, Rolls Royce and Associates, Boeing, ExxonMobil, NASA, Martin Marietta Energy Systems, US Dept. of Energy, Hitachi Ltd., British Petroleum Research Inst., Westinghouse-Bettis, LevelTech, GE Aviation, and Tokyo Electric Power Company.

## *Society's changing relationship with materials – key challenges*

Recent advances in the theoretical understanding of the structure and behaviour of materials, driven by new experimental techniques, new modelling tools (computers), and new models, have changed our fundamental relationship with materials - we are learning to predict the behaviour of materials under different conditions. This will allow us, ultimately, to deliberately design optimized materials for specific applications, rather than search for them in semi-empirical, inefficient, costly ways. Indeed, "the Age of Discovery in materials is drawing to a close, to be replaced by an Age of Design, in which human creativity will offer new materials and ways of creating them". [65]

**Two key challenges have emerged in MSE as a result of our evolving relationship with materials:**

1 **Model validation -** As our understanding of materials grows, we are developing tools and methodologies for computational materials design. Human beings have the ability to infer mechanisms from observed properties. This ability is critical for the development of computation tools for materials design, but it is not sufficient – we must validate our models and theories, by testing their predictions, and by confirming the mechanisms that underpin them. Model validation can only be accomplished through careful experiments. The unique knowledge obtained from neutron beam measurements is used to refine models, paving the way to improved products and reduced costs, and allowing innovative Canadian companies to compete successfully in the global economy.

2 **Material and component qualification -** We rightly demand more of our new materials – they should be more reliable, last longer, and perform better under more difficult conditions. Qualification refers to measurements and/or inspections undertaken to ensure that a material or component can perform its intended purpose satisfactorily (safely, reliably, economically). It is an activity that must be undertaken periodically throughout the lifetime of critical components. How many (more) flights can an airplane make before it must be retired? Is a landing gear system suitable for continued use after an unexpectedly hard landing? Is it safe to resume operations in a plant (chemical, manufacturing, power generation) after an unexpected failure? How do we prove to regulators that a new, more efficient material or process is suitable for a given application? How do we optimize processes? More fundamentally, how can regulators establish guidelines that ensure that the public is well protected? Neutron beam techniques provide clear answers to many of these questions – insights that can help prevent economic loss, ensure availability of critical services, and save lives.

The interactions of neutrons with matter lead to unique and powerful methods to address the critical issues of *model validation* and *material qualification*. The great benefits of neutrons in MSE stem from their ability to penetrate deeply (several cm) into most materials, allowing bulk materials, as well as multi-component devices and structures, to be studied in detail. Material behaviour under service conditions, and during fabrication is of particular interest. Here again, we draw on the penetrating power of neutrons, which can easily probe materials contained in a suitable sample environment that simulates the actual conditions encountered in the field. Neutrons also have a unique sensitivity to hydrogen, whose presence is known to severely impact the performance of many structural materials.

## *Neutron Diffraction for Materials Science and Engineering in Canada*

Neutron scattering methods in which Canadian researchers in Materials Science and Engineering have considerable expertise include macroscopic and intergranular stress mapping, crystallographic texture analysis, characterization of material heterogeneity, in-situ experiments to study load partitioning and phase transformations, and imaging methods. Some details are summarized here:

**Residual Stress scanning -** Engineering materials undergo complex processing schedules (melting and casting, heating and cooling, rolling, extrusion, welding, etc…). These processing steps lead to residual stresses, whereby one part of the material or component pushes or pulls against another part. [66] There is no external evidence of this 'inner turmoil' - we just see a chunk of stuff that sits quietly, for example, on a desk, or under the hood of a car. However, residual stresses affect the performance of mechanical parts because they superpose on (add to) the applied stresses that the component experiences in service, which can cause unexpected failures with potentially disastrous consequences. Residual stresses are not always bad - they can be tailored to benefit the intended application, provided we understand how they are produced.

Neutron diffraction is recognized by regulatory agencies as an excellent and viable technique for the measurement of residual stresses. The concept behind the method is simple. Many engineering materials (metals, alloys, ceramics) have a well-defined, orderly, periodic arrangement of atoms (a crystal structure). The atoms can be viewed as lying on sets of parallel planes with a characteristic spacing. In the unstressed condition, the plane spacing has a well-defined value, which can be measured directly by neutron diffraction. When the material is stressed (either internally or via externally applied forces), the plane spacing changes. The difference between the stressed and unstressed plane spacing is used to calculate strains, which are converted into stresses via simple relations.

The high penetrating power of neutrons makes them ideal for the evaluation of stress 'at depth' in engineering components. With careful use of apertures before and after the specimen, gauge volumes ranging from 1 mm$^3$ to 1000 mm$^3$ can be defined. The gauge volume is simply moved over a grid of locations deep inside components to map residual stresses in macroscopic materials or components. No other technique can accomplish this over the enormous range of sample sizes required - from small rivets a few millimetres in length to pipeline sections nearly a half metre in diameter.

Neutron stress scanning is non-destructive in that it is not necessary to disturb the internal stresses in order to measure them. This is in contrast with all non-diffraction techniques, which require that the part be machined, thereby relaxing the stress state we are seeking to measure.

The stress distributions measured by neutrons are directly comparable to those modelled with commercial finite element packages. Neutron residual stress mapping is thus an invaluable tool for validating and refining these models.

Recognizing the industrial and scientific importance of residual stress scanning, as exemplified in Canada, all of the major neutron laboratories in the world have now built, or are building, dedicated stress scanning instruments based on the Chalk River lead (Table 1). The superior design and construction of the primary Canadian stress-scanning machine (L3), were essential to establish the technology in the first place, and L3 remains the instrument to beat in the world.

Canadian macroscopic stress scanning activities have influenced a number of industries within Canada and abroad. Highlights include:

- Participating in NASA's (National Aeronautics and Space Administration) Columbia Accident Investigation Board.
- Evaluating the effectiveness of stress mitigation processes for the Yucca Mountain Project, where nuclear waste containers are being designed to survive 10,000 years
- Qualifying suppliers of nuclear materials to facilitate international sales of Canadian nuclear technology.
- Evaluating the effects of radiation on stresses on welds and joints, providing solid knowledge to make life-extension decisions for nuclear plants. [67]
- Measuring residual stresses in aeroengine components to understand failure. [68]
- Validating models the residual stresses fields to be expected in a turbine discs [69]
- Measuring stresses near the interface of diffusion-bonded composite. [70]
- Providing unique knowledge to allow a Canadian steel company to expand its market.

TABLE 2 - Materials Science and Engineering Diffractometers around the world.

| Country | Source type | Laboratory | Instrument name |
|---|---|---|---|
| France | Reactor | Institut Laue-Langevin | SALSA |
| Germany | Reactor | FRM-II | STRESS-SPEC |
| Germany | Reactor | HMI | E3 and E7 |
| Australia | Reactor | OPAL | Kowari |
| Switzerland | Continuous spallation | SINQ | POLDI |
| USA | Pulsed spallation | LANSCE, Los Alamos National Labs | SMARTS, HIPPO |
| UK | Pulsed spallation | ISIS, Rutherford-Appleton Lab | ENGIN-X |
| Japan | Reactor | JRR-3, Japanese Atomic Energy Agency | RESA |
| Japan | Pulsed spallation | J-PARC, Japan Spallation Neutron Source | "Ibaraki"<br>"Takumi-JAEA" |
| USA | Pulsed spallation | Spallation Neutron Source, Oak Ridge National Labs | Vulcan |
| USA | Reactor | NIST Center for Neutron Research | BT8 |
| USA | Reactor | HFIR, Oak Ridge National Labs | NRSF2 |
| Canada | Reactor | NRU, Chalk River Labs | L3 and E3 |

*The Canadian neutron beam laboratory has provided Marubeni Canada Ltd. with access to a unique measurement probe, which has provided a basis for business with clients in Japanese heavy industries. The Canadian expertise in neutron beam research is world-class and should be retained by ensuring there is a neutron source into the 21st century.*

*Mr. Jun Fukuhara,*
*President & C.E.O.*
*Marubeni Canada Ltd. (1999)*

**Intergranular strains -** Unlike macroscopic stress scanning, which measures the stress distribution on the scale of a component, intergranular strain measurements examine the strains that develop on a much finer scale – that of the crystals that make up the large majority of engineering materials. Neutron diffraction studies of intergranular stresses reveal load sharing behaviour or intrinsic thermal strains of various crystallographic orientations in monolithic materials and composites. Additionally, intergranular strain measurements are also of great importance for testing elastic-plastic models of the mechanical behaviour of polycrystalline aggregates at the grain level, which are critical to our interpretation of macroscopic stress maps and the understanding of processes such as metal forming. Such information is also important for lifetime performance predictions, particularly in cases where preferred orientations of grains (texture) may introduce anisotropy that influences macroscopic behaviours such as creep and growth.

**In-situ studies -** The penetration of neutrons makes possible in-situ experiments in which conditions such as temperature, atmosphere and mechanical loading can be applied to materials at the same time as neutron scattering reveals what is happening at the crystallographic level. The Canadian Neutron Beam Centre has been a leader in developing unique neutron-compatible sample environments and fixtures for in-situ tests. These include high-temperature, environment-controlled furnaces for use in understanding and optimizing thermomechanical processing schedules, a quenching furnace, fixtures for biaxial loading, humidity-controlled cells, devices for handling and studying geological ice, and a unique system for studying hydrogen-storage materials. Highlights of in-situ studies include:

- In-situ neutron diffraction measurements on pipes subjected to simulated underground loading conditions were central to a study of water main pipes. The neutron diffraction results were combined with finite element modelling to improve municipal inspection protocols in order to reduce the risk of catastrophic failures with high collateral damage. [71]

*Ipsco is a Canadian steel company whose product was barred from the bridge-building market because an old engineering code rejected their manufacturing method. Neutron scans of typical steel specimens from Ipsco revealed that the internal stresses of their product are not a concern. The neutron scattering results formed the basis of the case for changes to the code, thus opening a new market for their product.*

Neutrons can map stresses in a bent water main to validate computer models.

Figure 2.3.1 Making the right decision about fitness-for-service of older water mains requires solid knowledge. Replacing infrastructure too soon entails higher cost to taxpayers, but leaving pipes in place too long runs a risk of failure and damage to the other structures.

- One of the most exciting developments in in-situ testing has been the ability (since 1993) to measure the response to applied loads of different families of grains in polycrystalline metals and alloys. These measurements have revealed how stresses develop and change under controlled loading conditions around notches, holes and bends, and have been used to validate state-of-the-art computational models of polycrystal plasticity. [72]-[76]

- Fusion welding is one of the most common joining processes, but also a very complex one. In a world first at Chalk River, in-situ measurements of phase and stress evolution during Gas Tungsten Arc Welding (GTAW) of a plain carbon steel were made. [77]

**Crystallographic texture -** Most common materials, including metals, minerals, structural ceramics, semiconductors, and superconductors, are polycrystalline aggregates - they are made up of small (nanometre to centimetre) crystals, aggregated together to form a macroscopic piece. *Crystallographic texture* (or simply *texture*) deals with the crystallographic orientation of the component crystals (*grains*). The properties of the aggregate depend on the texture because the properties of the crystals are themselves anisotropic (they depend on the crystal direction in which they are measured). The nature of the boundaries between crystals (*grain boundaries*), which has a profound effect on material properties, is also naturally related to texture. Recognition of the importance of grain boundaries has led, in recent years, to a whole new field of study – grain boundary engineering. Examples of properties that depend on texture include the elastic properties, strength, ductility, fatigue life, toughness, magnetic permeability, and electrical conductivity (including superconductivity), and susceptibility to hydride cracking. Neutron diffraction is the most accurate method to analyze texture quantitatively, because neutrons can truly sample the bulk material, regardless of specimen orientation.

**Microstructural heterogeneity on varying length scales -** Microstructural heterogeneity may be introduced deliberately to facilitate a desired performance characteristic; more often it is an unwanted by-product of manufacturing processes which can affect performance adversely. In either case, the determination of such heterogeneity is of critical importance in many engineering and design applications. Neutrons are ideally suited to evaluating microstructural and crystallographic variations, a good example being the survey of microstructural variations across aluminum sheet, whose resulting rough surface is unsuitable for automotive body panels. [78]

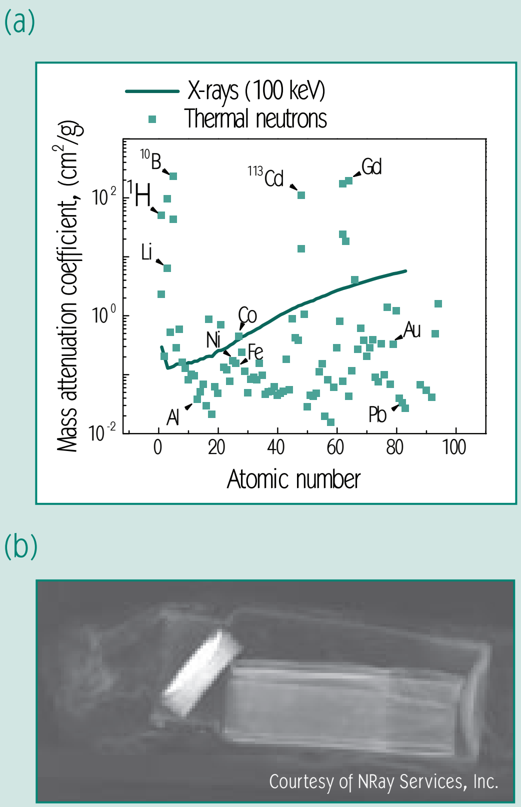
### *Neutron Imaging*

Analogous to X-ray radiography in medicine, neutron radiography is performed by shining a neutron beam onto a specimen, and recording the image on a suitable detector placed behind the specimen. A 2-D image of the internal structure of a material, component, device, or assembly is thus obtained non-destructively. Neutrons and X-rays interact differently with materials. In some cases they produce similar information, but often they produce different, complementary information. While X-ray attenuation scales directly with atomic number, neutrons are efficiently attenuated by only a few specific elements. When these few elements are present, neutron radiography is the most effective method for inspection. In other words, in many cases neutrons are the best, non-destructive way to see inside an object, component, or assembly.

For example, organic materials or water are clearly visible in neutron radiographs because of their high hydrogen content, while many structural materials such as aluminium or steel are nearly transparent. Figure 2.3.2(a) shows how various elements interact with X-Rays and neutrons.

Figure 2.3.2 (b) shows an image of an historic document, from the time of Louis Riel. In those days, important documents were stored by putting them in a bottle, sealing the bottle with a cork and wax, and wrapping the package in lead foil. X-rays would not be able to produce this image which proves the document inside was intact because the X-rays could not penetrate the lead foil. Even if they could, the paper would be nearly invisible to the X-rays.

Neutron radiography is used extensively in the geology and aerospace sectors as a non-destructive inspection technique for the inspection of aircraft turbine blades, or the examination of fluid behaviour in internal channels and cavities of engineering components, soil, rock and ceramics. Canadian company NRay Services Inc. (Dundas, Ontario) is a world leader in applying neutron radiography to engineering problems. NRay, a spin off of Atomic Energy Canada Ltd., uses the radiography facility at McMaster to conduct their work, but are currently looking for other facilities to expand their services. NRay have stated that they would build a new



Courtesy of NRay Services, Inc.

Figure 2.3.2 (a) X-Ray vs. neutron attenuation by atomic number. (b) An example of what that means: only neutrons see a historic paper document inside a lead-wrapped casing, demonstrating that the document is intact without opening the package.

world-class radiography facility in a new high flux reactor built in Canada.

Figure 2.3.3 shows an NRay neutron radiograph of the air-cooling channels in two aeroengine turbine blades. The blade on the left has obstructed channels, making it impossible to cool properly in service, which can lead to disastrous consequences.

In neutron tomography, a series of radiographs is taken with the specimen at different orientations with respect to the incident beam, and recombined to non-destructively generate a 3-D image of the internal structures and cavities of a component or device. The 3-D image can be used to accurately determine the internal dimensions of complex components, or to reveal flaws that can lead to failure. Figure 2.3.4 shows a detailed tomographic reconstruction of a CANDU reactor feeder pipe (in cross-section). The variations in the wall thickness in the figure arise from the pipe bending process, and can adversely affect the performance of the pipe. The pipe was not sectioned for these measurements.

## *Future Science and Impacts*

Materials and components in the future will have to meet new standards driven by environmental concerns (e.g. higher performance to weight ratios) and increasingly demanding environments. This applies to all industries that depend on improved materials and processes for improved efficiency, reliability, and performance.


Courtesy of NRay Services, Inc.

Figure 2.3.3 Neutron radiograph of air-cooled turbine blades

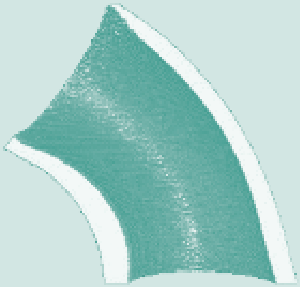


Figure 2.3.4 - Tomographic reconstruction of a bent feeder pipe.

Recently, the International Atomic Energy Agency (IAEA) recognized that as the world enters a new nuclear energy age, significant, but incremental changes to power reactor designs are placing materials under ever more demanding conditions. Generation IV reactors, with their higher operating temperatures and more corrosive media, will place even greater demands on materials. The IAEA has specifically recognized that neutron diffraction must play a role in the development of these materials, stating "…neutron based methods in particular have played and will continue to play an important role in research in materials science and technology… A materials development program will therefore play a major role in the design and development of new nuclear power plants, for the extension of the life of operating reactors as well as for fusion reactors." [79]

New instruments and methods are needed to drive new science, and to enable us to probe material behaviour at an unprecedented level of detail that will allow us to develop better predictive models of material behaviour, and to achieve higher performance, safety, and reliability. Neutron scattering techniques and facilities must advance in Canada to respond to advances in materials science and engineering. Instruments at a new Canadian Neutron Centre must be able to continue and improve on existing measurement capabilities. Overall, this means smaller, more intense neutron beams and better detection capabilities leading to faster and more efficient collection of high quality data. This will open up new fields of study, hitherto inaccessible to neutron beam methods, and where the unique properties of neutrons will provide new insights for progress.

**The white beam stress scanner -** Although the Canadian stress-scanning instrument, L3, has been the international benchmark for many years, other countries are now positioning their facilities to supersede our capabilities. The next-generation instrument for neutron-based Materials Science and Engineering in Canada will be a 'white beam' stress scanner. [80] This instrument will enable the measurement of many different crystallographic directions simultaneously, thus improving the efficiency and speed of measurements. The performance of a white-beam instrument at a high flux reactor source is expected to outperform time-averaged measurements on a spallation source instrument, while retaining the great advantage of superior spatial resolution. New fields of study can therefore be envisaged:

- With finer resolution and higher flux it will become possible to obtain two-dimensional maps around realistic cracks in full-scale components, as needed to understand the mechanisms underlying stress-corrosion cracking.

- Composite materials (e.g. metal matrix, cermets and ceramic matrix) and multiphase alloys have stress-strain interactions between the constituent phases, that can best be understood by simultaneous monitoring of strain response among phases during deformation, which is only possible with a broad-spectrum diffraction method.

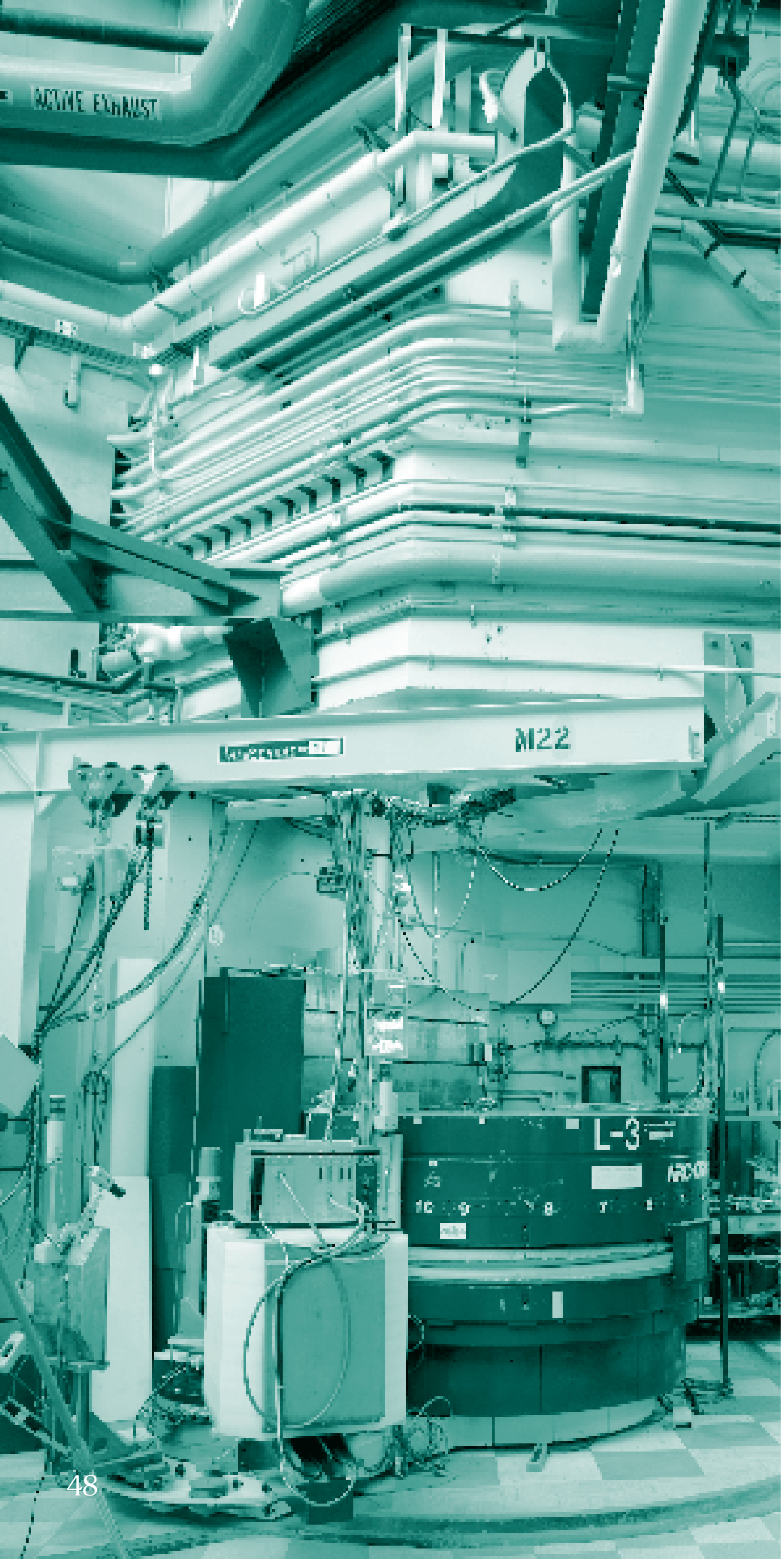
- Faster data collection would provide the opportunity to study microstructural evolution in real time for many systems to better understand manufacturing processes such as casting and forming.

- Interfaces internal to a component or a composite material are uniquely accessible to neutrons. Examples of this application exist, but obtaining data very close to the interface or at interfaces deep in large samples constitutes a significant challenge that can only be overcome using an optimized instrument. Interfaces are of interest in the studies of barrier coatings, composite structures that provide improved strength/weight ratios and smart composites.

- The white beam stress scanner will enable a new class of in-situ studies because of the higher data rates it will allow: better time resolution, lower volume fraction limits, the ability to study weakly scattering or more strongly absorbing materials.

- Able to acquire complete pole figures simultaneously at a number of (*hkl*) values, the white-beam scanner can also serve as a high throughput texture instrument that preserves the advantages of the current "classical" texture instrument.

**Scanning Neutron Microbeam -** As materials become more and more sophisticated and tailored to classes of applications, the ability to understand their macroscopic behaviour on the microscopic level is essential. At the leading edge of this field is the use of a neutron microbeam to probe stress and crystallographic orientation on a grain-by-grain basis. X-ray and electron microbeams are providing unprecedented knowledge of what happens in materials at length scales comparable to and below the size of the grains. However, these techniques are generally limited to the surface or very near surface, where the behaviour will be different. Only a neutron beam technique can provide this information at depth in full-scale components non-destructively (i.e. without sectioning the material so that subsurface material does not become the new surface material). Data



obtained at depth, resolved on the scale of grains, can provide unprecedented information on such localized phenomena as crack propagation (including stress corrosion cracking), ingress of foreign elements in materials (good or bad), and failure of interphase boundaries in composite materials. A neutron microbeam prototype was tested and proven at Chalk River through a collaboration of researchers from the NRC-Canadian Neutron Beam Centre, and Oak Ridge National Laboratory in the U.S. [81] Further development and practical implementation of this technique awaits the higher fluxes and dedicated white beam instrument design of a new Canadian Neutron Centre.

Technologically advanced materials such as shape memory alloys, magnetic shape memory alloys, smart materials, energy harvesting materials, and medical composites are all expected to benefit from spatially resolved measurements of microstructure within the material volume.

**Neutron Radiography and Tomography -** The Canadian Air Force uses neutron radiography to inspect certain composite flight control surfaces on their aircraft. These components are susceptible to water ingress and must be inspected periodically. The light shaded regions in Figure 2.3.5 reveal water inside the control surface of a Canadian CF-18 fighter jet. Neutron radiography is the most sensitive technique available for these inspections. The air force has set up a neutron radiography facility at the Royal Military College (Kingston, ON), which is capable of inspecting large surfaces. However, the facility uses a SLOWPOKE-2 reactor, which has a very low neutron flux, resulting in low quality images that require long exposure times. A dedicated radiography facility constructed as part of a new, multi-purpose research reactor would have a much higher flux yielding better images at shorter exposure times. It could also be designed to accommodate much larger specimens than are currently possible. Naturally, the instrument would also be suitable for tomographic studies. This capability would be an important asset for defence R&D,

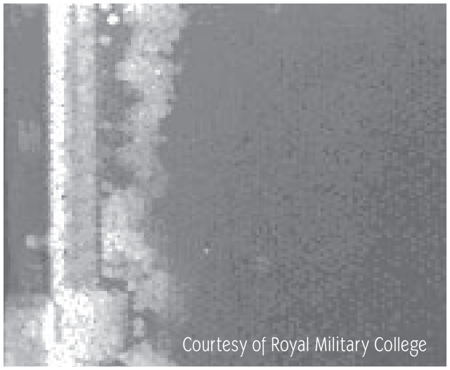


Figure 2.3.5 Detecting water inside a CF-18 component

as it would constitute an effective and efficient means to achieve safe and reliable operation of current and future aircraft fleets, which make heavy use of composite materials.

Research in neutron radiography has two main goals: to increase the speed at which images can be acquired, and to improve the quality of the images obtained. At present, in Canada, neutron radiographic images typically take several seconds or minutes to acquire. Recent advances worldwide have produced real-time imaging capabilities that approach moving picture frame rates (e.g. 15-30 frames per second), but many processes take place at higher rates than these. An effective solution for cyclic processes is stroboscopic data collection, in which multiple images are acquired at the same point in a cycle, over many cycles (it is assumed that the material does not evolve significantly over the number of cycles required to obtain a good-quality image). However, with a higher flux and dedicated radiographic instrumentation, real time images could be produced of single-shot moving components and fluids, and of material processes, such as injection moulding or casting, thus allowing expansion into new areas of engineering evaluation and development of fabrication processes. Imaging of hydrogen and water in real systems in real time (fuel cells) would also make effective use of one of the unique properties of neutrons. Real-time images of slow processes are already possible, but even these process rates are too high for current Canadian capabilities.

Several of the leading facilities around the world have installed a cold neutron radiography capability, which can produce a superior radiographic image. Other recent advances, such as phase contrast enhancement and energy selective imaging, also increase the quality of radiographs. The superior resolution and excellent detail provided by these emerging techniques are only possible with high-intensity neutron beams. A new neutron beam facility would allow the Canadian neutron radiography community to continue to develop these fields of research and provide an optimized instrument that would benefit the national scientific and engineering communities.

## 2.4 Thin Films and Surfaces - Nanostructures

The research community using neutron beam methods to study in thin films and surfaces has been growing in parallel with the development of neutron reflectometry at Chalk River. However, in 2002, a team of researchers from 13 universities, led by The University of Western Ontario, secured funding through a national program of the Canada Foundation for Innovation to construct Canada's first dedicated neutron reflectometer. This new instrument commenced operation in 2007, providing Canadians with a competitive facility to enable world-class research on phenomena that occur on the nanoscale across several disciplines. Neutron reflectometry has emerged, and its user community is expected to grow as university scientists become increasingly experienced in applying this experimental methodology to their programs of research and education.

### *Overview*

While materials are the building blocks of our world, and it is important to understand their structures and dynamics, the next step is to understand how materials interact with each other – that is, to explore what happens at surfaces and interfaces.

Surface science and thin film phenomena appear in the whole range of condensed matter physics. Neutron scattering has the unique advantage of being sensitive to isotopes (e.g. hydrogen and deuterium) and to magnetic structures. It has proven to be invaluable to polymer and biological sciences as well as magnetism. The large penetration depth of neutrons allows non-destructive evaluation deep inside the specimen and/or sample environments.

Neutron Reflectometry (NR) is emerging as a workhorse technique in the area of thin films and surfaces. It offers the unique capability of determining the chemical and magnetic profile in thin films. By using NR it is possible to map the distribution of a gas or liquid, to monitor the growth of an oxidation front, or to study the magnetic properties of magnetic films used in advanced information technologies. In the past five years there were more than 600 research articles in the 'INSPEC' data base that used NR.

### *Current thin film research*

Despite the fact that up to now only about 40% of the C5 spectrometer time was available for thin film studies, a very wide range of different scientific areas (e.g. corrosion, thin magnetic films, polymer films, and biocompatible coatings) was covered. The following list shows collaborations with Canadian researchers (corrosion, thin magnetic films, polymer films, biocompatible coatings) and international researchers (thin magnetic films and multilayers) as well as areas not yet explored at Chalk River but where NR has been applied very successfully elsewhere (giant magnetoresistance sensors, hydrogen storage, nanostructured materials) and where Canadians could use NR as a powerful tool for their research in the future:

**Corrosion -** Canadian scientists have used neutron scattering techniques to do corrosion related research. Their projects, some completed and some ongoing, fall into two categories: ( i ) investigation of reaction kinetics [83] and ( ii ) study of nature and growth of the passive oxide layer [84], [85] that provides protection against corrosion. Given that Canada has many industries that rely on corrosion prevention (e.g. ship building, oil and gas exploration, automobile manufacturing, and nuclear power to name a few) research on corrosion will continue in the future, and neutron scattering will continue to make its contribution by providing results that could not be obtained by any other method. Corrosion science is inseparable from elechtrochemistry (see below) as metals corrode via an electrochemically driven reaction;

**Electrochemistry -** Electrochemistry is the study of charge-transfer reactions that take place on the surface of solids, usually in contact with a liquid electrolyte solution. It encompasses technologically important topics such as batteries, fuel cells, electroplating and anodization. Since the chemical and physical changes are confined to the solid/liquid interface, electrochemistry naturally falls under the surfaces and interfaces research carried out with techniques such as neutron reflectometry. [86]

**Biocompatible implants -** Surfaces coated with tethered hydrophilic polymers such as polyethylene glycol, dextran and others are of interest to biomaterials science. By altering surface-protein interactions, it is possible to design implant materials to suit the local physiological environment as well as the intended function. Neutron experiments specifically designed to study biocompatible coatings have been carried out at Chalk River. In one such study, the protein-repelling efficacy, desirable for certain implants (e.g. artificial heart valves), of a coating was investigated as a function of chemisorption conditions [87]. The counter-intuitive results from neutron reflectometry have indicated the way to optimize the biocompatibility of future implants.

**Magnetic thin films, proximity effects -** Magnetic properties of materials, such as magnetic moments and magnetic anisotropies, are influenced by the surface and interface which, in thin films, might lead to a strong deviation from the properties of bulk material. Polarized Neutron Reflectometry (PNR) experiments have revealed an enhancement of the magnetization of iron films in contact with Ag, Au , and Cu [88] and a polarization of Pd films in proximity to Fe films. [89]

**Exchange-spring magnets -** Exchange-spring magnets are heterostructures that consist of hard and soft ferromagnetic layers combining the large anisotropy of the hard magnet with the large magnetic moment of the soft magnet. These systems are very attractive for applications requiring hard magnets, e.g. electric motors. Neutron diffraction [90] as well as PNR [91] was used to determine the complex magnetic structure of these systems. It is crucial to get this information in order to improve the theoretical understanding and as a second step, based upon these findings, to engineer new materials with the desired properties.

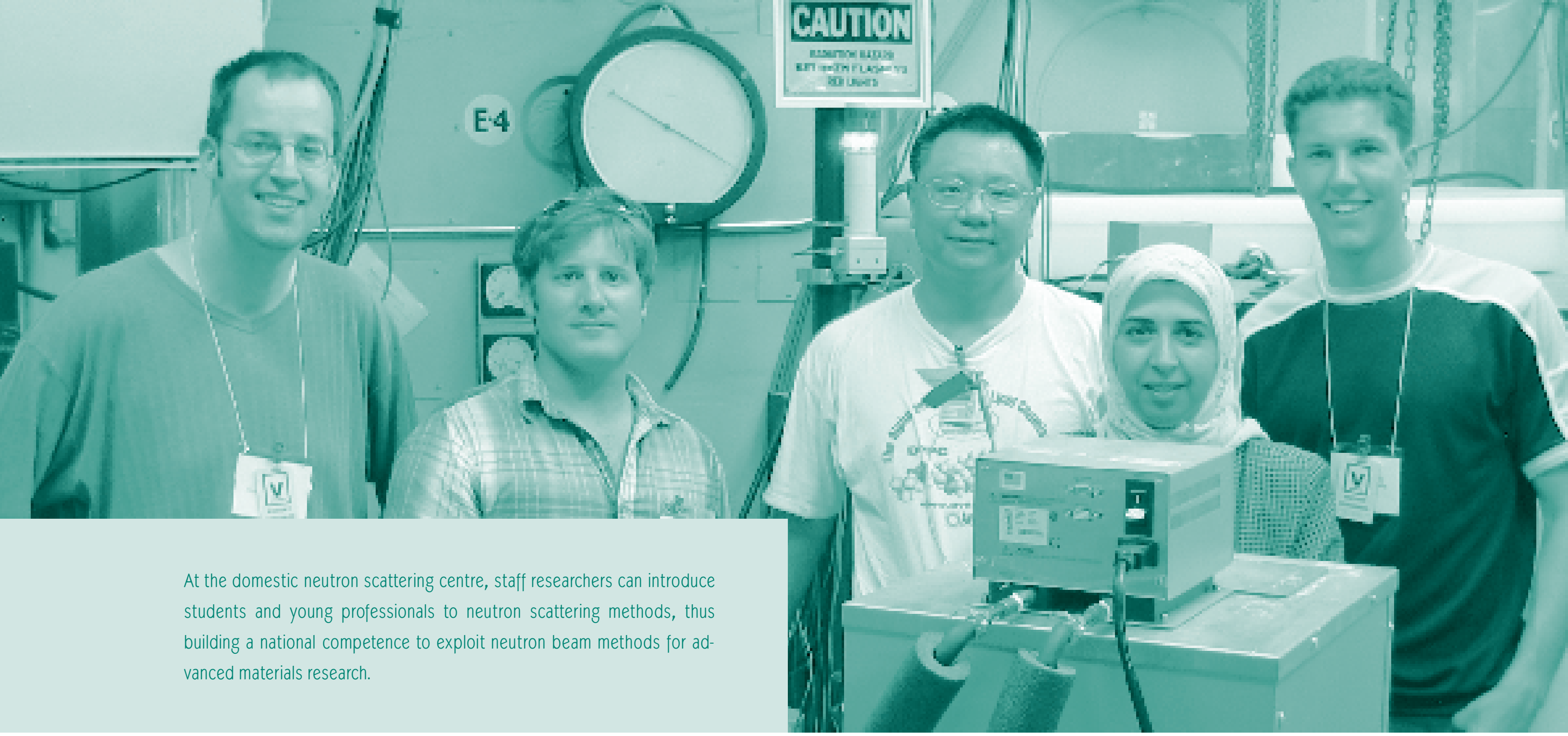
**Exchange-coupled multilayers and giant magnetoresistance sensors -** In 1989, the phenomenon called giant magnetoresistance (GMR) was discovered in layered structures composed of magnetic and non-magnetic layers [92]. For this discovery the Nobel prize 2007 in physics has been awarded to Peter Grünberg and Albert Fert. Nowadays all read heads used in computer hard disks are based on this GMR effect. PNR is the technique of choice to unambiguously determine the magnetic structure in these layered structures [93]. Furthermore, PNR allows one to perform a very precise analysis of the complex magnetic configurations in these thin film systems used in modern read heads. This enables researchers to optimize the performance of these GMR based sensors. [94]

**Spintronics -** A technology called spintronics (spin-based electronics) has emerged recently which is based on semiconductor technology exploiting the electron spin instead of the electron charge. Several proof-of-concept spintronic devices (e.g. the spin transistor) have been proposed already [95] and the focus of research is on finding materials with the needed properties to realize these new electronic devices. PNR can help us to understand the materials' properties by determining for example, the interdiffusion of layers, the magnetization profile, and elucidating the magnetization reversal processes as has been shown in Refs [96] and [97].

**Hydrogen in thin films -** Hydrogen in bulk metals and semiconductors has attracted considerable research interest. In recent years the focus has shifted to thin films because, as in the case of bulk materials, the interaction of hydrogen with the host film can lead to significant modifications of the electronic, magnetic, and structural properties [98]. NR was used to determine the hydrogen profile in a film along with the change of the structure and magnetic properties of the film due to the hydrogen cycling [99]. This information is crucial for development of hydrogen storage materials and hydrogen sensors.  Hydrogen absorption is important in predicting the corrosion lifetimes of metal components such as reactor pressure tubes and nuclear waste containers. NR has been applied to determine the hydrogen absorption during a corrosion process. [84]

**Nanostructured materials -** Due to the steady progress in lithography and deposition techniques it is possible to fabricate periodic magnetic nanostructures. These nanomagnets are of technological importance for high density magnetic data storage and magnetic sensors. Recent experiments using the newly developed technique of off-specular NR have shown that neutron scattering can deliver valuable information on the magnetic structure and magnetization reversal of these nano-scale objects.  [100]

**Internal structure of polymer films -** The strength of the interaction between a neutron and a hydrogen nucleus is very different from that between a neutron and a deuterium



At the domestic neutron scattering centre, staff researchers can introduce students and young professionals to neutron scattering methods, thus building a national competence to exploit neutron beam methods for advanced materials research.

nucleus. Therefore, by either using heavy water or deuterating certain functional groups of the polymer film to modify the neutron scattering contrast, the internal structure of a polymer film can be determined by NR [101]. It is very important to understand the interaction of a film with water, especially for films suitable for use as sensors or drug delivery vehicles. In the case of polyelectrolyte multilayers, NR helped to understand the swelling behaviour by revealing a non-uniform water distribution in the polyelectrolyte film. [102]

**Photoactive films -** There is currently considerable interest in thin films that respond to light in the ultraviolet and infrared bands of the electromagnetic spectrum. Such materials find application in telecommunication (as routers, couplers, filters, etc.) and the microelectronics industry (as photoresists), and can also be used as photoactuators or photonic band gap materials. These materials often cannot be studied using optical techniques, because their interaction with light would confuse the measurement. Recently at Chalk River, NR was successfully applied to investigate photomechanical effects in-situ (during laser illumination) in azo polymer films [104]. Surprisingly, the experiments showed two competing photomechanical effects in this system, one that causes expansion and one that causes contraction.

### *Impacts*

The largest economic impact of the aforementioned areas is certainly in the field of corrosion. The most recent study shows that the cost of corrosion in the USA for the year 1998 was $276 billion. [103] Taking the same percentage of the GDP the corrosion costs are about $ 35 billion per year for the Canadian economy. The advancement of knowledge on the mechanisms of corrosion and strategies to mitigate corrosion therefore provide high potential impact on the national infrastructure and the economy.

Scientific impacts are realized by advancing the fundamental understanding of the atomic, electronic, and magnetic properties of materials and their relationship to the physical properties of materials. Advancements are frequently accelerated by applying the unique advantages of neutrons for probing atomic, molecular and nanostructures. The opportunity to generate new knowledge through neutron reflectometry is illustrated by the fact that two CNBC researchers in collaboration with NR users from external institutions produced 33 articles in leading peer-reviewed international journals during the last 4 years.

The CNBC facility is now providing opportunities to educate PhD students and postdocs in the application of neutron reflectometry for research on phenomena at the nanometre scale. Over the last 5 years, neutron reflectometry results constituted a substantial part in 5 PhD theses: Oleh Tanchak, at McGill; Kevin Yager, at McGill; Larry Unsworth, at McMaster; Li Cheng, at McGill; and Firas Mansour, at The University of Western Ontario.

### *Future impacts, forecast*

The research activities in the area of thin films and surfaces have been growing continuously during the past two decades, especially in physics, chemistry, and biophysics. Because of its unique ability to map both chemical and magnetic profiles, NR will be heavily used in the future as a versatile tool for investigations on new materials with dimensions in the nanoscale. Economic impacts from NR experiments are most likely to arise in the field of corrosion (e.g. by developing anti-corrosive coatings), biophysics (e.g. biocompatible implants), chemistry (thin film sensors), or portable electricity generation and fuel storage systems (fuel cells and H-storage).

## 2.5 Soft Materials - Polymeric and Biomimetic

Internationally, the community applying neutron beam methods to soft materials (polymers, biomimetic systems) has grown tremendously, largely supported by cold-neutron beams and techniques such as small-angle neutron scattering and contrast matching through hydrogen-deuterium isotope substitution. In Canada, the NRU reactor does not have a cold source, and whenever researchers have needed small angle scattering they have availed themselves of foreign facilities, to the degree possible. There has been little opportunity to build much more than a centre of expertise at Chalk River, with some initial academic collaborations. However, anticipating a new Canadian Neutron Centre with a cold source and instruments capable of supporting world-leading research in soft materials, it is important to engage a new community of interest in this area, and to incorporate their perspective into this planning document.

### *Overview*

Soft materials encompass a broad range of condensed matter, including biological molecules, polymers, colloids, surfactants, and similar soft materials. They are relevant to the all branches of the life sciences, chemistry and physics, and have tremendous breadth of application (e.g., adhesives, paints, gels, pharmaceuticals, and liquid crystals). By examining the structure and dynamic properties of these materials, a better understanding of biological functions and materials engineering is attainable. Hydrogen, the most common element making up soft materials, fortuitously has a neutron scattering length that is considerably different from that of its heavy isotope, deuterium. The resulting capability of contrast variation makes low energy thermal and cold (i.e. long wavelength) neutrons excellent probes for the study of these normally delicate materials.

Soft materials self-assemble into a variety of structures ranging in size from tens of nanometres to micrometres. In such cases, longer wavelength (i.e. > 5Å) cold neutrons are used to elucidate the structural details of these macromolecular assemblies. Perhaps the most useful and widespread techniques employed in this discipline are small angle neutron scattering (SANS), neutron reflectometry (NR), and

Scientists employ a great number of probes to aid them in understanding, characterizing and improving materials. The importance of neutron scattering methods for soft materials research is a consequence of the special way that neutrons interact with hydrogen. However, for this domain of materials research, the neutron facility must also include a range of complementary tools to prepare specimens and carry out preliminary characterization.

neutron diffraction (ND). These technique have developed into powerful tools for the study of macromolecules in crystalline and amorphous or solution states, yielding information about size, shape, conformational changes, as well as molecular associations in solution – information needed to understand essential molecular interactions for chemical or biological function. To a lesser extent, techniques such as quasi-inelastic neutron scattering (QINS), neutron spin-echo (NSE) and backscattering (BS) are used to provide insights into the dynamical processes of these macromolecular assemblies.

The amount of research in soft materials with neutrons currently conducted in Canada is limited by the instrumentation available. For example, the CNBC does not have a dedicated SANS instrument, only a limited capability. As a result, researchers interested in using the above mentioned techniques presently do so at foreign laboratories. In fact, the bulk of the Canadian soft materials research needs - with regards to neutrons – are fulfilled at foreign laboratories. It should be pointed out, however, that a dedicated neutron reflectometer, was recently installed at Chalk River through a Canadian Foundation for Innovation (CFI) initiative led by the University of Western Ontario. This dedicated reflectometer will do much to nurture the nascent Canadian community interested in exploring soft thin films and interfaces, and is one of the steps taken by the CNBC in continuing to build a vibrant neutron scattering community in soft materials.

## *Current soft materials research*

The usefulness of neutron scattering techniques can be seen in the current research being done by Canadian researchers:

**Liposomes for drug delivery -** Encapsulating a drug in lipid-based vesicles improves the circulation half-life of the drug in vivo. Moreover, functionalised vesicles help target the drug to the sites of disease, greatly reducing side effects in patients. SANS has been used extensively to reveal aggregate morphologies, map out the complex structural phase diagrams of the different formulations of the lipid mixtures [105]-[107] and understand the spontaneous formation mechanism of such vesicles. [108] An ongoing research program is focusing on maintaining their stability and size after incorporation of drugs or medical imaging contrast agents.

**Hydrogen fuel cell membranes -** The heart of the Proton Exchange Membrane (PEM) Fuel Cell is a polymer membrane, where hydrophilic channels serving as paths for conducting ions are embedded in a hydrophobic matrix. SANS and the analogous small-angle X-ray scattering (SAXS) have been used to determine the block-copolymer structure of promising PEMs, trying to relate how the molecular architecture affects the efficiency of the membrane. [109], [110]

**Hydrogels -** Hydrogels are typically comprised of a sparse network of cross-linked polymers embedded in a fluid matrix; one very well-known example is simple gelatin. Poly(vinyl alcohol) solutions form hydrogels when thermally cycled between room temperature and –20 °C. These gels have desirable mechanical properties resembling to those of cardiovascular tissues and are used in dressing wounds, heart valve stents, etc. Canadian researchers are using SANS to examine the architecture of PVA gels under stress and shear. [111]

**Biological membranes -** Aligned stacks of lipid bilayers are used as models of cell membranes and are amenable to diffraction studies to determine their structure. Using deuterium labeling, the exact location of proteins [112], cholesterol [113] and other lipid components [114] are revealed in great detail.

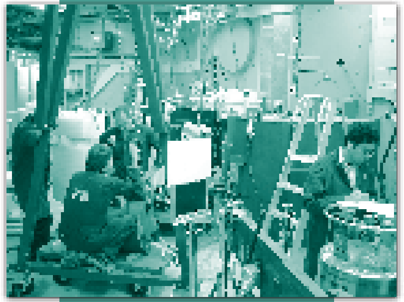
**Biocompatible Thin Films -** Immune response against foreign objects is always an important issue when it comes to organ transplants. Biocompatible thin films coating the surfaces of implant organs can prevent the adsorption of certain proteins, and thus reduce organ rejection. The water distribution and swelling of these thin films are two factors that determine their suitability in organ transplants. Neutron reflectometry is a technique capable of accurately determining the water profile and swelling behaviour of these thin films, and by doing so helping in the qualification of these materials for medical use [115].

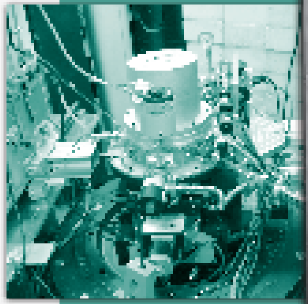
### *Impact*

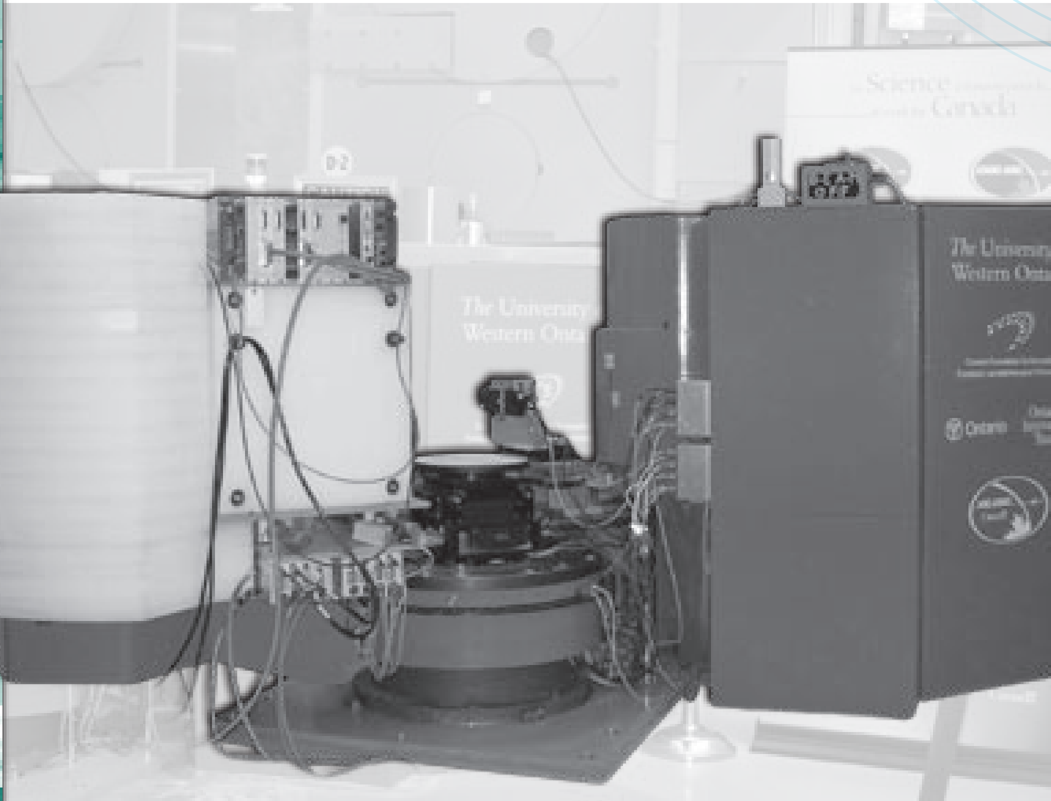
Demand for nano biotechnology in health care products is projected to jump ~50% annually through 2009, led by improved cancer and central nervous system therapies based on solubilization technologies. Diagnostic tests based on nanoarrays and quantum dots, and imaging agents based on superparamagnetic iron oxide nanoparticles will also see strong growth. The demands for nanotechnology medical products is estimated to grow by more than 17% annually to reach $53 billion in 2011 and for drug delivery and biomedical application will grow to $3.7 billion, up from $165 million in 2004. [116]

Techniques such as SANS are now commonly used in industrial polymer science applications research. It is of such value that ExxonMobil funded the NG7 30-m SANS instrument located at NIST Center for Neutron Research (Gaithersburg, MD). In the area of membrane research, the Cold Neutrons for Biology and Technology consortium, led by biophysicist Stephen White of UCI, received $5 million from the National Center for Research Resources of the National Institutes of Health to build the first-in-U.S. neutron-beam research station fully dedicated to biological membrane experiments. In 2005 the same group commissioned the Advanced Neutron Diffractometer/ Reflectometer (AND/R) instrument. The dual mission of the AND/R overlaps the thin-film reflectometry and membrane diffraction that the CNBC has been supporting at C5 (reflectometry) and N5 (diffraction) for several years. It probes the elusive structure and interactions of cell membranes and their components, gathering information key to improving disease diagnosis and treatment.

One achievement of the CINS community in 2007 was the opening of Canada's first Neutron Reflectometer. This scientific instrument was built with funds from the Canada Foundation for Innovation, the province of Ontario and the National Research Council. The project was led by the University of Western Ontario supported by 12 other universities across Canada. The reflectometer is a powerful new instrument for investigating thin films, surfaces and interfaces in materials. Studies by Canadians in this field have investigated polymers that change thickness under laser light (a potential computer storage technology), coatings on medical implants that resist the build-up of proteins to avoid blood clotting, and in-situ electrochemistry to examine how the corrosion process works.







VIP Ribbon-cutting, June 15, 2007: (left to right) Patrick Pilot (CFI), John Yakabuski MPP, Brian McGee (VP AECL), Cheryl Gallant MP, Pierre Coulombe (President NRC), Ted Hewitt (VP UWO)

# 3. NEUTRON BEAM INSTRUMENTS AND METHODS

At the 2006 Annual Meeting and Workshop of the Canadian Institute for Neutron Scattering [138], a preliminary list of neutron-beam instruments was developed. The instruments would support the scientific research identified earlier in the workshop, some instruments being suitable for experiments in several scientific areas. In Table 3, these instruments are grouped according to the type of neutron source they require: *thermal* being the general moderator of the research reactor, *cold* being a localized moderator at a temperature of about 20K and *hot* being a localized moderator at a temperature of about 2300 K.

The detailed specifications of any of these instruments would be the subject of further discussion with users and designers. The following sections will describe the general principles and applications of each type of instrument, so it can be understood how each would address the scientific requirements of the user community.

## 3.1 Control system and user interface

The control of neutron beam instruments, management of data and the interface with the user is a matter of great importance for every instrument of the neutron beam laboratory. The existing system at Chalk River evolved by iteration over a 40 year period, responding to the needs of researchers. It incorporates many excellent concepts and features, which should be retained. However, hardware and networking technologies have advanced more quickly than was possible to adopt in recent decades. Users increasingly feel that the interface presented to them at foreign neutron beam laboratories is more intuitive, and less prone to programming errors. A major rejeuvenation of the control and data management system should be included in the long-range plan for a new Canadian Neutron Centre.

TABLE 3 - List of neutron beam instruments identified at CINS AGM / Workshop 2006

| Thermal | Cold | Hot |
|---|---|---|
| Classical stress scanner | Quasi-Laue diffractometer | High-Q diffractometer |
| White-beam stress scanner | Classical SANS (pinhole) | High energy TAS |
| Diffractometer in a shielded facility | Reflectometer, vertical surface | |
| Thermal radiograph/tomograph | Reflectometer, horizontal surface | |
| Triple-axis spectrometer | Triple-axis spectrometer | |
| Ultra SANS (double crystal) | Disc chopper spectrometer | |
| Developmental station / texture / single | Low-Q powder diffractometer | |
| High-Res'n powder diffractometer | Backscattering spectrometer | |
| High-speed powder diffractometer | Spin Echo spectrometer | |
| | Depth Profiler | |
| | Developmental station | |

Each neutron beam instrument requires a local data acquisition system that enables automatic control of mechanical components, detector systems and a wide variety of add-on, ancillary equipment such as furnaces, cryostats, magnetic fields and loading devices. The new data acquisition system should be programmed through an intuitive, user-friendly interface to set specimen conditions and initiate data collection on a round-the-clock basis, to make maximum use of neutron beam time. The data should be automatically stored in a reliable archive system. Both the control and the data-storage functions of the data acquisition system should be accessible from remote sites through computer networks so as to minimise the time that users must be present near radiation-emitting equipment and maximise the convenience of interacting with an experiment from any location worldwide. Data may be transferred via the internet directly from the data storage system to the user's laboratory, anywhere in the world.

The interface between the neutron instrument hardware and the computer control must be reliable to ensure that neutron beam time is not wasted because of control system faults. Un-interruptable power supplies will be essential for angle-encoder read-outs, detector electronics and control computers.

The architecture of the control and data acquisition system must be flexible so that improvements in technology can be incorporated readily into the capabilities of the neutron beam laboratory. Having the ability to adapt to North American standards for data-storage formats and analysis routines would provide users a 'common look and feel' for experiments wherever they may occur in the continental network of neutron facilities.

## 3.2 Neutron Reflectometers

A neutron reflectometer measures the scattering-length density profile with a sub-nanometre resolution, as a function of depth to about 300 nm, and averaging over an optically-flat area on the order of a few cm$^2$. This fundamental measurement provides information about interface roughness, and gradients of atomic composition versus depth on the length scale of 0.5 nm to about 300 nm.

Neutron Reflectometry (NR) is emerging as an indispensable and popular technique for surface and thin-film science. With increasing demand for access world-wide, most of the latest neutron facility projects have one or more reflectometers in their instrument suite (e.g. 2 at the SNS *United States*, 3 at ISIS *United Kingdom*, 3 at FRM-II *Germany*, 1 at OPAL *Australia*). To serve the needs of the Canadian research community best, the building of two reflectometers was recommended at the CINS Annual General Meeting and Workshop held in October 2006 [138], one with a horizontal sample geometry optimized for samples with liquid/gas or liquid/liquid interfaces, the other one with a vertical sample geometry optimized for all other types of interface. Both reflectometers should be part of a 'day-one suite of instruments'.

New instrumentation ideas like extreme focusing monochromators (converging rays spanning a wide range, e.g. 11.4°, as implemented in the D3 Reflectometer at Chalk River) will be employed for both reflectometers to the full extent possible, i.e. as much as allowed by the beam geometry and the size of the cold source and guides. For the horizontal-sample reflectometer, this may require a special and dedicated guide whose width is much wider than its height. Another feature that should be explored is to exploit a broad wavelength band, either with a tuneable $\Delta\lambda/\lambda$ in the incident beam, or through a full-spectrum incident beam in combination with a set of analyzer crystals. A tunable $\Delta\lambda/\lambda$ can be realized by placing a supermirror reflector in a guide (to reflect out neutrons with $\lambda$ too long) in tandem with a cooled Be-filter (to reject neutrons with $\lambda$ too short). Adjusting the grazing angle of the reflector allows the variation of $\Delta\lambda$. 'Full-spectrum' approaches are under development at NIST, USA and

Undergraduate student André Gaudin from the University of Prince Edward Island learns how to set up an experiment on magnetoresistant thin films from NRC scientist Helmut Fritzsche.

LLB, France. Taking advantage of such innovative methods would increase the performance of these new reflectometers, by about 1 or 2 orders of magnitude compared to the current configuration at Chalk River. Combining optimum instrument design with a powerful reactor and a cold neutron source, would offer Canadian researchers two world-leading instruments, with performance equal or exceeding those at the most powerful research reactor (ILL, Grenoble, France) or the most powerful spallation source (SNS, Oak Ridge, USA).

There is currently no demand for time-resolved NR experiments among the CINS users. This may change within the next decade, leading to the question of monochromatic vs. time-of-flight (TOF) techniques. The following facts should be taken into account for addressing this question.

**1.** Both TOF and constant-λ techniques lead to data of similar quality when each scan is appropriately optimized, as demonstrated by tests at D17 of ILL. [139]

**2.** Although TOF enables NR without mechanical movements (and hence is more suitable for time-resolved experiments), it is so only if one wishes to measure reflectivity over a narrow dynamic range ($Q_{min}$:$Q_{max}$ ~ 1:5).

**3.** A monochromatic instrument that cycles continuously between $Q_{min}$ and $Q_{max}$, say, with 0.1 Hz frequency, while storing each neutron count q-stamped and time-stamped (i.e. without stopping for point-by-point counting) can essentially yield time-resolved data. However, an instrument of this kind is so far an unproven technology.

Finally, both reflectometers should incorporate an option for polarized neutrons. It is envisaged that polarized $^3$He filter technology will be well established at the time a new Canadian Neutron Centre is built, and that polarizing neutrons with this add-on technology will make no significant difference to the design of the reflectometers themselves.

### *Horizontal Scattering Geometry*

The University of Western Ontario led a consortium of 13 universities in a national proposal to the Canada Foundation for Innovation to build a dedicated neutron reflectometer, which was commissioned for operation at the NRU reactor beginning in 2007. The design is a constant-wavelength, variable-footprint, with an option for polarized neutrons and a choice of one-dimensional or two-dimensional detection of the scattered neutrons. This reflectometer holds the specimen with its surface-normal in the horizontal plane (surface itself held perpendicular to the ground), and so is not suitable for study of bulk liquid / vapour interfaces. However, it is an excellent tool to investigate all other interface types (solid-solid, solid-liquid, solid-vapour and buried interfaces) and is able to access high values of scattering vector, Q. The horizontal-scattering configuration is versatile for a wide range of nanomaterials research. This existing instrument was designed to be transferred from the 'D3' thermal-neutron beam line at the NRU reactor to a cold-neutron beamline at a new Canadian Neutron Centre. Transferring the D3 reflectometer to a cold neutron beam line will deliver at least an order of magnitude improvement in signal to background, which will enable researchers to work at the forefront in sensitivity and spatial resolution.

### *Vertical Scattering Geometry*

Many neutron facilities (e.g. HMI, Germany; ISIS, UK; ILL, France; SNS, USA) install a neutron reflectometer with a horizontal surface geometry, that is with the surface-normal vertical. This geometry is suitable for studying all types of interface, including liquid/vapour interfaces, but typically does not enable such a wide Q-range as in the horizontal-scattering configuration. This type of reflectometer enables the studies of thin films at air/liquid and liquid/liquid interfaces, which are important in the realms of soft matter and biology. Applications involve the study of the interaction of proteins with lipid monolayers, surface behaviour of surfactants, polymers and other amphiphiles at liquid/air and liquid/liquid interfaces.

## 3.3 Small Angle Neutron Scattering (SANS)

Small angle neutron scattering (SANS) probes structure in materials on the nanometre ($10^{-9}$ m) to micrometre ($10^{-6}$ m) scale. Structure on these length scales is critical to the performance of advanced engineering materials. For example, the toughness of high impact plastics depends on the admixture of stiff and flexible segments of polymer molecules on the nano-to-micro scale. Nanometre/micrometre structure, are also crucial to biological processes in cells, to the storage of information on magnetic disks, to the hardness of steels and superalloys, to the conduction of current in superconductors, and many other materials properties.

In the biological sciences, SANS is a powerful, albeit low-resolution structure method that can provide unique information on a diversity of biological systems. It is the most powerful technique for studying inherently disordered systems for which at best, high-resolution structures would be available only for individual components. For example, the function of many proteins is often intimately associated with a change in conformation, usually in response to the binding of a ligand or interaction with a receptor. SANS methods offer great potential in this field. Because of its dependence on geometric shape, scattering data can be extremely sensitive to domain orientations and hence to major conformational changes. Contrast variation studies are particularly useful for these studies. The way in which proteins fold to their final three-dimensional shape is one of the major unsolved problems in biology; therefore, methods for detecting the compactness of proteins are of great fundamental interest.

Presently, there are over 30 SANS instruments in operation worldwide, predominantly at reactor sources. There is currently no dedicated SANS instrument in Canada.

Although a few SANS experiments can be done on high-contrast materials at Chalk River using thermal neutrons (limited Q-range, $> 0.007$ Å$^{-1}$), most Canadian researchers find themselves having to go elsewhere to carry out their research. However, as a result of their great utility, SANS instruments are oversubscribed worldwide, making it very difficult to gain access. Perhaps for this reason, among the large pool of Canadian soft-materials researchers there are relatively few using SANS as an experimental technique. Through the use of cold (i.e. long wavelength) neutrons and tight beam collimation, state-of-the-art SANS instruments located at the CNC will be capable of probing structure on a length scales ranging from 1 nm to nearly 10,000 nm.

### *Classical Pinhole SANS*

Without a doubt, the 'classical pinhole' SANS instrument is one of the most popular and oversubscribed techniques at every neutron facility that offers it. SANS instruments are simple in design and versatile for interrogating specimens under realistic conditions (e.g., temperature, pressure, magnetic fields, pH and humidity). The classical 30m SANS instrument has a 15 m evacuated flight path before and after the specimen station, and is equipped with a two-dimensional detector whose position can be varied between 1 and 15 m with respect to the specimen. This setup provides great flexibility in scattering angle enabling this type of instrument to probe structures with length scales ranging from 1 nm to nearly 200 nm. However, to interrogate even larger structures, a $MgF_2$ focusing lens can reduce the projection of the straight though beam on the detector. [140] With this setup, the attainable minimum Q-value is ~ 0.001Å$^{-1}$, corresponding to a length scale of 500 nm.

An approach taken to increase the number of incident neutrons on the sample is to employ a multi-pinhole collimator, which converges multiple incident beams onto a single region of the detector. [141] The new VSANS (Very Small Angle Neutron Scattering) instrument is based on this concept and is presently under construction at NIST. Capitalizing on the availability of cold neutrons, the proposed CNC SANS instrument will support a wide spectrum of university, government and industrial researchers, particularly those in chemistry, biology and condensed matter physics.

The CNC SANS instrument will immediately be exploited by the strong Canadian biophysics and biomaterial communities who are interested in domain structures in membranes, drug membrane interactions and phase diagrams of phospholipid vesicles, biopolymers, hydrogels, etc. To accommodate the demand, it may be necessary to add a second 30 m SANS to the suite of instruments in the guide hall. At the time a second SANS is built, it may be evident that it should be optimized for a particularly active sector of the user community.

## *Ultra SANS*

Ultra small angle neutron scattering (USANS) is a technique for cases where information on material structure is needed over the size range from 0.1 m to 20 m. Although the techniques of choice for studying the structure of micron-sized particles are electron microscopy, light scattering and atomic force microscopy, there are, however, a number of cases where none of these techniques is applicable (e.g., low contrast and opaque materials (for light scattering), and magnetic structures). Applications can be found in colloid science (e.g., mixtures of particles, strongly correlated colloid crystals and micron sized particles), materials science

The ability of neutrons to penetrate materials is an essential factor to enable research about the time - evolution of surface chemistry by neutron reflectometry from metal thin films inside an aqueous electrochemical cell.

(e.g., filled polymers, cements and microporous media) and polymer science (e.g., constrained systems, emulsion and polymerisation). Ultra-SANS is the new capability most requested in Australia's new OPAL facility. [145]

A USANS instrument would be placed on a dedicated thermal beam port and use a combination of a pyrolytic graphite pre-monochromator - to select 2.4 Å neutrons - and multiple reflections from large silicon (220) perfect single crystals, before and after the sample to achieve the exquisite precision for measuring small angular deviations from the initial beam direction.

## 3.4 Stress Scanners

### *Classical monochromatic beam*

The basic stress-scanner is a double-axis diffractometer with a sample table capable of accommodating large objects (up to 1.5 tons) and moving them around reproducibly to within ~10 m in all three dimensions. Diffracted neutrons are detected with a position-sensitive $^3$He-counter, which should subtend at least 3 degrees in the scattering plane with high intrinsic resolution (~0.2° $2\theta$) and a range of ± 20 degrees out of the scattering plane, with modest resolution (~2°) to facilitate corrections of angular positions from the intersection of the Debye-Scherrer cone with a cylindrical detection plane. Computer-controllable beam-defining masks close to specimen location will define the sampling volume to a minimum spatial resolution of the order 0.2 mm wide and 1 mm high. The beam will be provided by an optimized monochromator assembly that delivers flexibility of wavelength range and resolution.

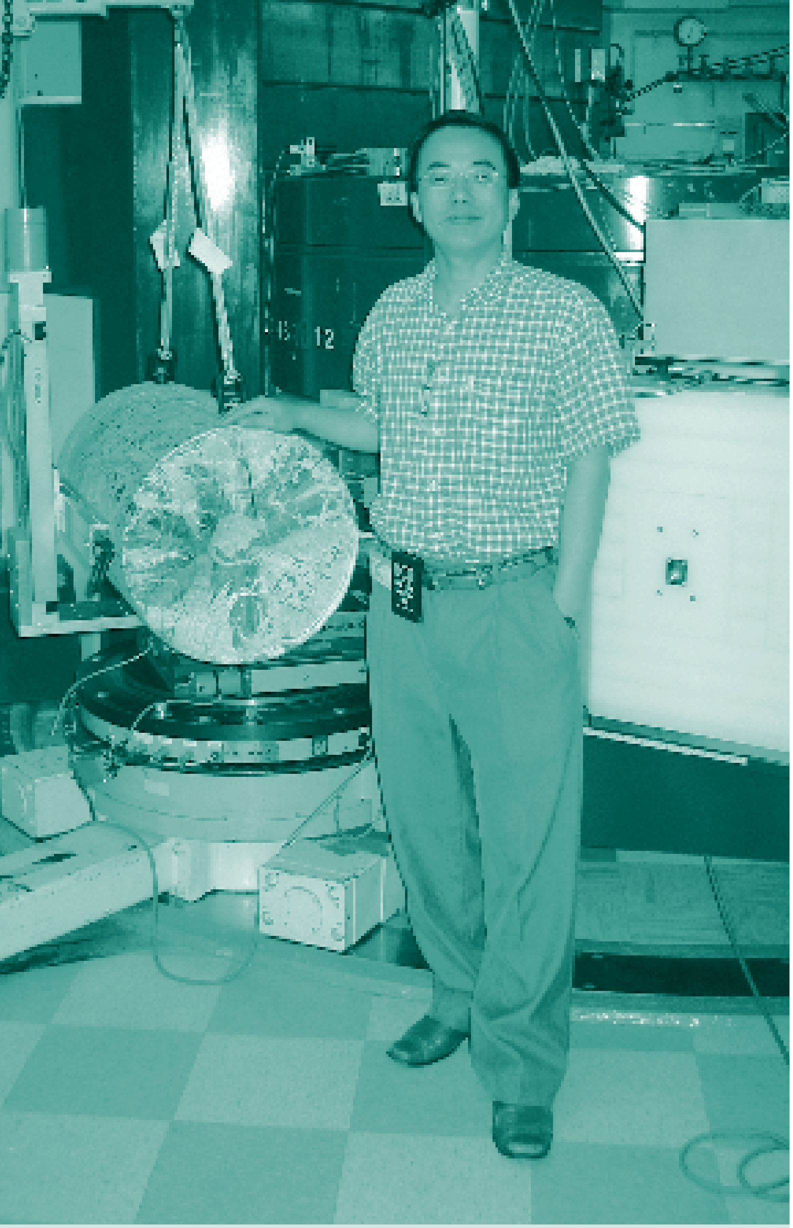
### *White Beam Stress Scanner*

Monochromatic beam or constant wavelength (CW) instruments (typically located at steady-state sources) and scanning-wavelength time-of-flight (SW-TOF) instruments (commonly found at pulsed sources) each have their own unique advantages and disadvantages when it comes to strain measurements. In the case of *in-situ* deformation, in which the purpose is to track the behaviour of several crystallographic directions, SW-TOF instruments have the advantage of surveying many {*hkl*} peaks with each pulse. Because of their design, SW-TOF instruments have a defined instrumental gauge volume (IGV), which imposes a limit on sample size, or at least a trade-off between sample size and spatial resolution. Typically a small number of radial collimators is used to define the dimensions of the IGV.

CW instruments, on the other hand, have the advantage that the IGV can be tailored, continuously over a wide range. The lower limit on the IGV dimension is imposed primarily by parallax to 0.2 to 0.3 mm in the scattering plane. Position sensitive detectors (PSDs) are used to reduce data acquisition times by collecting an entire Bragg peak with a single setting of the detector arm. The main disadvantage of a CW instrument is that for a given specimen direction only one {*hkl*} can be measured at a time. This is often sufficient for macroscopic strain scanning, but having additional {*hkl*} can be beneficial in that Type II (intergranular) stresses can be evaluated simultaneously. CW instruments using a monochromating crystal have incident beams with focused and defocused sides permitting only one strain direction to be measured at any given time.

It is desirable for scattering to occur at 90° so the IGV is a cube, or rectangular parallelepiped. In this way the sampled volume is independent of specimen direction. For SW instruments this requirement is easily satisfied, while for CW instruments this requires selecting a wavelength that places the scattering from the specimen at, or near 90°.

Presently, SW-TOF instruments are being favoured for fundamental research on materials science because there is a growing interest in *in-situ* deformation studies and the need to track several {*hkl*} to explore the interactions of crystallite orientations in a polycrystalline aggregate. A white beam instrument on a steady-state source provides an opportunity



The ability of neutrons to penetrate materials enables researchers to probe the interior of large specimens (such as this magnesium casting, which is 50 cm in diameter and a meter long) and to acquire 3-dimensional maps of internal residual stress, non-destructively.

to realize the benefits offered by both CW and SW-TOF instruments by performing wavelength discrimination after scattering from the sample, and thus extracting diffraction data from several {*hkl*} simultaneously.

## 3.5 Oriented-specimen diffractometers

### *Cold Laue microbeam*

Analysis of crystal structures in small specimens can be achieved rapidly via a 'Laue' – type instrument, where the incident neutron beam contains a broad range of wavelengths, and a two-dimensional detector collects diffracted reflections spread over a large solid angle. The instrument should be located in a guide hall, where a velocity selector will define the range of neutron wavelengths that are incident on the specimen. Accurate specimen orientation is computer controlled. Beam-defining elements will be designed to maximize the flexibility of applications of the instrument. A state-of-the art, high-resolution two-dimensional detector (e.g. an image-plate) will surround the specimen (cylindrical geometry) to maximize the data acquisition rate. The commercial availability and constant advances in such detectors are key defining elements for such instruments. The instrument will serve the scientific communities in biology, pharmaceuticals, coarse-grained materials, and soft-materials, as well as studies of organo-metallic compounds with large cells. A similar instrument on a cold guide, called IMAGINE, is currently being planned for the HFIR reactor at Oak Ridge National Laboratories, and the experience from its construction will greatly benefit the design of a cold neutron Laue system at Chalk River.

### *Thermal Laue diffractometer*

The Canadian user community will benefit from a 'white beam' Laue diffractometer on a thermal guide, similar in concept to VIVALDI at ILL. [117] However, to exceed VIVALDI's capabilities, a new instrument could incorporate the ability to focus the white beam using Kirkpatrick-Baez (K-B) mirrors. Although relatively new to neutron beams, researchers from the NRC-Canadian Neutron Beam Centre and Oak Ridge National Laboratory have shown that K-B mirrors can be used effectively for neutron scattering experiments. [118] Improvements in the design of these mirrors (e.g. improved focal length) are expected as the SNAP project at the SNS develops instruments for the new spallation source. Such mirrors will allow the neutron beam to be focused down to dimensions of a few tens of microns. As has been discussed in other parts of this document, the ability to focus on small, 'X-ray' sized crystals will enable neutron crystallography to be applied more widely, for example to determine the location of hydrogens and water molecules in bio-macromolecular materials with unit cells of up to 10,000 Å$^3$. The recently constructed KOALA instrument at ANSTO is the most modern analogue to this kind of instrument. Either a dedicated beam port, or an end guide position is required to have the maximum possible wavelength spread incident on the sample. [119] - [121]

The higher time-averaged flux of a new Canadian Neutron Centre, compared to the SNS, should make the thermal Laue diffractometer highly competitive internationally. K-B double focusing will deliver neutron fluxes that are higher than those now possible at VIVALDI. Provision of a removable upstream supermirror will be used to provide filtration of the incident spectrum, and can be used to switch the incident spectrum on the sample. With the mirrors removed, crystals with larger cross-sections can be examined, allowing for the rapid alignment of crystals for triple-axis work, which presently take many hours to align with Eulerian cradles on monochromatic beamlines.

An optimized beamline would require a cylindrical area detector system, most likely an image plate system, with pixel resolution of 200 x 200 $m^2$, or better. A $^3$He detector will also be provided for transmission measurements as part of the alignment of the sample in the fine beams. The sample table will be of sufficient dimensions and load capability to accommodate standard closed-cycle refrigerators and furnaces. Additionally, an encoded XYZ translation system with two arcs will be required to hold diamond anvil and other pressure cells.

### *Developmental station / texture / single crystal diffractometer*

A diffractometer with a tuneable monochromatic beam can be applied to assess the quality of a so-claimed single-crystal specimen and to align it in preparation for installation in a furnace or cryostat. It can also evaluate the mosaic spread and quality of crystal monochromators at various stages of development, or as a testing facility to align elements of multiple-crystal monochromators or analyzers. This instrument can support single-crystal neutron diffraction experiments or quantitative texture analysis for users from chemistry, physics and materials engineering disciplines.

The instrument will include two switchable monochromators: a) a perfect crystal and b) one with a mosaic spread in the range 0.5 - 1.0°. At the specimen location, there will be $\theta$ and $2\theta$ drives, an Eulerian cradle and an XYZ translator system, all under computer control. Collimation will be flexible to include various beam reductions and masks. A control program will automatically search orientation space to find diffraction peaks and optimize crystal alignment. Special tools will facilitate automatic transfer of the specimen to a standard cryostat mount while retaining the correct orientation. A scintillator / TV system will allow users to see crystal reflections during manual setup.

## 3.6 Powder Diffractometers

At modern neutron facilities, there are at least two powder diffractometers, one configured for high-resolution and good data collection efficiency and another configured for high efficiency with reasonable angular resolution. Users of the former focus on structure determination and refinement from conventional size samples, while the latter diffractometer would be employed in time resolved studies, research involving small samples, studies of magnetic structure - especially involving very small magnetic moments or small samples of isotopically substituted materials - and the monitoring of phase transitions on a fine temperature grid. The Canadian community would benefit from having both of the above-mentioned diffractometers. The performance parameters of these instruments should approach those set by DRACULA (high efficiency) and the Super D2B (high-resolution) instruments located ILL (France) or, similarly, the Wombat and Echidna instruments at ANSTO.

### *High efficiency diffractometer (HED)*

The high efficiency diffractometer's data collection rate should exceed current benchmarks set by GEM (ISIS, UK) and POWGEN (SNS, USA), by increasing the detector solid angle to at least 1 steradian utilizing two-dimensional detectors and implementing focusing monochromators to increase the flux on sample. Relative to CNBC's C2 diffractometer, performance enhancement could exceed two orders of magnitude.

One of the principal applications of the HED will be the detection of weak magnetic reflections and the mapping of magnetic phase transitions as a function of temperature and pressure. Compared to spallation source instruments (e.g. GEM and POWGEN), this type of experiment is better suited to instruments at reactors as they are better able to access low Q data. The investigation of small sample volumes, perhaps of the order of 10 mg, common for pressure studies or isotopically substituted samples, will also be a major activity at such a diffractometer. It is anticipated that the ability to handle such small sample volumes will make applications to high pressure attractive. At ILL's D20 facility, excellent data are being collected on the order of minutes on sample volumes of the order of 100 $mm^3$. The combined efficiency of a new HED and the CNC should be at least five times that of D20 and should approach the level of the planned DRACULA instrument (ILL, France). Experience from the design of the recently constructed Wombat diffractometer at ANSTO will be very useful. [122], [123]

### *High-resolution diffractometer (HRD)*

The high-resolution instrument, HRD, will use a large take-off angle (e.g. 135°) and good collimation to attain a maximum resolution, $d/d \sim 5 \text{ x } 10^{4}$, and an effective scattering angle range of between 3° and 160°. As with HED, detectors with a large solid angle will be utilized giving either real or quasi-2d information. This instrument will be used for the solution and refinement of crystal structures. Although the latter function is a mainstay of neutron powder diffractometers, it is anticipated that the former activity will increase greatly in parallel with developments in structure solution software. The recently constructed Echidna instrument (ANSTO) will be a good guide for the design and construction of such an instrument. [124]

### *Shielded Diffractometer*

Many experiments, particularly those of industrial interest, are challenging with regard to hazard management. For example, highly radioactive or toxic specimens and pressurized components all present an increased risk. In-situ measurements involving toxic solvents or toxic-reaction byproducts, or an operating engine will also lead to increased risk. By shielding a diffractometer in a reinforced isolated structure, built outside the reactor containment, with regulation-compliant ventilation, fire-protection, radiation-shielding and sound proofing, risks to personnel can be minimized. The protection of the shielding facility will permit neutron diffraction to be applied to a wide range of materials systems, serving the disciplines of chemistry, materials science and industry.

Example projects include:

- evaluation of radiation damage on crystal structures in nuclear alloys (aluminum, stainless steel, zirconium…), fundamental knowledge for fitness-for-service guidelines for continued safe operation of power plants
- phase transitions and solid-state reactions in nuclear fuels that are candidates for next-generation research and power applications

- non-invasive thermometry in operating gas turbine engines, to validate engineering models, and place safety margins on a firm foundation
- the structure factor of supercritical water at various conditions of pressure and temperature - as may play a role in the 'Generation IV' nuclear power technology of the coming decades.

Although the neutron diffractometer itself would be fairly standard, the ability to handle specimens in extreme conditions would constitute a unique experimental facility at the Canadian Neutron Centre, to which neutrons would be delivered by a thermal neutron guide.

### *Hot source diffractometer*

HED and HRD are priorities for the CNC, however, an instrument capable of accessing data that can be used to perform Neutron Pair Distribution Function (NPDF) analysis, would be an important capability for the CNC. Such an instrument requires a hot source to attain neutron wavelengths near 0.30 Å – 0.35 Å. Such wavelengths and a maximum scattering angle (2 ) of 160° (maximum Q > 30 Å) could be realized, making such an instrument competitive with those found at spallation sources. A good starting point would be the D4 diffractometer at the ILL, which supplies 0.35 Å neutrons. At such short wavelengths, large solid angle detectors will compensate for the lower source intensities. Such an instrument would be welcomed by the growing community of material scientists interested in the study of local order, for instance local site ordering, or Jahn-Teller distortions.

### *Cold-neutron diffractometer*

Usually, the low-Q region of traditional diffraction patterns is sparsely populated with Bragg peaks. However, many important materials form three-dimensionally ordered structures with lattice parameters much larger than those found in atomic crystals. The diffraction patterns from such materials may contain numerous peaks in the low-angle region, and the overlapping peaks at higher angles may defy straightforward analysis of the crystal structure. Dense populations of low-Q diffraction peaks may also occur if the material is a composite with many constituents, or if the symmetry of the crystal unit cell is low. A cold neutron powder diffractometer enables the resolution of low-Q diffraction data and facilitates the structural analysis of materials that may arise in condensed matter physics, chemistry, advanced materials, geology and biophysics. Examples of systems with large unit cells include inorganic molecular crystals, biomaterials that organize into cubic structures, complex magnetic structures and ordered alloys. Since complex magnetic structures may be a prime application for such a machine, it will be important to design the instrument to be able to handle both very low temperature stages such as $^3$He-$^4$He dilution equipment, and to fabricate the instrument so that magnet cryostats can be operated if desired. Instruments in this class include DMC at the swiss spallation source, SINQ.

The low-Q powder diffractometer will have a variable monochromator take-off angle, in the $2\theta_m$ range of between 40° and 130°. A selection of monochromator crystals will be used to maximize the flexibility of wavelength, resolution and intensity delivered to the specimen. For high intensity measurements, a pyrolitic graphite (0002), vertically focused monochromator, with take-off angles of 40.8° and 77.5°, will deliver neutrons that can be filtered by graphite or beryllium, respectively. For high-resolution, a germanium monochromator can be used at a take-off angle of 128° with switchable diffraction planes (111), (311), (400) and (511) delivering wavelengths 5.88 Å , 3.07 Å , 2.55 Å and 1.96 Å , respectively.

## 3.7 Neutron Spectrometers

Compared to other experimental techniques such as NMR, muon-spin-rotation and synchrotron X-ray scattering, inelastic neutron scattering provides the most complete information on how the space and time correlations (momentum and energy) of atoms and molecules are linked to the properties of materials. In addition since neutrons couple with comparable strength to both magnetic and structural degrees of freedom (and these two can be fully separated using polarized neutrons), magnetic inelastic scattering is a niche area for neutrons where it is unlikely that synchrotron X-rays will compete effectively in the foreseeable future.

In an inelastic neutron scattering experiment, the energy of the neutron is determined before and after scattering from the sample. Hence these experiments usually require monochromated neutrons incident on the sample as well as an analysis of the neutron energy after scattering by the sample. This is achieved by several methods such as Bragg scattering from single crystals (triple axis spectroscopy and backscattering instruments) and time-of-flight scattering (disc-chopper spectroscopy instrument). In addition, the quantum mechanical property of neutrons spin is exploited in spin-echo techniques, where no monochromatization is required. A wide range of energy and momentum transfers (and their respective resolutions) are provided by these techniques that are essential in studying different systems (from condensed matter to biological systems). In the following we describe the instruments that were discussed and prioritized at CINS AGM 2006 and 2007.

### *Triple-axis spectrometers*

A triple axis spectrometer (TAS) can be used to probe the scattering function at nearly any coordinates in energy and momentum space accessible by the spectrometer in a precise and controlled manner. Triple-axis spectroscopy has proved to be the most effective and diverse instrument among inelastic instruments. It was Canadian physicist Bertram Brockhouse who first developed [125] the brilliant TAS concept at NRX and NRU reactors located at Chalk River Laboratories (home of CNBC) about 50 years ago. The first results from the prototype triple-axis spectrometer were published in January 1955 and the first dedicated triple-axis spectrometer was built in 1956. Brockhouse shared the 1994 Nobel Prize in Physics for this development, which allowed elementary excitations, such as phonons and magnons to be observed. Since its original development, this technique has been used in studying excitations in many different areas such as condensed matter physics (magnetism and superconductivity and other quantum materials), in systems where lattice effects and critical phenomena are important, chemical physics and more recently also in the field of biophysics.

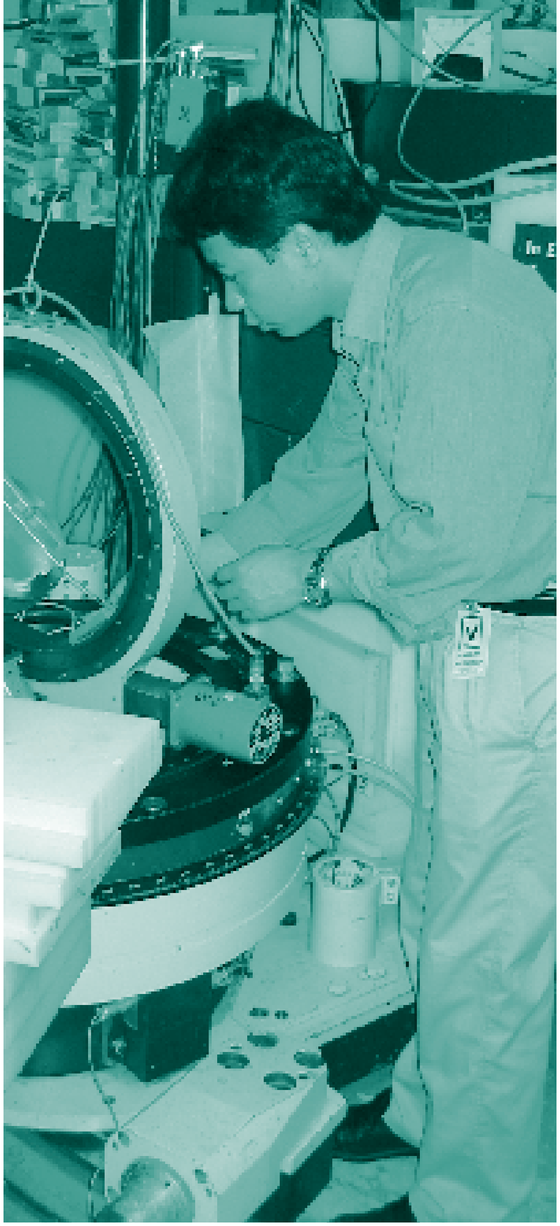
The triple-axis spectrometer is the workhorse for inelastic scattering studies [126] at steady-state neutron sources and consequently, one of the most important instruments at the CNC will be a triple-axis spectrometer. The basic instrument consists of three independently controlled axes of rotation for the sample, monochromator, and analyzer crystals. Over the past couple of decades there have been profound changes in design of TAS instruments all resulting in making this technique more effective [127], [128]. The use of large double focusing monochromators and analyzers have resulted in enhanced luminosity and made it possible to study very small single crystals (as small as 10 mm$^3$) while the rate of data collection has also been increased by 1-2 orders of magnitude. In addition new conceptual designs such as spectrometer multiplexing [129] and novel geometries [130] have now been materialized. Pursuit of the optimized design for TAS spectrometers has made them a very effective, complementary technique with the time-of-flight (TOF) instruments for single crystal spectroscopy at pulsed neutron sources.

In studying excitations, it is often crucial to be able to separate the magnetic and non-magnetic contributions in a clear and indisputable manner. This is possible if one uses polarized neutrons when performing inelastic experiments. The application of focusing and modern polarization techniques ($^3$He neutron spin filters) has significantly enhanced the sensitivity of polarized-neutron experiments. [131] In addition, there are new developments in the field of polarized neutrons such as zero-field full vector polarization analysis (Cryopad), [132] which enables three dimensional polarization analysis experiments. Such concepts are invaluable in solving the uniqueness problem associated with complicated magnetic structures (e.g. spiral vs. stripe order) and more complicated structures. It can also be used for inelastic scattering and the precise determination of the eigenvectors of magnetic excitations. Hence, polarization analysis is an essential feature for any triple-axis spectrometer that is built at the CNC.

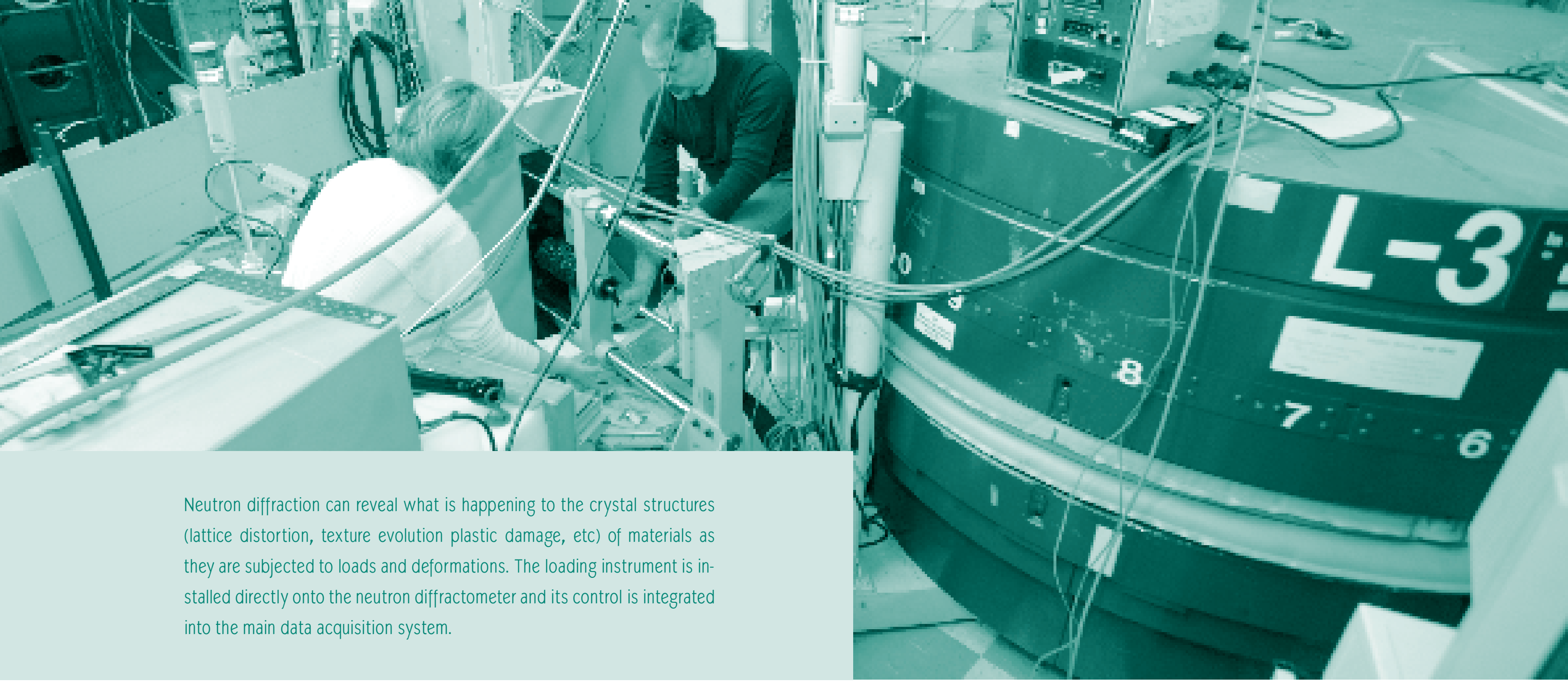
Triple-axis instruments can be located on beam lines that are served by any of the neutron sources: thermal, cold or hot. A few remarks can be made about each instrument:

**THERMAL** - A modern and optimized triple-axis spectrometer located at a thermal neutron beam tube at the reactor shielding face with accessibility to a large solid-angle, can be operated either in a high flux mode (i.e., double focusing monochromator and analyser), or in a traditional mode of operation with Soller collimators providing high resolution. This will be the workhorse TAS and will have the capability of energy transfers up to 100 meV with a best resolution of 0.2 meV. The use of double focusing, a multiwire detector (and/or area detector in combination with an array of independently controllable analyzer crystals), integrated shielding, and a polarized beam option should be included in its design. It is highly desirable to include a tuneable beam filter for higher harmonics provided by a velocity selector in front of the monochromator in order to circumvent the limitation imposed by graphite filter positions.

**COLD** - One of the unique opportunities presented by the CNC is the existence of a beam port that views the cold source directly and exits on the reactor face. This permits the extraction of a beam with a fairly wide angular divergence and does not impose the energy cut-off associated with the wavelength dependence of the critical angle of a



The ability of neutrons to penetrate materials enables them to sample the bulk volume of a specimen, nearly independently of specimen orientation. This bulk sampling generates superior analyses of crystallographic texture, enables the study of minority phases embedded in a matrix and minimizes contributions to the measurements from artifacts of surface preparation or contamination.



Neutron diffraction can reveal what is happening to the crystal structures (lattice distortion, texture evolution plastic damage, etc) of materials as they are subjected to loads and deformations. The loading instrument is installed directly onto the neutron diffractometer and its control is integrated into the main data acquisition system.

cold-neutron guide. A triple-axis instrument located on this beam would be the world leader for the investigation of heavy-fermion and high-temperature superconductors, amorphous materials and any other system with overdamped excitations. This optimized TAS instrument will provide an energy resolution of 0.08 meV and energy transfers of up to 15 meV. Its design should include double focusing, a polarized-beam option and a multiwire detector to extract the maximum flux possible from the cold source and offer the highest monochromatic flux of neutrons at the sample position for energies less than 25 meV available in the world. The detector section of the instrument will yield significant gains over the conventional triple-axis design through the use of a flexible analyzer array of independently controllable crystals and an area detector. Again the use of a tuneable beam filter provided by a velocity selector in front of the monochromator is highly desirable.

**HOT** - Measurements at high energy transfer and small momentum transfer - as required for example in the study of magnetic excitations - are made possible by the very high incident energies which would be available from a hot neutron source if a TAS was placed to view such a source in the CNC reactor.

### *Disc-chopper Spectrometer*

The disc-chopper, time-of-flight spectrometer (DCS) [133] is a particularly versatile instrument whose energy resolution can be adjusted to match the needs of an experiment without suffering a reduction in the accessible range of momentum transfer. DCS instruments were originally used for studying quasielastic scattering in molecular and related systems (such as diffusion in liquids and suspensions, kinetics of hydration reactions, and slow motions of large biological and macromolecular structures). However the application of existing instruments (such as NIST DCS) at reactor-based sources has proven to be immensely successful in other fields, such as exploring magnetic excitations. Condensed matter problems such as spin waves in frustrated Kagomé lattice antiferromagnets, ferromagnetism in bilayer copper oxides, spin-glasses and spin frustration, Haldane spin chains, and even heavy fermion superconductivity have also been tackled using this instrument. [134] Locating a disc-chopper spectrometer in the guide hall of CNC will provide high-resolution neutron spectroscopy support, of world class, to the diverse Canadian scientific community.

In the TOF technique, a polychromatic neutron beam is used and the time (and hence velocity) for the neutrons to travel from the source of the beam to the detector is measured. In an inelastic process where the neutron gains or loses its energy after interacting with the sample, a velocity change occurs which in turn results in a different arrival time at the detector. For DCS instruments, a combination of choppers is used (two synchronized choppers to define the incident beam energy, a third chopper to eliminate unwanted neutrons with velocities that are integral multiples of the desired neutron velocity, and a fourth chopper spinning at a lower speed to prevent frame overlap from different pulses). Such an instrument in the cold guide hall should be designed to provide high-energy resolution (~3 eV) and an incident energy of 0.3 to 25 meV. The sample will be situated in an argon-filled chamber that can accommodate a wide range of sample environments. Data acquisition is optimized by including a large number of detectors (~1000 high-efficiency $^3$He proportional counters) covering a large angular range, between -10 to 130 degrees, and detecting the scattered neutrons after traveling over a distance of about 4 metres. The detector angular range could be improved to provide better solid angle coverage and to employ a truly pixelated detector (metre long $^3$He tubes). This detector coverage would make DCS an expensive instrument. However such an instrument does serve a relatively large community - larger than require access to triple-axis spectroscopy.

It is expected that the new instruments in pulsed sources will improve on current TOF chopper capabilities by a large factor ~50 to 100. However, these instruments will be heavily oversubscribed, and hence a facility at which exploratory as well as detailed parametric studies (temperature and field dependence which are usually slow) can be done would be of general value.

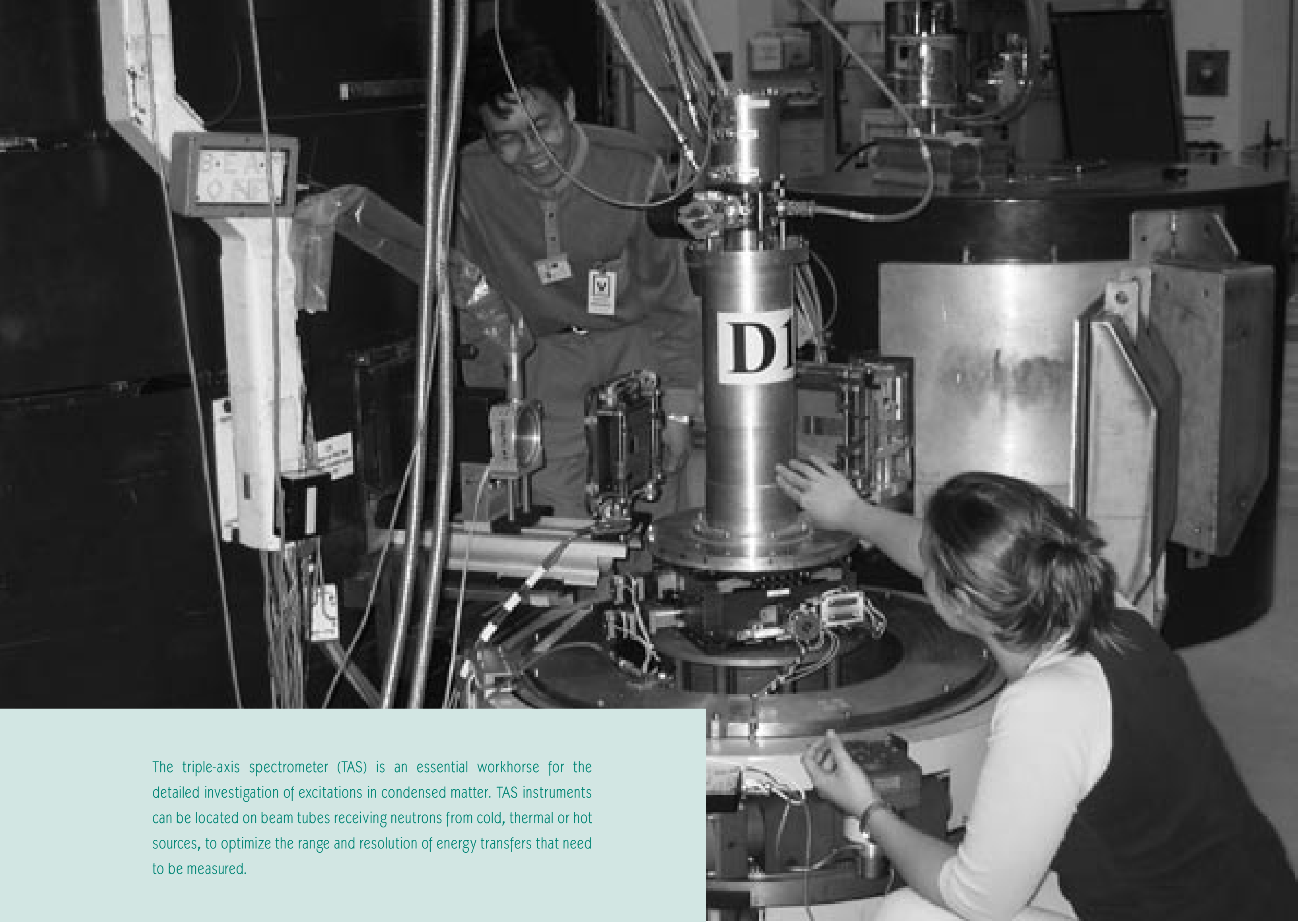
### *Backscattering*

The neutron backscattering technique, developed about 40 years ago, provides much higher energy resolution (~1 eV) than a cold TAS. With its superb energy resolution, backscattering is definitely helpful in the physics of condensed matter (study of quasielastic phenomena), as well as its well-known applications in molecular tunnelling, and rotational motion in biophysical systems.

A backscattering instrument [135] uses perfect single crystals (such as perfect Si or Ge with very narrow mosaic spreads) for monochromator and analyzer each at a fixed Bragg angle of ~90°. In the backscattering method, incident neutrons with different energies are produced by a Doppler drive attached to the monochromator. Since perfect single crystals are used as monochromators, one is able to change the neutron energy by changing the temperature of the crystals to vary the lattice spacing of the monochromator keeping the scattering angle fixed. Backscattering can provide 0.8- eV energy resolution, and transfers of up to 40 eV neutron energy gain or loss. The elastic momentum transfer can range from Q of 0.06 to 4 Å$^{-1}$. An array of Si analyzers and detectors gives a relatively broad momentum resolution of 0.02 to 0.2 Å$^{-1}$.

The backscattering instrument should be built in the cold guide hall and preferably located at the end of the guide. The long wavelength (3 - 10 Å) cold neutrons will maximize the range of time scales that can be probed with the instrument. Flight paths before and after the specimen need to be evacuated. Sample environments include temperature, pressure, magnetic fields, pH and humidity. In addition there should be a crystal orientation stage for single crystal studies.

The backscattering design provides more than a factor of 10 better energy resolution than can be achieved with the disc-chopper design and the intensity is higher. However, the instrument is not as flexible in Q range and energy transfer as the disc-chopper time-of-flight machine.



The triple-axis spectrometer (TAS) is an essential workhorse for the detailed investigation of excitations in condensed matter. TAS instruments can be located on beam tubes receiving neutrons from cold, thermal or hot sources, to optimize the range and resolution of energy transfers that need to be measured.

### *Spin Echo*

A hundred-fold increase in energy resolution is possible by the spin-precession (neutron spin-echo, NSE) technique [136], which exploits the fact that neutrons have a magnetic moment. Very high energy-resolution is achieved without the associated intensity losses from a backscattering geometry with nearly perfect crystals. Opposite-spin precession before and after the sample gives a polarization 'echo' whose breadth indicates the rate of relaxation processes on a much slower time-scale than is possible with conventional neutron spectrometers. The difference between the number of precessions before and after the sample is proportional to the change in the velocity of the neutron after interacting with the sample. The resolution of the neutron energy transfer is independent of the beam monochromatization since the precession of each neutron is measured. In the spin-echo technique, the time-dependent Fourier transform of the usual momentum-energy dependent scattering function is measured.

The spin-echo spectrometer can investigate time scales on the order of tens of nanoseconds (converting from the time domain, the NSE is able to achieve neV resolution). Applications include magnetic phase transitions in disordered systems, the influence of dipolar interactions on magnetic phase transitions, dynamics of the glass transition, lifetime of elementary excitations, transport phenomena in porous materials and quantum diffusion. NSE can be applied to problems in magnetism where the magnetic dynamics are slow, as occurs in spin glasses and other disordered magnets. The technique is complementary to optical correlation spectroscopy since it allows a large range of momentum transfer to be probed.

Because NSE relies on precise knowledge of the neutron spin, this technique is very sensitive to magnetic field pollution. Experience at several neutron facilities has underscored the importance of placing this type of instrument at the end of a guide at a location far from other instruments, or electrical motors, which generate stray magnetic fields and compromise measurements by the spectrometer.

### *Resonant spin-echo*

There have been recent developments in combining spin echo and TAS [137] techniques. Such an instrument (known as a resonance spin-echo spectrometer) uses the characteristics of each type of instrument to achieve very high-energy resolution at relatively high-energy transfer (not possible with either a conventional spin echo, or a conventional TAS alone). The implementation of this technique results in an increase in the energy resolution of a TAS instrument by at least one of magnitude. Consequently, performing inelastic experiments at high-energy transfers with a high resolution is possible by this technique. Interesting results on lifetimes of excitations, and how these change as materials undergo phase transitions (e.g. the lifetimes of phonons on entering superconducting states) have been obtained. Other applications include magnetic excitations, broadening of spin waves, study of the lineshape of the gap modes in singlet ground states and high resolution Larmor diffraction to measure changes in lattice constants with outstanding accuracy.

## 3.8 Real-space Imagers

A classical neutron radiography instrument is fairly simple: a collimated, large-area beam with a full spectrum of energies passes through a specimen and is more-or-less attenuated before exposing a neutron-sensitive film or pixelated detector. Images would be assessed visually to identify features of concern. Such an instrument could be installed on either a thermal or cold-neutron beamline and is likely to be of interest to a private enterprise that provides neutron radiography services to industry.

To go beyond this functional level, to enable quantitative measurements of intensity (as opposed to simple spatial variations of contrast), requires more sophisticated detection and analysis. Intensities must be collected by a detector that generates numerical values for further analysis - total neutron counts per pixel, with a spatial resolution better than 0.1 mm. The data acquisition system must be able to process large data sets from digitized images, providing immediate imaging as well as statistical analysis tools in an intuitive interface, suitable for experts and non-expert users. There should be a capacity for stroboscopic imaging, through which data collection can be gated by some cyclic positioning of a test component. Specimen-handling equipment should be flexible enough to handle a variety of loads and sample shapes. For the greatest penetration and lowest background, this quantitative radiograph should be located to receive a spatially homogeneous, large-area, cold neutron


Courtesy of NRay Services, Inc.

Neutron radiography reveals the detailed internal structure of a rose, non-destructively.

beam. Such an instrument can also be configured to generate tomographic images by rotating the specimen around a vertical axis and collecting quantitative radiographs at a selection of orientations.

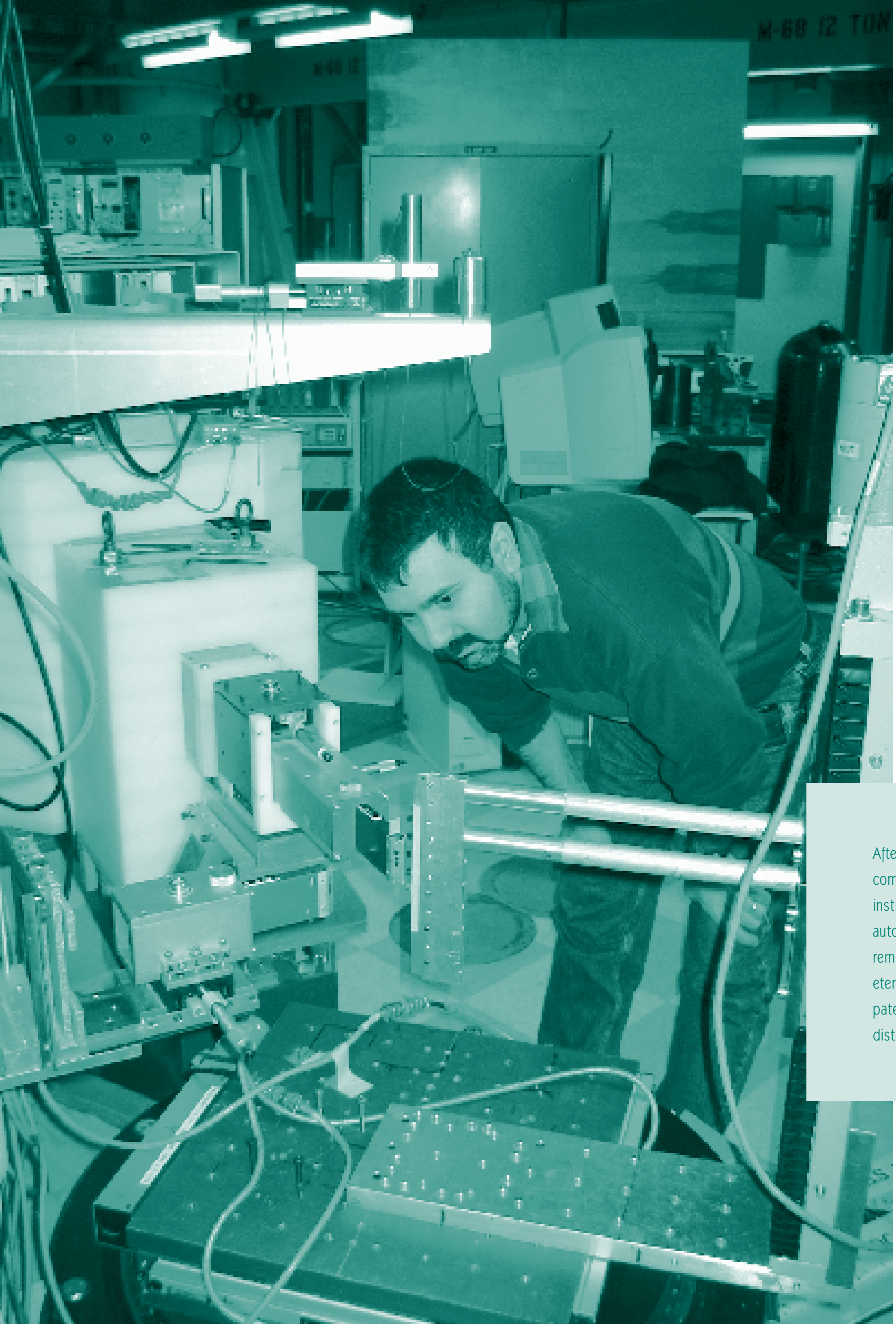
## 3.9 Atomic-resolution Holography

Traditionally, protein structures have been determined by X-ray diffraction of crystallized samples and more recently in the case of small to medium size proteins in solution, by nuclear magnetic resonance (NMR) spectroscopy. In the case of protein crystallography well-ordered crystals must be made available. Obtaining such crystals (i.e. long range translational and orientational order) constitutes a major obstacle, as many proteins, especially those associated with membranes, are very difficult to crystallize. Thus, the structures of such proteins are not known to atomic resolution. However, recently developed atomic resolution holography techniques present the possibility of resolving the structure of proteins, which at present, cannot be solved using traditional techniques (e.g. X-ray diffraction and solution NMR).

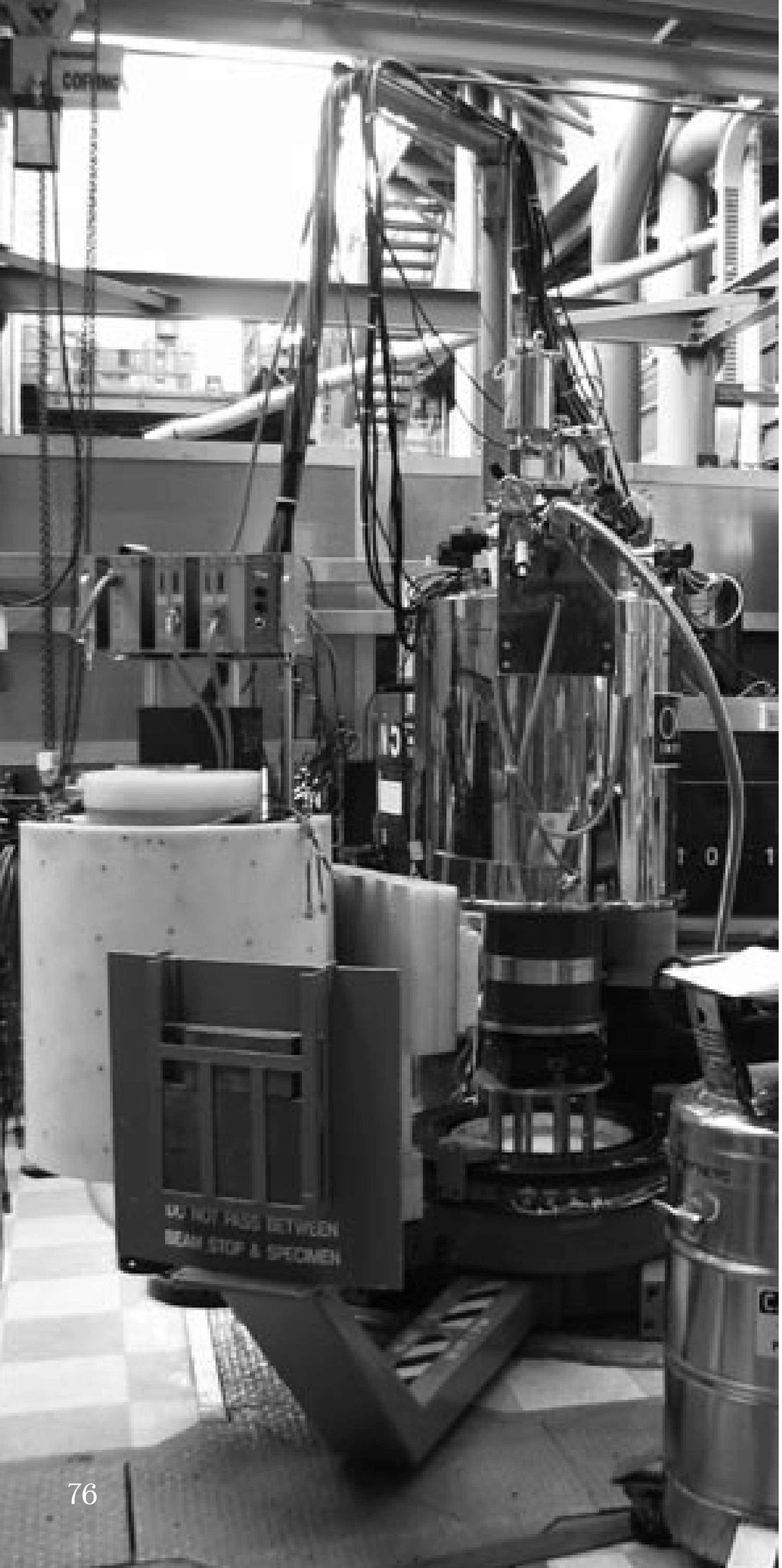
A high-resolution instrument suitable for neutron holography will be constructed on a cold neutron beam line (large unit cells) and will employ a cylindrical neutron sensitive image plate detector, capable of high spatial resolution with good homogeneity and a large dynamic range, and that subtends a very large angle at the specimen. The sample crystal will be mounted on a goniometer head on the cylinder axis. This diffractometer will not be unlike the LADI and VIVALDI instruments presently at ILL (France).

## 3.10 Relating Science Requirements to Instruments

A matrix can be defined to indicate how various neutron beam instruments and methods can provide support for research in various scientific domains. An example is found in



After precise alignment has occurred, computer control of neutron beam instruments enables 24/7 operation, automatic specimen selection, and remote control of spectrometer parameters, so that researchers can participate in collaborative experiments from distant locations.



a report of the Beam Facilities Consultative Group that formulated the instrumentation plan for the new OPAL reactor at ANSTO in Australia. [142] Their matrix is presented in Table 4.

The Canadian version of this matrix, Table 5, reflects the similarities and differences of the neutron beam user communities in each country. Australia and Canada have similar populations, and both are resource-based economies, which constitute the background for the scope and focus of national S&T priorities. Both countries are concerned about brain drain and attracting talented, highly qualified people back to Australia has been highlighted in news arising from their new OPAL reactor. On the other hand, the Canadian neutron laboratory is part of a North American network of 6 facilities, each of which has strengths in certain scientific domains, based on the expertise of staff and interests of the regional user community. Canadian researchers have relatively easy access to highly specialized instruments that may be located at only one of the 6 facilities, or to teams of experts in scientific areas that are not necessarily the focus of effort in Chalk River. The Chalk River facility has historic strengths in materials science, magnetism, and powder diffraction, and has chosen to focus growth in soft materials and thin-film / nanostructural phenomena – responding to interests of Canadian scientists and anticipating the expanded capabilities of a new Canadian Neutron Centre. The Chalk River neutron facility shares its research reactor with users who carry out nuclear technology R&D and who generate isotopes for industry and medicine. The Canadian user community is already vigorous and well organized through the Canadian Institute for Neutron Scattering (CINS), which has members spanning the spectrum from academia to industry, and which is highly multidisciplinary – covering physics, chemistry, materials science, earth science, biophysics and engineering. In Canada, neutron radiography is carried out by a private business, NRay Services Inc., and is not considered part of the main mission of CINS at this time. Possible clinical applications of neutron beams are

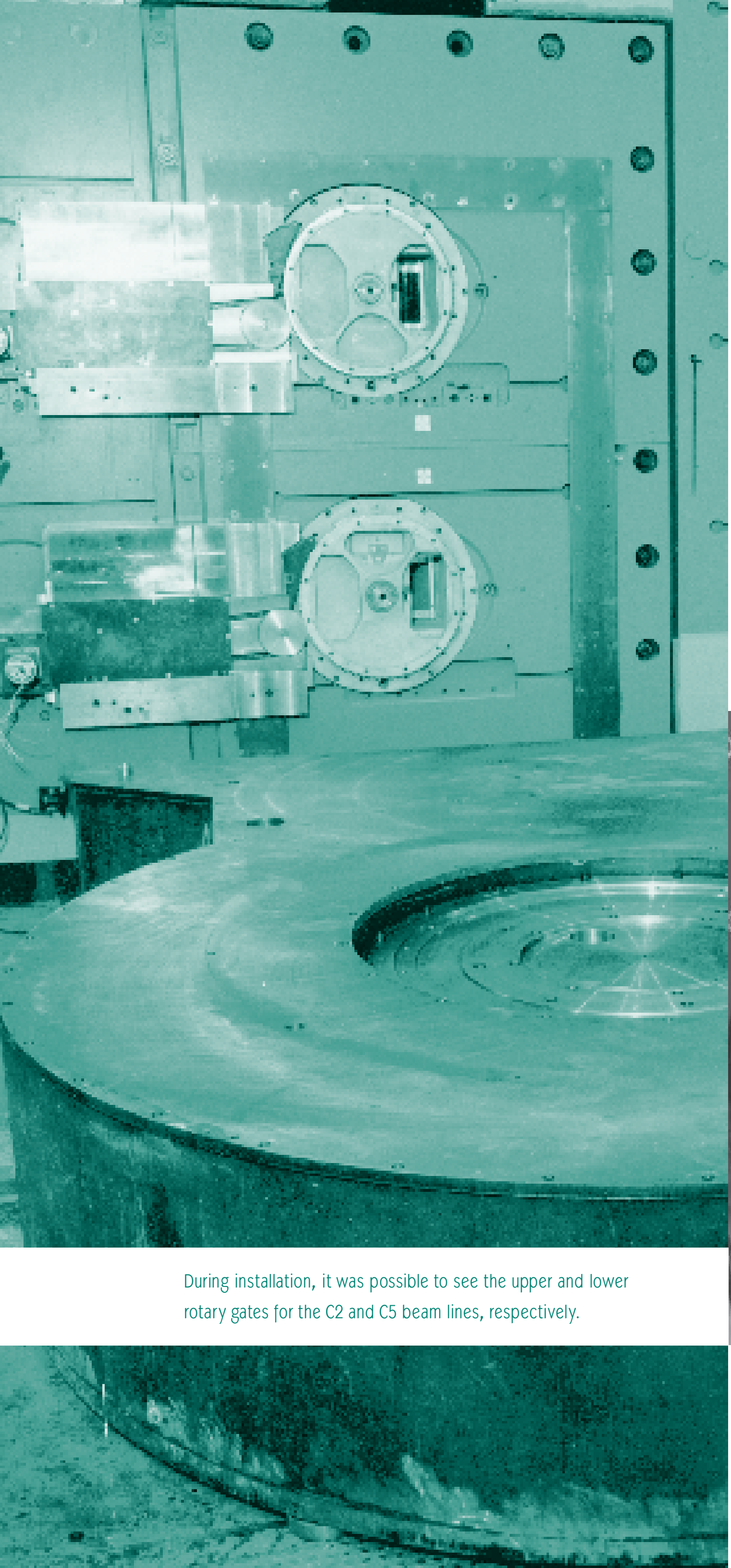
TABLE 4 - Relationship of neutron beam techniques to S&T domains – Australian view

| Scientific Domain<br>Neutron Beam Technique | Condensed matter physics | Disordered crystalline materials, Liquids & Glasses | Polymers & Soft matter | Structural chemistry & Materials science | Biology & Biotechnology | Earth & Environment sciences | Engineering science | Neutron optics & Fundamental physics | Clinical medicine |
|---|---|---|---|---|---|---|---|---|---|
| Small angle neutron scattering | ● | ● | ● | ● | ● | ● | | | |
| Neutron powder diffraction | ● | ● | | ● | | ● | ● | | |
| Inelastic neutron scattering | ● | ● | ● | ● | ● | | | | |
| Single crystal diffraction | ● | | | ● | ● | ● | | | |
| Neutron reflectometry | ● | ● | ● | ● | | | | ● | |
| Polarized neutrons | ● | ● | ● | | | | | ● | |
| Neutron spin echo | ● | ● | ● | | ● | | | | |
| Radiography/ Tomography | | | | | | | ● | | |
| Boron neutron capture therapy | | | | | | | | | ● |

also not considered part of the CINS mission. However, in both of these areas, it is recommended by CINS that a new Canadian Neutron Centre be designed with the power and flexibility to enable these other neutron-beam applications to be implemented in the future, should the interest arise from the driving communities. In Canada, polarized neutrons are assumed to be available as a feature of many instruments, and should not be associated with a unique instrument. Considering the foregoing, the level of demand from each Canadian neutron-beam user sector for each class of neutron instrument can be estimated as high (filled symbol), moderate (open symbol) or low (blank). This characterization of demand or applicability is a factor to consider when prioritizing instruments to be installed at a new Canadian Neutron Centre.

TABLE 5 - Applicability of neutron beam methods to S&T domains – Canadian view

| SCIENTIFIC DOMAIN<br>NEUTRON BEAM METHOD<br>may encompass multiple instruments | Materials Science | Engineering | Earth Science | Structural Chemistry | Polymer science | Biophysics | Thin Films and Surfaces | Magnetism / Quantum Materials |
|---|---|---|---|---|---|---|---|---|
| Triple-axis spectrometers | | | ○ | ○ | | | | ◐ |
| (Q,ω) surveying spectrometers | | | ○ | ○ | ○ | | | ◐ |
| High-resolution spectrometers | ○ | | ○ | ○ | ○ | | | ◐ |
| Oriented-specimen diffractometers | ◐ | ○ | | | ○ | ○ | ○ | ◐ |
| Powder diffractometers | ◐ | ◐ | ◐ | ◐ | ○ | | | ◐ |
| Stress scanners | ◐ | ◐ | | | | | | |
| Real-space Imagers | ◐ | ◐ | | | | | | |
| Small-Angle Neutron Scattering | ◐ | ○ | | ○ | ◐ | ◐ | ○ | ○ |
| Neutron Reflectometers | ○ | | | ○ | ◐ | ◐ | ◐ | ○ |
| Atomic-resolution Holography | ○ | | | ○ | ○ | ◐ | | |



The construction of the DUALSPEC instruments at Chalk River, jointly funded by NSERC and AECL, coincided with the establishment of a more formal user-facility access system, overseen by CINS.

During installation, it was possible to see the upper and lower rotary gates for the C2 and C5 beam lines, respectively.

DUALSPEC was commissioned in 1992


NRU
REACTOR

# 4. FACILITY REQUIREMENTS

## 4.1 The Neutron Source

The benchmark for a reactor-based neutron beam laboratory is the highly successful Institut Laue-Langevin (ILL) in Grenoble, France. The ILL claims the most intense neutron flux in the world for neutron beam research [134] $\sim 15 \times 10^{14}$ neutrons/cm$^2$/s, about five times the unperturbed core flux in the NRU reactor. When beam tubes are inserted into the core, a depression of flux occurs near the tube. For example, at the ILL, the perturbed flux at the nose of the beam tube (i.e. the primary source of neutrons entering the beam tube) is $\sim 12 \times 10^{14}$ neutrons/cm$^2$/s. Maximizing the perturbed flux that enters the beam tube is a primary concern for neutron beam applications.

Distance (r) from the source to the monochromator reduces intensity by $1/r^2$ unless guides can be exploited to retain flux and maintain an effective solid angle (divergence in the range 0.5° – 2.0°) as viewed from the downstream neutron beam instrument. Minimizing the distance from the nose of the beam tube to the neutron spectrometer would be desirable because the optimum solid angle can be achieved with the smallest source cross section, and the lowest background emission, while retaining the highest possible flux ahead of the nose.

At the NRU reactor, the selection of wavelength and resolution reduce the flux of thermal neutrons delivered to the specimen to the order of $10^6$ – $10^7$ neutrons/cm$^2$/s, which ultimately limits the range of experiments that can be undertaken for reasons of signal-to-background ratio.

As a source of thermal neutrons, the spectrum of neutron wavelengths from the NRU reactor gives the highest flux in the range 1.2 - 1.5 Å. The horizontal cold neutron source at the ILL, (6 litres of liquid deuterium at 25 K) enhances the flux of neutrons with wavelengths longer than 3 Å to a level of $8 \times 10^{14}$ neutrons/cm$^2$/s, which is much higher than can be obtained from a thermal spectrum. For an example of neutrons with a wavelength near 10 Å, the intensity gain from a cold neutron source, a factor of 20 to 30, can truly revolutionize the range of scattering experiments on materials with characteristic structures in the nanometre range, such as biological membranes, polymer coatings for medical implants, mesoporous media, layered electronic and optical devices and nanomagnetic multilayers.

Conversely, a hot source (eg. graphite at 2300 K, self-heated by radiation in the reactor core; or an undermoderated fission target) can enhance the flux of neutrons with wavelength less than 0.8 Å, good for applications in liquid and amorphous materials, or for spectroscopy at high energy transfers.

Neutron beam tubes within the reactor need to be designed with state of the art calculations, and with due consideration of the interplay with other tenants of the new, multipurpose neutron source that is envisioned. The main goals of beam tube design are to maximize the flux of neutrons delivered to neutron beam instruments, and to minimize contamination with fast-neutrons or gamma rays from fission in nearby fuel elements.

Canada's current neutron source is the NRU reactor at Chalk River Laboratories. Owned and operated by Atomic Energy of Canada Ltd. (AECL) the NRU reactor is a multipurpose facility; the neutrons that it generates are used by three very different science communities. Isotopes are produced for use in medicine and industry: NRU is the largest global producer of isotopes. Neutron beams from the reactor are used by CINS members in materials research across a host of scientific disciples. The conditions inside the core of NRU are used by AECL to test fuels and components for the CANDU reactor.

A summary of design parameters includes:

- aligning beam tubes to avoid direct viewing of fuel elements;
- placing the noses of re-entrant beam tubes in regions of high flux in the moderator;
- adjusting the cross sections of beam tubes to trade off the effect of displaced moderator, which depresses flux, with size of source, which can enhance flux;
- adjusting the aspect ratio of beam tube cross section to optimize the resolution versus flux of various neutron beam instruments;
- lining beam tubes with reflecting material, effectively to expand the solid angle viewed by the downstream neutron beam elements and thus to further enhance the flux delivered to the specimen; and
- evacuating beam tubes or filling them with helium to minimize the loss of neutrons through scattering or absorption along the flight path.

Because the neutron spectrometers incorporate large components of shielding, and therefore require substantial dimensions in height and width around the beam lines, the beam tubes must exit the reactor core at least 1 m above the level of the working floor, preferably in the range 1.25 m to 2.50 m above the main working floor. The possibility of bringing out beam lines at two different heights above the main floor, or even of having beam tubes that exit the reactor at an incline should be considered as a way to maximize the number of beam instruments close to the neutron source.

It is expected that additional beam lines will be developed over the lifetime of the neutron source, and that the configuration of various elements inside the reactor will be adjusted to meet evolving requirements of science and technology. For example, a single cold-neutron beam tube may need to be converted to a manifold that views the cold-neutron source but feeds a number of neutron guides for multiple neutron beam instruments that meet growing demand in coming decades. The design of the reactor core and the surrounding structure must be sufficiently flexible to enable occasional reconfiguration of beam layouts in the future, e.g. when a major refurbishment is undertaken. The large number of beam holes at different elevations in the NRU reactor is an example of a flexible design.

Operation of the neutron source needs to be consistent with the requirements of an international user facility, where professional scientists and students will travel from anywhere in the world to participate in experiments lasting from a few days to a few weeks. The reactor schedule needs to be predictable and reliable to enable orderly planning of user arrival, training, access, completion of an experimental plan and departure to clear the instrument for the following user. The neutron beams must deliver the maximum flux that is possible from the reactor, more than 75% of the year, to function as a competitive centre in an international network of neutron facilities.

Radiation levels at the face of the reactor wall need to be <10 μSv/hr of gamma rays and <1 neutron /cm$^2$ /s with the reactor at full power. The shielding that maintains these low external fields should be composed of optimal materials to minimize the distance from the neutron source to the neutron beam instrument. The working floor environment near the reactor must be engineered as a radiological zone in which visiting researchers with less than half a day of training can carry out neutron scattering experiments safely and unaccompanied, around the clock, with no expectation of contamination or exposure to significant radiation fields. It must be possible to shut off an individual beam line before radiation enters any component of a neutron beam instrument, so that construction or maintenance can be carried out safely on any component while the neutron source continues to operate and other scientific or industrial activities proceed as usual.

## TABLE 6 - Summary of Neutron Beam User Requirements for the Neutron Source

| Requirement | Quantitative Limits | Notes |
|---|---|---|
| Flux at the nose of all thermal beam tubes | $> 10 \times 10^{14}$ n / cm$^2$ / s | Same flux in moderator surrounding cold / hot sources |
| Number of thermal beam tubes exiting reactor wall | > 10 | Consider multiple elevations, instrument footprints |
| Thermal guide manifold | 1 | Serve up to 2 thermal guides |
| Cold neutron sources | 1, possible to add 2nd | 25 K, liquid hydrogen |
| Cold guide manifold | 1 | Serving up to 6 cold guides |
| Cold beam tube | 1 | For instrument at reactor wall, but can be converted to a second cold guide manifold |
| Hot neutron sources | 1 | Consider graphite block or undermoderated fission target |
| Hot beam tubes | 2 | |
| Geometry of beam tubes | 1.25 m < beam height above floor < 2.50 m<br>Minimal distance from nose of beam tube to neutron spectrometer<br>No fuel in line of sight | Consider multiple heights above working level, and slanted tubes to second working level.<br>Consider reactor shield materials to minimize wall thickness, tube length and cross section. |
| Flight paths | No nitrogen or argon along neutron flight paths/beam tubes/guides | Fully evacuated or filled with low-scattering gas, such as helium or $CO_2$ |
| Duty cycle of reactor | Capacity factor > 75%<br>Maximum flux to beam tubes at all times | Reliable schedule, published months in advance |
| Engineered radiological zoning | < 10 mSv/h at reactor face<br>< 1 neutron / cm$^2$ / s | Suitable zoning and layout for safe, unaccompanied access by trained visitors 24 / 7. |
| Beam gates | 1 per beam line, upstream of all neutron beam instrument components. | Reliable, maintainable, adequate for safe work inside instrument shielding while reactor is operating |

## 4.2 Neutron Beam Halls

Once neutron beams have emerged from the reactor source, they will either enter neutron beam instruments that are located immediately adjacent to the reactor, inside the Reactor Hall, or they will enter guides that transport them into a separate building (the Guide Hall) where many more neutron beam instrument are located. Because neutron beam instruments include a lot of radiation shielding, only a limited number of instruments that can be physically placed around the circumference of the reactor source. In the Guide Hall, however, the guides can fan out somewhat and provide more space for neutron instruments per source position in the reactor core. Since neutron instruments each cost about 1% of the reactor source, it is more cost effective to find ways to place more neutron instruments around the source than to build additional reactors or spallation sources. At the ILL there are currently 42 neutron beam instruments around a single, compact reactor core. Most modern neutron beam facilities include one or two guide halls, to capitalize on the ability to 'fan out' more instruments from a given neutron source.

### REACTOR HALL

The neutron beam instruments immediately adjacent to the neutron source, in the Reactor Hall, require substantial volumes of shielding to contain the superfluous radiation that is not directly associated with the experiments. Therefore, neutron beam instruments are inherently large, heavy objects with a footprint on the order of 20 $m^2$, and a mass in the range of 10 – 40 tonnes. Ancillary equipment, which is added to neutron spectrometers to impose conditions of interest on specimens, can also be heavy or large in volume. It is essential that the Reactor Hall be designed with adequate load capacity; with adequate floor area and headroom to manoeuvre equipment; and with cranes that can access any location on the floor for neutron beam experiments, or to service neutron beam instruments, with a capacity of up to 20 tonnes. There should be a minimum of 10 m of clearance between the face of the reactor's biological shield and the wall of the Reactor Hall working area. The ceiling should be at least 10 m from the working floor of the Reactor Hall.

The layout of the Reactor Hall should also provide 'natural' protection from the viewpoints of radiological safety and security for the nuclear facility, while minimizing impediments to neutron users entering their experimental area, bringing specimens and specialized ancillary equipment with them. An entrance / exit area should enable several operations to be conducted efficiently, such as:

- Confirming that personnel are authorized to enter the Reactor Hall;
- Acquiring personal protective equipment
- Identifying incoming equipment and approving it to enter the Reactor Hall;
- Assessing radioactivity prior to release of materials from the Reactor Hall;
- Transferring experimental equipment into and out of the Reactor Hall;
- Recording personnel dosimetry and assessing contamination;
- Providing decontamination facilities near at hand.

The Reactor Hall should be physically separated from other parts of the research reactor facility, such as:

- Reactor operations, control or maintenance
- Access to in-core experiments on nuclear materials and components
- Isotope research or production facilities

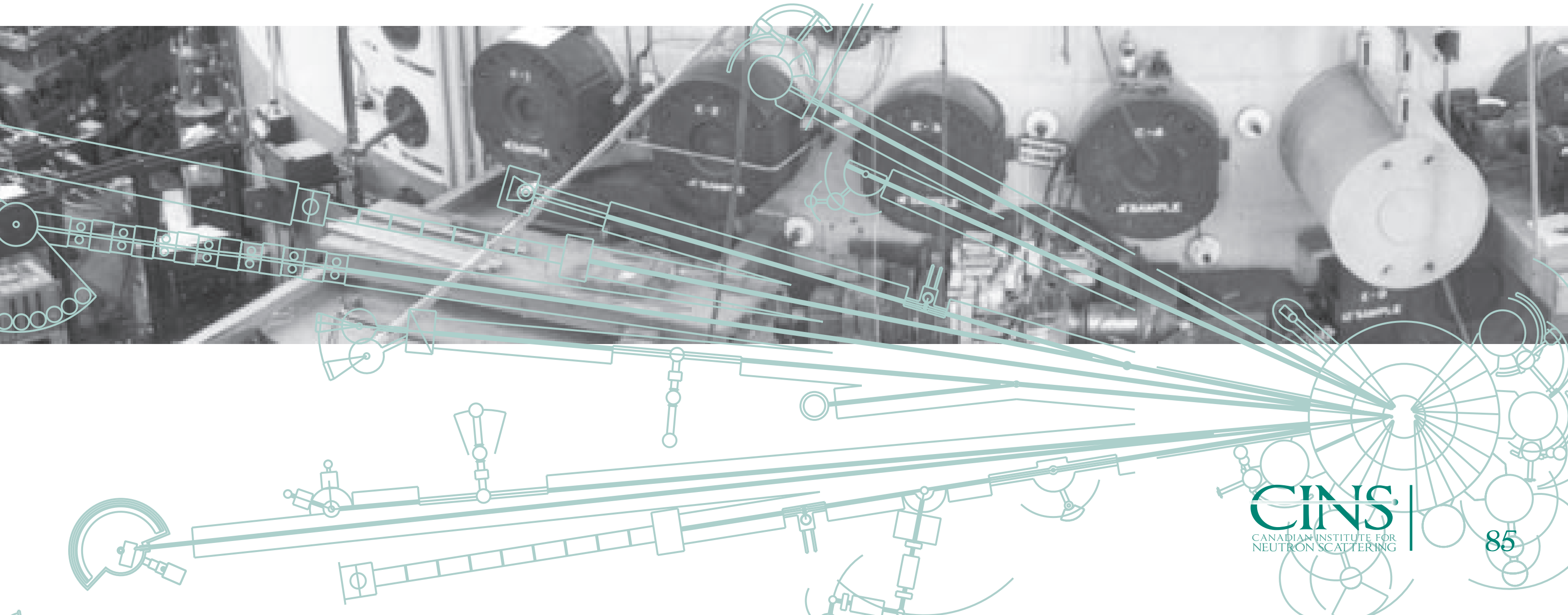
The separation should be such that a neutron beam user or student cannot, by accident or design, enter a zone for which he or she does not have appropriate training or security clearance. The separation should also be such as to minimize the probability of contamination spreading from in-core activities to the Reactor Hall, where neutron users work on neutron beam instruments.

## GUIDE HALL

Most modern neutron centres have a guide hall in which the majority of neutron beam instruments use cold neutrons. Cold neutrons, with long wavelengths and low energies can be transported effectively through Ni-coated or supermirror guides retaining good angular divergence (and total flux) over substantial distances from the cold neutron source inside the reactor. Guide halls are usually located as separate structures, outside of the reactor containment, with only the neutron guides penetrating from one zone to the other, via gates that can be shut in the event of an emergency. Several of the leading neutron centres have more than one guide hall, the second added part way through the life cycle of the neutron source as a cost-effective way to add neutron instrument capacity without the high cost of building a separate neutron source. Therefore, site selection for a new Canadian Neutron Centre should allow for the possibility of one Guide Hall at the outset with the possibility to add a second Guide Hall sometime in the second decade of operation.

Each Guide Hall should have interior dimensions at least 60 m in the direction radially outward from the cold neutron source, at least 30 m wide and a clear inside height of at least 10 m. The neutron guide sections must be aligned within a precision of a few hundredths of a degree and remain stable in relative position over 10s of metres. Several of the cold neutron beam instruments also demand very low vibrations, and long-term dimensional stability. Therefore, the foundation and floor of the guide hall must be designed to take advantage of stable underlying bedrock, to isolate the experimental areas from mechanical vibrations due to reactor machinery. The entire Guide Hall requires good control of temperature and humidity to retain reliable performance of the beam lines and instruments.

Over the lifetime of a new Canadian Neutron Centre, it is certain that there will be maintenance, upgrades, new instrument installations and experiments that require lifting of heavy components. Therefore lifting capabilities up to 20 tonnes must be available at all points on the floor of the Guide Hall.



Labs and workshops adjacent to the Guide Hall are where more complex experiments are assembled prior to moving onto a neutron spectrometer. Pictured here, an industrial sample is mounted on equipment that will apply large forces, and high temperatures. Once on a spectrometer, neutron measurements will show scientists how the material responds to these conditions.

## 4.3 Attached Laboratories and Workshops

The neutron beam facility will include laboratories and workshops to maintain and develop neutron instrument components or specimen-environment equipment as well as to prepare and handle specimens that must be produced on site, near the scheduled time of neutron scattering experiments.

These working areas should be integral parts of the CNC complex, for example attached to one side of the Guide Hall, to optimize the synergy of operational and developmental staff, whether scientific, engineering or technical. Examples of workshops needed to sustain operation and development of the neutron facility itself are listed here.

*Data acquisition, networking and control centre:* The CNC neutron laboratory will implement state-of-the-art information technology that enables secure, remote control of experiments, remote data analysis, high transfer rates, North American standard formatting, and mass archiving. It is expected that there will be a continuous requirement for upgrading, and reconfiguration as science and technology evolve during the lifetime of the CNC. A central location will be needed for design and testing of new installations, and as a hub for the networking of neutron instruments or other services (desktops, printers, phones, video conferencing, external data links, etc).

*Electronics workshop:* The CNC will continuously require the fabrication, testing and troubleshooting of numerous electronic parts for the control of the neutron instruments and integration of ancillary equipment, to keep pace with evolving scientific and technological requirements. Space will be required for storage of components, design workstations, assembly and testing benches and room for exemplars of key mechanical components to be set up for development or debugging of interfaces.

*Detector workshop:* Development, assembly, troubleshooting and repair of neutron or gamma detectors requires a clean environment, vacuum and gas-filling, electronics to diagnose signals and operate detectors, storage for radioactive test sources, cryogen handling capability, layout areas, wiring frames, and storage of stock materials or components.

*Design offices:* Design facilities will be required to maintain and upgrade neutron beam instruments, to develop new beam lines, and to develop one-off ancillary equipment for innovative experiments. Design offices require space for design workstations, assembly drawing layouts, drawing archives, and storage for reference information about materials or regulations.

*Furnace workshop:* This workshop will support furnace assembly and maintenance, including mechanical handling equipment, vacuum systems, gas flow controls, ventilation, leak detection, high power supplies, safe temperature control and monitoring. Associated with this workshop will be sufficient storage space for the full complement of ancillary equipment and spare components, organized for safe access as required. A well-ventilated working area of approximately 6 m x 6 m is needed for each system that is either being prepared for installation at a beamline or in a state of commissioning or repair. There will need to be at least 3 of these lay-down areas located on the same floor as the working level of the Guide Hall.

*Vacuum / cryogenic workshop:* The many experiments at ultra-cold temperatures require a dedicated support workshop. This workshop will support cryostat assembly and maintenance, including mechanical-handling equipment, vacuum systems, leak detection, power supplies, temperature monitoring and access to cryogenic fluids, with proper ventilation and other safety features. Associated with this workshop will be sufficient storage space for the full complement of ancillary equipment and spare components, organized for safe access as required. There must be a workspace large enough for safe handling and testing of large cryomagnets, and closed-cycle refrigeration systems. A well-ventilated working area of approximately 6 m x 6 m is needed for each system that is either being prepared for installation at a beamline or in a state of commissioning or repair. There will need to be at least 5 of these lay-down areas located on the same floor as the working level of the Guide Hall, to facilitate transportation of heavy, yet delicate cryogenic equipment to and from the beam lines, or into the Reactor Hall.

*Fabrication shop:* A small machine shop is an essential asset for adapting user specimens to neutron instruments, and to implement some designs for neutron instruments or ancillary equipment. The shop requires space and power for a suite of standard machine tools and fittings (turning, milling, grinding, cutting, drilling, and a joining station), work areas for assembly, plus storage of stock materials, fasteners, bearings, tools, and so on.

Neutrons can easily penetrate through the wall of a refrigeration unit and reach a sample of material inside that is being cooled. Specialized equipment enables physicists to measure material properties at temperatures very close to absolute zero and simultaneously subjected to a high magnetic field. Pictured here a technician prepares a cryomagnet for an experiment at -272°C, with a vertical magnetic field that is variable up to 9T.

*Engineering testing workshop:* Engineering materials research may involve large, heavy, complicated and sometimes dangerous specimens. A laboratory will be required for mechanical testing equipment development, including space to operate at least one universal testing machine, capability to test pressurized systems, and to handle heavy specimens, such as radioactive specimens in shielding. Space will be included for the full suite of ancillary equipment and spare parts, arranged for safe access. A working area of approximately 6 m x 6 m is needed for each system that is the subject of current work. There will need to be at least 2 of these lay-down areas located on the same floor as the working level of the Guide Hall.

With the increasingly multidisciplinary character of the Canadian user community, it is clearly necessary that laboratories be provided for on-site preparation of specimens by visiting researchers. For many types of experiments, the final preparation of the material to be studied must take place just prior to placing it in the neutron beam. Such support laboratories adjacent to the neutron guide hall provide the necessary work-benches, fume-hoods, storage, etc. of any modern, safe laboratory. Ideally, they should include characterization tools that complement neutron beam analyses, to qualify specimens prior to committing valuable neutron spectrometer time. Examples of these characterization tools include optical microscopes (phase detection and microstructural homogeneity), calorimeters (phase detection and verification of purity), bench-top X-ray scattering (quality of interfaces, phase detection or verification, and complementary contrast to neutrons) and light scattering equipment (to complement SANS).

Examples of laboratories that are needed to facilitate the research outlined in the early sections of this plan, include:

- An adequately functional chemistry laboratory for biological and soft-matter specimens that are ‘perishable’ and/or require preparation on-site. Such samples may have requirements for ultra-pure water, chemical supply and safe storage, refrigerators and freezers, liquid handling, centrifugation, pH metering, specialized lighting, glassware, balances, and optical microscopes.

- Heat treatment facilities to simulate the evolution of materials for engineering or earth sciences, including convective-air furnaces, controlled gases, vacuum, salt bath, fluidized sand bath, ventilation, fume hood, glove box, computer control and monitoring.

- A chemical preparation lab, with fume hood, glove box, chemical storage, access to cryogenic equipment, sink, balance and grinding equipment.

- A designated laboratory for X-ray and light scattering equipment will include power, cooling, safety features and space for X-ray powder diffraction, reflectometry, and small angle scattering as well as for dynamic light scattering instruments. These facilities provide on-site verification of specimens, or complementary contrast and Q-range in proximity to the neutron facility, but need to be treated with care as radiation-scattering instruments.

## 4.4 Offices and Meeting Rooms

Offices for research staff members should be large enough to accommodate the occupant, with space for one or two visitors to hold a discussion behind a closed door. The offices should be arranged immediately adjacent to the guide hall, and can be on an upper floor. At startup, there will need to be office space for about 30 research staff members, and 20 engineering / technical staff members. In due course, it is expected that the neutron beam laboratory will expand to twice this size.

In addition, there need to be spaces for visiting researchers and students, longer-term post-doctoral researchers associated with the facility, who may be accommodated in a more 'open-concept' space. Longer-term visiting faculty members (e.g. on sabbatical, or term-appointments at the facility) should be provided with offices.

The scientific process is more than just data collection at an instrument and analysis in an office. There need to be facilities for larger groups to meet and discuss results or for events of education and outreach. This requires meeting rooms that can accommodate 10 (2), 30 (2) and 100 (1) people, as well as a lecture facility that could handle up to 300 guests, with adjacent space for reception and refreshments. These meeting facilities should be adjacent to the Guide Hall.

Finally, the reception of visiting researchers and students requires adequate space for a large group (e.g. up to 100) to wait indoors, and work stations for parallel processing of several individuals through any required procedures, such as security clearance, badge issuance, signing of entry agreements, receipt of accommodation instructions, and so on. With adequate infrastructure in place, these administrative actions can be completed quickly and efficiently, while maintaining a sense of welcome and organization for visitors.

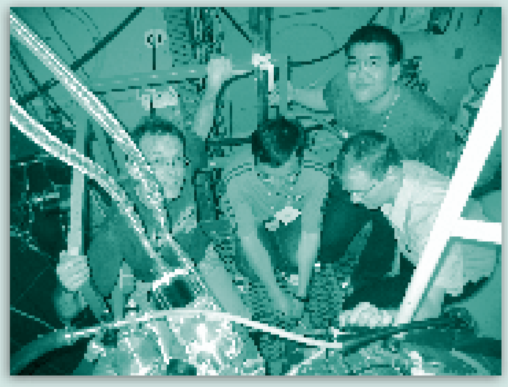
## 4.5 Accommodation

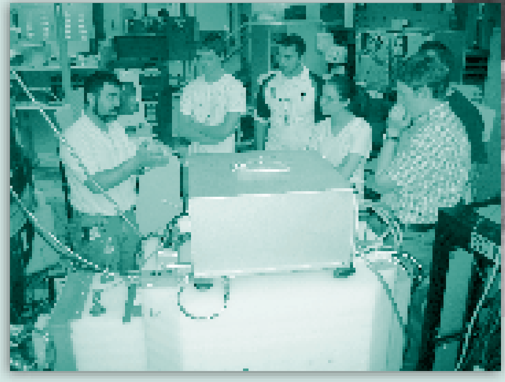
Users of specialized and large-scale scientific facilities, whether high-energy particle physics labs, astronomy observatories, or neutron scattering labs, are often engaged in what is colloquially known as 'suitcase science', i.e. where users travel from their home institution and stay for a period at the facility to conduct their research. Increasingly, instruments can be operated remotely, and data can be acquired and analyzed from an individual researcher's home institution. Nevertheless, the Canadian Neutron Centre is expected to deliver its greatest impact by providing an environment where facility staff, visiting scientists and students will share the same environment, work with common experimental tools, exchange ideas and knowledge across a wide range of disciplines and experience the full spectra of scientific activity – from discovery to problem solving, from academia to industry, from theory to instrumentation, and from experimental planning to publication in scientific literature. The underlying concept is to create an environment similar to a continuous scientific workshop, rather than a simply a remote source of data.

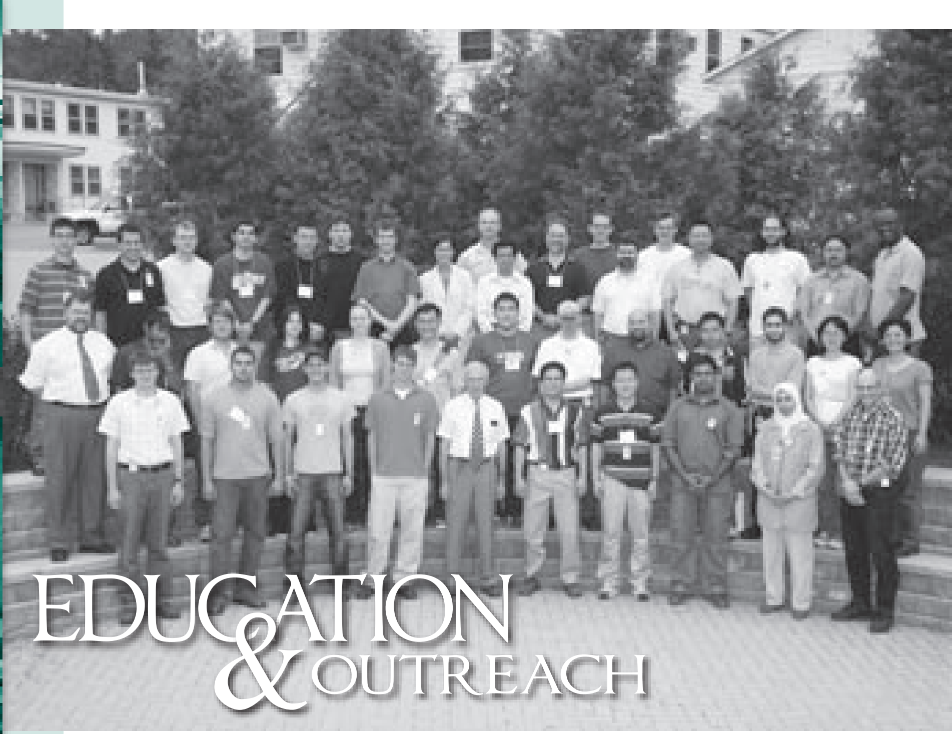
The model for accommodating visiting researchers varies widely across the world. Some facilities provide accommodation and charge users a small fee for their upkeep, while others provide local accommodations free of charge. There are instances where a third party operates a hotel on site, inside whatever security perimeters may be established, so that, once checked-in, the visitor can move freely from accommodation to the laboratory for the duration of their stay. For facilities that do not offer on-site accommodation, visiting scientists and students must arrange their own accommodation in distant hotels, incurring a significant cost for the research as well as an additional inconvenience or burden of travel to and from the laboratory itself. The Canadian user community requires access to some minimal, low-cost, on-site accommodation for visiting researchers and students. Many experiments require round-the-clock supervision, and having easy access to the laboratory at irregular hours can be helpful to relieve the stress of travel between accommodation and laboratory during experiments that last several, uninterrupted days. The availability of low-cost, nearby accommodation is important for existing neutron researchers and for attracting researchers new to neutron scattering. For scientists considering neutron scattering for the first time, available accommodation will remove logistical obstacles, and create a welcoming atmosphere for scientists to consider investing their time in accessing the facility.

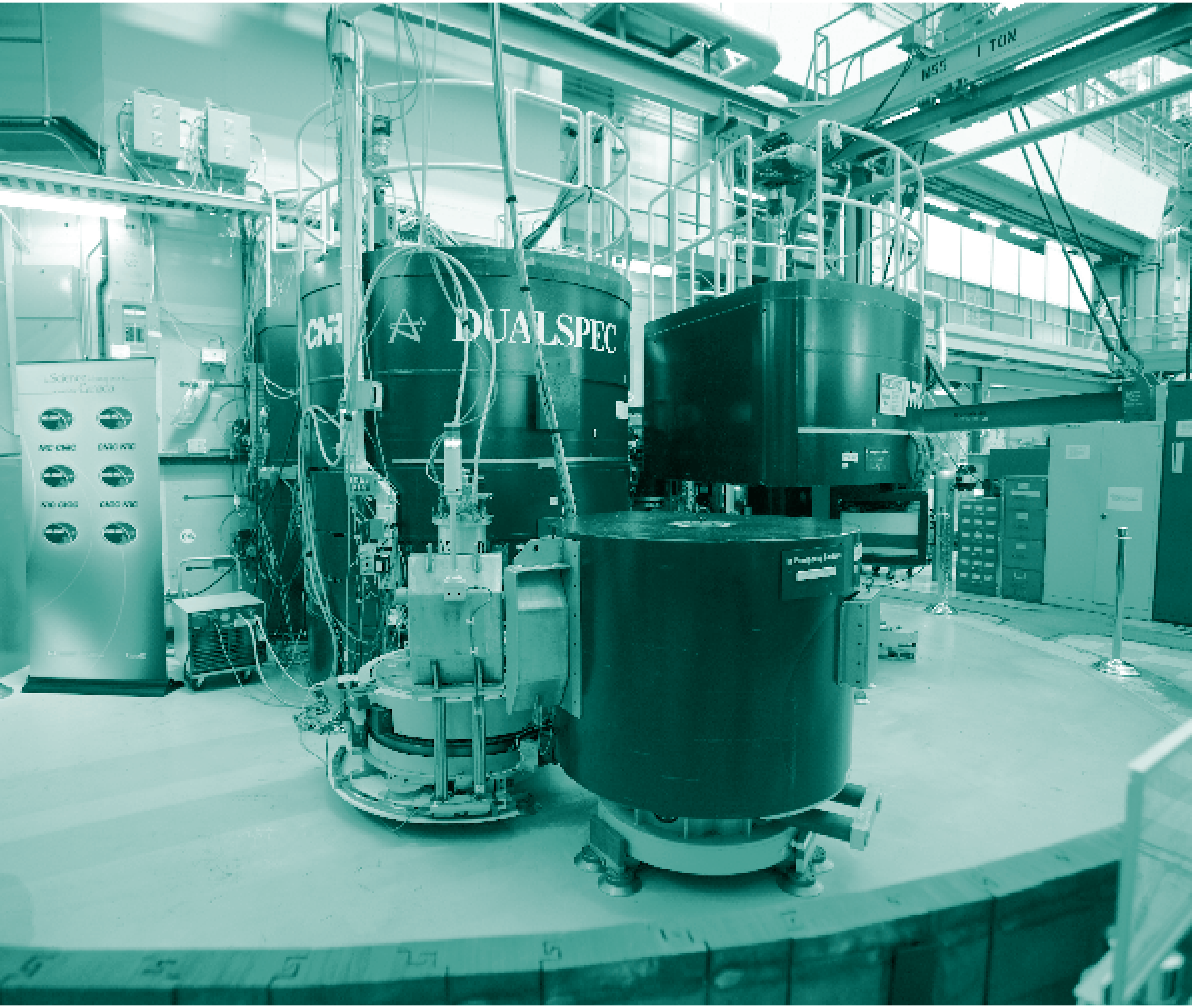
# EDUCATION & OUTREACH

One benefit of a national centre for neutron-based research that can accommodate visiting groups of scientists professors and students, is the role it plays in education and training of highly qualified people. The regular summer schools at the NRC Canadian Neutron Beam Centre pictured here, are one example of that educational activity. The presence of a national centre with a strong mandate for education and outreach encourages the development of a lively scientific community in Canada, in a way that access to foreign neutron sources does not.





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## 4.6 Governance and Management

How a future Canadian Neutron Centre is governed and managed will have a direct effect on its value as a research facility for the neutron scattering community. It is therefore worth identifying a few requirements for management and governance along with the physical and technical requirements that the community has for the CNC.

### PARTICIPATING IN A MULTIPURPOSE SCIENCE FACILITY

Current consideration is being given to a future Canadian Neutron Centre that will be designed and constructed as a multipurpose science facility. The neutron scattering community supports that concept as one that has brought a useful cost/benefit balance to Canada in the past, and may be the pathway to a more competitive neutron flux than could be achieved in a single-purpose neutron beam facility. A single-purpose neutron beam facility must secure funding to support the full cost of the neutron source plus the associated neutron beam facility. The ILL, with a full staff of about 450 people, has a total operating budget of about $100M, to support 42 neutron beam instruments. [135] The cost to operate the source alone is about half of this. Since a single source can provide neutrons for several R&D programs, the Canadian practice at the NRU reactor has been, effectively to divide the operating cost for the source among various mission elements: isotope production, nuclear R&D, and neutron beams for materials research. If a future Canadian Neutron Centre continues as a multipurpose neutron source, this may be a cost effective option for Canada to benefit from neutrons for a full spectrum of scientific and industrial needs. However, it will be essential to establish a governance arrangement that respects the requirements of each user community and is able to balance the operation of the facility so as to satisfy them all to the extent possible.

### GOVERNANCE

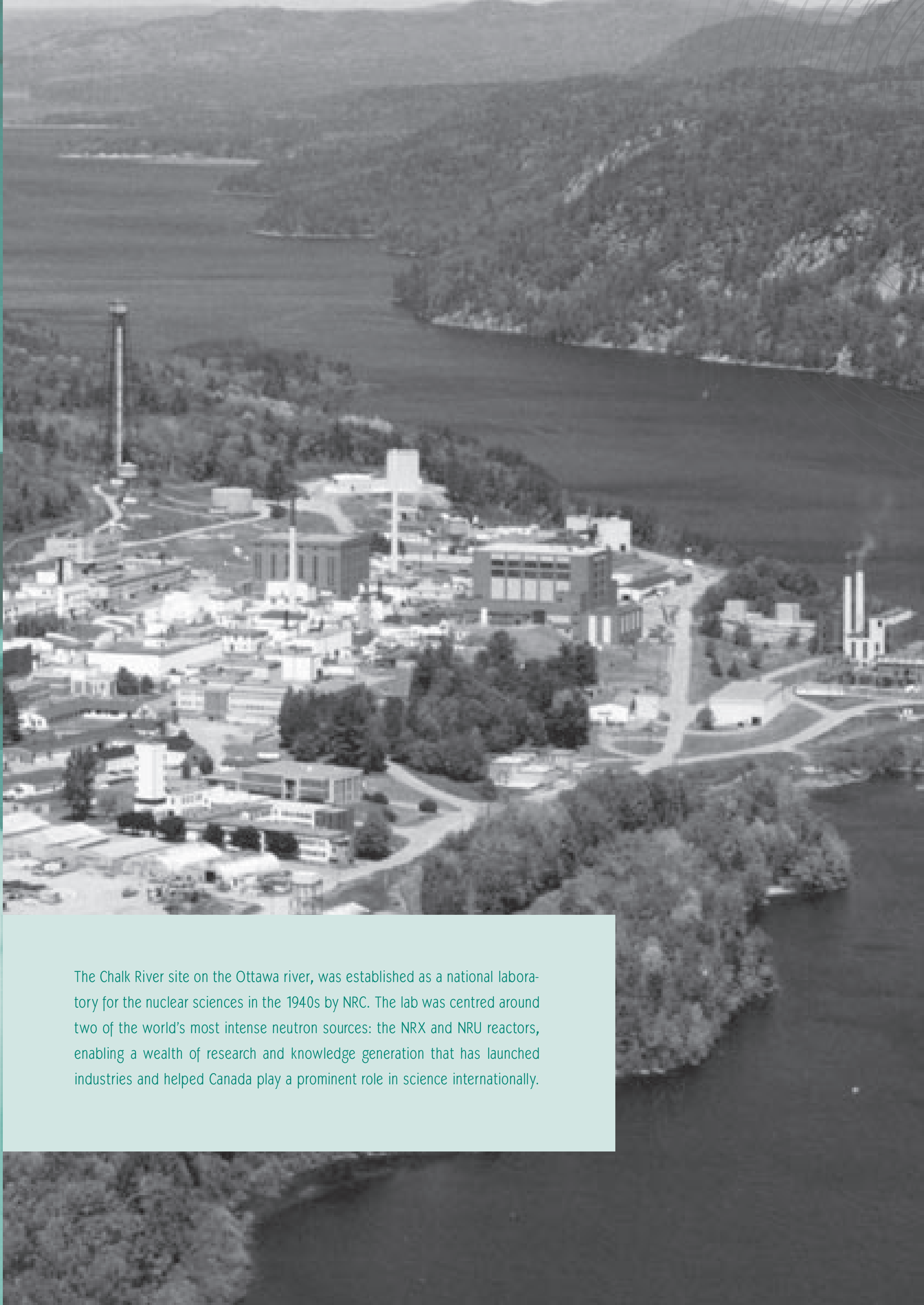
For the neutron scattering community it is important that the governing body be familiar with the goals of a neutron beam laboratory operating in a future CNC. Those goals include:

- being a unique and powerful scientific resource that is accessible by professors and students across Canada
- playing a role in the international network of neutron beam labs, welcoming foreign scientists and, by exchange, opening up the international network to Canadian scientists
- applying neutron beams to projects for industrial clients that help improve their business
- operating at full power on a predictable and reliable duty cycle

Those goals can be broadly classed as education (development of highly qualified people) innovation (giving Canadians the tools to develop new materials and technologies) competitiveness (supplying knowledge to companies to give them a business advantage) and cost-effectiveness through orderly management.

### OPERATING FUNDING

The operating costs of the CNC could be allocated according to the various scientific missions it is fulfilling. The production of isotopes, the support of the nuclear power industry and the support of the neutron scattering community could be allocated part of the operating costs. Equal roles in the financing of the CNC would help to supply balance in its governance. An agency or institution that represents the neutron beam user community could hold the funding contribution towards a logical portion of the operating cost of the neutron source itself (not just the attached neutron beam laboratory), and therefore participate in the governing structure as a key stakeholder. However it is accomplished, the neutron beam community needs a mechanism to express its priorities and influence both the operating framework and future capital developments within the neutron source they are sharing with other users.



The Chalk River site on the Ottawa river, was established as a national laboratory for the nuclear sciences in the 1940s by NRC. The lab was centred around two of the world's most intense neutron sources: the NRX and NRU reactors, enabling a wealth of research and knowledge generation that has launched industries and helped Canada play a prominent role in science internationally.

# 5. PRIORITIES

The overarching priority of CINS is to secure a new neutron source for Canada. This source must deliver world-class thermal and cold-neutron flux into many beam lines, with capacity for future expansion to respond to emerging science and technology. It must be mandated and governed to deliver the maximum benefit for Canadian science, industry and education for the next 50 years.

Assuming that this main priority is met, further consideration is needed to choose the suite of neutron beam instruments to install at the new Canadian Neutron Centre, to maximize the scientific impact of Canada's neutron beam user community.

## 5.1 Considerations

The CINS community first addressed the need for long-term planning and prioritization of neutron beam facilities in the early 1990s. [8] Since then, there has been an on-going discussion about how best to choose the instruments that will deliver the greatest value to the Canadian scientific community, and how to sequence their installation over time, recognizing that the needs of science and technology will evolve over the decades that a new neutron source is expected to operate. Two basic approaches are possible. The first favours those instruments that meet the research needs of the current Canadian users of the Chalk River facilities – an enhancement of the status quo, at least as a starting point – with some emphasis being placed on instruments that would be unique in the world. This approach would enable the Canadian neutron scattering community to both retain its international leadership position and attract and recruit the most sophisticated condensed matter researchers to our facility. The second strategy envisages a distribution of instruments and methods that supports the profile of research averaged over all international neutron laboratories. This latter approach would provide broader coverage and a new domestic capacity for Canadian users, especially those who must currently visit foreign laboratories to access facilities that are not available at Chalk River.

Other considerations used to establish instrument priorities include:

- the size of the current and potential user community
- growth trends in the Canadian neutron user community
- oversubscription rates at similar instruments in other neutron laboratories
- quality of the research that is supported by the instrument
- potential for positive socio-economic impacts arising from knowledge obtained from a given class of instrument or research
- effectiveness of the instrument for education of highly-qualified personnel
- identification of a champion to lead an instrument development team

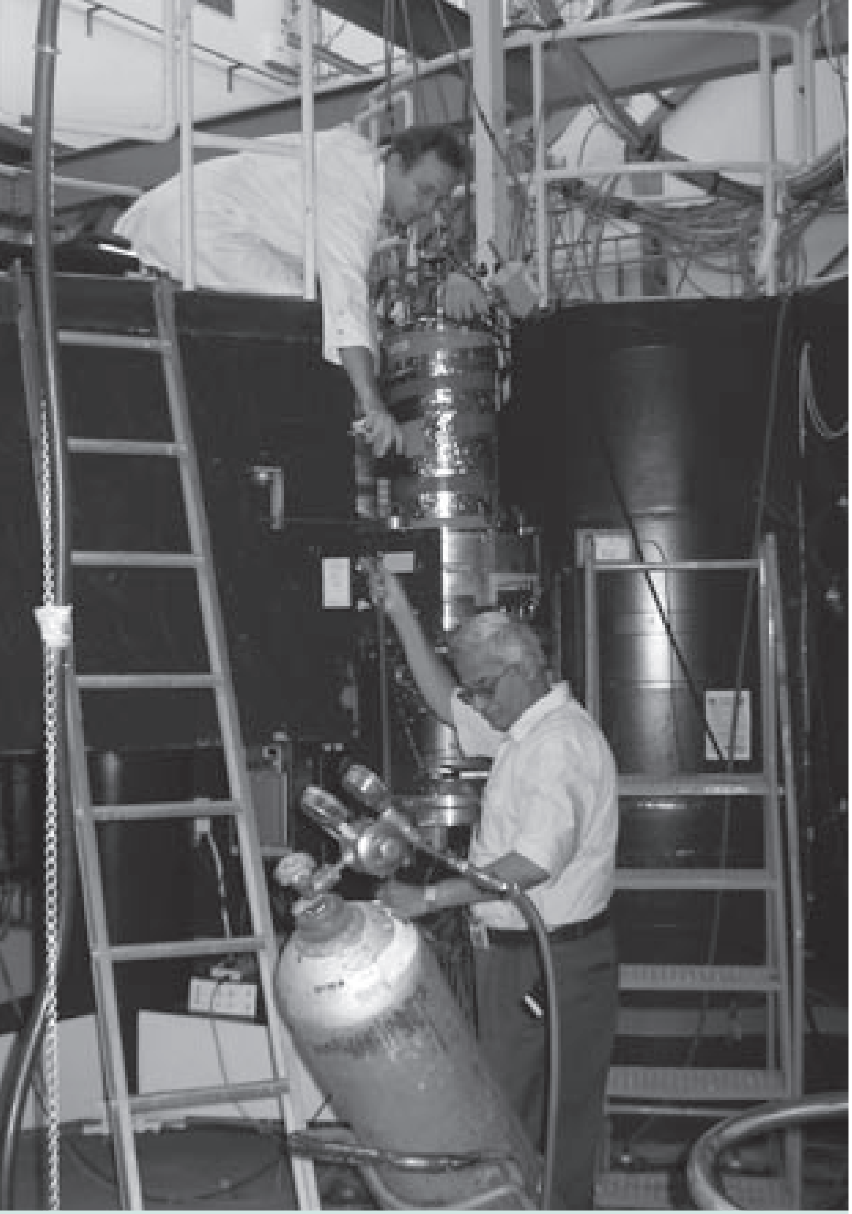
It is clear that the strength and diversity of the Canadian neutron scattering community is sufficient that the initial suite of instruments should be chosen to support and enhance existing research programmes rather than developing a general purpose collection. Indeed, as we completed the analysis using the criteria identified here, we found that the high priority instrument group that emerged represented a powerful facility that will be available as the new reactor comes on-line, and that the second round of instruments that would be developed shortly after initial operations commence, will place us firmly on the map for many years to come.

## TABLE 7 - Prioritization of instruments by subject-based working groups (WGs)

| Instrument | Source | Section | Comments |
|---|---|---|---|
| Reflectometer (Horizontal geometry) | Cold | 3.2 | Multiple WGs placed in top 3 Exists in Canada (D3) |
| Reflectometer (Vertical geometry) | Cold | 3.2 | Multiple WGs placed in top 3 Exists outside Canada |
| Triple-axis (polarized) | Thermal | 3.7 | One WG placed in top 3 Exists in Canada (C5) - can be advanced |
| Single-crystal texture / development station | Thermal | 3.5 | One WG placed in top 3 Exists in Canada (E3) |
| White-beam stress scanner | Thermal | 3.4 | One WG placed in top 3 Exists nowhere - innovative approach |
| High-efficiency powder diffractometer | Thermal | 3.6 | One WG placed in top 3 Exists in Canada (C2) - can be advanced |
| High-resolution powder diffractometer | Thermal | 3.6 | One WG placed in top 3 Exists in Canada (C2) - can be advanced |
| Low-Q powder diff. | Cold | 3.6 | One WG placed in top 3 Exists outside Canada |
| Disc chopper spectrometer | Cold | 3.7 | One WG placed in top 3 Exists outside Canada |
| Classic SANS | Cold | 3.3 | Multiple WGs placed in top 6 Exists outside Canada - very popular[3] |
| Ultra SANS | Thermal | 3.3 | Multiple WGs placed in top 6 Exists outside Canada |
| Triple-axis (polarized) | Cold | 3.7 | Multiple WGs placed in top 6 Exists outside Canada - can be advanced |
| Laue single crystal instrument (sub-mm) | Thermal | 3.5 | Multiple WGs placed in top 6 Exists outside Canada - can be advanced |
| High-Q powder diffractometer | Hot | 3.6 | One WG placed in top 6 Exists outside Canada |
| Triple-axis (polarized) | Hot | 3.7 | One WG placed in top 6 Exists nowhere - innovative approach |
| Shielded Diffractometer | Thermal | 3.6 | One WG placed in top 6 Exists outside Canada - can be advanced |
| Radiograph / tomograph | Thermal | 3.8 | One WG placed in top 6 Exists inside Canada - can be advanced |
| Backscattering, High-res'n Spectrometer | Cold | 3.7 | One WG placed in top 6 Exists outside Canada |
| Spin-echo spectrometer | Cold | 3.7 | One WG placed in top 6 Exists outside Canada[4] |

[3] Most facilities with SANS machines have more than one of these high-throughput instruments.

[4] Requires special attention to magnetic noise arising from surrounding instruments and infrastructure.



The determination of structure is the first step towards understanding phenomena in many materials. Diffraction methods constitute the most powerful probes of structure at the scale of atoms, molecules and nanostructures. Canada's scientific capacity in this area of materials research leaped forward in 1992, when the powerful C2 powder diffractometer (pictured above) was commissioned.

## 5.2 Recommendations of CINS AGM / Workshop 2007

At the CINS Annual General Meeting in 2007, five working groups were defined to represent the subject areas described in sub sections 2.1-2.5: (1) Excitations in Condensed Matter, (2) Crystallographic Analyses, (3) Materials Science and Engineering, (4) Thin Films and Surfaces – nanostructures, and (5) Soft Materials – polymeric and biomimetic. These working groups (WGs) then identified the instrument priorities based on their research needs, for neutron beam instruments as listed in Table 3, and described in Section 3. The top three instruments in each group's list were collected first, and the second three instruments in each group's list were collected next. The results are presented in Table 7, with comments.

## 5.3 Analysis of Priorities

If we combine the data on domains served by various instrument types (Table 5) with the priorities established by the working groups (Table 7), then we can divide the possible instruments into three broad categories.

The first group contains the 'High' priority suite of instruments to be built and commissioned in parallel with the reactor construction project. These instruments are the workhorse facilities that underpin the majority of the neutron beam research carried out by the Canadian neutron scattering community. The 'High' priority instrument group includes two thermal powder diffractometers, one each optimised for efficiency and resolution, a thermal triple-axis machine with polarisation capability and a white-beam stress-scanner. These four instruments, combined with the vertical sample reflectometer, replace the existing suite, currently located at NRU, with state-of-the-art machines that will immediately serve as a critical resource for the research programmes of Canadian users. The current facility at NRU only provides beams of thermal neutrons, greatly restricting

## TABLE 8 - Canadian user recommendations of neutron instrument priorities - 2007

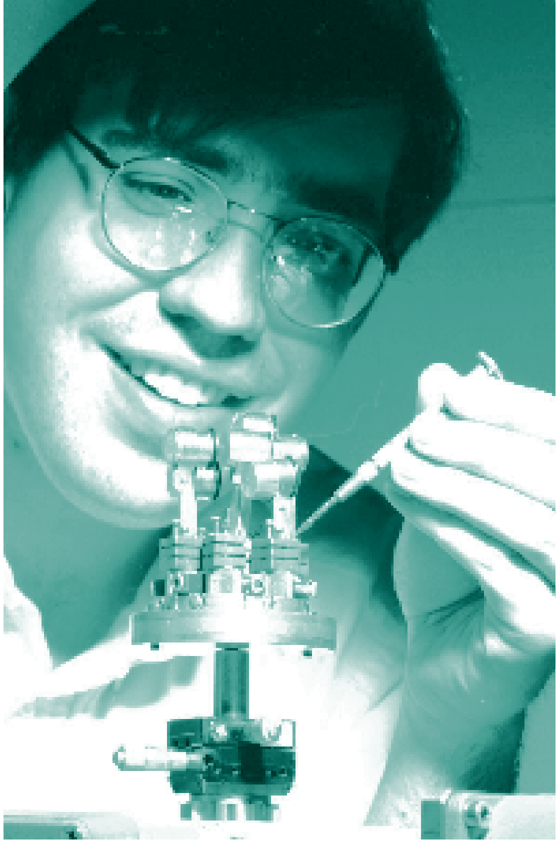
| High Priority | Medium Priority | Low Priority |
|---|---|---|
| T – Powder diffractometer (High efficency) | C – Second pinhole SANS | C – Backscattering spectrometer |
| T – Powder diffractometer (High resolution) | T – Ultra SANS | C – Spin-echo spectrometer |
| T – Triple-axis spectrometer (polarized) | T – Laue single crystal (sub-mm) | H – Powder diffractometer (High Q) |
| T – White-beam stress scanner | C – Powder diffract (Low Q) | H – Triple-axis spectrometer (polarized) |
| C – Reflectometer Vertical sample | C – Triple-axis spect (polarized) | T – Radiograph / tomograph |
| C – Reflectometer Horizontal sample | | T – Neutron holography |
| C – Classic Pinhole SANS | | |
| C – Disc chopper spectrometer (DCS) | | |
| T – Single-crystal / texture / development diffractometer | Labels indicate the 'temperature' of the neutron source required for each instrument (T=Thermal, H = Hot, C = Cold). | |

the areas of research that can be supported. There was a clear recognition, among all working groups, that a cold source to feed low-energy neutrons to suite of instruments was a high priority. This is reflected in the second group of instruments in the 'High' priority suite. Here we find two reflectometers; one versatile system covering a wide q-range with a vertical sample geometry, the second instrument dedicated to liquid-gas and liquid-liquid interfaces with a horizontal sample plane. The classic SANS instrument opens up the world of nano and mesoscopic structures, gels and colloids that appear in polymer chemistry and biologically relevant systems. Cold SANS instruments are consistently over-subscribed at every facility where they are built and results from this basic instrument are central to a rich variety of materials science. A high resolution DCS spectrometer rounds out the list of first-run cold instruments. The 'High' priority list is completed by a thermal development station. This flexible multi-purpose instrument will be used to evaluate and align single crystal samples. It will support instrument design projects that will arise both as the 'Medium' priority suite is developed and also to enable improvements to the first group. By placing this instrument at the end of a guide, and enclosing it in a shielded environment, it will also be possible to study specimens that present significant hazards while minimising the risks to both personnel and equipment.

The detailed sequencing of the instruments in the 'Medium' and 'Low' priority groups is far less certain than that established for the 'High' priority group. It is likely that the second round of instrument design would not start until the first group are being commissioned; about eight years after the start of the CNC project. The new research opportunities that the CNC will provide through its state-of-the-art instrumentation will attract a new generation of neutron beam users to Canada. As a result, both the make-up and the research interests of the Canadian community will change. However, some trends are clear, and so an outline of the future can be sketched.

SANS instruments are consistently over-subscribed, so either a second pinhole SANS (on the cold source) or an Ultra-SANS (on the thermal source) will be part of the second round. Similarly, the push towards working with ever smaller crystals will likely lead to the development of a need for sub-mm Laue capability. With a cold source already in place, a low-energy triple-axis machine and a powder diffractometer for extreme low-q diffraction studies would be natural extensions to the primary suite. All of these instruments were ranked highly by one or more of the working groups and have been built at other facilities where they serve quite wide communities of users.

In the 'Low' priority group, we find the highly specialised instruments such as the backscattering and spin-echo machines that serve a relatively narrow community, but yield data that cannot be obtained by other means. These instruments are critically important to those who depend on them, but need a significant commitment to champion and build. Similarly, while a hot source can provide very short wavelength neutrons that can be used to access diffraction data at high momentum or energy transfers, it is unclear whether such work is better done at a pulsed spallation source. However, several reactor-based hot sources are in operation with successful instruments. The proposed hot source and associated instruments might constitute unique elements of the 'Canadian' contribution to the global network of neutron scattering facilities, enabling structural studies of amorphous materials, such as liquids and glasses, and also high energy excitations in unconventional crystalline solids.



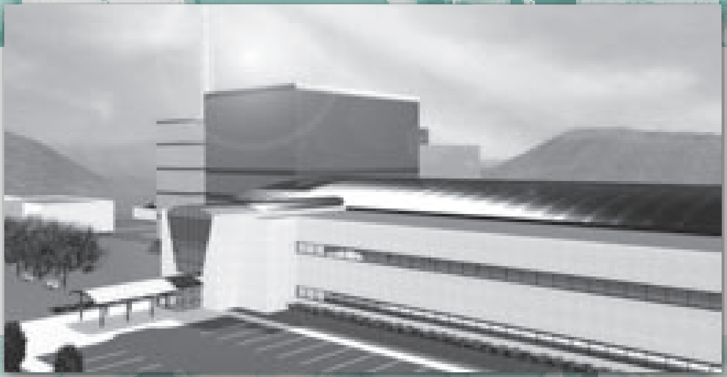
The final two instruments appearing on the 'Low' priority list received their low ranking because today's neutron beam user community does not currently exploit such instruments in their research. However, the CNBC is actively engaged in feasibility tests and demonstrations of both techniques, exploring possible ways to integrate these neutron beam methods into a future neutron facility. Neutron radiography or tomography may require leadership from a separate community of neutron beam users – those interested in industrial or medical imaging. While neutron holography is a newly discovered technique that offers the promise of revolutionizing our capability to determine structures of membrane-associated proteins that have defied attempts to prepare as crystals suitable for traditional diffraction analysis.

## 5.4 Summary

It is worth noting that the Canadian suite of instruments proposed here spans a very wide range of neutron-based methodologies. It includes a solid mix of demonstrated work-horse instruments with some more adventurous concepts such as the next-generation white-beam stress scanner. We also include a (Q, )-surveying instrument, following the successful experience of the DCS at NIST, and envision an important role for such a facility in the North American context. The Canadian neutron user community is open to the possibility of several radically new instrument concepts including neutron holography for atomic resolution imaging and a hardened spectrometer environment for hazardous systems. The diversity of the proposed instrument suite reflects the strengths and depth of our research community.

Having pioneered neutron scattering, Canada maintains a large footprint on the international landscape of materials research with neutron beams. We know what we need to retain our leading presence in the field. We know what is required to attract talented scientists of the highest quality to choose Canada as the place to live and express their scientific creativity for the benefit of society. In carrying out this plan for neutron scattering to 2050, we believe Canada will reinforce its world class capacity for excellence in materials research, and deliver impacts across the scientific spectrum from discovery to innovation.

# The next 50 YEARS wide open with Opportunity



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# Acronyms

AECL – Atomic Energy Canada Limited
AND/R – Advanced neutron diffractometer/reflectometer
ANDI – Applied Neutron Diffraction for Industry
ANSTO – Australian Nuclear Science and Technology Organization
BS – Backscattering
CFI – Canada Foundation for Innovation
CINS – Canadian Institute for Neutron Scattering
CMR – Colossal magnetoresistance
CNBC – Canadian Neutron Beam Centre (NRC program)
CNC – Canadian Neutron Centre (new neutron facility)
CW – Constant wavelength
DCS – Disc-chopper Spectrometer
DOP – Dioctylphthalate
GDP – Gross domestic product
GMR – Giant magnetoresistance
GTAW – Gas tungsten arc welding
HED – High efficiency diffractometer
HFIR – High Flux Isotope Reactor
HRD – High-resolution diffractometer
HTSC – High temperature superconductivity
IAEA – International Atomic Energy Agency
IGV – Instrumental guage volume
ILL – Institute Laue-Langevin
INS – Inelastic neutron scattering
INSPEC – Database of scientific publications
IPSCO – Steel company
IVACO – Steel company
KDP – Potassium dihydrogen phosphate
LLB – Laboratoire Leon Brillouin
MDSN – MDS Nordion, a medical company
MRI – Magnetic resonance imaging
MSE – Materials Science and Engineering
NCNR – National Center for Neutron Research
ND – Neutron diffraction
NIST – National Institute for Standards and Technology
NMR – Nuclear magnetic resonance
NPDF – Neutron pair distribution function analysis
NR – Neutron reflectometry
NRC – National Research Council
NRU – National Research Universal Reactor
NRX – National Research Experimental Reactor
NSE – Neutron spin echo
NSERC – Natural Sciences and Engineering Research Council
OPAL – Open Pool Australian Light-water Reactor
PEM – Proton exchange membrane
PNR – Polarized neutron reflectometry
PSDs – Position sensitive detectors
PVA – Poly vinyl alcohol
PVC – Polyvinylchloride
QINS – Quasi-inelastic neutron scattering
SANS – Small-angle neutron scattering
SAXS – Small-angle X-ray scattering
SDW – Spin density wave
SINQ – Swiss spallation neutron source
SMA – Shape memory alloy
SMEs – Small and medium-sized enterprises
SNS – Spallation neutron source
SW-TOF – Scanning-wavelength time-of-flight
TAS – Triple-axis spectrometer
USANS – Ultra small-angle neutron scattering
TOF – Time-of-flight
UCI – University of California, Irvine
VSANS – Very small-angle neutron scattering
WGs – Working groups
YBCO – Yttrium barium copper oxide

*In carrying out this plan for neutron scattering to 2050, we believe Canada will reinforce its world class capacity for excellence in materials research, and deliver impacts across the scientific spectrum from discovery to innovation.*

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