CINS

PLANNING TO 2050
FOR MATERIALS RESEARCH WITH NEUTRON BEAMS IN CANADA
2015 UPDATE

Canadian Institute for Neutron Scattering

About the Canadian Institute for Neutron Scattering (CINS):

CINS is a not-for-profit, voluntary organization that represents the Canadian scientific community of neutron beam users and promotes scientific research using neutron beams. Individual members include university faculty, professional scientists and engineers, research technicians, post-doctoral fellows and graduate students. Members include 400 individuals, of which 250 are from over 40 Canadian institutions in 7 provinces, including over 60 university departments from 32 universities. The university departments include broad representation from physics, chemistry, life sciences, earth sciences, materials science, and engineering. Our membership also includes 150 individuals from over 80 foreign institutions from 19 countries.

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Canadian Neutron Beam Centre

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CANADIAN INSTITUTE FOR NEUTRON SCATTERING

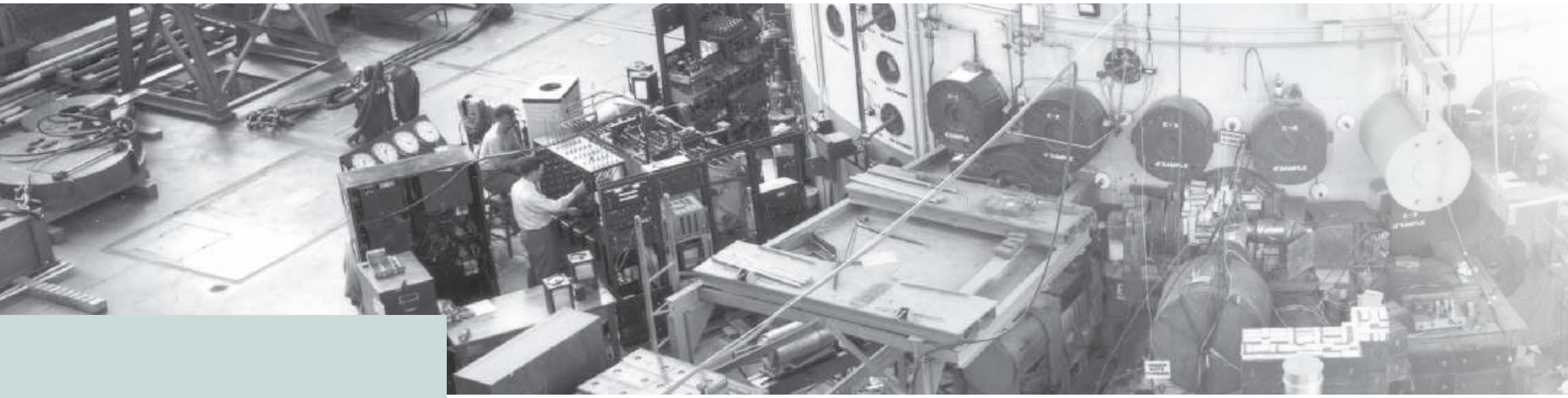
Planning to 2050 for Materials Research with Neutron Beams in Canada

2015 UPDATE

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.



Executive Summary

In "Planning to 2050", Canadian scientists describe materials research and development with neutron beams and recommend how to maximize its future value to Canada. The plan lays out the priorities of the community of physicists, chemists, engineers, earth and resource scientists, and life scientists who use neutron beams in Canada. These priorities have resulted from consultative democratic processes that have taken place over more than a decade.

The centrepiece of the plan is the construction of the Canadian Neutron Centre (CNC), a world-class neutron source with associated laboratories and infrastructure. The CNC will surpass the National Research Universal (NRU) reactor—planned to be permanently shut down in 2018—in the production of neutrons for materials research. In addition, the CNC could potentially continue the NRU reactor's functions in nuclear energy research or the production of isotopes for industry and medicine.

Canada enjoys a strong history in research with neutron beams, starting with the Nobel Prize–winning work of Bertram Brockhouse in the 1960s and continuing today.

The Importance of Neutron Beams

Neutron beams are versatile and irreplaceable tools for materials research. They enable fundamental scientific exploration and education, and can be applied in many sectors, including the aerospace, automotive, and manufacturing sectors, as well as in Canada's four priority areas: energy, environment, health, and communications. Everything around us, even the human body, is made of materials whose behaviour needs to be understood. By improving our understanding of the way that materials work, we can have positive impacts on every aspect of our lives.

Canadian Research with Neutron Beams

Research using neutron beams in Canada is carried out at a large centralized facility, but consists of many individual projects driven by research groups from universities, industry, and government laboratories across Canada and around the world.

Canada's primary neutron source is the NRU reactor at Chalk River Laboratories. The CNBC operates six neutron beam instruments surrounding the NRU reactor. These instruments direct neutrons from the reactor onto materials of interest.

Canada's neutron source is a highly valuable element of Canada's infrastructure for science and industry. Given that eight to ten years may be required to design, build, and license a new facility, a decision to secure a new neutron source is urgent.

Canada's neutron source is the NRU reactor at Chalk River Laboratories. This multipurpose facility supports science and industry in three distinct areas: (1) it supplies neutrons for the Canadian Neutron Beam Centre (CNBC) for materials research across a host of scientific disciplines; (2) its core provides a test environment for fuels and components for nuclear power technologies such as the CANDU reactor; and (3) it is the largest global producer of isotopes for applications in medicine and industry.

Canada enjoys a strong history in research with neutron beams, starting with the Nobel Prize–winning work of Bertram Brockhouse in the 1960s and continuing today. Innovative neutron instruments developed in Canada have been replicated at every major neutron beam centre worldwide. These include the neutron stress scanner, developed by scientists at Chalk River in the 1980s, and Brockhouse's triple-axis spectrometer (TAS). Today, the CNBC is a world leader in areas such as stress measurement for industry, powder diffraction, and the study of quantum materials with polarized neutrons.

The Canadian community of researchers who employ neutron beams maintains an international reputation for innovation and for the direct engagement of industry clients.

Examples of impacts on industry and society include:

- Helping the Canadian nuclear industry to manage the cracking of feeder pipes to ensure safe, reliable, and economical operations of power stations;
- Helping automotive and aerospace companies to increase the reliability of materials and repair methods used in critical components such as engines;
- Helping the oil and gas industry to improve the reliability of components subjected to high pressures during fracking operations, and to create inspection techniques to inform decision-making about replacing sections of pipeline; and
- Helping to develop a technology now being commercialized to save substantially on the high energy costs of producing the main bleaching agent used by the paper industry.

The CNBC has an excellent record of training highly qualified people. It also helps to connect Canadian scientists to a global network of neutron laboratories, thereby fostering collaborations with scientists from over 100 institutions in 20 countries.

Canada's Need for a New Neutron Source

Canada's NRU reactor has been operating since 1957. Although the NRU reactor was the world's best research reactor when it was built, Canada's capabilities have fallen behind in some areas—most notably in its lack of a source of cold neutrons, which are in the highest demand because they are especially useful for nanotechnologies and for health and life sciences.

In February 2015, the Government of Canada announced [1.1] that Canadian Nuclear Laboratories (CNL) will operate the NRU reactor until March 31, 2018, subject to relicensing. At the conclusion of this period, the reactor will be placed in a state of storage with surveillance until decommissioning.

With the upcoming permanent closure of the NRU reactor, the Canadian neutron scattering community is faced with a grave challenge. Without a domestic neutron source, Canada will be on the verge of losing its competency in neutron scattering science and technology. Relying on foreign facilities for access to neutron beams has major disadvantages and limitations. From similar experience in other countries, it is certain that attempting to maintain a 'virtual neutron beam centre', without a domestic neutron source, will result in the loss of neutron beam expertise. Challenges include: costs associated with securing access; difficulties in attracting and retaining expertise and in training highly qualified personnel; an unclear role in supporting the user community; difficulty with performing proprietary research; and an inability to direct the research and facilities toward Canada's strategic needs. Given that eight to ten years may be required to design, build, and license a new facility, a decision to secure a domestic neutron source is urgent.

Canada is not alone. Many foreign neutron facilities are also approaching the end of their lifespans. In fact, the total capacity of neutron sources in OECD countries will decrease over the next ten years, even though the global demand for neutron facilities is growing and several new foreign facilities are being built.

One benefit of a national centre for research using neutron beams—in this case, a facility that can accommodate visiting groups of scientists, professors, and students—is the role it plays in the education and training of highly qualified people. The CNBC hosts regular summer schools. The presence of a national neutron 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 alone does not.

Our Vision for a New Canadian Neutron Centre (CNC)

We envision a new world-class facility, referred to as the Canadian Neutron Centre. Whether the neutron source is multipurpose or single-purpose, a reactor or a spallation source, the CNC would be designed to surpass the capabilities of today's facility to a time horizon of about 2050.

The proposed CNC would be a vital part of Canada's infrastructure for science and industry. While a facility dedicated to materials research using neutron beams would maximize its scientific output, Canada's rich experience with the NRU reactor shows us that a single, multipurpose reactor can perform each of these three missions: (1) materials research using neutron beams; (2) materials testing in the reactor core for the development of nuclear power; and (3) isotope production for industry and medicine.

Through the materials research mission, the CNC will:

- Reassert Canada's international leadership in research using neutron beams by enhancing areas in which Canada is strong but in which it currently lags, such as the application of neutron beams to the study of nanotechnologies and life sciences;
- Retain and expand Canada's national hub that fosters innovation in the application of neutron beams, in order to respond to Canada's research priorities while evolving according to national goals and policies;
- Educate and develop skills for thousands of highly qualified people, while also attracting highly qualified people to Canada;
- Sustain and increase proprietary neutron research by Canadian industries, in order to develop new industrial materials and products and to access wider markets;
- Support tens of thousands of individual science projects over its lifetime; and

- Foster scientific exchange in the global research community as part of a worldwide network of facilities for materials research.

Should Canada decide to continue other missions beyond neutron scattering, a multipurpose facility can achieve an excellent balance of economics and performance by serving these additional functions:

- Providing commercial research and development (R&D) services for the nuclear power industry to support the international fleet of CANDU reactors, as well as Canada's own nuclear industry, which has an estimated economic impact of over $6 billion per year, by enabling the testing of fuel and components under conditions representing a power reactor;
- Enabling Canada to develop more advanced nuclear power technologies and to effectively participate in the Generation IV International Forum; and
- Providing commercial irradiation services for non-nuclear industries, such as doping materials for computer chips and producing materials for the medical diagnosis and treatment of patients in Canada and around the world.

The Chalk River Laboratories site on the Ottawa River was established as a national laboratory for the nuclear sciences in the 1940s by the National Research Council. The lab was centred around two of the world's most intense neutron sources, the National Research Experimental (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. Through the presence of this true national centre for neutron scattering, scientists in universities and industries across Canada have had access to the very best scientific tools. Today, Canada has an historic opportunity to once again establish a world-class national laboratory that supersedes the aging facilities at Chalk River Laboratories.

An Environment for Science at the CNC

Science is a human endeavour. It is not just about facts, tools, and facilities. Science thrives on curiosity about nature and the free exchange of ideas between individuals.

We will create an environment that attracts highly qualified people, that strongly contributes to their education, and that facilitates the needs of their research. It will foster the exchange of ideas and knowledge between staff and visiting scientists who will continuously flow through the centre. To accommodate scientists who travel from across Canada and around the world to participate in experiments, the CNC will operate at full power on a reliable schedule. If a multipurpose facility, the CNC will need a governance arrangement that respects the needs of each user community.

The Neutron Source: The CNC must include a neutron source that delivers world-class neutron flux into many beam lines. A major advance will be a source of cold neutrons, which are in high demand worldwide for the study of life sciences, soft materials, and nanotechnology. A flexible design will allow the addition of beam lines in the future.

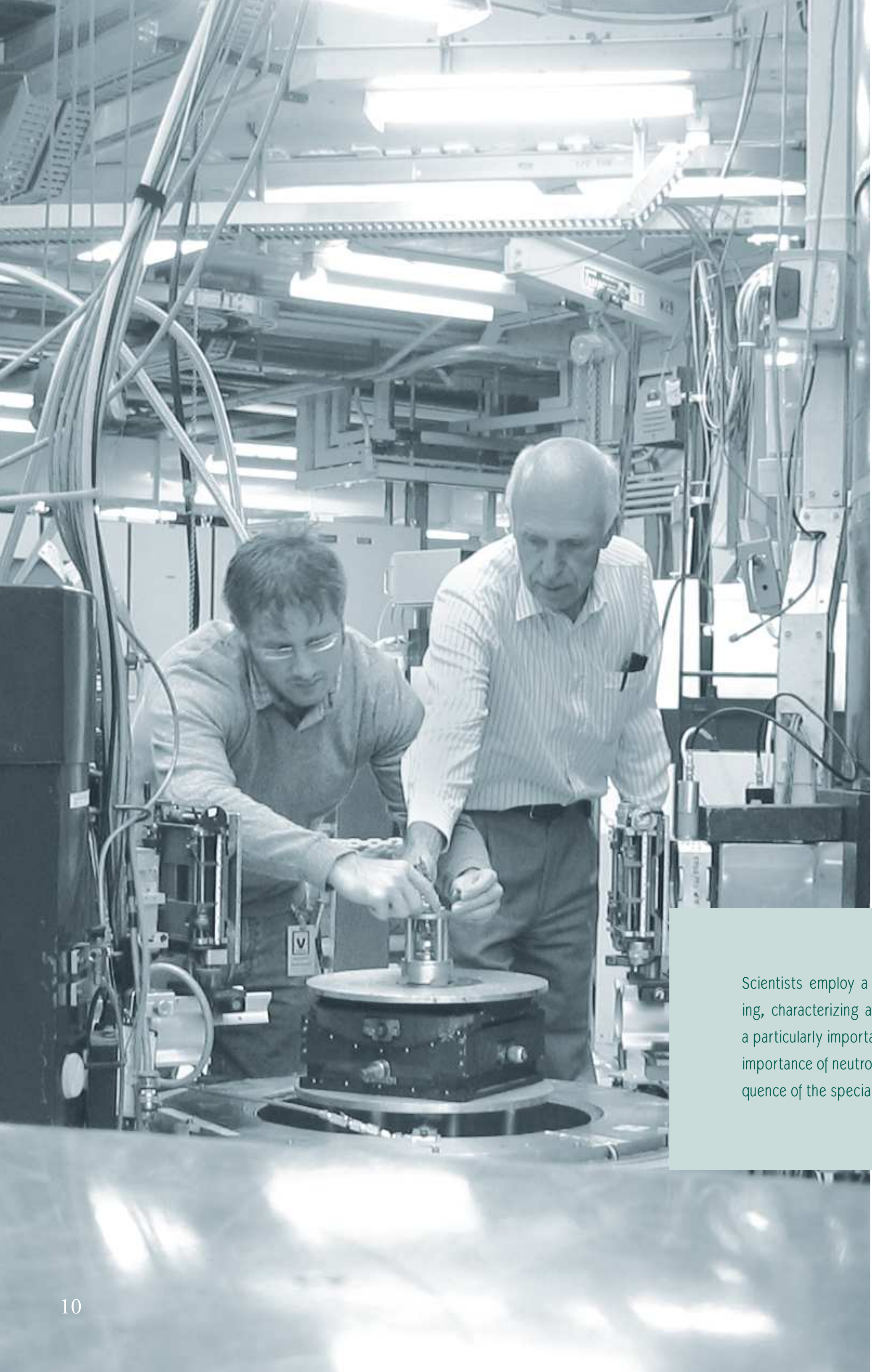
Neutron Beam Halls and Instruments: To perform many simultaneous experiments, a suite of neutron beam instruments will be housed in neutron beam halls. The reactor hall will be adjacent to the reactor in order to allow maximum neutron flux by being near the source. One or more guide halls in nearby buildings will increase the number of instruments possible by reducing instrument crowding at the source, although a high neutron flux to each instrument will be achieved using state-of-the-art neutron guiding technology. The planned suite of instruments will offer world-class performance and will introduce capabilities that are currently unavailable in Canada.

Attached Facilities: The CNC complex will include much more than the reactor and instruments. There will be office spaces and meetings rooms to enhance scientific collaboration; laboratories for on-site preparation of specimens by visiting scientists; workshops and working areas for the design, construction, testing, maintenance, and repair of specialized equipment; and a modern data acquisition, networking, and control centre that is able to adapt to future technologies.

Conclusion

Canadians contribute significantly to the world's knowledge of materials, and Canada receives much knowledge in return. Thanks to the contributions of industry, academia, and government, Canada reaps a wide array of benefits that range from health to wealth to well-being. As our domestic neutron source, the new CNC will be a versatile and irreplaceable part of the future of materials research in Canada.

The CNC will yield high value to Canada by planning for the human side of science, as well as by providing world-class scientific instruments. It will be an environment designed to generate ideas and promote the exchange of information. On behalf of the Canadian neutron beam user community, "Planning to 2050" outlines ways to maximize the new CNC as a world-class facility for materials research—one that will deliver impacts across the spectrum from discovery to innovation.



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. That includes people, food, energy technologies, the Earth and our environment, and infrastructures to transport water and goods. It also includes buildings, computers, airplanes, and cars, as well as devices for medicine, communication, entertainment, and everything else.

Materials are pervasive, although 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.

LED lights are an example of success in materials research, providing us with energy-efficient and environmentally friendly light sources. The invention of a key enabling technology, the blue light–emitting diode, was honoured with the 2014 Nobel Prize in Physics.

Other recent Nobel Prize in Physics awards illustrate how materials research underpins our everyday experiences. The 2009 prize honoured the inventions of fibre optics and CCD sensors, which are the backbones of broadband internet and digital cameras. The 2007 prize honoured the discovery of a phenomenon that enables computer hard drives, called giant magnetoresistance (GMR). The 2010 prize honoured ground-breaking experiments with graphene, a new material expected to lead to breakthrough applications in computers and touch screens; when combined with plastics, it may also be used to create new super-strong yet lightweight materials.

Materials research has been leading to transformational advances for centuries. In the 19th century, materials development was fundamental to steam-powered locomotion, which pushed the limits of materials to withstand certain temperatures and pressures and to support trains on thousands of kilometres of steel rails. The steam engine made possible the rapid expansion of North America and enabled people to travel so quickly that 'local time' could no longer be measured practically with reference to noon as the local solar zenith. In fact, Canadian Sir Sandford Fleming defined time zones to enable the orderly scheduling of the trains, and 'jet lag' was born!

In the mid-20th century, vacuum tubes were the unit of logic and the precursors to today's computers. At that time, engineers envisioned building vast computers to perform calculations. However, a fundamental shift occurred with the development of the transistor, which could be made exquisitely small and yet perform the same function as vacuum tubes. 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 instances of materials research—were also necessary steps towards the new technology. Today's computers out-perform the computers in the wildest dreams envisioned at that time, and now include handheld packages that play movies on demand, let you call work from anywhere, help you navigate your way home, and enable you to access your bank from the other side of the planet.

We hardly realize it, but our human experience has been shifted tremendously by materials research and development, which has continually produced advances to bring us into the information age of today.

In this document, references to 'materials' should be understood to include the following: (1) structural materials (e.g. metals, alloys, ceramics, or composites that are used to build machines and infrastructures); (2) functional materials (e.g. nanostructures that store gases, help chemical reactions to occur with less energy, or filter toxins from air and water, as well as crystal structures that change shape or magnetic alignments, which can be exploited in batteries, information storage, and other useful applications); and (3) soft materials (e.g. plastics, membranes, proteins, gels, and complex fluids like milk and blood).

Similarly, references to 'materials research' should be understood to encompass a full range of scientists and scientific disciplines, a few illustrations being:

- Biophysicists investigate the nanostructures that occur naturally in cells and tissues in order to provide fundamental clues that may offer more accurate directions for research on life processes, diseases, and therapies than is possible from large-scale clinical studies alone;

- Condensed matter physicists are trying to track down some of the challenging phenomena at the frontiers of knowledge, which could introduce a new technological revolution through advances in such things 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;

- 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, and more reliable materials cost-effectively;

- Earth scientists acquire a firm understanding of the temperature and pressure responses of minerals, which enables conclusions to be made about geological history and the condition of planet Earth; and

- Polymer chemists develop thin film coatings that make medical implants safe and reliable, as well as new organic electronics, membranes for fuel cells, and much more.

The importance of materials research is that materials underpin every aspect of the human experience. Indeed, discoveries of new materials or refinements of existing materials constitute the essential building blocks for advancements 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. Notably, neutron beams are a particularly important and irreplaceable part of the 'scientific toolkit'. For example, materials engineers need the penetrating power of neutron beams to examine the stresses deep inside critical industrial components that x-rays cannot penetrate. Biophysicists need the gentle probing of neutron beams to unravel the structures within biological membranes under lifelike conditions. Chemists need the sensitivity of neutrons to hydrogen to develop fuel cells and hydrogen storage materials. Physicists need the electrically neutral and magnetic properties of neutrons to better understand superconductivity (SC) and the magnetic structures of materials.

The world science community recognized the great importance of neutron beams when it awarded Bertram Brockhouse and Clifford Shull the Nobel Prize in Physics in 1994 for pioneering the use of neutron beams to probe materials. The place of neutron beams as valued scientific tools is manifested today in a global network of about 20 national neutron beam facilities operating around the world. These points are explored further in later sections.

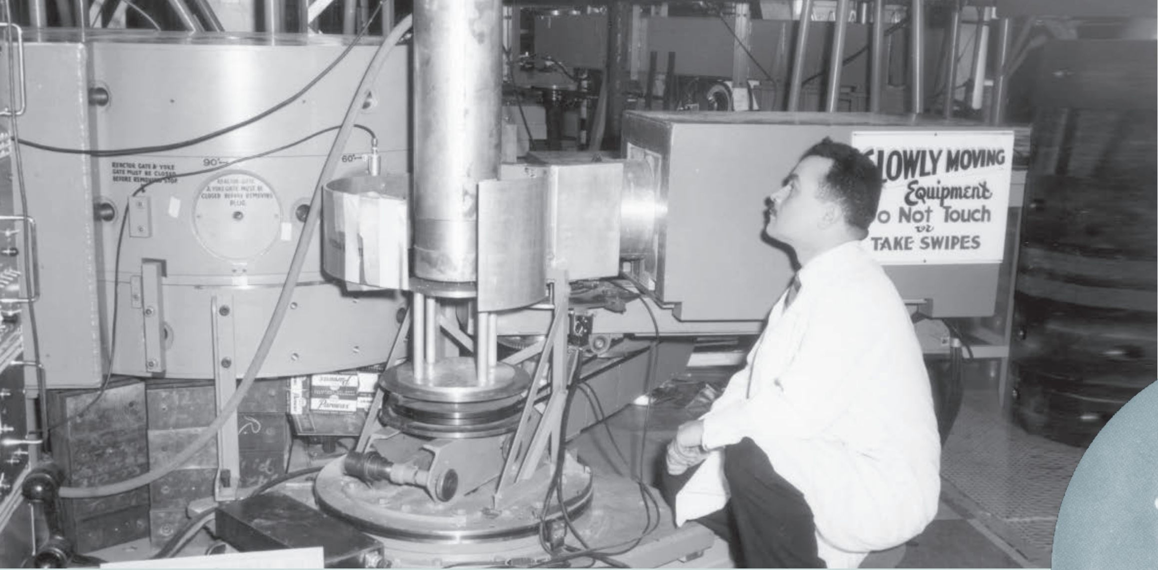
Neutron beams are irreplaceable for materials research because of the special way that neutrons interact with matter. All matter is made of atoms, which can be arranged either in orderly (crystalline) solid structures or in random (amorphous) structures in the solid, liquid, or gaseous states. Neutrons are sub-atomic particles that interact (1) with the nuclei of atoms and (2) 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 nuclear magnetic resonance (NMR), microscopy, ultrasonics, muon spin resonance, or electromagnetic radiation (e.g. laser light, x-rays, or gamma rays). This is not to diminish the importance of these other techniques, but to highlight that neutron beams provide another window for investigating materials—a window that sometimes reveals complementary information that is essential for the final understanding of how materials behave.

The way neutrons scatter from atoms (i.e. by changing their direction, energy, or 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 (1) in all kinds of materials, such as metals, minerals, ceramics, composites, polymers, lipid membranes, and peptides; (2) in all kinds of states, such as crystals, powders, liquids, gels, and colloids; and (3) in all kinds of applications, such as aerospace, automotive, energy, environment, medicine, communications, manufacturing, fundamental scientific exploration, and education.

Neutrons are neutral, spin-½ sub-atomic particles that interact (1) with the nuclei of atoms through short-ranged strong interaction, and (2) 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 neu-

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.

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Neutrons are penetrating but non-destructive

The typical energies of thermal neutrons are measured in the milli-electron volt (meV) range; their energies are a million times less than x-rays of corresponding wavelengths in the range of 1-10 angstroms (Å). Although these neutron energies are very 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 thus determine the centre of mass of an atom that is 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 (i.e. deuterium), a property that can be exploited to unravel the complex structures of biological materials and polymers in which 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 else to eliminate them from the signal through means such as 'contrast-matching' the particular feature with the surrounding solvent.

1.3 Canadian Neutron Beam Research – Stature and Status

In 1994, Canadian scientist 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 (TAS), developed at Chalk River Laboratories in the 1960s, has been replicated at neutron beam research centres worldwide, and it continues to serve as a primary instrument for exploring the frontiers of condensed matter physics. In the mid-1980s, 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 is now called the Canadian Neutron Beam Centre (CNBC). As a piece of our national science infrastructure, the CNBC is accessible to the research community that is represented by the Canadian Institute for Neutron Scattering (CINS), which includes established users as well as students and first-time users. Over the three-year period from 2011 to 2013, about 240 researchers from industry, government laboratories, and academia (i.e. 70 university departments spread across 30 Canadian universities in 7 provinces) participated in research dependent on access to the CNBC's 6 neutron beam lines. The CNBC enables industrial research in sectors such as nuclear energy, aerospace, automotive, oil and gas, defence, and primary metal production.

Industry accesses neutron beams for materials research because the resulting knowledge often impacts safe, reliable, and economic operations. A primary example was an extended research program in partnership with Atomic Energy of Canada Limited (AECL) and the CANDU Owners' Group (COG) over a ten-year period to manage the cracking in feeder tubes in CANDU nuclear reactors. The research program followed two forced outages of the Point Lepreau Nuclear Generating Station in 1997 and 2001, which together cost over $50 million. Stress analyses using neutron beams made key contributions to several outcomes, including: (1) the regulator was assured during these outages that the station could be restarted safely, thus avoiding further unplanned down-time costs; (2) China was assured that it could continue with the $4 billion construction of two reactors at Qinshan without the need for costly mid-construction design changes; (3) New Brunswick Power was able to make informed decisions regarding the timing of its $1 billion project to refurbish the Point Lepreau station in 2008 and regarding its ongoing management activities of

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.

> *"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*

the cracking, which cost as much as $5 million per year; (4) the broader nuclear power industry gained sufficient knowledge to assure the regulator that the feeder cracking was manageable at all stations, and also saved substantial time and resources during outages either by focusing the scope of the feeder inspections or by establishing other means to manage the cracking; and (5) the industry was able to develop materials and maintenance methods to provide high confidence that the observed feeder cracking will not be a significant concern at any new reactors or at any existing reactors after they are refurbished.

Further examples of the CNBC's recent impacts on industry, society, and research at the leading edge of science and technology include the following instances:

- Hydro-Quebec's research institute (IREQ) accessed the CNBC to understand a new cathode material used to produce sodium chlorate for the paper industry, and is now commercializing technology that is expected to save substantial amounts of energy for the industry, estimated at over $6 million per year;
- Major automotive companies in partnership with university teams have accessed the CNBC to improve the reliability of materials in lightweight vehicle engines while reducing manufacturing costs;
- Major aerospace companies have accessed the CNBC to improve the reliability of jet engines by examining stresses in turbine discs and blades made using new welding methods;
- Schlumberger, a multinational oil and gas company, accessed the CNBC recently to improve the reliability and reduce the costs of fracking by examining stresses in prototype fluid ends—a key component that must withstand harsh conditions and that is costly to replace;
- Defence Research and Development Canada has accessed the CNBC for several projects to advance national defence, including qualifying a new repair method for large ship propellers and assessing the structural integrity of submarine hulls to support the life-extension of our fleet;
- Several research groups from Canadian and foreign universities access the CNBC to make fundamental discoveries about superconductivity, which could lead to energy-saving technologies. (Notably, one such group has been recognized with the Brockhouse Canada Prize for Interdisciplinary Research in Science and Engineering);
- Researchers from Queen's University are accessing the CNBC to build a fundamental understanding of magnetic Barkhausen noise (important as a non-destructive, high-speed indicator of defects in buried gas pipelines) to evaluate fitness-for-service, to inform decisions

about costly maintenance activities, and to help avoid catastrophic accidents;

- Researchers from McMaster University accessed the CNBC to make the first direct experimental observation of rafts in a fluid lipid membrane; and

- Researchers from Brock University accessed the CNBC to understand the biological roles and functions of several membrane-associated molecules, including: (1) a protein that relieves symptoms of respiratory distress syndrome in premature babies; (2) vitamin E; and (3) an anti-microbial agent.

Canadian researchers maintain an international reputation for innovation in neutron beam instruments and methods. Through continual improvement, the L3 neutron stress scanner at the CNBC is still a world-leading instrument for metallurgical engineering, and plans are being developed for a next-generation 'white-beam' stress scanner. At the leading edge of North American neutron instruments are the CNBC's C2 powder diffractometer with 800 channels, as well as the CNBC's C5 polarized beam triple-axis spectrometer. Examples of innovation in methods include the world-first demonstration of molecular holographic imaging, as well as modifying a triple-axis spectrometer to perform small angle neutron scattering to partially compensate for the lack of a cold neutron source. One important application of neutron holography may be to enable molecular structure determinations to high resolution in the class of membrane-associated proteins (about one-third of known proteins), which are difficult to fully crystallize and therefore have often defied detailed characterization. Such a capability would have a major impact on the understanding of structure and function for the life sciences.

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

Although recognized for its excellence in some areas of science and technology, Canada's neutron beam facility has fallen behind laboratories in other nations that have acquired decades of experience with cold neutron beams, which are especially powerful for research in soft materials, life sciences, and nanotechnologies. Canada's existing National Research Universal (NRU) reactor does not include a cold neutron source, so there is relatively little experience with techniques such as small angle neutron scattering (SANS), neutron reflectometry (NR), high-resolution neutron spectroscopy, and spin-echo spectrometry, among others. 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 (e.g. fields related to the structures and dynamics of proteins and other polymers in solution).

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 4 user facilities in North America, 12 in Europe, 5 in Australasia, and a few others. There have been some recent closures of aging facilities, for example in Denmark (Risø), Germany (Jülich), the U.S. (Argonne and Brookhaven), and Sweden (Studsvik). To expand capacity for neutron beam experiments and to meet growing demands, some new facilities are currently under construction or have recently been completed, such as in Japan ($2.4 billion), Australia ($350 million), the U.S. ($2.2 billion), Germany ($750 million), and Sweden ($2.5 billion). This activity demonstrates a widespread recognition of the social and economic benefits arising from materials research using neutron beams.

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.

A domestic neutron facility connects Canadian scientists from dozens of universities and laboratories to a global network of neutron facilities and attracts international scientific collaborators. In the last three years, the CNBC has enabled the Canadian science community to conduct projects with collaborators from over 20 countries. 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 four neutron scattering user facilities 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 U.S. is located at the National Institute of Standards and Technology (NIST). With over 20 neutron instruments and a staff of 100, the NIST Center for Neutron Research has 2000 research participants each year and can only supply half of the demand for its beam time [1.2]. As a result of the 2006 American Competitiveness Initiative [1.3], the NIST Center for Neutron Research is undergoing a substantial expansion. It has constructed a new building, added a second cold source, and is installing five new instruments to allow it to accommodate experiments from an additional 500 scientists each year.

It is sometimes suggested that we send Canadians to foreign neutron beam facilities instead of building a new national centre. However, international experience in attempting to maintain 'virtual neutron beam centres', where the real sources are elsewhere, has uniformly resulted in the 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 as a result 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

“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. Bruce D. Gaulin (McMaster University), Past President of the CINS and of the Neutron Scattering Society of America

respond to the specific research interests of the Canadian user community. Access to foreign neutron facilities by experienced Canadian neutron researchers cannot substitute for our current situation of having an established national neutron user program.

Sometimes an analogy is drawn from Canadian astronomers and nuclear particle physicists, who are accustomed to remotely accessing or travelling to foreign facilities in lieu of access to a state-of-the-art domestic research facility. But astronomy and particle physics are unlike materials research in that they are strongly influenced by the facility that can see into space the farthest or achieve the highest energy. Internationally, science in these other domains has reached the point where facilities must be enormous multi-national undertakings to be at the leading edge. This is the realm of ‘big science’, where Canada has few opportunities, on its own, to build world-class telescopes or particle accelerators.

Surprising for many, a neutron facility is not ‘big science’; it does not require a massive investment to answer a relatively small number of fundamental questions. In contrast, a neutron beam facility enables tens of thousands of individual scientific projects for a large user community over its lifetime. It is well within the grasp of a single nation like Canada to build a world-class neutron beam facility that would contribute to the global neutron beam capacity.

A domestic neutron beam facility can be tuned to meet Canada’s strategic science and technology (S&T) priorities and to enable Canadian industries to study practical questions, such as how to make an aircraft safer or how to make steel manufacturing more competitive. Without major ongoing investments similar in scale to the cost of a domestic facility, Canadian priorities would exert little influence at foreign-owned neutron facilities. Conducting proprietary neutron beam research at foreign facilities is currently difficult for Canadians, and it could not be sustained for the long term as a Canada-based service to industry in the absence of a domestic facility.

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 the CNBC has been outstanding. In the last three years, there were 125 visits by young, highly qualified people to the laboratory, including 14 post-doctoral fellows and 65 students, many of whom visited more than once. The Canadian students came from 18 universities in 6 provinces. In addition to those already counted, many other young, highly qualified people attended workshops and biennial summer schools to engage with hands-on research measurements at the CNBC.

Growing Highly Qualified *People*

Engineering graduates Stephanie Stafford (Kinectrics Inc.) and Jessica Hiscocks (Nu-Tech Precision Metals Inc.) 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

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

- Training, including industrial safety training and radiological self-protection training, is provided to enable them to work safely, particularly in terms of working 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, performing 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 institutions, and also provides a deeper understanding of techniques, their applications, and their limitations;

- Once adequately trained, students are able to operate neutron spectrometers by themselves, and (depending on technical complexity) they often change specimens and conditions of specimen environments (e.g. 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, often with follow-up discussion when the student returns to his or her home institution, is a further enhancement of the student's learning; and

- Opportunities to join researchers and other visitors in informal settings provide the student with networking opportunities that can help in later career development, as science is essentially a human activity involving the exchange of ideas and collaborative efforts.

> *"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), Past President of CINS*

Through access to the domestic neutron scattering centre, students gain insight into a multidisciplinary scientific and engineering environment quite different from the academic situation at their home institutions. They gain in-depth exposure to a powerful and versatile experimental method for materials research at a world-class facility. Through access to the national centre, students may be inspired to persist towards careers in advanced materials research; they may also gain confidence that they will find opportunities—in Canada

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

—to apply their knowledge and express their creativity through 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 part of their thesis work, an expanded Canadian Neutron Centre will see this number triple or quadruple in the future.

1.6 The Prospect of a New Canadian Neutron Centre (CNC)

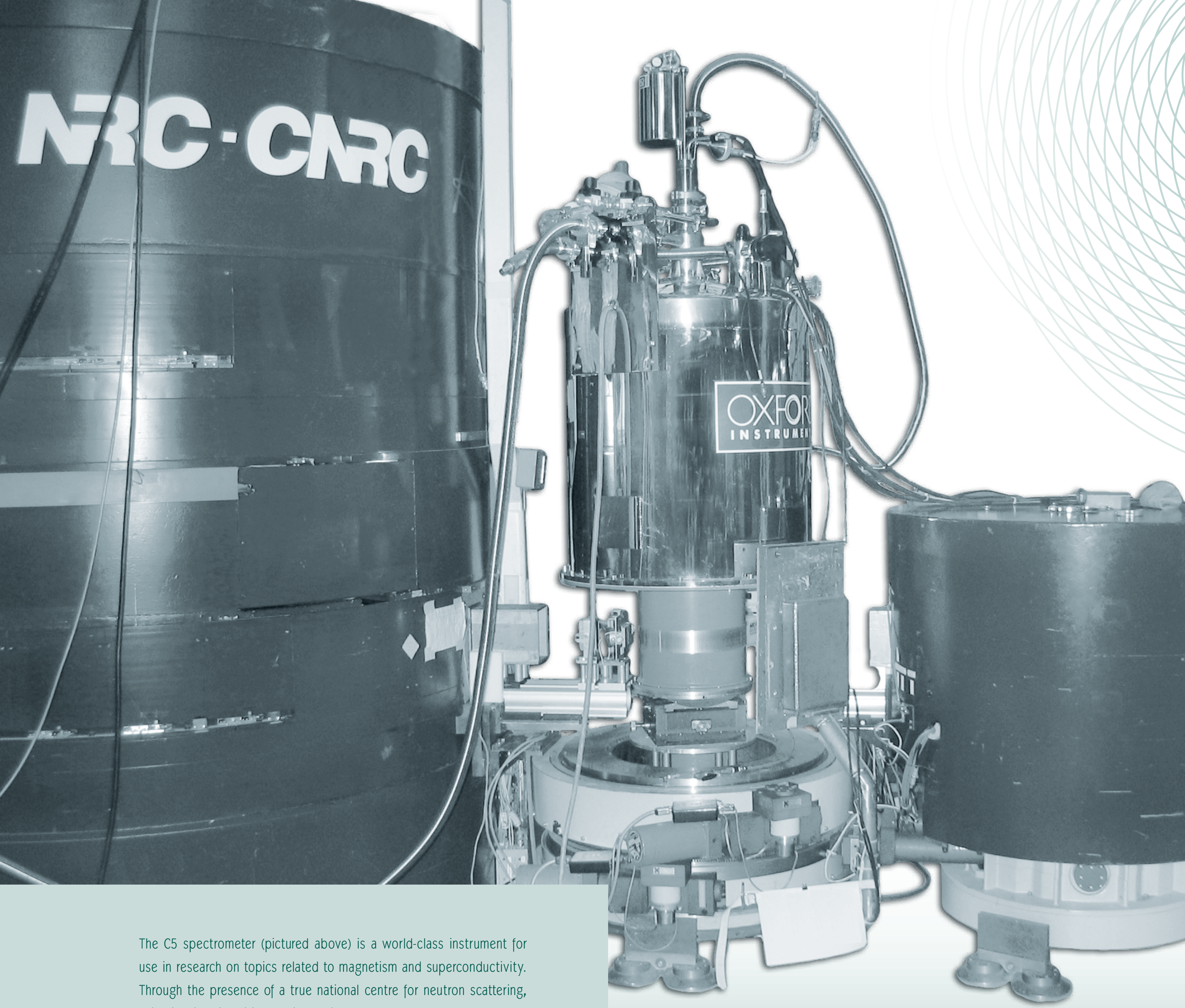
We envision a new world-class facility, referred to as the Canadian Neutron Centre (CNC). Whether the neutron source be multipurpose or single-purpose, a reactor or a spallation source, the CNC would be designed to surpass the capabilities of today's facility to a time horizon of about 2050. Having learned from over 60 years of experience with the National Research Experimental (NRX) and NRU reactors at Chalk River Laboratories, and from 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.

A new CNC must include at least one cold neutron source, as well as a suite of cold neutron instruments that will enable research on soft materials and nanotechnology as never before possible in Canada. The next generation of instruments and methods at the CNC can be built upon the foundation of Canada's leading presence in certain areas of neutron beam research. The world-class CNC should begin with about 10 beam lines and expand over time to about 25 beam lines. These facilities will enable thousands of research projects by Canadian and foreign users, and will help to educate over 2000 new highly qualified people for jobs at the forefront of knowledge-intensive industries.

The need to replace and surpass the NRU reactor's capabilities has long been recognized by academics, industry, committees, and the authors of various studies, both national and international [1.4–1.12]. The NRU reactor, which has been operating for over 58 years and is the oldest major research reactor in the world, is now planned to be permanently shut down in 2018. It is now an urgent matter to complete the analyses of Canada's need for replacement capabilities and to begin construction of new facilities.

Because the NRU reactor is a multipurpose science facility, there have been many economic, health, and social impacts arising from its operation—impacts that go beyond the results of materials research with neutron beams. The NRU reactor supported the development of the medical isotope industry and continues to produce Tc-99m, the most commonly used medical isotope in nuclear medicine, as well as Co-60 for cancer treatments and other isotopes with medical or industrial applications. These isotopes are used for the treatment and diagnosis of over 20 million patients in 80 countries annually. NRU also provides a test bed for the nuclear power industry. The current fleet of CANDU reactors, which generate one-sixth of Canada's electricity, could not have been designed and built without the essential knowledge gained through NRU. According to the Canadian Nuclear Association [1.13], that industry today represents over $5 billion of annual economic activity by 150 companies, and it directly provides 25 000 highly paid jobs—4000 of which are held by highly qualified personnel.

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



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 Laboratories therefore tend to be associated with one of five scientific communities or areas of interest: (1) excitations in condensed matter; (2) crystallographic analyses; (3) materials science and engineering; (4) thin films and surfaces, particularly nanostructures; and (5) soft materials, particularly polymers and biological materials. 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 originally drafted the following sub-sections following discussions held at the CINS's 2006 and 2007 Annual General Meetings (AGMs). The content was subsequently updated and approved by the members at the 2014 AGM. Each sub-section below 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.

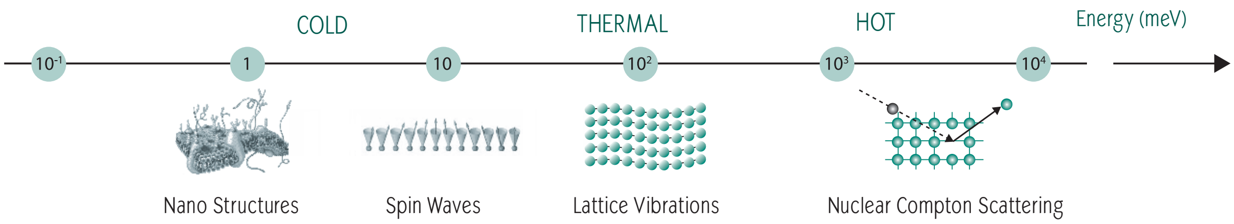
2.1 Excitations in Condensed Matter

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 education. Canada's scientific presence in this area of materials research can be traced back to the pioneering work of Nobel Prize–winning 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 those 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 the energy states of condensed matter as opposed to structures. One of the most important properties of neutrons is this: by virtue of their mass, neutrons with de Broglie wavelengths appropriate for determining the structure of materials (i.e. 1–4 Å) possess energies typical of the low-energy excitations of condensed matter (i.e. 5–80 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

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



spanning temperature ranges from about 20 Kelvin (K) to about 2000 K. Speaking of energy in terms of temperature, neutrons with lower energies are referred to as ‘cold’, and those with higher energies as ‘hot’. Figure 2.1.1 shows what types of phenomena can be measured by neutron scattering and provides a comparison of the temperature and meV energy scales.

Understanding low-energy excitations (i.e. those of up to 80 meV or so) lies at the heart of contemporary materials physics and chemistry. Quantum mechanics, our most accurate fundamental physical theory, makes very specific and 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), which are very well matched to the typical energies of neutrons. Therefore, when a neutron creates or absorbs an excitation, it loses or gains enough energy such 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 its initial energy (whereas ‘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 Bertram Brockhouse, co-recipient of the 1994 Nobel Prize in Physics 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” [2.1].

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 along the same direction); by measuring the change of polarization on scattering, magnetic excitations can be distinguished from non-magnetic ones.

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.

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 possible at the sample, and by using detection systems that can simultaneously measure neutrons scattered over a range of angles and 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. Furthermore, 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 on 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 Science and Technology, the Economy, and Society

The invention of the triple-axis spectrometer 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 liquids. In the 1980s, the use of INS to study much bigger molecules (i.e. 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 had 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. Soon after their discovery, diffraction experiments 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 [2.2], and the theory has enabled the intelligent design of other SMA materials. The first commercial application of the material was a shape-memory coupling for piping (e.g. oil line pipes for industrial applications, water pipes and similar types of piping for consumer applications, etc.). The late 1980s saw the introduction of the SMA 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, about half of all peripheral vascular stents currently available are manufactured with Nitinol.

Canadian expertise in INS for magnetism and quantum materials is applied to numerous sub-topics, such as those discussed in the sub-sections below.

High-temperature Superconductivity in Cuprates and Pnictides: The discovery of high-temperature superconductivity (HTSC) in 1986 in copper-based materials (known as cuprates) sparked a new interest in the field of superconductivity (SC). Despite a large number of studies on HTSC, there is still no consensus on the mechanism responsible for superconductivity. Thus, these materials still remain one of the most challenging problems facing condensed matter physicists today. The discovery of SC in antiferromagnetic (AF) iron-based materials (so-called pnictides) in 2008 [2.3] was shocking and exciting, since no one expected to observe SC in the presence of iron with strong magnetism [2.4]. This broke the 20-year monopoly held by the cuprates.

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 these materials is that their superconducting transition temperature (Tc) is much higher than the classical, low-temperature superconductors. The record Tc for HTSC is now about 165 K at high pressures—more than halfway to room temperature. 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 that of liquid nitrogen instead of liquid helium, which is much more expensive than liquid nitrogen 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, as well as to boost utilities' efficiencies and to eventually help in reducing greenhouse gas emissions and pollution [2.5];
- Enabling large amounts of energy to be stored for peak demand times, as well as greatly enhancing the usefulness of energy sources that are not available on demand 24/7 (e.g. wind power and solar energy) [2.6];
- Enabling magnetically levitated transportation, for which research and development is strong in the U.S., Japan, China, and Germany [2.7];
- Making possible a 'table-top' magnetic resonance imaging (MRI) machine as a routine medical diagnostic tool [2.8]; and
- Implementing a superconducting electronic device, known as a Josephson junction, which could serve as the basis of the next generation of supercomputers [2.9].

For both classes of cuprate and pnictide superconductors, of particular interest is understanding the nature of any spin and/or charge ordering in these materials for their entire phase diagrams. Neutron scattering has played a vital role in exploring fundamental properties of the charge carriers and testing current theories of HTSC for cuprates [2.10–2.16]. Neutron scattering measurements have also been quite instrumental in revealing important details of the magnetic properties of pnictide superconductors [2.17–2.22].

While parent compounds of cuprates and pnictides are different (i.e. magnetic insulators vs. magnetic metals), neutron scattering measurements have indicated that, similar to cuprates, superconductivity in pnictides occurs near an antiferromagnetic phase. The pnictides possess simpler crystal structures than cuprates and appear more accessible to theorists. Thus, it is hoped that a full understanding of their fundamental properties will aid to unlock the mystery of superconductivity in cuprates and other unconventional superconductors.

The intense research performed globally on HTSC has been beneficial not only for the dramatic improvement of existing theoretical and experimental approaches, but also for the development of new ones. This includes neutron scattering methods used to measure magnetic excitations. The challenging requirements of performing such experiments on HTSC (e.g. relatively small crystals, the weakness of the inelastic signal) have prompted efforts to increase the performance of triple-axis spectrometers through higher flux at the sample and increased detector capability; they have also stimulated efforts to further the development of wide-angle time-of-flight (TOF) spectrometers with higher flux.

Worldwide, the current market for HTSC wire is estimated to be U.S. $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 Tc, 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 the other electrons provide; rather, they have an extra interaction where they can still flow like 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 [2.23], 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. Notably, neutron scattering is the key method for investigating the peculiar magnetic properties of these systems, and could therefore help to answer many questions.

One outstanding problem in the physics of heavy fermion materials is that the nature of the order parameter that sets in below T_0 = 17.5 K in URu_2Si_2 still remains unknown [2.24]. Neutron scattering has been instrumental in determining the properties of the hidden order state, and in testing current theories of hidden order. A detailed neutron scattering study did not find [2.25] any evidence for orbital currents predicted by theory. Instead, evidence for spin activation was found, and it was demonstrated [2.26, 2.27] that the large drop in entropy below T_0 is due to the gapping of the spin spectrum, as seen by neutron scattering. The dynamic incommensurate spins have been interpreted [2.26] as the response of an itinerant rather than a local spin system, and made a connection to a Fermi surface nesting. These studies showed that the paramagnon dispersion above T_0 follows the spin wave dispersion for $T < T_0$, indicating that the exchange interaction between uranium moments does not change across T_0. The main characteristic of the phase transition was found to be a dramatic decrease of the electronic damping of longitudinal fluctuations below T_0. All these findings support hidden order theories that are based on itinerant spins rather than localized spins. Recent neutron scattering experiments have placed strict and well-defined constraints on hidden order theories [2.28] with in-plane magnetic dipole moments [2.29].

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 to be in the same sector of condensed matter physics research as are HTSC and heavy fermion systems. Classic examples are elemental chromium

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.

and low-dimensionality $FeGe_2$ [2.30]. There are also examples of materials that are neither HTSC nor heavy fermion systems, but are correlated and show SDW magnetism (e.g. $V_{1.973}O_3$) [2.31]. 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 interest recently, as they exhibit an extreme form of quantum behaviour at low temperatures. These materials have 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. Because the ground state of these materials is non-magnetic, they display no elastic magnetic neutron scattering other than possibly diffuse scattering. 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. Canadian researchers used INS to induce an excitation from the ground state to the first and second excited states in TiOBr, in order to calculate the energy difference (i.e. the 'energy gap') between these states [2.32]. $KCuF_3$ is another example, which shows evidence of a crossover between one- and two-dimensional behaviour in the magnetic excitation spectrum [2.33]. In contrast, chains of S=1 (not S = 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 [2.34]. 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 [2.35, 2.36]. A more recent area of study involves how orbital and spin momenta couple to give rise to low-dimensional physics on typically three-dimensional lattices, such as in clinopyroxene and spinel systems. These systems usually have higher transition temperatures that approach room temperature (e.g. T_c = 210 K in $NaTiSi_2O_6$) [2.37].

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 the 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, including electronics, optics, medicine, and many others. As an example, one could consider electronics, where the ever-growing complexity of microprocessor and memory chips over the past few years has led to a large chip density—and, hence, to the very small dimensions of individual electronic components (i.e. 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.

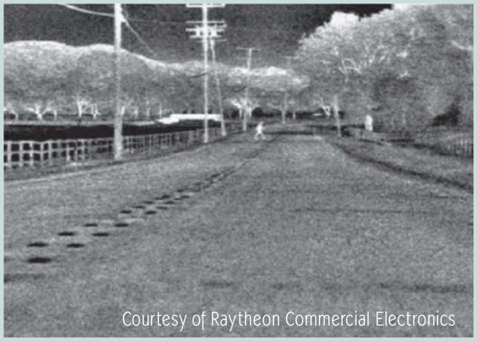


Figure 2.1.2 Pyroelectric Imaging. Lighter colors correspond to warmer temperatures.

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 magnetic moments cannot find a simple low-energy configuration; 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 $Ho_2Ti_2O_7$, have magnetic rare-earth ions arranged on networks of corner-sharing tetrahedra. An in-depth review of the many exotic ground states exhibited by systems with this frustrated lattice was written by [2.38]. At low temperatures, these materials cannot find a conventional long-range ordered state, but rather each finds a distinct exotic disordered state (e.g. a 'spin liquid' state for $Tb_2Ti_2O_7$ and a 'spin ice' state for $Ho_2Ti_2O_7$). On the application of an appropriate magnetic field, the spin liquid state of $Tb_2Ti_2O_7$ can be caused to order (complete with well-defined spin excitations), characterized, and ultimately understood through INS [2.39].

More recently, studies have focused on 'quantum spin ices' wherein the exotic frozen short-range ordered state observed in $Ho_2Ti_2O_7$ is induced by quantum fluctuations. $Pr_2Zr_2O_7$ [2.40], a material thought to be a quantum spin ice, presents researchers with a means of observing magnetic excitations, or 'monopoles'. An analogous 'quantum spin liquid' state has also been observed in $Yb_2Ti_2O_7$, although the exact nature of this ground state remains unclear [2.41]. Canadian researchers, in collaboration with theorists from the U.S., are pioneering this recent field of study, having fit data obtained from INS in magnetic fields to quantitatively extract the entire Hamiltonian (an equation of fundamental importance to understanding the behaviour of any system) for the first time [2.42].

Like in low-dimensional systems, orbital effects can also couple with the magnetism on geometrically frustrated lattices. 'Spin glasses', the magnetic analogue of structural glasses, are characterized by frozen in, randomly oriented magnetic moments—much like how structural glasses lack long-range periodic order. For years it was thought that chemical disorder is a prerequisite for spin glass behaviour [2.43]. That is why it was so surprising to find spin glass behaviour in nearly 'disorder-free' materials such as $Y_2Mo_2O_7$ [2.44]. INS experiments by Canadians at Chalk River Laboratories on powder [2.45] and on a single crystal of $Y_2Mo_2O_7$ [2.46] show clear freezing of the spins into a unique isotropic short-range ordered arrangement that cannot be explained by any of the conventional magnetic models used for other spin glasses.

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 (e.g. dilute paramagnets). Thus, there is great potential to not only achieve low temperatures in space-limited situations, but also to develop a new generation of environmentally friendly refrigerators.

Topological Materials: Recent years have seen the birth of a new area in quantum mechanics: topological insulators [2.47]. Crystalline solids usually fall into two broad categories—namely, metals and insulators—discerned by their ability to conduct electric current. Technologically important semiconductors bridge the line between these two and exhibit characteristics of both to a degree that can be controlled by external means. The physics of these basic states of quantum matter has long been thought to be thoroughly understood, and this understanding—formulated in the standard band theory of solids—constitutes one of the founding pillars of modern physics. In topological insulators, however, the bulk is an insulator, while the surface hosts an exotic metallic state with special topological properties. Not only can the electrons on the surface of a topological insulator flow with little resistance, but their spin and direction are also intimately related (i.e. the direction of the electron determines its spin, and vice versa) [2.48]. First understood theoretically in 2005 [2.49], a topological insulator was discovered experimentally in 2008 [2.50]. This discovery has the potential to revolutionize spintronics and quantum computing [2.51]. In addition, this discovery spurred further understanding of various topological quantum materials, including topological superconductors and Weyl semimetals. In particular, the 5d transition metal oxides (e.g. iridium oxides and osmium oxides with strong spin-orbit coupling) have recently been the subject of intense theoretical and experimental studies as potential candidates for realizing various topological quantum phases [2.52, 2.53]. Again, neutron scattering experiments have been critical in determining the magnetic properties of these materials [2.54–2.56].

Colossal Magnetoresistance: Discovered in 1993, colossal magnetoresistance (CMR) is a phenomenon of greatly reduced electrical resistance in the presence of a magnetic field. Chemically, CMR materials are similar to high temperature superconductors with the exception 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 (i.e. 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 [2.57] 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, France) and Peter Grünberg (Forschungszentrum Jülich, Germany) for the discovery of giant magnetoresistance.

Ferroelectrics: Ferroelectric 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 anywhere from a few to a few dozen or more capacitors, this application alone represents a huge technological and economic impact. Ceramic disk capacitors made of $BaTiO_3$, a ferroelectric material, are simple to manufacture and have captured more than half of the ceramic capacitor market. Transparent ferroelectric crystals are commonly used for the doubling, tripling, and quadrupling of laser frequencies, and also as electro-optic modulators, Q-switches, Pockels cells, etc.

Ferroelectric materials also exhibit two other important properties: piezoelectricity (i.e. the generation of voltage when compressed); and pyroelectricity (i.e. the 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 megahertz (MHz). Piezoelectrics are also used for medical imaging and treatments (e.g. ultrasound), underwater navigation and detection (e.g. sonar and hydrophone arrays), and nano-precision motion (e.g. actuators), just to name a few important applications. Pyroelectrics are at the heart of infrared detectors and thermal imaging devices used for firefighting, 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 [2.58]. Since then, many materials, both existing

TABLE 1 - Comparison of energy ranges for various spectrometers, including the triple axis spectrometer (TAS).

Instrument Type (Name, Location)	Max. Energy Transfer (meV)	Best Resolution (meV)
Modern thermal TAS (C5, CNBC[a])	100	0.2
Cold TAS (SPINS, NCNR[b])	10	0.06
Chopper spectrometer (MAPS, ISIS[c])	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)

a=Canadian Neutron Beam Centre, Canada; b=NIST Center for Neutron Research, U.S.; c=ISIS pulsed neutron and muon source, U.K.

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

and 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 20 years later, predicting how the dielectric constant would vary as the frequency of the lowest energy atomic vibration changed 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 at Chalk River Laboratories [2.59].

Thermoelectrics: The thermoelectric effect describes the phenomenon of a voltage when a temperature gradient is established between two adjoined semiconductors. This effect is completely reversible and can be used in solid state refrigerators; Peltier coolers take advantage of the inverse thermoelectric effect. Thermoelectric materials such as chalcogenides (i.e. materials with negatively charged S, Se, and Te) are used in space exploration missions for electric power generation. Thermoelectric devices are completely silent, owing to a lack of mechanical parts, and are extremely reliable; for instance, Voyager I continues to operate off of uninterrupted radioisotope thermoelectric power after nearly 40 years.

Beyond space travel, thermoelectric generation on Earth has found special niche markets, mainly for use as cathodic protection, as backup generators able to work at all times of day and in all weather conditions, and as a means of converting wasted heat back into energy. However, thermoelectrics are plagued with having low efficiency and high material cost. Studying why thermoelectrics work is central to solving these problems in order to implement thermoelectrics for new uses, such as wearable electronic or medical devices. Heat is carried throughout the material through collective atomic motions called phonons. In fact, INS was developed by Canadian Bertram Brockhouse precisely to study these types of dynamics; PbTe, an excellent thermoelectric material, was one of the first systems to be studied using INS at Canada's NRU reactor [2.60]. Today, due to modern cold moderators, chopper technology, and advances in computation and software, these dynamics have been revisited when new insight into old problems has come to light [2.61]. The dimensionless figure of merit generally describes how good a thermoelectric a certain material is. Today, the highest dimensionless figure of merit is nearly triple what it was over 50 years ago when INS was first developed.

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 backscattering 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.

Next Generation Nuclear Fuels: The physical properties of uranium oxide and uranium nitride are of great interest not only because of the highly correlated electronic nature of these materials, but also because of their technological application as nuclear fuel. For such applications, it is important to understand the mechanisms by which thermal transport occurs. Neutron scattering measurements of atomic vibrations (i.e. phonons) enable scientists to directly examine the connection between microscopic thermal transport via phonons and macroscopic thermal conductivity. Hence, INS provides the microscopic benchmark needed to understand thermal transport mechanisms. In a surprise discovery while studying the phonon spectra of these materials, some of the most beautiful real-world examples of the quantized harmonic oscillator have been discovered in uranium nitride by Canadian researchers using neutron scattering—a fantastic proof-of-principles study of introductory quantum mechanics [2.62]. The neutron scattering study of phonons in uranium oxide has demonstrated [2.63] that the phonon density of states measurements are stringent tests for ab initio simulations of phonon physics, and has also indicated a further need for advances in theory to address the lattice dynamics of uranium oxide.

Polymers: INS has provided insights into the excitations of polymers, such as the 'plasticizing effect' that occurs when the additive dioctylphthalate (DOP) is added to polyvinylchloride (PVC) [2.64]. 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 (NSE) 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 [2.65]. 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 [2.66], magnetic copper ions were combined with quinoxaline bromide—$Cu(C_8H_6N_2)Br_2$—to form a spin ladder, which is made from two spin chains that interact more strongly with each other than with 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 on 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 (QENS) is needed to obtain quantitative values for diffusion rates. In one example of such a study [2.67], 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.

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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). First proposed in 1986 [2.70] by J. Smith and colleagues, this technique was applied immediately to a number of proteins, notably myoglobin and hemoglobin, with continuing applications today [2.70].

One property that sets them apart from inorganic compounds is that 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 the relatively slow large-scale diffusion of atoms and is measured with quasi-elastic neutron scattering. The study of diffusion requires neutron backscattering or spin-echo spectrometers, which Canada does not have at this time. Consequently, there are few Canadian examples in this field of research, which is currently dominated by U.S. and European scientists. Part of the motivation for this document is the hope that a new Canadian neutron centre would be better able to provide the facilities needed for more research relevant to the 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 the early triple-axis spectrometer, or TAS (i.e. Brockhouse's machine and those not much different from his), excitations with energies in the range of 5−30 meV were 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 to draw attention to the minimum energy transfer available, but to make 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 via the introduction of '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 (at a temperature of about 20 K), which is located inside the reactor vessel and 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, and spin-echo spectrometers). Even the traditional TAS has been revised in order to increase the detected neutron intensity [2.71]. Table 1 compares the energy windows for various machines to those of a modern thermal TAS.

In combination, a number of these spectrometers can probe excitations spanning over seven orders of magnitude (i.e. up to 2000 meV for a chopper spectrometer and down to less than 2 × 10 4 meV for a spin-echo spectrometer), making inelastic neutron scattering a very powerful and flexible tool for materials research.

Software is also of primary concern to INS researchers. Greater computational power and new multinational collaborations such as the Mantid project [2.72] have resulted in advances in data compilation and manipulation software. Using such software, it is now possible to collect, visualize, and manipulate the entire four-dimensional (Q, E [meV]) coordinate set of data obtainable using a single instrument with a single material. Software ingenuity is rapidly increasing the accessibility of INS to the average non-specialized neutron user, in much the same way that powder diffraction is used today. High-calibre computing facilities and a department dedicated to software development is critical to the success of any new neutron source in Canada.

Canadian perspective

Canada has three TAS instruments, including the DUALSPEC instrument at the C5 beam line, which was partially funded by the Natural Sciences and Engineering Research Council of Canada (NSERC). DUALSPEC 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 current problems; they can do only part of their experiments at home, while having 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 above, including high-temperature superconductivity, heavy fermion systems, frustrated magnets, and low-dimensional and quantum magnetism. Problems at today's leading edge often require access to lower energy excitations like those observed in superconductors or in slow-moving large polymer molecules. Thus, types of spectrometers are needed to access different ranges of momentum and energy transfer that span seven or eight orders of magnitude.

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

2.2 Crystallographic Analyses

The CNBC's C2 powder neutron diffractometer continues to attract a strong user base within the Canadian community and abroad. It remains the most efficient reactor-based powder instrument in North America, and its value is enhanced by excellent ancillary equipment consisting of several cryostats and furnaces. Since the last survey, which included research activities up until around 2007, there have been at least four significant new developments that have expanded opportunities for diffraction at C2. Two of the most important have been the provision of a sample cell for use with highly absorbing materials [2.73] and the addition of a Heliox probe [2.74] that extends the temperature range to 0.34 K. In addition, a new furnace for *in situ* experiments on hydrogen storage materials has been built and commissioned along with special sample cells [2.75]. Another important development is a shielded sample mount capable of safely housing active samples of up to 80 rem/h (0.8 Sievert/h) on contact, allowing diffraction measurements on samples that have been exposed to high radiation fields and have themselves become highly active. This provides the capability to study things such as a variety of post-irradiated fuel compositions—an important aspect for nuclear reactor fuel development.

The great strengths of powder neutron diffraction vis à vis x-ray diffraction are: (1) the ability to accurately detect and refine the positions of light (i.e. low atomic number) atoms (e.g. H, Li, and O) in the presence of heavy atoms; (2) the ability, in favourable cases, to distinguish between atoms of nearly the same atomic number (e.g. Fe and Mn, Sc and Ti, O and N, Yb and Lu, etc.); (3) the ease of use of sample environments such as furnaces and cryostats for the study of phase transitions; and (4) the ability to solve and refine magnetic structures, including the quantitative measurement of magnetic moments. In the following section, highlights of some Canadian research activities using C2 will be presented.

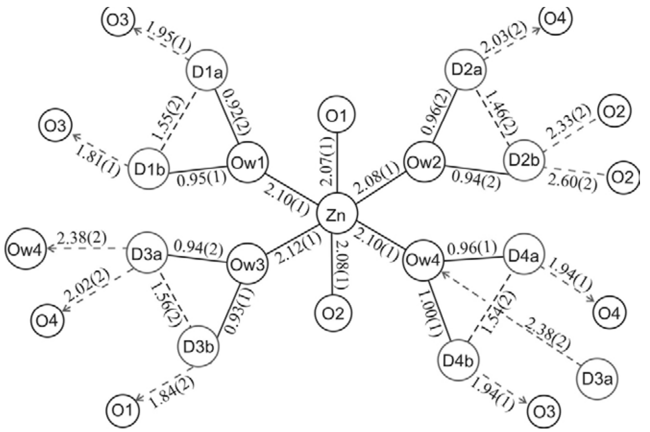


Figure 2.2.1. The hydrogen bond network in $ZnSO_4 \cdot 4D_2O$ [2.76].

Canadian Research Activities Using C2

The positions of H atoms and their participation in hydrogen bonding is a perennial issue in hydrated minerals. R.C. Peterson (Queen's University) and his group have used C2 data in the study of a number of hydrates belonging to the rozenite group of minerals, such as $ZnSO_4 \cdot 4D_2O$, $ZnSO_4 \cdot 6H_2O$, and $MnSO_4 \cdot 4H_2O$ [2.76]. In these materials, the Zn^{2+} and Mn^{2+} ions are in octahedral coordination, connected by a hydrogen bonding network. While hydrogen positions derived from single crystal x ray data were available for these rozenites, it was possible to obtain much more accurate and precise positions from the neutron powder data. The results for $ZnSO_4 \cdot 4D_2O$ are show in Figure 2.2.1.

In Figure 2.2.1, note the highly asymmetric nature of the D–O bonds, which involve short (~0.95 Å) and long (1.9–2.3 Å) segments. In some cases (i.e. D2b and D3a), a single D ion forms a "bifurcated" hydrogen bond involving one short and two long bonds.

Neutron diffraction was used to determine site occupations in two transition metal oxide systems. In the first instance, the groups of M. Bieringer (University of Manitoba) and A. Petric (McMaster University) studied the solid solution between the spinel structure oxides Mn_3O_4 and $CuMn_2O_4$ [2.77]. Such compositions are reported to have excellent catalytic properties for oxygen reduction and are candidates for the cathode in solid oxide fuel cells. Both Cu^{2+} and Mn^{3+} are strong Jahn-Teller ions with octahedral site preferences, and it is problematic to predict a priori the site occupations in spinel, which has one tetrahedral and two octahedral sites per formula unit. By taking advantage of the strong contrast in neutron scattering lengths (i.e. b = 3.6 fm for Mn, and b = 7.6 fm for Cu), it was possible to determine unambiguously the site preferences for several compositions within the solid solution. As well, the measurements could be done *in situ*—a great advantage given that data on quenched samples had been shown to be unreliable indicators of site ordering. In the other example, the group of J. Greedan (McMaster University) has carried out extensive studies on a series of brownmillerite oxides of the composition $Ca_{2-x}Sr_xFe_{2-x}Mn_xO_5$, in which there are also octahedral and tetrahedral sites for the transition metal cations, this time in the ratio of 1:1. Again, it was of interest to determine the site preferences for Mn^{3+} (i.e. b = 3.6 fm) and Fe^{3+} (i.e. b = 9.4 fm), and the refinements unequivocally showed the expected strong octahedral site preference of Mn^{3+} [2.78].

In certain cases, neither x-ray nor neutron diffraction alone are sufficient to provide a complete structural solution. However, one can exploit the complementary nature of these two probes to considerable advantage. An excellent example is provided by a member of the dugganite series, namely $Pb_3TeCo_3V_2O_{14}$, which crystallizes in the non-centric P321 space group and is of interest due to its potential multi-ferroic behaviour. Here, the presence of very heavy elements such as Pb and Te render difficult the refinement of accurate positions of the oxide ions using x-rays, while the essential invisibility of V to neutrons (i.e. b = 0.44 fm) creates a parallel dilemma for neutron diffraction. The group of C.R. Wiebe (University of Winnipeg) was able to solve the crystal structure of this complex material using simultaneous refinement of data from both a synchrotron x-ray source (i.e. the 11 BM at the Advanced Photon Source) as well as C2 [2.79]. The resulting structure is shown in Figure 2.2.3.

The most active area of research involving C2 over the past few years has been the study of magnetic phase transitions and magnetic structures. In part, this reflects the enhanced opportunities in the area of highly absorbing materials made possible by the availability of the short pathway sample cell mentioned at the beginning of Section 2.2. Typically, magnetic scattering data for such materials are obtained either by use of 'hot source' neutrons of short (i.e. ~0.5 Å) wavelengths, or via x-ray resonant scattering at a light source. The former approach has the disadvantage of the scarcity of hot source neutrons (as none are available in North America) and low resolution, while the x ray methods cannot measure

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

magnetic moments. Thus, C2 is the only North American neutron resource for such experiments. D.H. Ryan (McGill University) and collaborators from Université de Montréal, McGill University, and McMaster University have studied a large number of Gd and Eu based intermetallic compounds. Among the most interesting examples is very recent work on the half-Heusler intermetallic, GdBiPt, which is a candidate antiferromagnetic topological insulator [2.80]. These collaborators were able to solve its magnetic structure—namely, that below T_N = 9 K, the Gd moments are arranged in ferromagnetic planes parallel to the face diagonal of the chemical unit cell, which couple antiferromagnetically to adjacent planes. Such a layered magnetic structure is thought to be a necessary criterion for realization of the antiferromagnetic topological insulating state. It should be noted that these data were collected on a 150 mg sample.

Intermetallics containing Eu^{2+} (isoelectronic to Gd^{3+}, 4f7, S = 7/2) are also possible now at C2. The absorption cross-section for Eu is about 10% of that for Gd (but still 102 times greater than for most elements) and requires the short pathway-length cell. $EuFe_2P_2$ with the $ThCr_2Si_2$ structure is closely related to the superconducting iron pncitides. The group of D.H. Ryan (McGill University) was able to show that the Eu moments order ferromagnetically in this material below T_c = 30 K [2.81]. This result is in stark contrast to isostructural $EuFe_2As_2$, in which the Eu moments form a planar antiferromagnetic structure.

As mentioned at the beginning of Section 2.2, C2 is now capable of measurements below 1 K, and this opportunity has been exploited by J.M. Cadogan and D.H. Ryan to determine the magnetic structure of $Er_3Cu_4Si_4$. With the Heliox insert and cell, data were taken to 0.34 K, as shown in Figure 2.2.2. There are two Er sites with very different magnetic behaviors. Er(2d) sites order commensurately at 14 K with k = (0 1/2 0) and a moment of 8.7 μB at 0.34 K. On the other hand, the Er(4e) moments begin ordering at only 3.3 K, which is described by an incommensurate k = (0

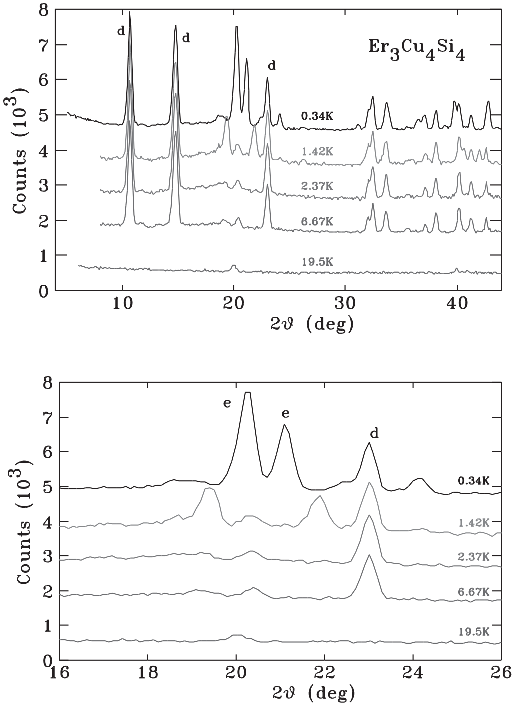


Figure 2.2.2 (Top Left) C2 data for $Er_3Cu_4Si_4$ taken with the Heliox sample cell at various temperatures. Reflections due to the Er(2d) sites and Er(4e) sites are indicated [2.82].

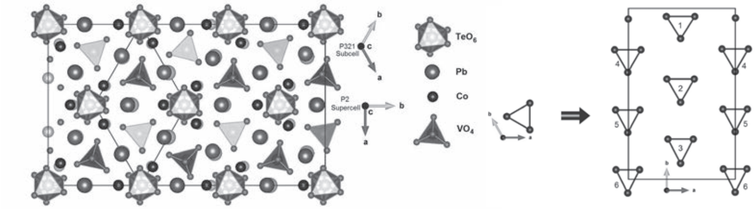
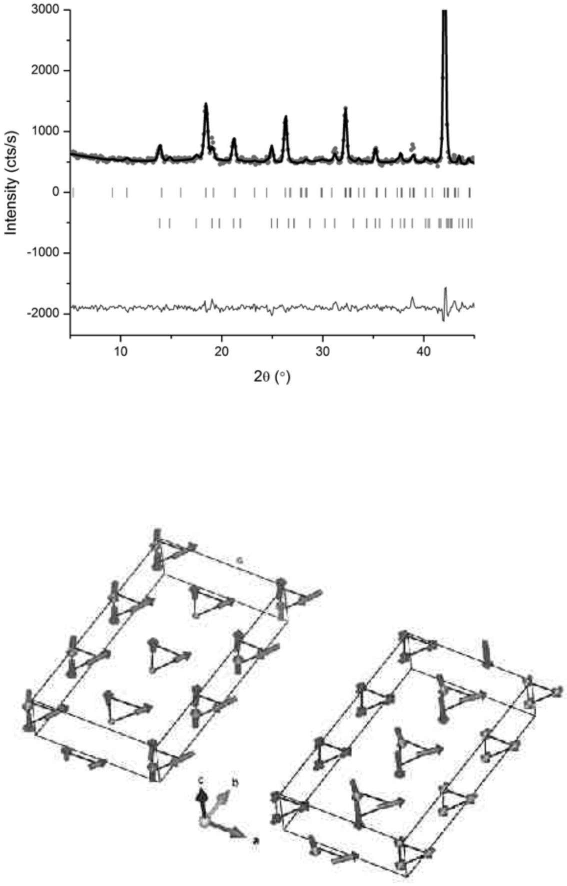


Figure 2.2.3 - (Bottom) The crystal structure of $Pb_3TeCo_3V_2O_{14}$ showing the relationship between the idealized P321 cell and the distorted P2 cell of six times the volume. (Right) The Co^{2+} trimers, now isosceles triangles, in P2 [2.83].

0.876 0) and a much reduced moment of only 4.4 μB until ~0.8 K, below which commensurate k = (1/3 1/2 1/2) order locks in with an eventual moment at 0.34 K of 8.8(2) K [2.82].

C2 has also seen extensive use to aid in the unraveling of quite complex magnetic structures in several oxide materials. In the dugganite $Pb_3TeCo_3V_2O_{14}$, mentioned above, the magnetic Co^{2+} ions form an unusual set of trimers, which in turn form a hexagonal net, introducing geometric frustration. The crystal structure is shown in Figure 2.2.3. There are two magnetic phase transitions occurring at T_{N1} = 8.6 K and T_{N2} = 6.0 K. Below T_{N1}, the Co spins appeared to order according to an incommensurate wave vector, k_1 = (0.752 0 1/2). A commensurate, but very odd, k_2 = (5/6 5/6 1/2) appeared to describe the magnetic structure below T_{N2}, implying a magnetic cell that is 72 times the volume of the chemical cell. It was then discovered that the crystal structure was very weakly distorted to a monoclinic symmetry, P2, with a chemical supercell six times the volume of the P321 cell. Using ultra high–resolution neutron data from the WISH instrument at the ISIS pulsed neutron and muon source in the U.K., in combination with C2 data, it was possible to solve the magnetic structures associated with



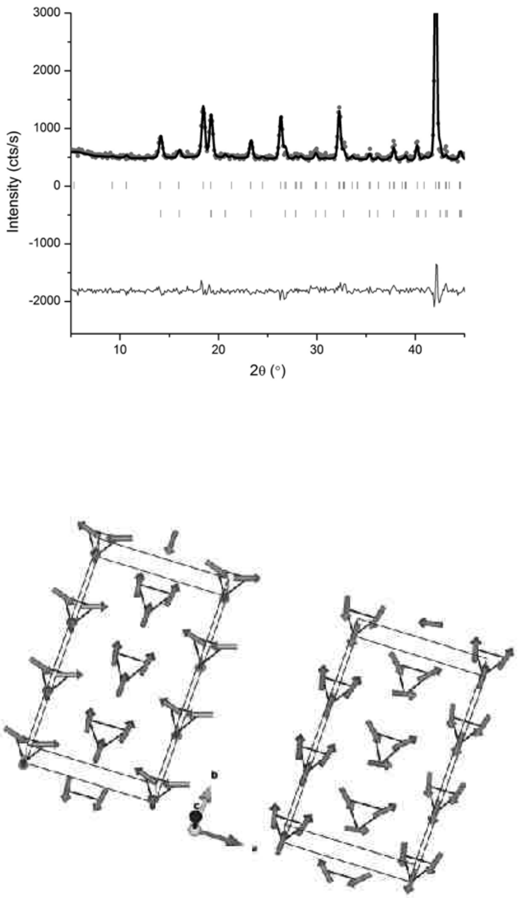
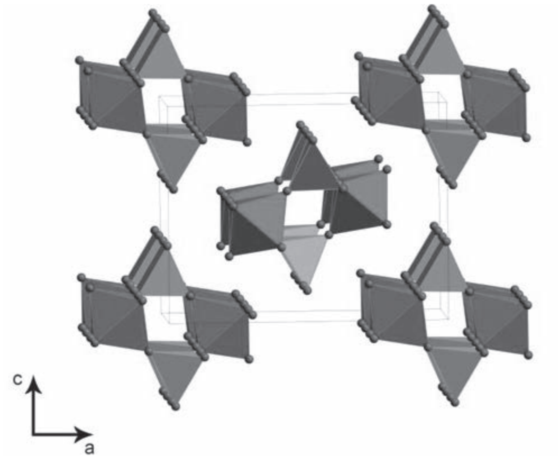


Figure 2.2.4 (a) (Top) Refined magnetic structure below 8 K for $Pb_3TeCo_3V_2O_{14}$. k_1 = (1/2 0 1/2) [2.83].

Figure 2.2.4 (b) (Top) Magnetic structure below 6 K for $Pb_3TeCo_3V_2O_{14}$. k_2 = (1/2 1/2 1/2) [2.83].

Figure 2.2.5. View of the crystal structure of $BaYFeO_4$ along the b axis. The square planar FeO_5 units are in orange, and the FeO_6 octahedral units are in green [2.84].



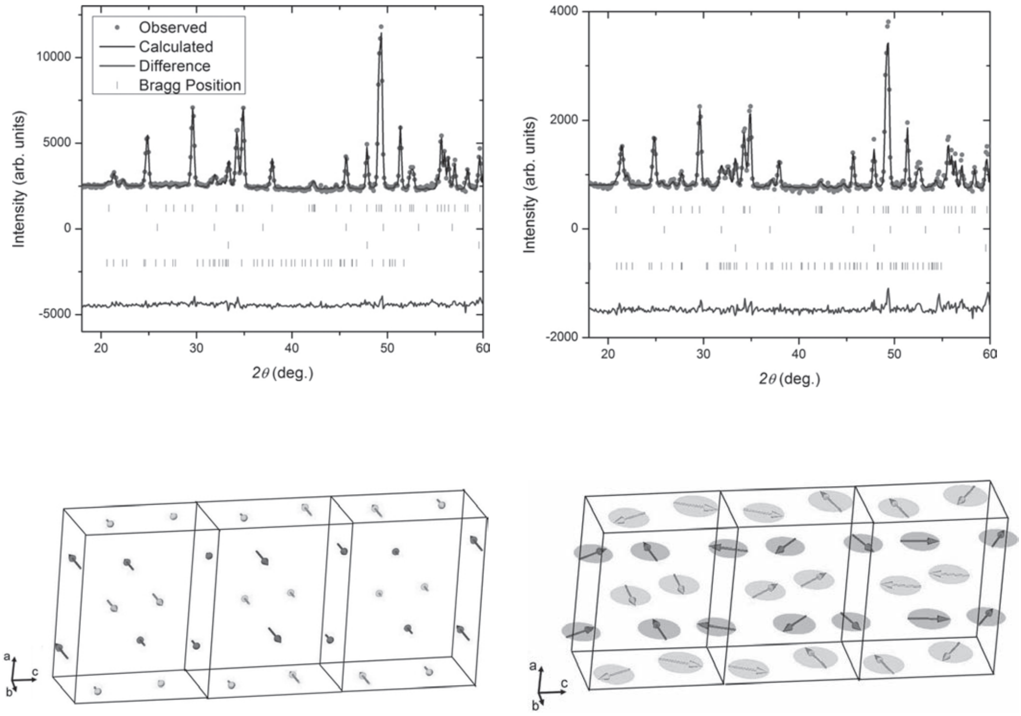


Figure 2.2.6. (Left) The refined C2 data (top) for the spin density wave structure (bottom) at 38 K. (Right) The refined C2 data (top) for the cycloid structure at 6 K (bottom) [2.84].

both transitions, as shown in Figures 2.2.4(a) and 2.2.4(b), with propagation vectors k_1 = (1/2 0 1/2) for T_{N1} and k_2 = (1/2 1/2 1/2) for T_{N2}, the directions of which are indicated by the thick arrows. In P121, the Co trimers form isosceles triangles rather than equilateral triangles [2.83].

In a collaboration with S. Derakhshan (California State University, Long Beach), the magnetic structure of a new Fe oxide, $BaYFeO_4$, was solved. In spite of the apparently simple stoichiometry, the structure of this material is complex, consisting of relatively isolated columns of four membered rings each consisting of corner-sharing FeO_5 square planar units and FeO_6 octahedral units, as shown in Figure 2.2.5 [2.84].

Again, there are two apparent magnetic phase transitions: T_{N1} = 47 K and T_{N2} = 36 K. C2 data were used to solve the magnetic structures in both regimes. In the range 36 K < T < 48 K, a commensurate k_1 = (0 0 1/3) structure was found, best described as a spin density wave with moments fixed along the b axis. Meanwhile, below 36 K, there was an incommensurate k_2 = (0 0 0.35) structure set in a cycloid with the moments now in the bc plane, as shown in Figure 2.2.6.

C2 Upgrade

While still performing admirably, the existing powder diffractometer, C2, was designed and constructed in the early 1990s and has some limitations and potential reliability problems. This 20-year-old BF3 based detector is starting to show alarming signs of fatigue, as it already has several faulty wires that are not possible to troubleshoot or replace.

Recognizing the impact that the C2 diffractometer has on numerous research fields, the community is strongly recommending and supporting an upgrade of the instrument. This will allow the CNBC to continue to provide reliable, internationally competitive neutron powder diffraction services for many years to come.

Replacing both the detector and the monochromator would effectively result in a new instrument that will provide a significantly higher rate of data acquisition and better quality data than the current setup, placing us at a truly competitive level internationally. One can envision a five-fold increase in the data acquisition rate just by replacing the present detector with a state-of-the-art ^3He based detector. This increase factor rises from (1) expanding the solid angle of the detector from the current 80° to 120−140°, a larger vertical acceptance angle than the current detector, as well as (2) the greater efficiency of ^3He as compared to BF_3 in capturing neutrons. Replacing the simple monochromator with a focusing multi-crystal assembly would increase the intensity of the beam impinging on the specimen by a factor of two to five times.

The proposed new instrument also necessitates the design and fabrication of a new sample table and detector shielding. The sample table will allow new sample environments to be accommodated for research on materials over a wider spectrum of conditions (e.g. magnetic field, pressure, temperature, chemical environment, etc.) than previously possible.

The performance improvements offered by the new instrument would allow the CNBC to: (1) continue to provide reliable powder diffraction services; (2) accommodate more visiting scientists; (3) improve the quality of powder diffraction services (i.e. the quality of data); (4) decrease costs of services to industry, since the same measurements would require less beam time; and (5) make it possible to observe time-dependent phenomena on a time scale that is not achievable with the current setup.

2.3 Materials Science and Engineering

The materials science and engineering (MSE) 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

IVACO recently expanded its steel plant at L'Orignal, Ontario, partly because of research using the CNBC that enabled it to add value to its products.

"Having detailed, fundamental knowledge of the strain and stress states in our customer's deformed steel parts allowed us to add value to our products and gain an edge over our competitors."

- Dr. Nicholas Nickoletopoulos, General Manager at Ifastgroupe and Sivaco Wire Group (IVACO), 2013

experimental tools. Therefore, the majority of community members are 'occasional adopters'. These researchers may have some experience with x-ray or electron diffraction, but they 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 to collaborate with a neutron scattering expert to plan and execute an experiment to meet their research objectives. Canada's contribution of neutron beam methods to fundamental materials science and engineering has developed synergistically with the emergence of the program entitled 'Applied Neutron Diffraction for Industry', which began in the mid-1980s.

Overview – How Neutrons Support Materials Science and Engineering

Materials science and engineering 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, 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 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 fee-for-service work at the Canadian Neutron Beam Centre since the mid-1980s. The CNBC has continued to hone its capabilities to put neutrons to work for industry and society by enhancing industry competitiveness and stability, as well as by ensuring public safety and reliable services (e.g. rail, aerospace, automotive, and power generation and distribution services) to the public.

Nemak Canada is developing technologies, now close to being implemented, using neutron scattering that will speed production times and reduce energy usage, thereby saving millions in manufacturing costs. In one line of this research, neutrons are used to reveal stresses in engine blocks before, during and after stress relief to determine whether the heat treatment process can be simplified without compromising reliability.

MSE also delivers on the protection and security needs of society. Materials research in this realm requires access to the same broad spectrum of advanced research capabilities. However, beyond materials research, protection and security requires the ongoing development of inspection and monitoring capabilities.

In terms of MSE, over 200 proprietary reports have been provided to clients including: Pratt & Whitney Canada; Alcan International; Sydney Steel Corp.; Syncrude; Welding Institute of Canada; Ontario Power Generation; IPSCO; IVACO; Dynetek; Rolls Royce and Associates; Boeing; ExxonMobil; Hitachi Ltd.; BP Institute; Westinghouse–Bettis; LevelTech; GE Aviation; Tokyo Electric Power Company; NASA; Atomic Energy of Canada Ltd.; Defence R&D Canada (Atlantic); Martin Marietta Energy Systems; NRC Aerospace; U.S. Department of Energy; and other government departments. An overview of the impacts these measurements have had on some of the Canadian companies on this list is presented in Section 1.3.

Society's Changing Relationship with Materials – Key Challenges

Recent advances in the theoretical understanding of the structure and behaviour of materials, as driven by new experimental techniques, new modelling tools (i.e. computers), and new models, have changed our fundamental relationship with materials—namely, we are learning to predict the behaviour of materials under different conditions. This will ultimately allow us to deliberately design optimized materials for specific applications, rather than search for them in semi-empirical, inefficient, and costly ways. The new field of integrated computational materials engineering is emerging as a comprehensive approach to the design of components from basic fundamentals. 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" [2.85].

Two key challenges have emerged in MSE as a result of our evolving relationship with materials: (1) model validation; and (2) material and component qualification.

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 and the ongoing development of methods, subject materials, and conditions seen in the fabrication of components and the conditions experienced during service. The unique knowledge obtained from neutron beam measurements is used to refine models, paving the way for improved products at reduced costs while also allowing innovative Canadian companies to compete successfully in the global economy.

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—all while minimizing our environmental impact. At the same time, worldwide competition drives industry to meet these ever-increasing demands as cost-effectively as possible. Thus, simply over-designing is no longer an acceptable option. Qualification refers to measurements or inspections undertaken to ensure that a material or component can perform its intended purpose satisfactorily (i.e. safely, reliably, and 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 chemical, manufacturing, or power generation plant after an unexpected failure? How do we prove to regulators that a new, more efficient material or process is suitable for a given application? Can we save money by refurbishment rather than building something new—and still ensure safe, reliable operation? 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.

Protection, Security, and Forensics

Worldwide, nations are making investments in research and technologies that will aid in the protection and security of their citizens against chemical, biological, radiological, nuclear, and explosive (CBRNE) events caused by accidents or wilful acts. CBRNE events refer to the uncontrolled release of chemicals, biological agents, or radioactive contamination into the environment, as well as explosions that cause widespread damage [2.86].

Materials research improves the performance of the materials used to defend citizenry and protect first responders against CBRNE agents. Technologies developed for materials research using neutrons have been adopted as technologies for inspection and monitoring. Forensics seeks to scientifically reveal evidence to establish events or origin of materials in order to identify the intentional or unintentional perpetrators.

The interactions of neutrons with matter lead to unique and powerful methods to address the critical issues of model validation and materials qualification. The great benefits of neutrons in MSE stem from their ability to penetrate deeply (i.e. several centimetres) into most materials; this allows 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.

These same unique properties of neutrons enable the non-destructive investigation of forensic artefacts, leaving them available for subsequent investigation or as intact evidence. Similarly, neutrons make it possible to investigate hazardous or unknown materials in containments [2.87]. In these endeavours, neutrons reveal the unseen.

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; deformation and phase transformations; and imaging methods. Some details are summarized in the subsections below.

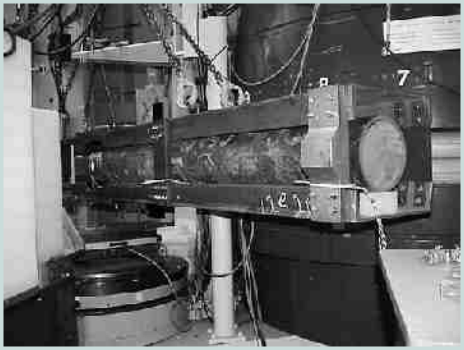
Residual Stress Scanning: Engineering materials undergo complex processing schedules (e.g. melting and casting, heating and cooling, rolling, extrusion, welding, etc.). These processing steps lead to residual stresses, whereby one part of the material or component pushes or pulls against another part [2.88]. There is no external evidence of this 'inner turmoil'—we just see a chunk of stuff that sits quietly on a desk, for example, or under the hood of a car. However, residual stresses affect the performance of mechanical parts because they superpose on (i.e. add to) the applied stresses that the component experiences while 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 (e.g. metals, alloys, ceramics) have a well-defined, orderly, periodic arrangement of atoms (i.e. 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 unstressed and stressed 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 1–1000 mm^3 can be defined. The gauge volume is simply moved over a grid of locations deep inside of components to map residual stresses in macroscopic materials or components. No other technique can accomplish this over the enormous range of sample sizes required—which varies from small rivets a few millimetres in length to pipeline sections nearly half a metre in diameter.

Neutron stress scanning is non-destructive in that it does not have 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 or highly specialized custom-developed finite element packages. Neutron residual stress mapping is thus an invaluable tool for validating and refining these models (see Figure 2.3.1).



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.

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
Swedan	Pulsed spallation	ESS	BEER
U.S.	Pulsed spallation	LANSCE, Los Alamos National Laboratory	SMARTS, HIPPO
UK	Pulsed spallation	ISIS, Rutherford-Appleton Laboratory	ENGIN-X
Japan	Reactor	JRR-3, Japanese Atomic Energy Agency	RESA
Japan	Pulsed spallation	J-PARC, Japan Spallation Neutron Source	Ibaraki, Takumi JAEA
U.S.	Pulsed spallation	Spallation Neutron Source, Oak Ridge National Laboratory	Vulcan
U.S.	Reactor	NIST Center for Neutron Research	BT8
U.S.	Reactor	HFIR, Oak Ridge National Laboratory	NRSF2
Canada	Reactor	NRU, Chalk River Laboratories	L3 and E3

The industrial and scientific importance of residual stress scanning, as exemplified in Canada, has been widely recognized. Thus, all of the major neutron laboratories in the world have now built, or are building, dedicated stress scanning instruments based on the Chalk River Laboratories example (see Table 2). The superior design and construction of L3, the primary Canadian stress scanning machine, were essential to establish the technology in the first place, and L3 remains the benchmark instrument in the world.

Canadian macroscopic stress scanning activities have influenced a number of industries within Canada and abroad. Some highlights are listed in Section 1.3.

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—namely, 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 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 (i.e. texture) may introduce anisotropy that influences macroscopic behaviours such as creep and growth [2.89].

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:

- One of the most exciting developments in terms of *in situ* testing has been the ability to measure the response to applied loads (including biaxial 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. Advances in our capabilities are such that multiaxial loading, as well as loads combined with various environmental conditions, have allowed *in situ* testing to come much closer to realistic conditions [2.90–2.95];

- Fusion welding is one of the most common joining processes, but it is also a very complex one. In a world first at Chalk River Laboratories, *in situ* measurements of phase and stress evolution during the gas tungsten arc welding of plain carbon steel were made [2.96]; and

- *In situ* studies that focus on processes related to the fabrication of aluminum engine blocks and cylinder heads, including solidification, stress-relief processes, and alloy development, are helping the industry to realize higher fuel econo my vehicles [2.97, 2.98].

Hydrogen Sensitivity: Hydrogen is present practically everywhere, and it penetrates easily into many important engineering materials such as steel, titanium, aluminum, and zirconium, often resulting in damage that adversely influences material performance. Understanding how hydrogen enters materials and the form that it takes (e.g. whether it dissolves in the host matrix, forms a separate hydride phase, or develops into gas pockets) can help develop mitigation strategies and establish fitness-for-service guidelines to ensure the safe operation of critical systems. Neutrons are sensitive to the presence of hydrogen in materials—often at the level of a few parts per million—because hydrogen scatters neutrons very strongly. As a result, neutron scattering has become a powerful technique to study how hydrogen enters materials and how it causes damage. Thanks to the high penetrating power of neutrons, measurements are often performed *in situ* and under realistic conditions of temperature, pressure, and atmosphere, thereby resulting in valuable quantitative data.

Crystallographic Texture

Most common materials, including metals, minerals, structural ceramics, semiconductors, and superconductors, are polycrystalline aggregates. As such, they are made up of small (i.e. 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 (i.e. grains). The properties of the aggregate depend on the texture, because the properties of the crystals are themselves anisotropic (i.e. they depend on the crystal direction in which they are measured). The nature of the boundaries between crystals (i.e. grain boundaries), which has a profound effect on material properties, is also naturally related to texture. In recent years, recognition of the importance of grain boundaries has led 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), as well as 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. Highlights of neutron diffraction studies of texture include:

- Texture measurements revealed that an anisotropic yield surface led to the formation of 'dog ears' on aluminum beverage cans, which would cause a plant shutdown. Plant shutdowns were thus avoided by optimizing the texture;

- Zirconium alloy components used in nuclear power plants are given favourable mechanical properties by specifically tailoring the developed texture. Extensive texture measurements and modelling supported the development of these components, and have also been used to qualify them for use in the nuclear industry; and

- Magnesium alloys are of great interest for lightweighting vehicles. The development and validation of computer models of the forming process that incorporate texture were critical to the development of alloys capable of being stamped into automotive body panels.

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 [2.99].

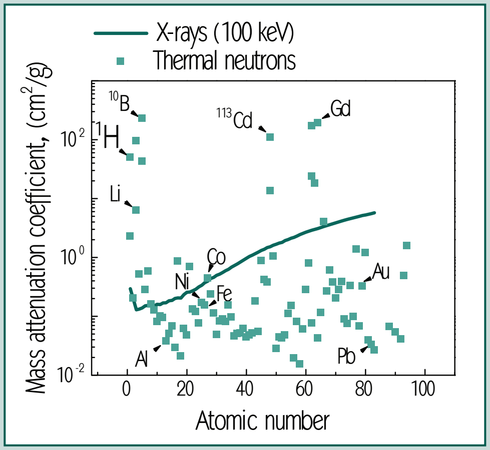
Neutron Imaging

Analogous to x-ray radiography in medicine, neutron radiography is performed by shining a neutron beam onto a specimen and then recording the image on a suitable detector placed behind the specimen. A two-dimensional 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 yet 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 and water are both clearly visible in neutron radiographs because of their high hydrogen content, while many structural materials such as aluminium and 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 a neutron radiograph image of an historic document from the time of Louis Riel. In those days, important documents were stored by putting them in

(a)



(b)

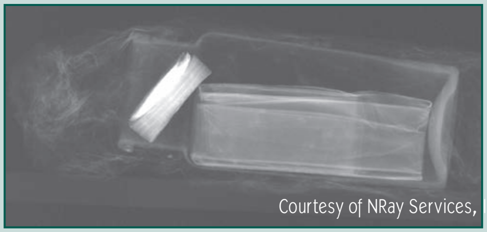


Figure 2.3.2 (a) X-Ray vs. neutron attenuation by atomic number. (b) An example of what that means: only neutrons see a historic paper document inside a lead-wrapped casing, demonstrating that the document is intact without opening the package.

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 that 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 such things as the inspection of aircraft turbine blades, as well as the examination of fluid behaviour in the internal channels and cavities of engineering components, soil, rock, and ceramics. In fact, the European community is building a radiography beam line as one of the two first instruments at the European Spallation Source because of the demand for, and the scientific and cultural impacts of, neutron imaging [2.100]. Canadian company NRay Services Inc. based in Dundas, Ontario is a world leader in applying neutron radiography to engineering problems. NRay, a spinoff of Atomic Energy of Canada Limited, uses the radiography facility at McMaster University to conduct its work. NRay has stated that they would build a new 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 is revealed to have obstructed channels, making it impossible to cool properly while in service, which can lead to disastrous consequences.

In neutron tomography, a series of radiographs is taken of the specimen at different orientations with respect to the incident beam, and then recombined to non-destructively generate a three-dimensional image of the internal structures and cavities of a component or device. The three-dimensional image can be used to accurately determine the internal dimensions of complex components, as well as 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 of 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.

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 increasingly 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” [2.101].

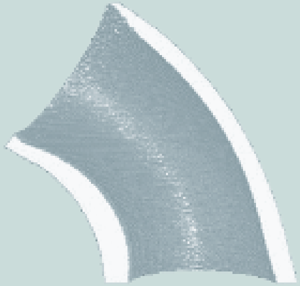


Figure 2.3.4 - Tomographic reconstruction of a bent feeder pipe.

Neutron radiograph of air-cooled turbine blades; the blade on the left is revealed to have obstructed channels.

New instruments and methods are needed to drive new science. Such advancements will enable us to probe material behaviour at an unprecedented level of detail, thereby allowing 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 to improve on existing measurement capabilities. Overall, this means smaller, more intense neutron beams and better detection capabilities, ultimately leading to the faster and more efficient collection of high-quality data. This will open up new fields of study hitherto inaccessible to neutron beam methods, 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 [2.102]. 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. Both the Institut Laue-Langevin (ILL) in France and the NIST in the U.S. are pursuing the development of a white beam stress scanner. New fields of study can therefore be envisaged based on the following considerations:

- With finer resolution and higher flux, it will become possible to obtain two-dimensional maps around realistic cracks in full-scale components, as required to understand the mechanisms underlying stress-corrosion cracking;
- Composite materials (e.g. metal matrixes, cermets, and ceramic matrixes) and multiphase alloys have stress-strain interactions between the constituent phases, which can best be understood by simultaneous monitoring of strain response among phases during deformation. Such monitoring 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, in order 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 within 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-to-weight ratios, and smart composites;

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

- It will be possible to acquire complete pole figures simultaneously at a number of values on the Miller indices (i.e. {hkl} values) relating to planes in crystal lattices. The white beam stress 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 the 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 localized phenomena such as crack propagation (including stress-corrosion cracking), ingress of foreign elements (good or bad) in materials, and failure of interphase boundaries in composite materials. A neutron microbeam prototype was tested and proven at Chalk River Laboratories through a collaboration of researchers from the Canadian Neutron Beam Centre and Oak Ridge National Laboratory in the U.S. [2.103]. 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 Royal Canadian Air Force uses neutron radiography to inspect certain composite flight control surfaces on its aircraft. These components are susceptible to water ingress and must be inspected periodically. The light shaded regions in Figure 2.3.5, a neutron radiograph, 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 in Kingston, Ontario that 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, multipurpose research reactor would have a much higher flux, thus yielding better images at shorter exposure times. It could also be designed to accommodate much larger specimens than are currently permitted. Naturally, the instrument would also be suitable for tomographic studies. This capability would be an important asset for defence research and development (R&D), as it would constitute an effective and efficient means to achieve the safe and reliable operation of current and future aircraft fleets, which make heavy use of composite materials.

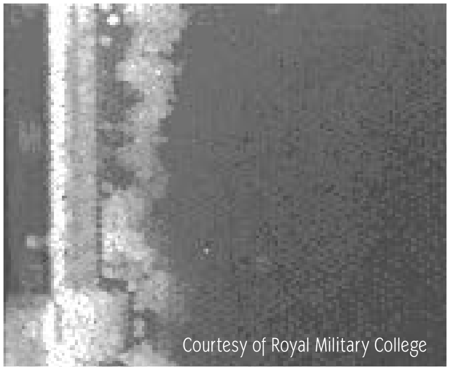


Figure 2.3.5 Detecting water inside a CF 18 fighter jet component using neutron radiography; the light shaded regions reveal water inside the control surface.

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 even higher rates than that. 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 higher flux and dedicated radiographic instrumentation, real-time images could be produced of single-shot moving components and fluids, and also of material processes (e.g. 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 and in real time (i.e. in 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 cold neutron radiography capabilities, which can produce superior radiographic images. 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 while providing an optimized instrument that would benefit the national scientific and engineering communities.

Maximizing the Penetration Advantage

Scientific and engineering pursuits should always rely on the results obtained through the use of complementary techniques. The non-destructive character of neutron radiography plays well into this, as other experimental methods can still be employed on the very same sample after a neutron experiment. Moreover, all applicable neutron methods could be employed before moving on to destructive examination methods.

The high penetration of neutron radiography also makes it possible to investigate samples within various sample environments. Experiments have taken this a step further and performed measurements on samples in hazardous environments that have been contained to minimize the risk to personnel. Such experiments have been performed using a container and a sample specific to the particular *in situ* test.

A recent set of experiments has demonstrated that such containment can be designed, and protocols developed, to examine unknown samples using multiple neutron methods [2.87]. Combined with other non-neutron methods, a forensics sample or a specimen that has emerged through a CBRNE event can be investigated.

2.4 Thin Films and Surfaces – Nanostructures

The research community that uses neutron beam methods to study thin films and surfaces has been growing in parallel with the development of neutron reflectometry (NR) at Chalk River Laboratories. 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 (CFI) to construct Canada's first dedicated neutron reflectometer, the D3. This new instrument commenced operation in the summer of 2007, providing Canadians with a competitive facility to enable world-class research on phenomena that occur on the nanoscale across several disciplines. Since its commissioning, the D3 reflectometer contributed to 33 peer-reviewed journal articles as of September 2014.

Overview

Materials are the building blocks of our world. While 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.

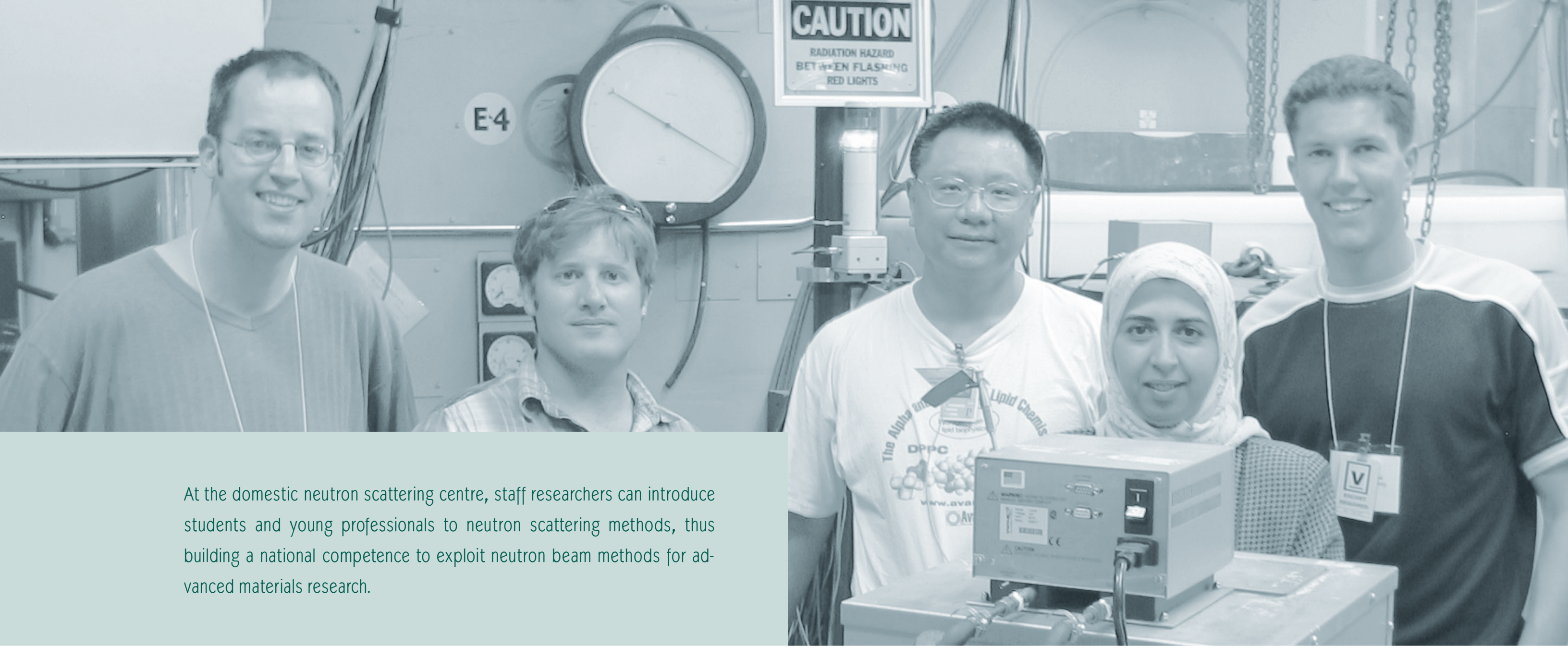
Surface science and thin film phenomena appear across the whole range of condensed matter physics. Neutron scattering has the unique advantage of being sensitive to isotopes (e.g. hydrogen and deuterium) and to magnetic structures. It has proven to be invaluable to polymer and biological sciences, as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

Neutron reflectometry 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 of thin films. Researchers can do such things as map the distribution of molecules at a gas-to-liquid interface, monitor the growth of a reaction front, and study the magnetic properties of magnetic films used in advanced information technologies—just to name a few of the research frontiers made accessible by NR.

Current Thin Film Research

A wide range of different scientific areas (e.g. corrosion, supercapacitors, thin magnetic films, hydrogen storage, polymer films, and biophysics) have been assisted in the past decade through NR experiments at Chalk River Laboratories. The following sub-sections draw attention to various collaborations with Canadian and international researchers. They also point to areas not yet explored at Chalk River Laboratories, but where NR has been applied very successfully elsewhere (e.g. giant magnetoresistance sensors, lithographically structured materials), as well as 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. These projects—some completed and some ongoing—fall into two categories: (1) investigation of reaction kinetics [2.104], and (2) study of the nature and growth of the passive oxide layer [2.105, 2.106] 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 generation, 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



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.

by any other method. Corrosion science is inseparable from electrochemistry (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-to-liquid interface, electrochemistry naturally falls under the surfaces and interfaces research carried out with techniques such as neutron reflectometry [2.107]. NR and electrochemical impedance spectroscopy experiments can be performed at the same time on the same sample [2.108], which gives valuable information on the structure and electrochemical properties of the sample.

Biocompatible Implants: Surfaces coated with tethered hydrophilic polymers (e.g. polyethylene glycol, dextran, etc.) 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 Laboratories. In one such study, a coating's protein-repelling efficacy, which is desirable for certain implants (e.g. artificial heart valves), was investigated as a function of chemisorption conditions [2.109]. The counter-intuitive results from neutron reflectometry have indicated the way to optimize the biocompatibility of future implants.

NR experiments supported the existence of a relatively thick continuous phase of water stemming from within an anti-fouling monoethylene glycol silane adlayer. In contrast, this physically distinct (from bulk) interphase is much thinner and only interfacial in nature for the less effective adlayer lacking internal ether oxygen atoms. These results provided further insight into the link between antifouling and surface hydration [2.110].

Magnetic Thin Films, Proximity Effects: The magnetic properties of materials (e.g. 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 [2.111], as well as a polarization of Pd films in proximity to Fe films [2.112].

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 [2.113], as well as PNR [2.114] and the application of both techniques on an identical sample [2.115], were used to determine the complex magnetic structure of these systems. It is crucial to get this information in order to improve theoretical understanding and then, based on 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 [2.116]. For this discovery, the Nobel Prize in Physics was awarded to Peter Grünberg and Albert Fert in 2007. 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 of these layered structures [2.117]. 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 [2.118].

Spintronics: Recently, a technology called spintronics has emerged, which is based on semiconductor technology exploiting the electron's spin instead of its charge. Several proof-of-concept spintronic devices (e.g. the spin transistor) have been proposed already [2.119], and the focus of research is on finding materials with the necessary properties to realize these new electronic devices. Work at Chalk River Laboratories has investigated the magnetic properties of thin MnSi films and was able to confirm the existence of a new magnetic phase called skyrmion [2.120].

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, incorporation of hydrogen within the host film can lead to significant modifications of the electronic, magnetic, and structural properties [2.121, 2.122]. NR was used to determine the hydrogen profile in a film, along with the change of structure and magnetic properties of the film due to the hydrogen cycling [2.122]. This information is crucial for the development of materials for hydrogen sensors.

Thin films have been used as model systems to study the properties of hydrogen storage materials. At Chalk River Laboratories, Mg based alloys have been investigated extensively [2.123–2.125]. The NR experiments clearly showed that: (1) a Ta-Pd bilayer catalyst improved the sorption kinetics; and (2) Mg alloys work better than pure Mg because of a homogeneous hydrogenation, a result of avoiding the hydride layer that blocks further hydrogen intake in pure Mg [2.126].

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 the corrosion process [2.105].

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

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.

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 nanoscale objects [2.127].

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 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 [2.128]. 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 has helped to understand the swelling behaviour by revealing a non-uniform water distribution in the polyelectrolyte film [2.129].

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 the telecommunication sector (e.g. as routers, couplers, filters, etc.) and in the microelectronics industry (i.e. 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. At Chalk River Laboratories, NR was successfully applied to investigate photomechanical effects *in situ*, during laser illumination, in azo polymer films [2.130]. Surprisingly, the experiments showed two competing photomechanical effects in this system: one that causes expansion and the other one contraction.

Impacts

The largest economic impact of the aforementioned areas is certainly in the field of corrosion. A 2001 study funded by the U.S. Congress, with oversight by the Federal Highway Administration and support from NACE International, provided broad research on direct and indirect costs for U.S. industry sectors. The results of the study indicated the estimated annual direct cost of corrosion in the U.S. to be $276 billion [2.131]. Taking the same percentage of GDP, the corrosion costs would be about $35 billion per year for the Canadian economy. The advancement of knowledge about the mechanisms of corrosion and strategies to mitigate corrosion therefore provide high potential impact on the national infrastructure and economy.

Scientific impacts are realized by advancing the fundamental understanding of the atomic, electronic, and magnetic properties of materials and their relationship to physical properties. Advancements are frequently accelerated by applying the unique advantages of neutrons for probing atomic and molecular structures, as well as nanostructures. The opportunity to generate new knowledge through neutron reflectometry is illustrated by the fact that, as of September 2014, the new D3 reflectometer was used to produce 33 peer-reviewed articles since its commissioning in 2007. Furthermore, during these years, D3 has provided the opportunity to educate many graduate students, doctoral candidates, and postdoctoral fellows in the application of NR for research on phenomena on the nanometre scale. D3 experiments have been a substantial part in the Masters theses of Murray Wilson (Dalhousie University) and Natalia Pawlowska (University of Toronto), as well as the PhD theses of Chris Harrower (University of Alberta), Eric Karhu (Dalhousie University), and Drew Marquardt (Brock University).

Future Impacts and 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 into new materials with dimensions on the nanoscale. Economic impacts from NR experiments are most likely to arise in the field of corrosion (e.g. anti-corrosive coatings), biophysics (e.g. biocompatible implants), chemistry (e.g. thin film sensors), and portable electricity generation and fuel storage systems (e.g. fuel cells and hydrogen storage).

2.5 Soft Materials - Polymeric and Biomimetic Materials

Neutron beams have become indispensable tools for the study of structures and dynamics in polymeric and biological materials. An advantage of neutron over x-ray beams is that molecules or molecular groups can be highlighted through hydrogen–deuterium isotope substitution. Neutron beams can access the nanometre length and nanosecond time scales relevant in these materials through elastic and quasi-elastic neutron scattering techniques. Under the lead of John Katsaras, Mu-Ping Nieh, and Norbert Kučerka, the Canadian Neutron Beam Centre has developed an international reputation for soft and biological materials research.

While the NRU reactor provides a very intense beam of thermal neutrons, experiments in soft materials often benefit from neutrons of long wavelength and smaller energy—that is, from so-called cold neutrons. These slower neutrons are better adapted to the intrinsically slower dynamics and longer length scales as compared to crystalline or magnetic materials. 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, as well as to incorporate its perspective into this planning document.

Overview

In contrast to crystalline materials, polymeric and biological materials are classified as soft materials because of their inherent disorder. Their molecules are not arranged on regular lattice sites and are more or less free to diffuse. Soft materials include biological molecules, polymers, colloids, and surfactants, among others. They are relevant to all branches of the life sciences, chemistry, and physics, and they 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. By replacing hydrogen with deuterium, certain molecules or functional groups can be highlighted in neutron scattering experiments. The resulting capability of contrast variation makes neutrons excellent probes for the study of these normally delicate materials.

Soft materials self-assemble into a variety of structures ranging in size from nanometres to micrometres. As the corresponding dynamics cover time scales from picoseconds to microseconds, soft materials can be considered multi-scale materials. The most widespread techniques employed in this discipline are small angle neutron scattering (SANS), neutron reflectometry, and neutron diffraction. These techniques have developed into powerful tools for studying the structure of macromolecules, yielding information about size, shape, and conformational changes, as well as molecular associations in solution—information needed to understand essential molecular interactions for chemical or biological function. Dynamic techniques such as quasi-elastic neutron scattering (QENS), neutron spin-echo (NSE), and backscattering (BS) are used to provide detailed insights into the dynamic processes of these macromolecular assemblies.

Canada has a strong and internationally renowned soft matter community. At the Canadian Neutron Beam Centre, research in soft materials with neutrons is conducted on two neutron instruments: (1) the newly built, CFI-funded reflectometer; and (2) a triple-axis spectrometer. The CFI initiative was led by the University of Western Ontario. The triple-axis spectrometer has been optimized for small angle diffraction and diffraction experiments in soft materials. However, soft matter research with neutrons in Canada is currently strongly limited by the instrumentation available and by the unavailability of a cold source to produce long wavelength neutrons. As a result, many researchers presently conduct experiments at foreign laboratories. There is a huge potential to unleash, however; the availability of dedicated and optimized soft materials experimental neutron facilities in Canada would very likely create a vibrant and successful neutron scattering community in soft materials.

Current Soft and Biological Materials Research

Neutron beams can provide unique information about soft and biological materials, and they are often the technique of choice to determine molecular structure and organization in these materials. The importance and usefulness of neutron scattering techniques can be seen in the current research being done by Canadian researchers, discussed in the subsections below.

Liposomes for Drug Delivery: Encapsulating a drug in lipid-based vesicles improves the circulation half-life of the drug in vivo. Moreover, functionalized 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, to map out the complex structural phase diagrams of the different formulations of the lipid mixtures [2.132–2.134], and to understand the spontaneous formation mechanism of such vesicles [2.135]. An ongoing research program is focusing on maintaining their stability and size after the incorporation of drugs or medical imaging contrast agents. A flow cell to conduct neutron diffraction experiments on bicellar mixtures aligned by an *in situ* temperature controllable shear flow has recently been developed in a collaboration between the CNBC and the University of Connecticut, and is now available for experiments [2.136].

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 in an effort to relate how the molecular architecture affects the efficiency of the membrane [2.137, 2.138].

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 253 K. These gels have desirable mechanical properties resembling those of cardiovascular tissues, and thus are used in applications such as dressing wounds, heart valve stents, etc. Canadian researchers are using SANS to examine the architecture of PVA gels under stress and shear [2.139].

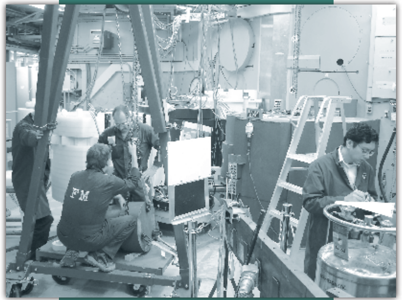
Biological Membranes: The impact of neutron scattering on membrane research is intimately connected with the capability to prepare biomimetic membrane systems. The composition of these synthetic membranes can be well controlled to mimic certain types of cells and tissues. By further using aligned bilayers, in-plane and out-of-plane structure can be determined with high (i.e. sub-nanometre) resolution under relevant physiological conditions. Using deuterium labeling, the exact location of things such as proteins [2.140] can be determined. Research at the CNBC recently revealed that cholesterol is found in the centre of polyunsaturated lipid bilayers [2.141, 2.142], while the commonly used 'umbrella model' assumes an alignment parallel to the lipid acyl chains. By localizing vitamin E in lipid membranes, the molecular mechanism of its protective, antioxidant properties was revealed [2.143, 2.144]. Experimental evidence for coexisting gel and fluid domains in lipid membranes was observed using neutron diffraction [2.145]. The neutron instrumentation at the CNBC turned out to be particularly suited to study the organization of cholesterol in so-called lipid rafts and its impact on lipid organization [2.146–2.149].

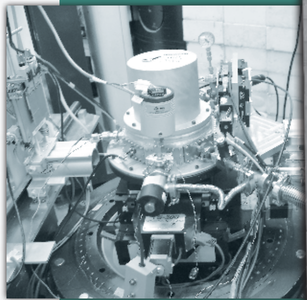
Biocompatible Thin Films: Immune response against foreign objects is always an important issue when it comes to organ transplants. Biocompatible thin films coating the surfaces of implant organs can prevent the adsorption of certain proteins, and thus reduce organ rejection. The water distribution and 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 is able to help in the qualification of these materials for medical use [2.150, 2.151].

Impact

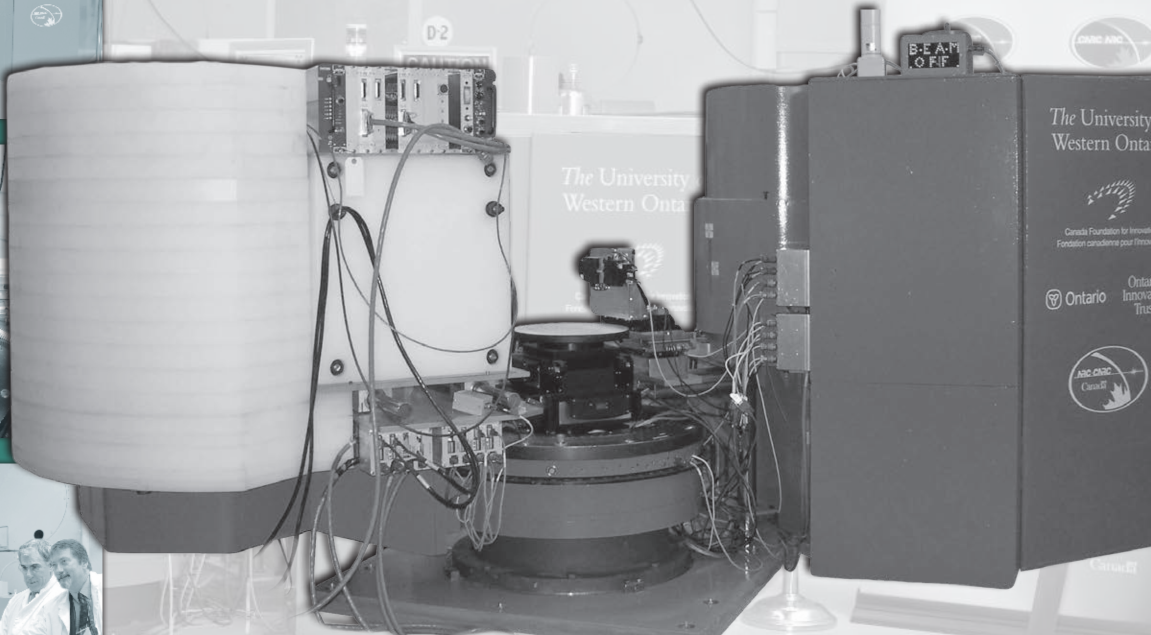
Demand for nano biotechnology in healthcare products is projected to significantly increase in the future, as led by improved cancer and central nervous system therapies based on solubilization technologies. Diagnostic tests based on nanoarrays and quantum dots, as well as imaging agents based on superparamagnetic iron oxide nanoparticles, will also see strong growth. The demand for nanotechnology medical products in the U.S. is estimated to grow by more than 17% annually to reach $34 billion in 2014, while drug delivery and biomedical applications are expected to reach $224 billion by 2017 [2.152].

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 the NIST Center for Neutron Research in the U.S. In the area of membrane research, the Cold Neutrons for Biology and Technology consortium, led by biophysicist Stephen White (University of California at Irvine), received $5 million from the National Center for Research Resources of the National Institutes of Health to build the first neutron beam research station in the U.S. 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 structures and interactions of cell membranes and their components, gathering information that is 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 AGM and Workshop of the Canadian Institute for Neutron Scattering [3.1], a preliminary list of neutron beam instruments was developed. The list was endorsed again at the 2014 AGM [3.2]. The instruments would support the scientific research identified in the 2006 workshop, with 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, with thermal being the general moderator of the research reactor, cold being a localized moderator at a temperature of about 20 K, 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 describe the general principles and applications of each type of instrument in order to provide an understanding of how each would address the scientific requirements of the user community.

3.1 Control System and User Interface

The control of neutron beam instruments, the management of data, and the interface with the user are all matters of great importance for every instrument in the neutron beam laboratory. The existing system at Chalk River Laboratories evolved by iteration over a 40-year period in response to the needs of researchers. It incorporates many excellent concepts and features that 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 rejuvenation of the control and

TABLE 3 - List of neutron beam instruments identified at the CINS's AGM and Workshop in 2006 and endorsed again at the CINS's AGM in 2014.

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

data management system should be included in the long-range plan for a new Canadian Neutron Centre.

Each neutron beam instrument requires a local data acquisition system that enables the 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, in order 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 minimize the time that users must be present near radiation-emitting equipment, and also to maximize 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 strategy for developing a data acquisition and control system is to work in collaboration with neutron facilities and similar scientific control systems from around the world, in order to build a system specialized to our needs. The international community provides a large library of off-the-shelf, open source components that have proved their reliability through many years of usage. By becoming active members of this community, we can take advantage of these off-the-shelf components. Becoming active community members also means contributing ideas and components back into the community, thereby not only improving our capability, but also contributing to the field of engineering and building control and data acquisition systems.

Working within the community means that, wherever possible, we use accepted standards. This includes standards for data storage formats, communication protocols, and device interfaces, among others. Using accepted standards provides a number of advantages, including: the ability to use existing products and components; the ability to provide the user with an interface that is similar to that encountered at other neutron facilities; and the ability to access a wider pool of readily available expertise when hiring or contracting for control system engineers.

With the rapid evolution of technology and devices, any control and data acquisition system must be sufficiently flexible and adaptable to take advantage of new devices that provide new capability. This includes not only smart scientific devices, but also new approaches to user interfaces. Our current control system was designed long before the internet, tablets, and smart phones were conceived. The devices and technologies that will be available over the next few decades are impossible to predict. The control system cannot be rigid in its assumptions about the technology available. It must be designed with the flexibility to adapt and integrate new technologies as they come on line.

3.2 Neutron Reflectometers

A neutron reflectometer yields data to determine the scattering length density profile of a flat sample as a function of depth to about 300 nanometres (nm). This fundamental result 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 an indispensable and popular technique for surface and thin film science. With increasing demand for access worldwide, most of the latest neutron facility projects have one or more reflectometers in their instrument suites (e.g. there are two at the SNS in the U.S., five at ISIS in the U.K., three at FRM-II in Germany, and one at OPAL in Australia). To best serve the needs of the Canadian research community, two reflectometers were recommended at the CINS's AGM and Workshop held in October

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

2006 [3.3]. These were: (1) a reflectometer with a horizontal sample geometry optimized for samples with liquid-to-gas or liquid-to-liquid interfaces; and (2) a reflectometer with a vertical sample geometry optimized for all other types of interfaces. Both reflectometers should be part of a 'day-one' suite of instruments.

New instrumentation ideas like extreme focusing monochromators that converge rays spanning a wide range (e.g. 11.4°, as implemented in the D3 reflectometer at Chalk River Laboratories) will be employed for both reflectometers to the fullest 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 the ability 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 neutrons whose λ is too long) in tandem with a cooled Be filter (to reject neutrons whose λ is too short). Adjusting the grazing angle of the reflector allows the variation of $\Delta\lambda$. 'Full-spectrum' approaches are under development at the NIST in the U.S. and at Laboratoire Léon Brillouin (LLB) in France. Taking advantage of such innovative methods would increase the performance of the new reflectometers by about one or two orders of magnitude as compared to the current configuration at Chalk River Laboratories. Combining optimum instrument design with a powerful reactor and a cold neutron source would offer Canadian researchers two world-leading instruments, with performance equal to or exceeding those at the world's most powerful research reactor, located at the Institute Laue-Langevin (ILL) in France, as well as the world's most powerful spallation source, the Spallation Neutron Source at Oak Ridge National Laboratory in the U.S.

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

- 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 the ILL [3.4];
- Although TOF enables NR without mechanical movements (and hence is more suitable for time-resolved experiments), this is so only if one wishes to measure reflectivity over a narrow dynamic range (i.e. Q_{min}:Q_{max} ~1:5); and
- A monochromatic instrument that cycles continuously between Q_{min} and Q_{max} with, say, a 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 an unproven technology thus far.

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 not significantly complicate the design of the reflectometers.

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 design 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 (with the surface itself held perpendicular to the ground), and so is not suitable for the study of bulk liquid-to-vapour interfaces. However, it is an excellent tool to investigate all other interface types (i.e. solid-to-solid, solid-to-liquid, solid-to-vapour, and buried interfaces) and is able to access high values of the 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 beam line 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. Helmholtz-Zentrum Berlin, or HZB, in Germany; ISIS in the U.K.; the ILL in France; and the SNS in the U.S.) install a neutron reflectometer with a horizontal surface geometry (i.e. with the surface normal vertical). This geometry is suitable for studying all types of interfaces, including liquid-to-vapour interfaces, but typically does not enable such a wide Q range as in the horizontal scattering configuration. This type of reflectometer enables the study of thin films at air-to-liquid and liquid-to-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, as well as the surface behaviour of surfactants, polymers, and other amphiphiles at liquid-to-air and liquid-to-liquid interfaces.

3.3 Small Angle Neutron Scattering

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 or micrometre structure is also crucial to such things as biological processes in cells, the storage of information on magnetic disks, the hardness of steels and superalloys, the conduction of current in superconductors, and many other materials properties.

In the biological sciences, SANS is the most powerful technique for studying the structure of native proteins and complexes and for rapidly analyzing structural changes in response to variations in external conditions. 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. 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 [3.5].

Thanks to advances in instrumentation and computational methods over the last decade, the amount of experimental SANS data involving proteins is increasing dramatically. In response, the freely accessible Small Angle Scattering Biological Data Bank was developed at the European Molecular Biology Laboratory in Germany to handle the growing amount of experimental data [3.6].

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 Laboratories 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 scale 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). For reactor sources, the classical 30 m 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

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.

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 through beam on the detector [3.7]. With this setup, the attainable minimum Q-value is ~0.001 $Å^{-1}$, corresponding to a length scale of 500 nm.

One 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 [3.8]. The new Very Small Angle Neutron Scattering (vSANS) instrument is based on this concept and is presently awaiting construction at the NIST. Capitalizing on the availability of cold neutrons, the proposed vSANS instrument will support a wide spectrum of university, government, and industrial researchers, particularly those in chemistry, biology, and condensed matter physics. The vSANS instrument will immediately be exploited by the strong Canadian biophysics and biomaterials communities that are interested in domain structures in membranes, drug–membrane interactions, and phase diagrams of phospholipid vesicles, biopolymers, hydrogels, etc. To accommodate the demand, it was deemed necessary to add an additional 10 m SANS in the second NIST guide hall in 2012.

In addition, long flight path SANS is available at spallation sources, where they have the additional advantage of the widest Q range of data in a single instrument configuration because of the multiple wavelengths of the neutron beam. For example, LoKI is a broadband SANS instrument planned for the European Spallation Source that has been fast-tracked through into engineering design. Its situation and time-of-flight design (i.e. 10 m of collimation and additional 10 m sample-to-detector distance, with the sample position 20 m from the moderator), as well as its large solid angle of detector coverage, put it on target to achieve 10 times the neutron flux of the current leading reactor-based instrument.

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 a number of cases where none of these techniques is applicable (e.g. when using low-contrast and opaque materials in the case of light scattering, or when using magnetic structures). Applications can be found in colloid science (e.g. mixtures of particles, strongly correlated colloid crystals, and micron-sized particles), materials science (e.g. filled polymers, cements, and microporous media), and polymer science (e.g. constrained systems, emulsion, and polymerisation). USANS is the new capability most requested in Australia's new OPAL facility [3.9].

An ultra SANS instrument would be placed on a dedicated thermal beam port and would 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.

Use in Energy Extraction

Recent USANS studies have looked at how methane and water penetrate pores in the Barnett Shale, an increasingly important source of natural gas in North America. Natural gas is held in tiny pores and can be best accessed by horizontal drilling and hydraulic fracturing techniques. Understanding the nature of the pores will provide clues to making gas extraction more efficient [3.10]. The microstructure of rock plays a critical role in many geologic processes, including the movement of water and natural gas, as well as in technological processes such as CO2 sequestration and gas shale recovery. USANS has recently characterized shallowly buried quartz arenites from the St. Peter Sandstone, and has discovered that nanoscale porosity is far more important than previously thought in fluid–rock interactions [3.11].

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.

3.4 Stress Scanners

Classical Monochromatic Beam

The basic stress scanner is a double-axis diffractometer with a sample table capable of accommodating large, heavy objects (i.e. up to metres in dimension and weighing two tonnes) and moving them around reproducibly to within ~10 μm in all three dimensions. Diffracted neutrons are detected with a position-sensitive ^{3}He counter, which should subtend at least 3° in the scattering plane with high intrinsic resolution (~0.2° 2θ) and a range of ± 20° 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) that 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 are 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 0.2−0.3 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 Type I (i.e. macroscopic) strain scanning, but having additional {hkl} can be beneficial in that Type II (i.e. 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 a rectangular parallelepiped. In this way, the sampled volume is independent of specimen direction. For SW instruments, this requirement is easily satisfied; for CW instruments, however, this requires selecting a wavelength that places the scattering from the specimen at or near 90°. CW instruments are often designed so that other scattering angles can be used when there is an advantage to do so, while SW instruments tend to be fixed in angles.

Presently, SW TOF instruments are being favoured for fundamental research in materials science because there remains a great deal of interest surrounding *in situ* deformation studies, as well as 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 to realize the benefits offered by both CW and SW TOF instruments by performing wavelength discrimination after scattering from the sample, thereby extracting diffraction data from several {hkl} simultaneously.

CW stress scanners are sometimes configured for the measurement of crystallographic texture by adding two more sample orientation angles and possibly a device to automate changes of sample. A white beam instrument configured in the same manner would enable simultaneous measurement of so-called pole figures, dramatically reducing the time required to obtain texture data.

White beam stress scanner designs are being pursued by NIST and the ILL.

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 of, and constant advances in, such detectors are key defining elements for these instruments. The instrument will serve the scientific communities in biology, pharmaceuticals, coarse-grained materials, and soft materials, as well as studies of organometallic 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 Laboratory in the U.S., and the experience from its construction will greatly benefit the design of a cold neutron Laue system at Chalk River Laboratories.

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 the ILL [3.12]. However, to exceed

VIVALDI's capabilities, a new instrument could incorporate the ability to focus the white beam using Kirkpatrick Baez (K-B) mirrors. Researchers from the Canadian Neutron Beam Centre and Oak Ridge National Laboratory have shown that K-B mirrors, although relatively new to neutron beams, can be used effectively for neutron scattering experiments [3.13]. 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 (e.g. to determine the location of hydrogen and water molecules in bio-macromolecular materials with unit cells of up to 10 000 $Å^3$). The recently constructed KOALA instrument at the Australian Nuclear Science and Technology Organisation (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 [3.14–3.16].

The higher time-averaged flux of a new Canadian Neutron Centre, as 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 also 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; presently, it takes many hours to align crystals with Eulerian cradles on monochromatic beam lines.

An optimized beam line would require a cylindrical area detector system, most likely an image plate system, with pixel resolution of 200 × 200 μm^2 or better. A ^3He 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 function as a testing facility to align elements of multi-crystal monochromators or analyzers. This instrument can support single-crystal neutron diffraction experiments and quantitative texture analysis for users from the chemistry, physics, and materials engineering disciplines.

The instrument will include two switchable monochromators: (1) a perfect crystal; and (2) one with a mosaic spread in the range of 0.5−1.0°. At the specimen location, there will be θ and 2θ 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 to 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 abovementioned diffractometers. The performance parameters of these instruments should approach those set by DRACULA (high-efficiency) and the Super D2B (high-resolution) instruments located at the ILL in France or, similarly, the Wombat and Echidna instruments at ANSTO in Australia.

High-efficiency Diffractometer (HED)

The data collection rate of the high-efficiency diffractometer (HED) should exceed current benchmarks set by the GEM at ISIS in the U.K. and the POWGEN at the SNS in the U.S. This can be done by increasing the detector solid angle to at least 1 steradian, utilizing two-dimensional detectors, and implementing focusing monochromators to increase the flux on the 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 (e.g. 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 the 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 at the ILL. Experience from the design of the recently constructed Wombat diffractometer at ANSTO will be very useful [3.17, 3.18].

High-resolution Diffractometer (HRD)

The high-resolution diffractometer (HRD) will use a large take-off angle (e.g. 135°) and good collimation to attain a maximum resolution, $\Delta d/d \sim 5 \times 10^{-4}$, and an effective scattering angle range of between 3−160°. As with HED, detectors with a large solid angle will be utilized, giving either real or quasi-two-dimensional 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 at ANSTO will be a good guide for the design and construction of such an instrument [3.19].

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, toxic-reaction by-products, or an operating engine will also lead to increased risk. Risks to personnel can be minimized by shielding a diffractometer in a reinforced isolated structure built outside the reactor containment, with regulation-compliant ventilation, fire protection, radiation shielding, and soundproofing. 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 and materials science, as well as industry. Example projects include:

- Evaluation of radiation damage on crystal structures in nuclear alloys (e.g. aluminum, stain less steel, zirconium) and 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 in order to validate engineering models and place safety margins on a firm foundation; and

- 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

While HED and HRD are priorities for the CNC, 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 0.30−0.35 Å. Such wavelengths and a maximum scattering angle (2θ) of 160° (maximum Q > 30 $Å^{-1}$) 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 materials scientists interested in the study of local order (e.g. local site ordering and Jahn-Teller distortions).

This proposed instrument takes on a higher priority at this time in view of the recent U.S. Department of Energy decision to curtail the user program at the Lujan Center, which greatly restricts access to their NPDF instrument—arguably, the best of its type in not only North America, but internationally as well.

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 (e.g. ^{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 the DMC at the Swiss Spallation Neutron Source (SINQ).

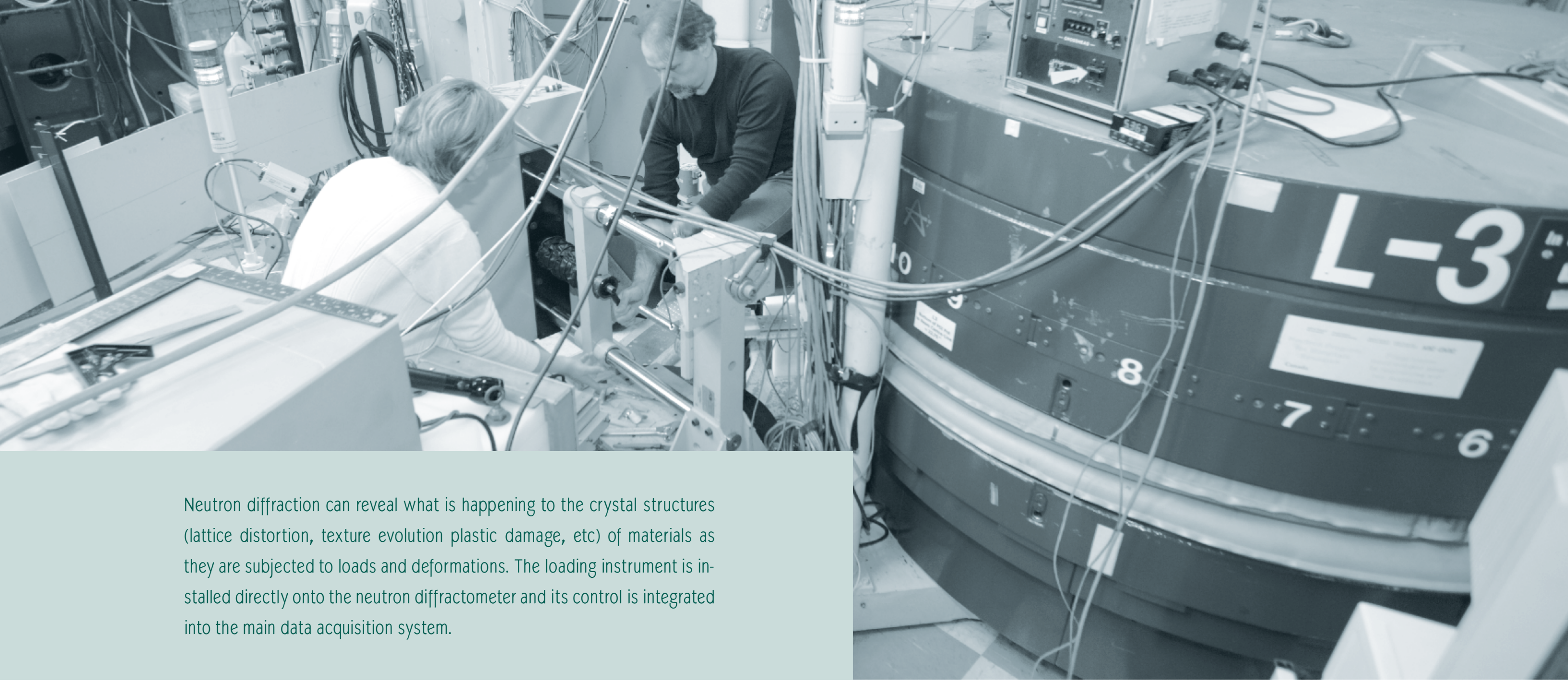
The low-Q powder diffractometer will have a variable monochromator take-off angle in the $2\theta_m$ range of 40−130°. A selection of monochromator crystals will be used to maximize the flexibility of wavelength, resolution, and intensity delivered to the specimen. For high-intensity measurements, a pyrolytic 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 of 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 nuclear magnetic resonance (NMR), muon spin rotation, and synchrotron x-ray scattering, inelastic neutron scattering provides the most complete information on how the space and time correlations (i.e. 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—an area 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 instruments). In addition, the quantum mechanical property of neutron spin is exploited in spin-echo techniques, where no monochromatization is required. A wide range of energy and momentum transfers

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.

(and their respective resolutions) is provided by these techniques, which are essential in studying different systems (e.g. from condensed matter to biological systems). In the following sub-sections, we describe the instruments that were discussed and prioritized at CINS's 2006 and 2007 AGMs. This selection was reaffirmed at CINS's 2014 AGM.

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 tool among inelastic instruments. It was Canadian physicist Bertram Brockhouse who first developed [3.20] the TAS concept at the NRX and NRU reactors located at Chalk River Laboratories (home of the 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 (e.g. magnetism, superconductivity, and other quantum materials); in systems where lattice effects and critical phenomena are important; in chemical physics; and, more recently, in the field of biophysics.

The triple-axis spectrometer is the workhorse for inelastic scattering studies [3.21] at steady-state neutron sources. 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 the design of TAS instruments, all resulting in making this technique more effective [2.71, 3.22–3.30]. The use of large double focusing monochromators and analyzers has resulted in enhanced luminosity and has made it possible to study very small single crystals (i.e. 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 [3.31–3.36] and novel geometries [3.37, 3.38] have now materialized. Pursuit of the optimized design for TAS spectrometers has made them a very effective, complementary technique for use with time-of-flight instruments for single crystal spectroscopy at pulsed neutron sources.

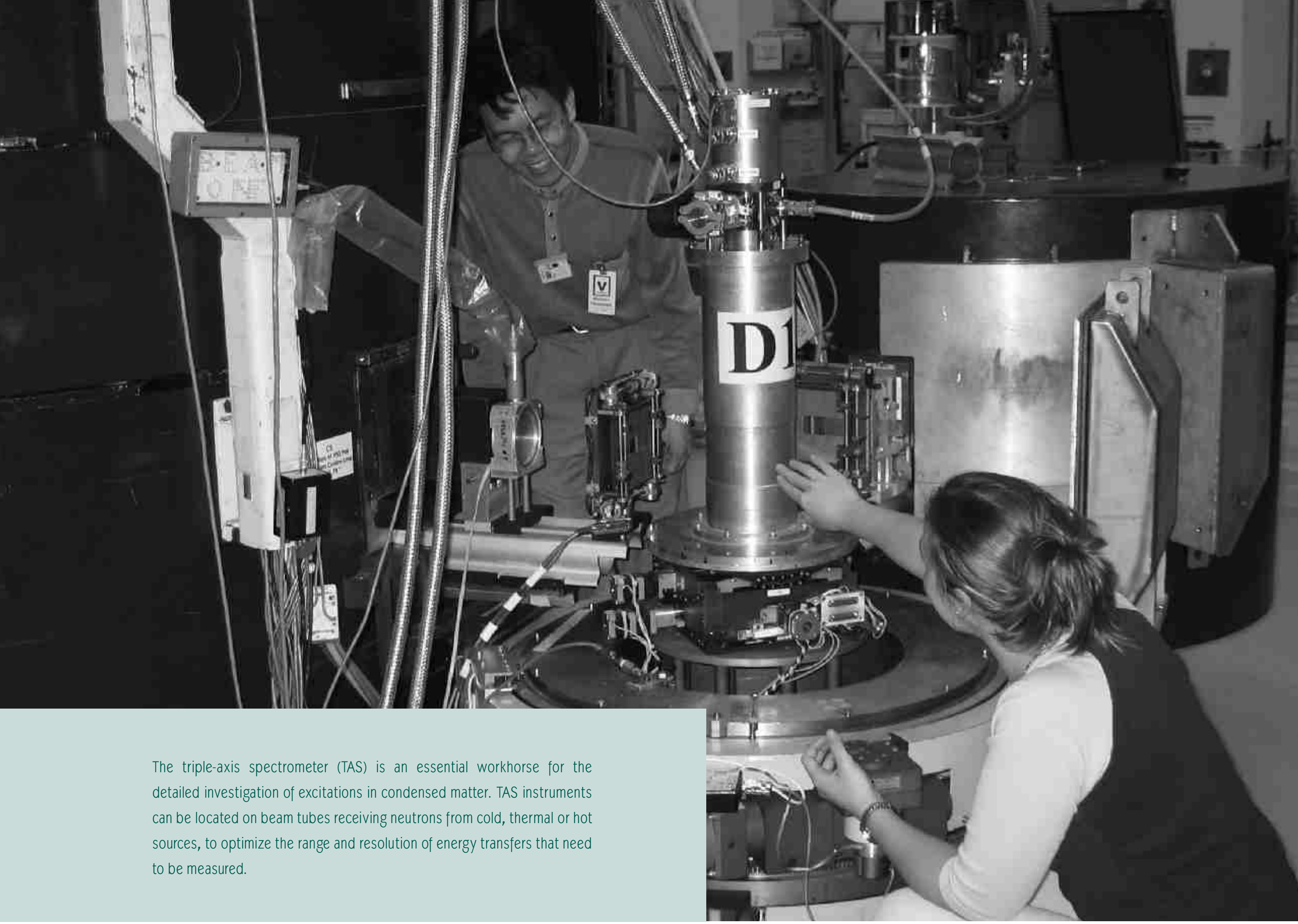
In studying excitations, it is often crucial to be able to separate the magnetic and non-magnetic contributions in a clear and indisputable manner. This is possible if one uses polarized neutrons when performing inelastic experiments. The application of focusing and modern polarization techniques (e.g. ^{3}He neutron spin filters) [3.39] and focusing heusler monochromator and analyzers [3.40] has significantly enhanced the sensitivity of polarized neutron experiments [3.41, 3.42]. In addition, there are new developments in the field of polarized neutrons such as zero-field full vector polarization analysis (Cryopad) [3.43, 3.44], which enables three-dimensional polarization analysis experiments. Such techniques are invaluable in solving the uniqueness problem associated with complicated magnetic structures (e.g. spiral vs. stripe order) and other 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 are made about each instrument in the sub-sections below.

Thermal Source: 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 analyzer) 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 or an area detector in combination with an array of independently controllable analyzer crystals or both, 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 Source: 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, while it does not impose the energy cut-off associated with the wavelength dependence of the critical angle of a 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 of 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 Source: 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 that would be available from a hot neutron source if a TAS was placed [3.45] to view such a source in the CNC reactor.



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.

Disc-chopper Spectrometer

The disc-chopper (time-of-flight) spectrometer (DCS) [3.46, 3.47] 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 quasi-elastic scattering in molecular and related systems (e.g. diffusion in liquids and suspensions, kinetics of hydration reactions, and slow motions of large biological and macromolecular structures). However, the application of existing instruments (e.g. the NIST's DCS) at reactor-based sources has proven to be immensely successful in other fields, such as in exploring magnetic excitations. Condensed matter problems (e.g. 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 [2.27, 2.39]. Locating a disc-chopper spectrometer in the guide hall of CNC will provide world-class high-resolution neutron spectroscopy support to the diverse Canadian scientific community.

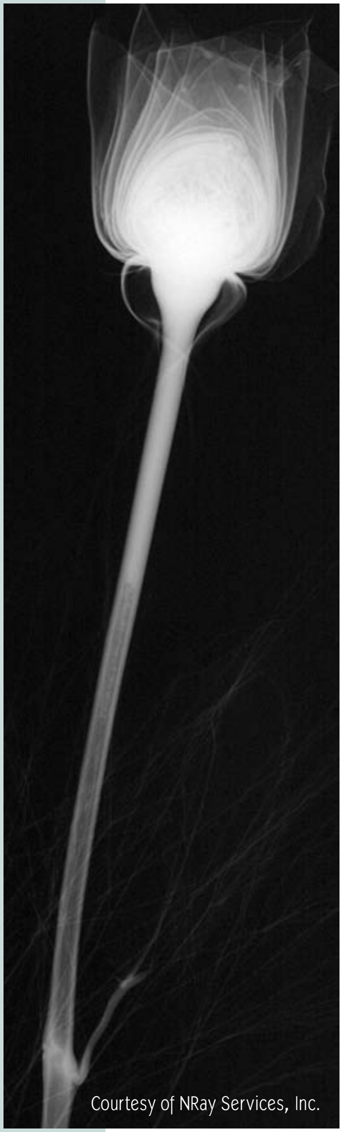
In the TOF technique, a polychromatic neutron beam is used, and the time (and, hence, velocity) for the neutrons to travel from the source of the beam to the detector is measured. In an inelastic process where the neutron gains or loses its energy after interacting with the sample, a velocity change occurs, which in turn results in a different arrival time at the detector. For DCS instruments, a combination of four choppers is used (i.e. 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 of about 3 electron volts (eV) and an incident energy of 0.3−25 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 (i.e. about 1000 high-efficiency ^{3}He proportional counters) covering a large angular range between 10 to 130°, and detecting the scattered neutrons after travelling over a distance of about 4 m. The detector angular range could be improved to provide better solid angle coverage and to employ a truly pixelated detector (i.e. metre-long ^{3}He tubes). This detector coverage would make DCS an expensive instrument. However, such an instrument does serve a relatively large community—one that is larger than the community that requires access to triple-axis spectroscopy.
It is expected that the new instruments in pulsed sources will improve on current TOF chopper capabilities by a factor of about 50 to 100. However, these instruments will be heavily oversubscribed; hence, a facility at which exploratory as well as detailed parametric studies (including 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 (i.e. the study of quasi-elastic phenomena), as well as its well-known applications in molecular tunnelling and rotational motion in biophysical systems.

A backscattering instrument [3.48–3.50] uses perfect single crystals (e.g. perfect Si or Ge with very narrow mosaic spreads) for the 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 micro-electron volts (μeV) energy resolution and transfers of up to 40 μeV neutron energy gain or loss. The elastic momentum transfer can range from a Q of 0.06 to 4.0 Å^{-1}. An array of Si analyzers and detectors gives a relatively broad momentum resolution of 0.02−0.2 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 neu trons 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.



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

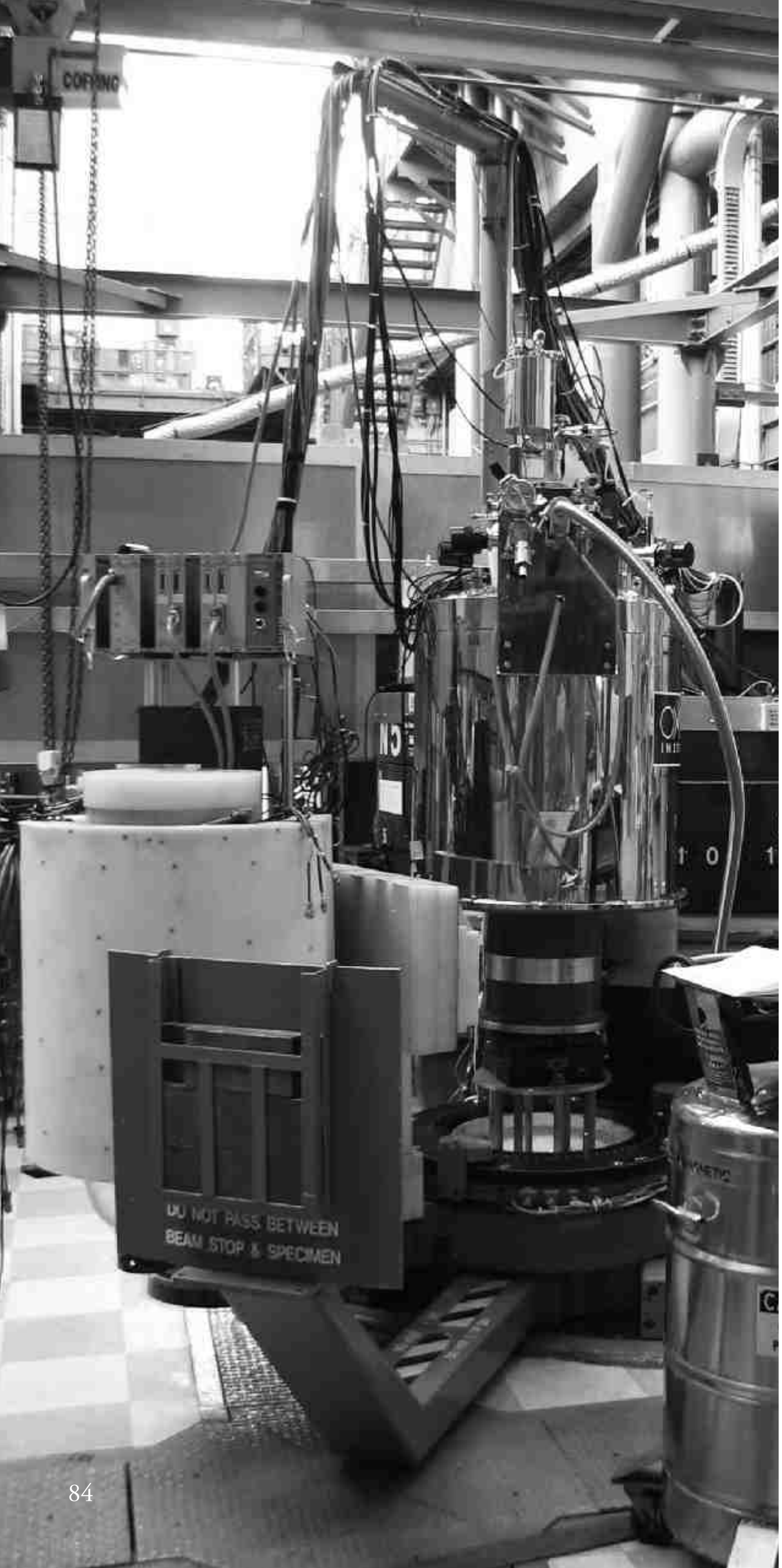
The backscattering design provides much better energy resolution (i.e. by more than a factor of ten) than can be achieved with the disc-chopper design, and the intensity is higher as well. However, the instrument is not as flexible in Q range and energy transfer as the disc-chopper time-of-flight machine.

Spin-echo

A hundred-fold increase in energy resolution is possible with the spin-precession (i.e. neutron spin-echo, or NSE) technique [3.50, 3.51], which exploits the fact that neutrons have a magnetic moment. Very high-energy resolution is achieved without the associated intensity losses from a back-scattering 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 nano-electron volt (neV) resolution. Applications include magnetic phase transitions in disordered systems, the influence of dipolar interactions on magnetic phase transitions, dynamics of the glass transition, the 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

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.



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 [3.50, 3.52–3.55] 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—something 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 magnitude. Consequently, performing inelastic experiments at high-energy transfers with a high resolution is possible using this technique. Interesting results on lifetimes of excitations, as well as on 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.

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 beam line and is likely to be of interest to a private enterprise that provides neutron radiography services to industry.

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 beam line and is likely to be of interest to a private enterprise that provides neutron radiography services to industry.

Applications of neutron imaging—encompassing radiography, computed tomography, and real-time and spectroscopic imaging—have been increasing in scope over recent years, finding use in cultural studies, archeology, plant biology, biomedicine, nuclear forensics, and materials science and engineering. To go beyond the 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—i.e. total neutron counts per pixel, with a spatial resolution better than 0.05 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 both expert 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 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. There should be a capability to image using thermal neutrons and cold neutrons, and to obtain energy-dependent data.

3.9 Atomic-resolution Holography

Traditionally, protein structures have been determined by the x-ray diffraction of crystallized samples, and more recently—in the case of small- to medium-sized proteins in solution—by nuclear magnetic resonance 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). It 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 the ILL in 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 a report of the Beam Facilities Consultative Group that formulated the instrumentation plan in 1998 for the new OPAL reactor at ANSTO in Australia [3.56]. Their matrix is presented in Table 4. The first set of seven neutron scattering instruments (part of the OPAL construction project) was completed in 2007 [3.57]. An additional seven instruments were added during the period 2008–2013. This major expansion of the instrument suite was accompanied [3.57] by a significant investment in infrastructure required to support these instruments (e.g. sample environments, ^{3}He polarizers/analyzers, and the National Deuteration Facility).

The Canadian version of this matrix, shown in 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 the OPAL reactor has been successful in attracting talented, highly qualified people back to Australia.

On the other hand, the Canadian neutron beam laboratory is part of a North American network of five user facilities, one of which is expected to wind down in 2015 [3.58]. Each facility has strengths in certain scientific domains, based on the expertise of staff and the 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 five facilities; they also have access to teams of experts in scientific areas that are not necessarily the focus of efforts at Chalk River Laboratories.

The Chalk River Laboratories facility has historic strengths in materials science, magnetism, and powder diffraction, and has chosen to focus growth in soft materials, thin films and nanostructural phenomena (in response to the interests of Canadian scientists, and anticipating the expanded capabilities of a new Canadian Neutron Centre). The reactor at Chalk River Laboratories is shared 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, low-flux neutron radiography is carried out by a private business, NRay Services Inc., at the McMaster Nuclear Reactor. Neither Canadian facility is exploring possible clinical applications of neutron beams at this time. However, a new Canadian Neutron Centre should be designed with the power and flexibility to enable world-class, high-flux imaging and to explore clinical applications should the interest arise. In Canada, polarized neutrons are assumed to be available as a feature of many instruments, and should not be associated with a unique instrument.

TABLE 4 - Relationship of neutron beam techniques to science and technology domains – Australian view [3.56].

Neutron beam technique \ Scientific domain	Condensed matter physics	Disordered crystalline materials, liquids and glasses	Polymers and Soft matter	Structural chemistry and materials science	Biology and biotechnology	Earth and environment sciences	Engineering science	Neutron optics and 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									●

TABLE 5 - Applicability of neutron beam methods to science and technology domains – Canadian view.

Neutron beam method (May encompass multiple instruments) / Scientific domain	Materials Science	Engineering	Earth science	Structural chemistry	Polymer science	Biophysics	Thin films and surfaces	Magnetism / quantum materials
Triple-axis spectrometers			○	○				●
I(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	○			○	○	●		

Level of demand: high = filled symbol; moderate = open symbol; or low = blank

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

Section 4.1, below, was developed after discussions at the 2006 and 2007 Annual General Meetings of the Canadian Institute for Neutron Scattering. Since then, a number of significant changes and developments have occurred that will have important implications on the kind of neutron source that Canada could be operating beyond the lifetime of the NRU reactor. These include:

- The announcement by the Government of Canada to permanently shut down the NRU reactor in 2018 [1.1];
- The announcement by the Government of Canada to stop the production of the medical isotope molybdenum-99 by means of the NRU reactor in 2016 [4.1];
- The now complete restructuring of AECL into Canadian Nuclear Laboratories [4.2] and the uncertainty about whether the future mandate for the Chalk River Laboratories site will require a research reactor [4.3];
- The proposal by the Province of Saskatchewan, made in 2009, to build a research reactor mainly for neutron scattering [4.4]; and
- Instrument developments at the McMaster Nuclear Reactor (i.e. the MAD, commissioned in 2010 [4.5], and a SANS instrument, with secured funding from CFI and partners, currently in the design stage).

The changing landscape makes it prudent to fully consider and evaluate all possible neutron sources for Canada at this critical time. In order to have a meaningful discussion related to the neutron source options at the CINS's 2014 Annual General Meeting, the CINS Science Council asked Dr. Zin Tun of the Canadian Neutron Beam Centre to prepare a discussion paper where all options for a future neutron source were considered. The discussion paper [4.6] identified the following options:

- A multipurpose research reactor;
- A dedicated research reactor for neutron beams;
- An upgrade of the McMaster research reactor; and
- A spallation neutron source.

At the end of the discussion session, it was unanimously agreed to establish a subcommittee to explore in detail the costs and benefits of the neutron sources that were identified in the discussion paper. The subcommittee, comprised of the Science Council and chaired by Dr. Zin Tun, reported back its findings to the CINS community in 2015 [4.7].

Canada's current neutron source is the NRU reactor at Chalk River Laboratories. Operated by Canadian Nuclear Laboratories (CNL), 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 CNL to test fuels and components for the CANDU reactor.

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 [4.8] at ~15 × 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 ~12 × 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 (i.e. divergence in the range of 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 reduces 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 of 1.2−1.5 Å. The horizontal cold neutron source at the ILL (6 L of liquid deuterium at 25 K) enhances the flux of neutrons with wavelengths longer than 3 Å, to a level of 8 × 10^{14} neutrons/cm^2/s, which is much higher than can be obtained from a thermal spectrum. For neutrons with a wavelength near 10 Å, the intensity gain from a cold neutron source—i.e. a factor of 20 to 30—can truly revolutionize the range of scattering experiments on materials with characteristic structures in the nanometre range (e.g. biological membranes, polymer coatings for medical implants, mesoporous media, layered electronic and optical devices, and nanomagnetic multilayers).

Conversely, a hot source (e.g. graphite at 2300 K that is self-heated by radiation in the reactor core, or an under-moderated fission target) can enhance the flux of neutrons with a wavelength of less than 0.8 Å, which is good for applications in liquid and amorphous materials, as well as 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 also to minimize contamination with fast neutrons or gamma rays from fission in nearby fuel elements.

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 ratios of beam tube cross-sections 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 of 1.25−2.50 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 the evolving requirements of science and technology. For example, in the coming decades, 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 in order to meet the growing demand. Thus, 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 microsieverts (μSv) per hour 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 summarizes the neutron beam user requirements for the neutron source at the CNC.

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 (i.e. inside the reactor hall), or they will enter guides that transport them into a separate building (i.e. the guide hall), where many more neutron beam instruments will be located. Because neutron beam instruments include a lot of radiation shielding, only

TABLE 6 - Summary of neutron beam user requirements for the neutron source at the Canadian Neutron Centre.

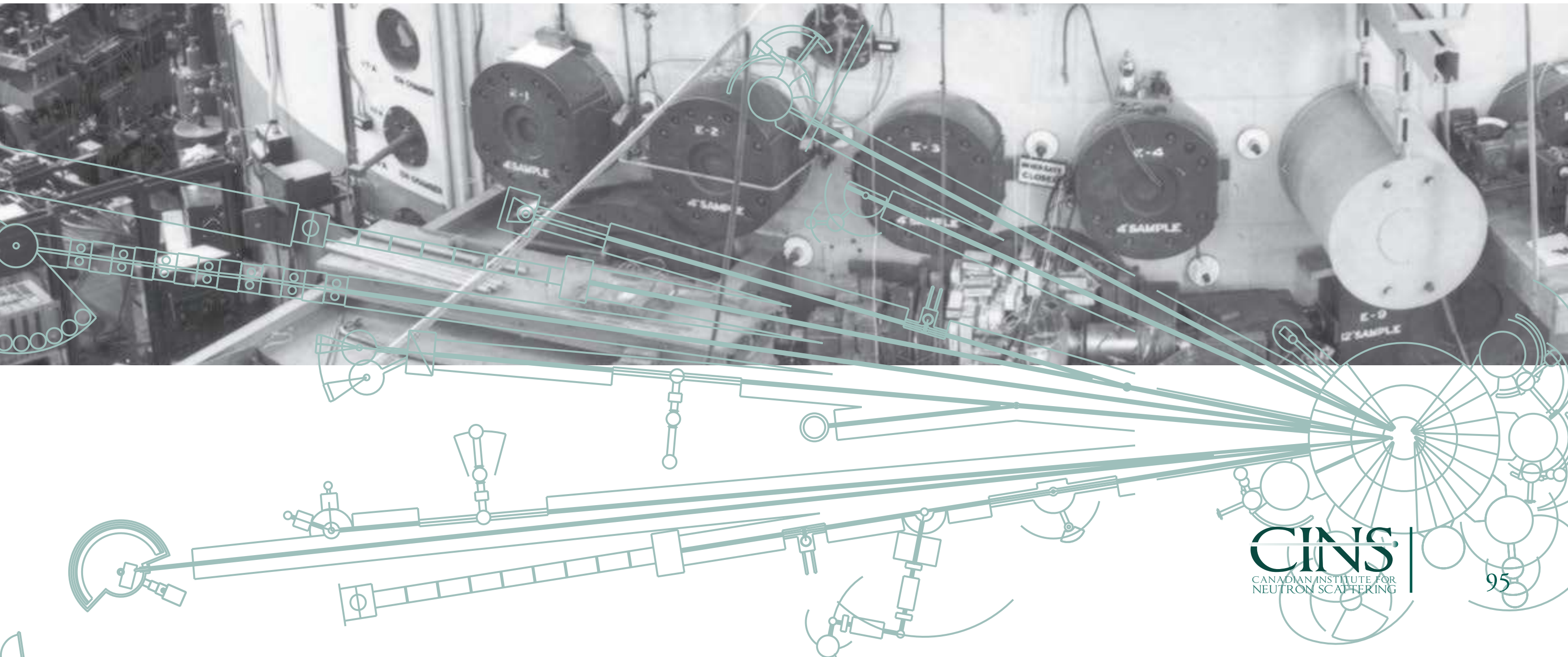
Requirement	Quantitative Limits	Notes
Flux at the nose of all thermal beam tubes	> 10 x 10^{14} n / cm^2 / s	Same flux in moderator surrounding cold / hot sources
Number of thermal beam tubes exiting reactor wall	> 10	Consider multiple elevations, instrument footprints
Thermal guide manifold	1	Serve 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 minimal distance from nose of beam tube to neutron spectrometer No fuel in line of sight	Consider multiple heights above working level and slanted tubes to second working level 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% Maximum flux to beam tubes at all times	Reliable schedule, published months in advance
Engineered radiological zoning	< 10 mSv/h at reactor face < 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

a limited number of instruments can be physically placed around the circumference of the reactor source. In the guide hall, however, the guides can fan out somewhat to provide more space for neutron instruments per source position in the reactor core. Since neutron instruments each cost about 1% of the cost 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 in the reactor hall, immediately adjacent to the neutron source, 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 thus essential that the reactor hall be designed to have the following: adequate load capacity; adequate floor area and headroom to manoeuvre equipment; and 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 the experimental area (and often bringing specimens and specialized ancillary equipment with them). An entrance and exit area should enable several operations to be conducted efficiently, such as:




M55 1 TON
DUALSPEC
NRC·CNRC
CNRC·NRC
In Emergency Contact:

- 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; and
- 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; and
- 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 so 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, with the second having been added partway through the lifecycle 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 one guide hall at the outset, with the possibility of adding a second guide hall sometime in the second decade of operation.

Each guide hall should have interior dimensions of 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 tens 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 in order 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 the lifting of heavy components. Therefore, lifting capabilities of up to 20 tonnes must be available at all points on the floor of the guide hall.

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 just before the scheduled time of the neutron scattering experiments.

These working areas should be integral parts of the CNC complex (e.g. attached to one side of the guide hall) to optimize the synergy of operational and developmental staff, whether scientific, engineering, or technical. Examples of workspaces needed to sustain operation and development of the neutron facility itself are discussed below.

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.

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 the design and testing of new installations, and to act as a hub for the networking of neutron instruments and other services (e.g. desktop computers, 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 the integration of ancillary equipment, in order to keep pace with evolving scientific and technological requirements. Space will be required for the storage of components, design workstations, and assembly and testing benches; there must also be room for exemplars of key mechanical components to be set up for the development or debugging of interfaces.

Detector Workshop

The development, assembly, troubleshooting, and repair of neutron or gamma detectors require a clean environment. Also required are vacuum and gas-filling capabilities, electronics to diagnose signals and operate detectors, storage for radioactive test sources, cryogen handling capability, layout areas, wiring frames, and storage for stock materials and 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

The furnace 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 × 6 m is needed for each system that is either being prepared for installation at a beam line or in a state of commissioning or repair. There will need to be at least three 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 will 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, while also providing 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 the safe handling and testing of large cryomagnets, as well as for closed-cycle refrigeration systems. A well-ventilated working area of approximately 6 m × 6 m is needed for each system that is either being prepared for installation at a beam line or in a state of commissioning or repair. There will need to be at least five 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 for implementing some designs for neutron instruments or ancillary equipment. The shop requires space and power for a suite of standard machine tools and fittings (e.g. turning, milling, grinding, cutting, drilling, and joining stations), as well as work areas for the assembly and storage of stock materials, fasteners, bearings, tools, and so on.

Engineering Testing Workshop

Engineering materials research may involve large, heavy, complicated, and sometimes dangerous specimens. A laboratory will be required for the development of mechanical testing equipment, including space to operate at least one universal testing machine, as well as capability to test pressurized systems and to handle heavy specimens (e.g. 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 × 6 m is needed for each system that is the subject of current work. There will need to be at least two 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 will provide the necessary equipment (e.g. work benches, fume hoods, storage, etc.) for a modern, safe laboratory. Ideally, they should include characterization tools that complement neutron beam analyses in order 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); benchtop 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:

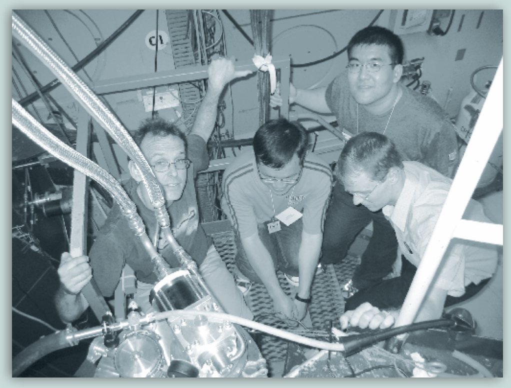
- Heat treatment facilities to simulate the evolution of materials for engineering or earth sciences, including convective air furnaces, controlled gases, vacuums, salt baths, fluidized sand baths, ventilation, fume hoods, glove boxes, and computer control and monitoring;

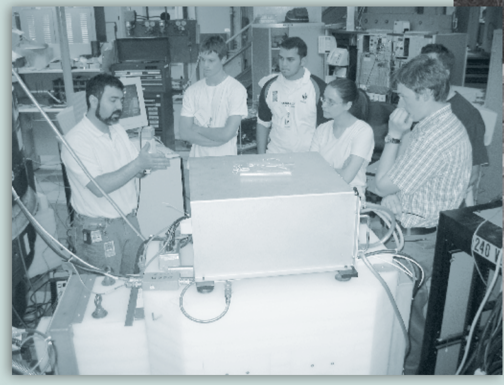
- A chemical preparation lab with a fume hood, a glove box, a sink, chemical storage, access to cryogenic equipment, and balance and grinding equipment; and

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

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.

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 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.





EDUCATION & outreach

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, which should be arranged immediately adjacent to the guide hall, can be on an upper floor. At startup, there will need to be office space for about 30 research staff members and 20 engineering and technical staff members. In due course, it is expected that the neutron beam laboratory will expand to twice this size.

In addition, spaces must be available for visiting researchers, students, and 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. those 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. Thus, facilities must be available for larger groups to meet and discuss results, as well as for education and outreach events. This requires meeting rooms that can accommodate 10 (2), 30 (2), and 100 (1) people, as well as a lecture facility that can 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, as well as work stations for the parallel processing of several individuals through any required procedures (e.g. security clearance, badge issuance, signing of entry agreements, receipt of accommodation instructions, etc.). 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 laboratories, astronomy observatories, or neutron scattering facilities—are often engaged in what is colloquially known as 'suitcase science' (i.e. where users travel from their home institutions to 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 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 accommodation 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, visitors can move freely from accommodation to laboratory for the duration of their stay. For facilities that have no 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 who are new to neutron scattering. For scientists considering neutron scattering for the first time, available accommodation will remove logistical obstacles and will create a welcoming atmosphere for scientists to consider investing their time in accessing the facility.

4.6 Governance and Management

How the 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 management and governance requirements (in addition to the physical and technical requirements discussed above) that the community has for the CNC.

Participating in a Multipurpose Science Facility

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.

Current consideration is being given to a future Canadian neutron facility that will be designed and constructed as a multipurpose science facility. The neutron scattering community supports this concept as one that has brought a useful cost–benefit balance to Canada in the past—and that 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 $100 million to support 42 neutron beam instruments [4.9].

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 (i.e. isotope production, nuclear R&D, and neutron beams for materials research). If the 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 the future CNC. Those goals include:

- Being a unique and powerful scientific resource that is accessible to academics and students across Canada;

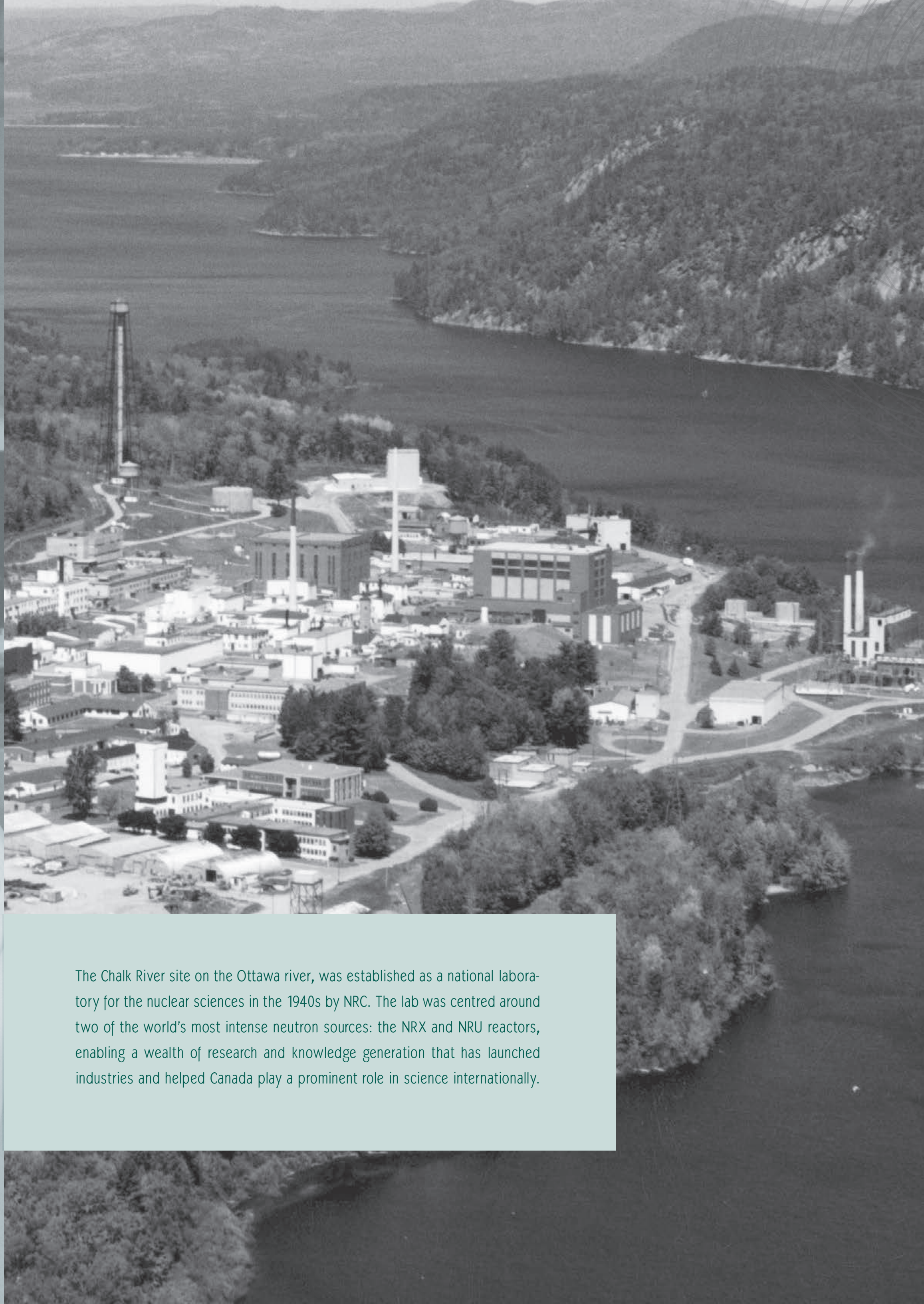
- Playing a role in the international network of neutron beam laboratories, welcoming foreign scientists, and, in exchange, opening up the inter national network to Canadian scientists;
- Applying neutron beams to projects for industrial clients so as to help improve their business; and
- Operating at full power on a predictable and reliable duty cycle.

Those goals can be broadly classed as education (i.e. the development of highly qualified people), innovation (i.e. giving Canadians the tools to develop new materials and technologies), competitiveness (i.e. 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 all 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 could participate in the governing structure as a key stakeholder. Regardless of how it is accomplished, the neutron beam community needs a mechanism to express its priorities and to influence both the operating framework and future capital developments within the neutron source it is sharing with other users.

The neutron beam community will need a mechanism to express its priorities and influence both the operating framework and future capital developments within the neutron source they will share 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 the Canadian Institute for Neutron Scattering (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 (CNC) 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 [1.4]. Since then, there has been an ongoing discussion about how best to choose the instruments that will deliver the greatest value to the Canadian scientific community, as well as 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 current Canadian users of the Chalk River Laboratories facilities—in other words, it is 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 Laboratories.

Other considerations used to establish instrument priorities for the new CNC include:

- The size of the current and potential user communities;
- 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 the education of highly qualified personnel; and
- Identification of a champion to lead an instrument development team.

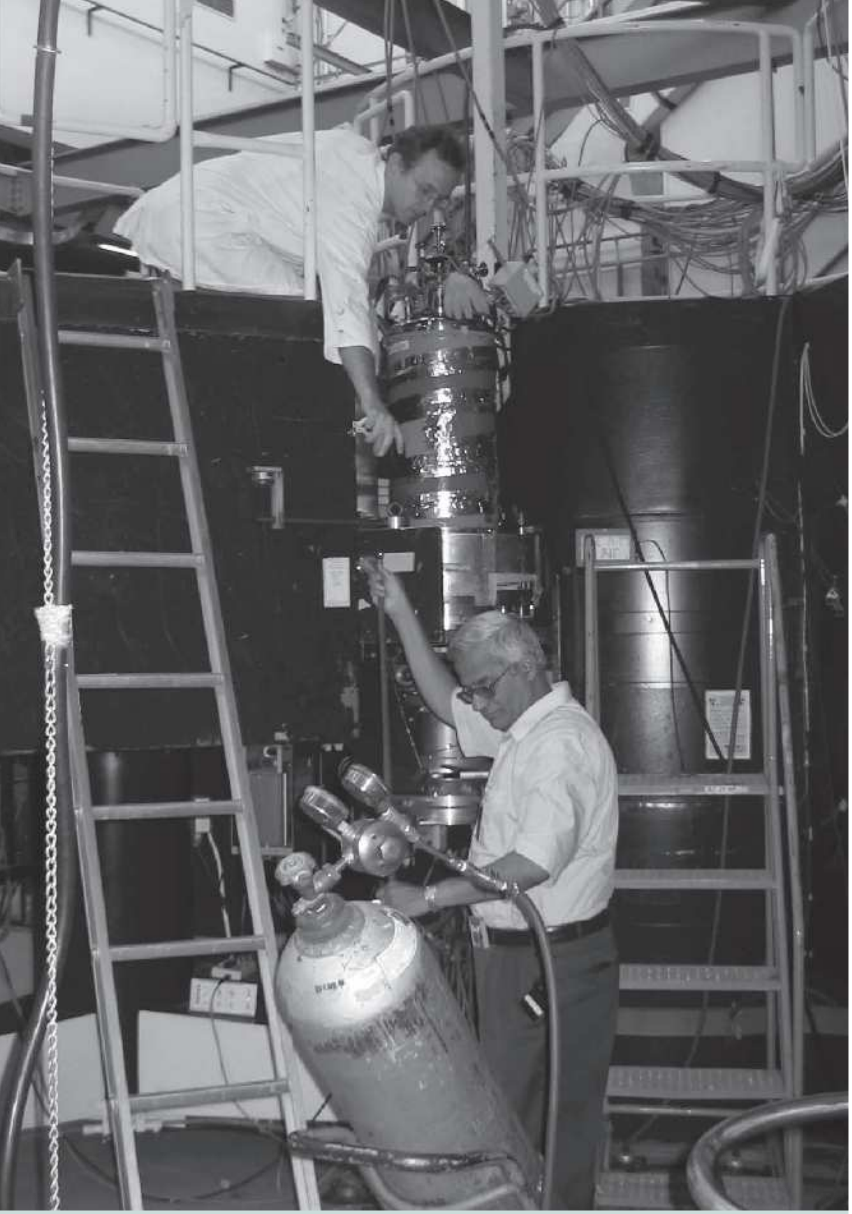
It is clear that the strength and diversity of the Canadian neutron scattering community is sufficient, and that the initial suite of instruments should be chosen to support and enhance existing research programs rather than to develop a general purpose collection. Indeed, as we completed the analysis using the criteria identified here, we found that the

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 spectrometer (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 diffractometer	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
Classical 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 spectrometer (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 spectrometer (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.

high priority instrument group that emerged represented a powerful facility that will be available as the new reactor comes on line; the second round of instruments, which would be developed shortly after initial operations commence, will place us firmly on the map for many years to come.

5.2 Recommendations of CINS AGM / Workshop 2007

At the CINS's Annual General Meeting in 2007, five working groups (WGs) were defined to represent the five subject areas described above, in Sub-sections 2.1–2.5. These are: (1) excitations in condensed matter; (2) crystallographic analyses; (3) materials science and engineering; (4) thin films and surfaces, particularly nanostructures; and (5) soft materials, particularly polymers and biological materials. These working groups then identified instrument priorities, based on their research needs, for the neutron beam instruments listed in Table 3 and described in Section 3, above. The top three instruments identified by each group were collected first, and the second three instruments identified by each group 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 (see Table 5) with the priorities established by the working groups (see Table 7), then we can divide the possible instruments into three broad priority categories: 'high', 'medium', and 'low' (see Table 8).

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 in-

TABLE 8 - Canadian user recommendations for 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)	Labels indicate the 'temperature' of the neutron source required for each instrument (T = Thermal, H = Hot, C = Cold).	
T – Single-crystal / texture / development diffractometer		

cludes two thermal powder diffractometers (one optimized for efficiency and the other for resolution), a thermal triple-axis machine with polarization capability, and a white beam stress scanner. These four instruments, combined with the vertical sample reflectometer, will replace the existing suite (currently located at the NRU reactor) with state-of-the-art machines that will immediately serve as a critical resource for the research programs of Canadian users.

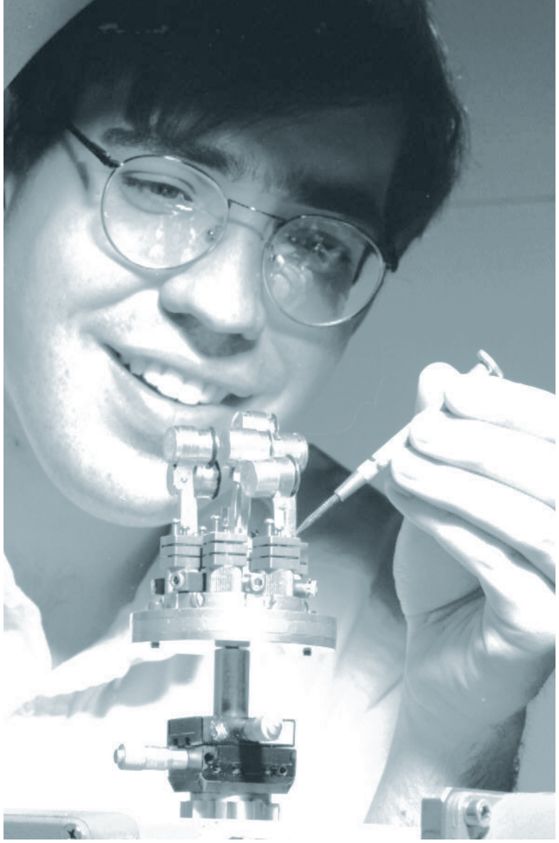
The current facility at NRU only provides beams of thermal neutrons, which greatly restricts the areas of research that can be supported. There was a clear recognition, among all working groups, that a cold source to feed low-energy neutrons to the suite of instruments was a high priority. This is reflected in the second group of instruments in the 'high' priority suite. Here we find two reflectometers—the first a versatile system covering a wide Q range with a vertical sample geometry, the second instrument dedicated to liquid-to-gas and liquid-to-liquid interfaces with a horizontal sample plane. The classical 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 oversubscribed 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 multipurpose instrument will be used to evaluate and align single crystal samples. It will support instrument design projects that will arise as the 'medium' priority suite is being developed, and will also 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 minimizing 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 was being commissioned (i.e. 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 makeup and the research interests of the Canadian user community will change. However, some trends are clear, so an outline of the future can be sketched.

SANS instruments are consistently oversubscribed, 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 of instruments. 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 of 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 so-called 'low' priority group, we find the highly specialized instruments such as the backscattering and spin-echo machines. Although these machines serve a relatively narrow community, they yield data that cannot be obtained by other means. These instruments are critically important to those who depend on them, but they need a significant commitment to champion and build. Similarly, while a hot source can provide very short wavelength neutrons that can



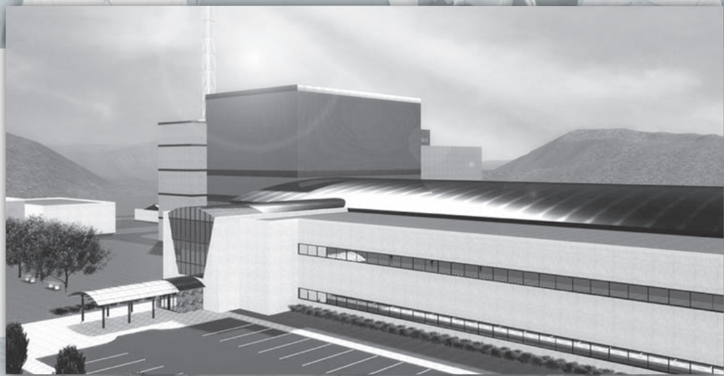
be used to access diffraction data at high momentum or energy transfers, it is unclear whether such work is better done at a pulsed spallation source. However, several reactor-based hot sources are in operation with successful instruments. The proposed hot source and associated instruments might constitute unique elements of the Canadian contribution to the global network of neutron scattering facilities, enabling structural studies of amorphous materials (e.g. liquids and glasses), and also high-energy excitations in unconventional crystalline solids.

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 workhorse instruments along with some more adventurous concepts, such as the next-generation white beam stress scanner. It also includes a (Q, ω) surveying instrument, following the successful experience of the DCS at the NIST. We 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 that Canada will not only reinforce its world-class capacity for excellence in materials research, but also deliver impacts across the scientific spectrum, from discovery to innovation.

The next 50 YEARS wide open with *Opportunity*



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CINS Contributors to This Plan

At the 2006 Annual General Meeting of the CINS (held October 13–15, 2006 at the University of Western Ontario), a workshop was included to spark a discussion about the long-range planning for neutron beam research requirements to a time horizon of 2050. A subcommittee was appointed to lead the first draft of the Plan. At the 2007 Annual General Meeting (held October 26–27, 2007 at Queen's University), a 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 content provided by the perspective working groups. The Plan was published in 2008 [http://www.cins.ca/docs/CINSweb_2008.pdf].

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2015 update to this plan

In the summer of 2014, Prof. Dominic Ryan, CINS President at the time, asked the CINS Science Council [http://www.cins.ca/people.html#sci] to lead the task of updating the Plan to not only include new and exciting scientific developments and future research directions, but also to reflect and plan for the changing environment. The updated draft, including a discussion paper on neutron source options, was sent to CINS members and posted on the CINS website prior to the 2014 AGM (held November 14–15, 2014 at the University of Toronto). At the AGM, the updated scientific programs portion and the Neutron Beam Instruments and Methods section of the updated draft were endorsed. In addition, it was unanimously agreed to establish a subcommittee to explore in detail the costs and benefits of the possible neutron sources, and to report back their findings to the community in 2015 (see Section 4).

The contributors to the updated draft are:

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Acronyms

AECL – Atomic Energy Canada Limited
AGM – Annual General Meeting
AND/R – Advanced neutron diffractometer/reflectometer
ANDI – Applied Neutron Diffraction for Industry
ANSTO – Australian Nuclear Science and Technology Organization
BS – Backscattering
CBRNE – Chemical, Biological, Radiological, Nuclear, and Explosive
CFI – Canada Foundation for Innovation
CINS – Canadian Institute for Neutron Scattering
CMR – Colossal magnetoresistance
CNBC – Canadian Neutron Beam Centre
CNC – Canadian Neutron Centre (new neutron facility)
CNL – Canadian Nuclear Laboratories
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
KDP – Potassium dihydrogen phosphate
LLB – Laboratoire Leon Brillouin
MDSN – MDS Nordion, a medical company
MRI – Magnetic resonance imaging
MSE – Materials Science and Engineering
NCNR – NIST Center for Neutron Research
ND – Neutron diffraction
NIST – National Institute for Standards and Technology, USA
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
QENS – Quasi-elastic neutron scattering
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

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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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