



National Research Council Canada Canadian Neutron Beam Centre 2009-2010 Biennial Report to the Canadian Institute for Neutron Scattering

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The National Research Universal (NRU) reactor is the neutron source for the Canadian Neutron Beam Centre. The NRU reactor was shut down for maintenance from May 14, 2009 until August 17, 2010.



### Experimental Reports / Online

The experimental reports from the CNBC's community of international users are presented in the language in which they were written.

These reports are available on the web site of the Canadian Institute for Neutron Scattering:

http://www.cins.ca/expreports.html

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CNBC is Canada's contribution to a global network of about twenty neutron beam laboratories that leverages international collaborations and facilitates exchange of people and knowledge.

# THE NRC CANADIAN NEUTRON BEAM CENTRE (CNBC)

### Large-scale scientific infrastructure

The National Research Council Canadian Neutron
 Beam Centre (NRC-CNBC) enables researchers to
 use neutron beams as tools for world-class materials
 research, which provides new understandings of
 materials and improves products for businesses.

Each year, over 200 scientists, engineers and students from universities, government labs and industry participate in research that depends on access to the CNBC's six neutron beamlines. Over a typical five-year period, CNBC research participants include more than 700 individuals from over 60 departments at about 30 Canadian universities, and from over 100 foreign institutions in over 20 countries. The CNBC enables industrial research in sectors such as nuclear energy, aerospace, automotive, oil and gas, defence and primary metal production. The CNBC typically provides more than 85% of its neutron beam time to the user community.

NRC helps clients effectively exploit large-scale scientific infrastructure. As a part of this NRC business line, the CNBC leads and enables Canada's neutron beam competency by developing innovative neutron beam instruments and methods, performing in-house research, training students and ensuring access to the CNBC's facilities by a wide range of users and clients. The CNBC is Canada's contribution to the global network of about twenty neutron beam laboratories that leverages international collaborations and facilitates the exchange of people and knowledge. In addition to enabling research, each element of Canada's large-scale science infrastructure, including the CNBC, is a stimulating platform for science outreach to foster a national culture of innovation.

### **OUR USER COMMUNITY**

Researchers from these Canadian universities or from these countries illustrate the breadth of the CNBC's user community.



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# HOW A NEUTRON BEAM FACILITY WORKS

### Overview of an Experiment

Researchers come from all over Canada and the world to probe materials with neutron beams to find solutions to challenges in health, industry, and science. From the initial inquires into the feasibility of an experiment to the final interpretation of results, CNBC scientists and technical staff provide support to our users to ensure that this national resource is accessible to any user.

As neutrons pass through a material, the material changes the properties of the beam, such as the direction, energy, or magnetic polarization. By detecting these changes, researchers can deduce certain properties of the material such as atomic structure or stress.

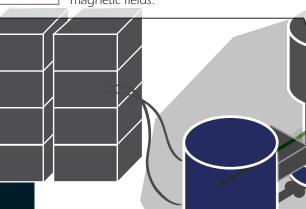


#### **User Arrival**

A researcher travels to the CNBC, typically after preparing a sample of a material for study. In some cases, samples may be prepared on site.



A sample material is placed in the emerging beam. As the neutrons pass through, the material changes the properties of the beam, such as the direction, energy, and magnetic polarization. Typically, the beam is scattered in many directions. A chamber around the material controls conditions such as temperature, pressure, or magnetic fields.



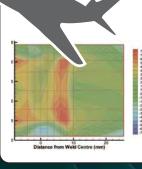
#### **Data Analysis**

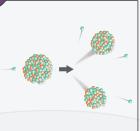
Data analysis typically continues after a user travels back to their home institution. CNBC scientists follow up with the users to assist with the analysis and interpretation of results.



### User Interface and Electronics

A specialized electronic system controls each portion of the beam line and collects the experimental data. Workstations provide the user interface to control the experiment and perform preliminary data analysis.



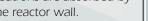


#### **Neutron Production**

Neutrons are tiny particles that reside in atoms. When uranium atoms are split in the reactor core, neutrons are released in every direction with a large spectrum of energies.

#### **Beam Production**

Several tubes through the reactor wall allow some neutrons to exit in the shape of a beam. Excess neutrons are absorbed by the reactor wall.





#### **Beam Preparation**

A crystalline material diffracts the beam, that is, it divides the beam according to the energies of the neutrons. A channel is positioned to allow only neutrons of a certain desired energy to proceed to the sample material. The remaining neutrons are absorbed in the wall of the large cylinder encasing the crystal.



#### **Neutron Detection**

A mobile detector system determines the intensity of the scattered beam in various directions.

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## THE NRU REACTOR RETURNS TO SERVICE

#### **DIRECTOR'S MESSAGE**

"A medical disaster", "Closed reactor spurs rush to avoid isotope shortages", "Isotope lapses unacceptable", "End of the road for world's oldest reactor?"

These were some of the headlines in the days after the National Research Universal (NRU) reactor at Chalk River, Canada was shut down to repair a leak on May 14, 2009—halting research, as well as medical isotope production. Because medical isotopes are radioactive elements with short half-lives, they cannot be stockpiled for future use. Since the NRU reactor produces 30-40% of the world's supply of the most common medical isotope (i.e., molybdenum-99), a global shortage resulted from its shutdown.

When the full scope of the necessary repairs was determined, some predicted it would spell the end for the world's oldest major research reactor. However, AECL Nuclear Laboratories rose to the challenge of effecting a first-of-a-kind repair using remote welding and imaging tools, to safely repair the reactor vessel from inside the core. After 15 months, AECL Nuclear Laboratories returned the reactor to high-power operation on August 17, 2010.

Canada's neutron-scattering community was hard hit while the NRU reactor was shut down, because this reactor is Canada's primary domestic source for neutron beams. It is the essential hub for the CNBC, which fosters our national competency in neutron scattering by facilitating access to neutron beams by students and researchers from universities, industries

John Root, Director NRC Canadian

**Neutron Beam Centre** 

Our overarching issue and concern remains the long-term prospect for Canada's source of neutrons.

and government labs from across Canada and abroad. The CNBC's beamlines are like spokes of a wheel surrounding the reactor. The diagram, "How a Neutron Beam Facility Works" on page 6, illustrates an example beamline.

To mitigate the shutdown's impact on Canadian science, and in particular, university research programs, the CNBC cooperated with other international neutron beam facilities. Twenty experiments were displaced because they were either in progress or scheduled when the reactor went down. The CNBC worked on behalf of scientists whose beam time was displaced, to acquire alternate beam time. The CNBC asked for 112 beam days; several facilities in the USA, Germany and Australia responded to our need and were able to cover 35% of the beam time requested. Their generous accommodation of our urgent situation was much appreciated. Of course, this response could not be sustained because neutron facilities worldwide are heavily oversubscribed.

The Natural Sciences and Engineering Council (NSERC) also helped to mitigate the impact of the shutdown by allowing a limited reallocation of funds to subsidise travel by Canadian university users and our scientists to the foreign laboratories. The availability of travel support was advertised through the CINS mailing list and on the CINS website.

Interestingly, only eight Canadian individuals took advantage of the available incentives to use foreign facilities during the shutdown period, far less than the 80 to 100 individuals who travel to Chalk River in a typical year to participate in neutron scattering

experiments. The "unplanned experiment" of a prolonged outage of the NRU reactor may lead one to conclude that a domestic hub of neutron facilities and expertise is essential to sustain and foster a strong neutron-scattering community.

The CNBC team took advantage of the opportunity presented by the prolonged shutdown to accelerate needed maintenance and upgrades, especially those that would be very challenging to undertake while the reactor is operating.

Upon restart, our neutron beam user program returned to full capacity within a month. I would like to thank our staff and users for maintaining communication and engagement throughout this period of uncertainty, ensuring that recovery of activity was very prompt. Applications for beam time are welcome at any time. Proposal forms are located at www.cins.ca.

The Canadian Nuclear Safety Commission recently announced a call for public input to a proposal to operate the NRU reactor to 2021. This timeframe could allow some overlap of operation until a replacement facility has been built and operated for an initial period. In the meantime, the CNBC will rejuvenate and expand its competencies in neutron scattering research, by building new neutron beam facilities, developing applications of neutron scattering to new areas of science and technology, and providing support for Canada's lively and growing neutron-scattering community.

John Root, Director NRC Canadian Neutron Beam Centre

Niki Schrie, the CNBC's Operations Manager, coordinates the user program, which welcomes students and scientists from across Canada and around the world every year.

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Post-doc Peter Kalisvaard resumes experiments with the D3 Neutron Reflectometer after the NRU restart, to learn about hydrogen storage in nano-structured Mg-alloy materials (with Professor David Mitlin, University of Albertal

## **2009-2010 STATISTICS**

The CNBC's capacity over the two years of 2009 and 2010 was 1212 beam days. This beam time was divided among 78 experiments and the six available beamlines.

During 91% of this time, the CNBC neutron beam instruments were occupied by the projects of users who came from Canadian universities, foreign institutions, government laboratories or industry. The remaining 9% of beam time was occupied by CNBC-driven projects to develop innovative neutron scattering methods, novel applications to new areas of science or to contribute to research at the cutting edge of condensed matter science.

Despite the 15-month shutdown, the CNBC retained strong engagement with the user community. There were 235 CNBC research participants in 2009 and 229 in 2010. These individuals were from 45 university departments spread among 24 universities in six Canadian provinces (Alberta, British Columbia, Manitoba, Nova Scotia, Ontario and Quebec).

The user community remained highly leveraged with foreign collaborations, with 102 research participants from foreign institutions in 2009 and 110 in 2010. In these two years, there was a total of 187 individual research participants from 85 foreign institutions in 21 countries (Armenia, Australia, Austria, Belarus, Belgium, Brazil, China, Croatia, France, Germany, Italy, Jamaica, Japan, the Netherlands, Poland, Russia, Slovakia, Sweden, Switzerland, the United Kingdom and the United States).

Drew Marquardt, a Brock University graduate student, learns to use neutron beams at NRC-CNBC following the restart of the NRU Reactor, to observe the behaviour of Vitamin E.



### CNBC User Statistics

Community Function	Indicator	2008	2009 <sup>1</sup>	2010¹
Access	Number of users. <sup>2</sup>	161	96	87
Canadian Access	Users from Canadian institutions.	75%	72%	76%
Participation	Research participants. 3	258	235	229
Leverage of International Collaboration	Research participants from foreign institutions.	39%	43%	48%
Canadian Academic Participation	Canadian universities represented by research participants.	18	19	18
Academic Participation Across Disciplines	Canadian university departments represented by research participants.	37	32	32
Education of Highly Qualified People	Students and post-docs who visited the CNBC to conduct research	44	22	20

### CNBC Facility Statistics

Statistic	Definition	2008	2009 <sup>1</sup>	2010¹
Capacity	Available beam time (beam -days).	1830	606	606
External Usage	Beam time occupied by external users.	88%	90%	92%
International Exchange	Beam time occupied by solely foreign users.	17%	32%	17%
Average Experiment Duration	Beam time (beam - days) per allocation.	15.5	13.7	17.3

<sup>&</sup>lt;sup>1</sup>The NRU reactor was shut down from May 14, 2009 to August 17, 2010.

<sup>&</sup>lt;sup>2</sup> A user during a given year is defined as an individual who either visited the CNBC during the year to conduct an experiment, or is a co-proposer of an experiment that ran during the year.

<sup>&</sup>lt;sup>3</sup> Å research participant during a given year is an individual who was a user during the year, or is a co-author of a paper resulting from work carried out at the CNBC that was published during the year.

### Resources for the Canadian Neutron Beam Centre

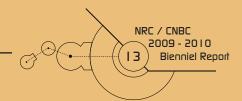
#### In-Kind Contribution

Source	Value <sup>1</sup>	Mission	Description
Atomic Energy of Canada Limited (AECL)	\$7 M	Major R&D Infrastructure	This in-kind contribution is an attributed cost of providing neutrons to the CNBC through AECL's operation of the NRU reactor.

### Direct Operating Funds

Source	Fraction	Mission	Description	
National Research Council (NRC)	60%	Major R&D Infrastructure	The CNBC is a major, national resource for strategic R&D by academia, industry and government labs.	
		Global Reach	The CNBC leverages Canadian participation in the global network of neutron beam facilities.	
Natural Sciences and Engineering Research Council (NSERC)	30%	University Research	The CNBC is unique in Canada as a major resource for R&D by more than 50 university departments across Canada.	
		Training Highly Qualified People	The CNBC helps train about 40 graduate students and post-docs annually by providing 'hands-on' access to neutron beams for their research programs.	
Industry	10% ± 5%	Direct Socio-economic Impact	The CNBC carries out proprietary research projects to add value to Canadian industry by providing knowledge needed to improve products, determine fitness-for-service, meet regulations, or enhance public safety. The CNBC charges fees for service on a full cost-recovery basis.	
Other Partners	3%	R&D Partnerships	The CNBC leverages targeted research networks and collaborations.	
Totals				
\$4 M	Direct Operating Funds.			
\$11 M	Direct operating funds plus attributed cost of neutrons.			

<sup>&</sup>lt;sup>1</sup>All figures are estimates based on a typical year.



### FEATURED ARTICLE

### Neutrons Reveal Unseen Secrets

December 9, 2009 Chalk River, Ontario

Scientists at the NRC Canadian Neutron Beam Centre (CNBC) in Chalk River have handled metal ranging from pieces of the ill-fated Challenger and Colombia Space Shuttles to train rails implicated in ecological disasters in Alberta. In these cases and others, their goal was to find out what went wrong.

But knowing what goes on inside metals even before such failures occur can help the designers and engineers that use them. This is why Dr. Ron Rogge and his colleagues are helping Defence Research and Development Canada (DRDC) Atlantic—one of seven DRDC establishments operated by the Department of National Defence—make Canadian submarines safer.

Dr. Rogge says X-rays are a well-known way to measure surface stress in metals non-destructively. But X-ray devices that can be made portable see less than a millimetre into steel.

By contrast, a technique called neutron diffraction residual stress measurement can see far deeper into metals, to map their internal stresses at the atomic level. Since surface and internal stresses may differ greatly, this technique can give a more complete picture of the strains created as submarines are welded together.

"The challenge is that neutron scattering requires a huge neutron source, such as at Chalk River," Dr. Rogge says. "It's not a portable technique, so the equipment cannot be taken to submarines, which are thousands of miles away at coastal naval bases.

However, the testing of relatively small pieces of metal, typically between 2 cm and 70 cm square, can reveal a great deal."

When shipbuilders weld curved metal plates together to form boat hulls, this leaves residual tensions internally because the liquefied metal in a weld cools at a different rate than the solid parts it joins. In this way, internal tensions pre-load a hull with stresses that reduce the amount of external stress the hull can take before failing.

"Wherever you have a weld, there will be stresses, unless there was a subsequent stress-relieving treatment," says Dr. Rogge. "There is only one non-destructive technique for looking at stresses deep inside material, and that is with neutrons."

Submarine captains who may need to sail and dive their boats close to their limits require a clear picture of the basic strengths and potential weak points that can be found even in newlybuilt vessels. To help obtain a clear picture, DRDC Atlantic has often asked Dr. Rogge's team to help it assess the as-built condition of and different kinds of repairs made to Canadian submarines.

Over time, corrosion thins and weakens the hightensile–strength, steel, hull plates of submarines. To keep boats working at their original rated depths, shipyards use a technique called weave welding to overlay new material and increase a submarine hull's thickness. Since any welding adds new strains to a hull, the team's research seeks to find what techniques work best. This project remains

### NEUTRONS AT WORK FOR INDUSTRY

Neutrons have some unique properties that make them an ideal probe for industrial research:

- They penetrate deeply into dense materials such as metals and alloys.
- They interact with nuclei of atoms, enabling the precise measurement of stresses in materials and components.
- They can probe material samples that are held under realistic conditions of pressure, temperature and stress.
- They are non-destructive; they do not damage the specimen under examination.

underway, and no results have been published yet. But it was, in fact, a particular submarine refit that led to one of Dr. Rogge's more unusual naval jobs.

In 2000, Canada took delivery of the first of four British Navy Upholder-class submarines and renamed them the Victoria class. During a recent half-life refit of the former HMS Unseen, renamed HMCS Victoria, naval technicians removed small sections of plate and welded in new pieces as part of a platform upgrade. Since the replacement occurred at an unusual place in the boat's structure, at a point crossed by one of the submarine's critical main circumferential welds, DRDC Atlantic scientists took the old piece to the CNBC for analysis. This was a rare chance to test a part of the original submarine in ways that could not be done on the full hull, even in dry dock.

"The old piece happened to have some interesting metallurgical details," says Rod McGregor, the engineer at DRDC in Victoria. "One of them was that circ-seam weld, for which NRC-CNBC is perfectly suited to give us a full, through-thickness characterization."

"There is an ongoing effort to re-evaluate the ultimate submarine operational limits using the latest computational methods, which requires explicit understanding of the physical character of the pressure hull," adds McGregor. "This was an exclusive opportunity to assess the strength and stresses of both the hull metal and the original manufacturer's weld, to help validate the models we're using to predict fatigue life and operational limits."



DRDC Engineer Rod McGregor checks an HMCS Victoria hull plate sample at CNBC in Chalk River.

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### **NEW MINERAL**

### In Honour of Lachlan Cranswick

(1968-2010)

Lachlan Cranswick (1968-2010) who worked at the NRC CNBC located at Chalk River Laboratories is being honoured posthumously for his scientific work in crystallography.

As a crystallographer and mineralogist, Lachlan specialised in applying neutron beams to the studies of materials science, structural chemistry, magnetism and geology. He assisted many scientists and students from universities across Canada and abroad to apply these scientific tools to advance their research programs. Lachlan Cranswick was passionate about ensuring access to the highest quality facilities for those scientists.

Mr. Cranswick's accomplishments have been honoured in the naming of a new mineral, "cranswickite".

Small deposits of cranswickite were found near Calingasta, Argentina while testing an instrument that is scheduled to be aboard the next NASA mission to Mars. Professor R.C. Peterson of Queen's University analysed samples and determined cranswickite to have the chemical composition MgSO4 · 4H2O with a new atomic structure previously unobserved in nature.

Mr. Cranswick disappeared from
his home in January 2010 and an
extensive search failed to find any trace of
him. His body was discovered months later in the
Ottawa River. After hearing of his disappearance,
Dr. Peterson applied to the International
Mineralogical Association to have the new mineral
named "cranswickite". The association approved
the name and published a short description in
Mineralogical Magazine in August. Dr. Peterson
has submitted the full scientific description of

cranswickite for publication in the journal, American Mineralogist.

Mr. Cranswick began his career at the Australian Commonwealth Scientific and Industrial Research Organisation, where he became an expert in X-ray diffraction measurements and data analysis in the early 1990s.

Although he did not have a Ph.D., he was granted a postdoctoral research associate position at the Daresbury synchrotron in the UK in 1997 because of this expertise in both diffraction and computing methods. There he developed what had been a national collaborative computer project for small molecule and powder diffraction, known as CCP14, into a project that became internationally renowned.

In 2003, he joined the CNBC, where he excelled in providing access to neutron beams for other scientists and in improving the methods for neutron diffraction to better serve these clients.

Early on, Lachlan embodied the spirit of openness and sharing of information. He gave freely of his time and knowledge to help the science of others through spreading information. At his own expense, he began sending out CDs of freely available crystallographic software (NEXUS) to institutions in developing countries that were without web connectivity, a practice he continued throughout his career. He was active in promoting scientific

knowledge and cooperation through writing

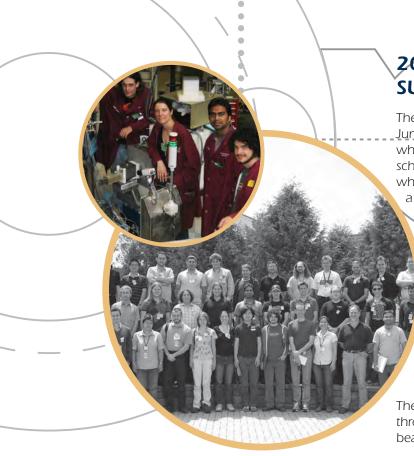
book chapters on powder diffraction,
editing newsletters, organising powder
diffraction workshops and helping
to organize conferences for the
International Union of Crystallography
(IUCr) and the American
Crystallographic Association. He was
a member of the Canadian National
Committee for Crystallography and
chaired the IUCr's Commission on
Crystallographic Computing.

Although only 41 when he disappeared, he co-authored at least 53 papers, including a heavily cited work on a superconducting material and one that reports "doing the impossible"—neutron diffraction on

impossible"—neutron diffractio

gadolinium compounds.

Deposits of cranswickite in Argentina. Photo courtesy of Dr. Ron Peterson.



### 2009 NEUTRON SCATTERING SUMMER SCHOOL

The 10th Neutron Scattering Summer School was held in June 2009 despite the extended outage of the reactor, which began almost exactly a month before the start of the school. The registered participants were polled concerning whether they wished to continue anyway. There was a strong positive response and CNBC welcomed 30 attendees.

The summer school was officially run by the Canadian Institute for Neutron Scattering, the body representing Canadian neutron-scattering users, and was held at Chalk River, with many CNBC scientists participating in teaching. Prominent neutron scatterers from Canadian universities also gave presentations: Bruce Gaulin (McMaster), Mario Bieringer (Manitoba), Maikel Rheinstädter (McMaster), Dominic Ryan (McGill), and Rick Holt (Queen's).

The school offered a balance of theory and experiment through lectures, hands-on activities at the neutron beamlines, and data analysis.

### MCMASTER ALIGNMENT DIFFRACTOMETER (MAD)

There is now a neutron spectrometer at the McMaster Nuclear Reactor located at McMaster University. The spectrometer is a teaching aid for graduate students to learn the basics of neutron diffraction and has a high enough neutron flux to align single crystals—the only such instrument at a Canadian university. Being able to align crystals locally will prepare users to make more efficient use of beam time allotted for experiments at higher flux facilities such as at the CNBC or foreign facilities.

The realisation of the McMaster Alignment Diffractometer (MAD) is the result of a partnership between the CNBC and McMaster that was funded through the Canadian Foundation for Innovation. A total of \$400K was allocated for this project; participants joked that it was called MAD because they had to be out of their minds to try to build an instrument on such a shoestring budget!

McMaster Alignment
Diffractometer, as installed
at the McMaster Nuclear
Reactor in May 2009.

Yet the project succeeded by drawing on CNBC resources and expertise for materials, equipment and project management, which included coordination of design, manufacturing,

assembly, testing and installation. Some of this work was outsourced to AECL or to other NRC facilities including NRC Design and Fabrication Services. The CNBC also donated the control system from its N5 spectrometer. The N5 control system was not needed because the NRU reactor was shutdown and because CNBC was building a new control system to operate N5 after the NRU reactor returned to service.

This project was completed with the installation of the control system, and a successful calibration scan on aluminium powder was performed on April 15, 2010.

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### **EXPERIMENTS**

### Toward a hydrogen economy: Investigating hydrogen storage properties of thin MgAl films

A future economy that uses hydrogen as an energy currency rather than oil and gas will depend on materials with the ability to absorb, store and release hydrogen efficiently. Magnesium and its alloys are amongst the most promising candidates for solid-state hydrogen storage applications, owing to their high hydrogen capacity of 7.6 wt.% and their low cost. However, an operating temperature of about 300 °C that is currently required for these materials is too high for vehicles, and ways of reducing the temperature are being investigated.

Ongoing research at the CNBC in collaboration with David Mitlin (University of Alberta and the NRC National Institute for Nanotechnology) investigates the effect of catalysts on lowering the operating temperature in thin films. Neutron reflectivity (NR) has proven to be a powerful tool for profiling the hydrogen or deuterium content, with nanometre resolution, in the distinct layers that constitute thin films. It has recently been shown using the NR technique employed at the CNBC that the use of a Ta/Pd bilayer catalyst on a Mg<sub>70</sub>Al<sub>30</sub> film layer improves its kinetic properties, leading to hydrogen desorption at 100 °C compared to 170 °C for a single Pd layer.

Such an experiment was interrupted in May 2009 when the NRU reactor shut down, and this research had to be continued at foreign neutron beam facilities, namely NIST (USA) and HZB (Germany). The researchers found that the Mg<sub>70</sub>Al<sub>30</sub> films can be made to store hydrogen up to 5 wt. % under the mild constraints of room temperature and a pressure of 1.3 bar, using a Ta/Pd bilayer as a catalyst under certain geometrical conditions. The effect of adding the Ta layer between the Pd and MgAl was very large; it allowed observable absorption at a pressure ten times lower than on the Ta-free sample, without affecting the storage capacity.

### Continuing to Train Highly Qualified People

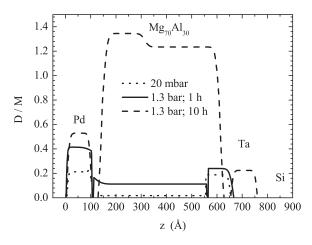
When the NRU reactor shut down in May 2009, Katharina Fritsch was on day three of a 14-day experiment at the C5 spectrometer at the CNBC. Katharina is a Ph.D. student of Bruce Gaulin at McMaster University. She was studying a magnetically dilute kagome staircase material, (Co<sub>1.x</sub>Mg<sub>x</sub>)<sub>3</sub>V<sub>2</sub>O<sub>8</sub>.

However, with the support of the CNBC, some discretionary beam time at NIST Centre for Neutron Research was obtained, and the experiment was performed in August 2009 on the triple-axis spectrometer, SPINS. Dr. Zahra Yamani, CNBC research officer, attended the experiment, providing her expertise and support during the experiment. Obtaining the discretionary beam time and being able to perform the experiment in a timely manner has allowed Katharina to make progress toward a major part of her Ph.D. thesis.

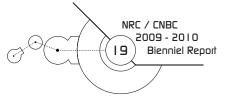




Illustration of the structure of the film with the single Pd catalyst layer (left) and the Ta/Pd catalyst bilayer (right).



Deuterium-to-metal ratio along the depth in the sample ( $Si/Ta/Mg_{70}Al_{30}/Pd$ ).



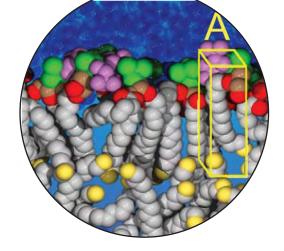


### Continuing International Collaborations

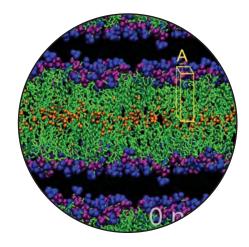
The shutdown displaced experiments scheduled for an on-going collaboration with Robert Birgeneau (University of California at Berkeley) and Stephen Wilson (Boston College). Preliminary data obtained on the N5 spectrometer at the CNBC showed the potential presence of magnetic critical fluctuations near the antiferromagnetic phase transition in the iron pnictide parent compound BaFe, As,. When follow-up measurements at the C5 spectrometer were displaced, the NIST Center for Neutron Research (NCNR) granted some of its discretionary beam time to allow this research to continue. Dr. Zahra Yamani, CNBC research officer, travelled to the NCNR to help finish a critical component of their study. Timely access to the NCNR enabled the successful completion of the project in a highly competitive and fast moving field.

## Enhancing Simulations of Biological Membranes through Experiment

The war on infectious bacteria may depend on replacing or enhancing our traditional antibiotics. Designing biomolecules that bind to membranes of bacteria and not the membranes of human cells may lead to such a success. Bruno Tomberli (Brandon University) and Chris Gray (University of Guelph) simulate the binding of biomolecules to bacterial-like and mammalian-like membranes. The accuracy of these simulations depends highly on our knowledge of the fundamental structure of the membranes obtained experimentally, including the lateral area per molecule. However, some discrepancies exist between the published values determined by X-rays and neutrons separately. Therefore, the researchers teamed with Dr. Norbert Kucerka, CNBC research



Simulated biomembranes: distant (left) and close (right) views.

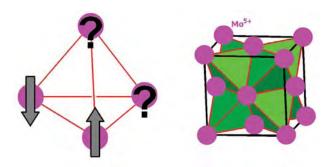


officer, and Stefan Kycia (Guelph) to develop a method to determine these values from simultaneous analysis of both X-ray and neutron data, and to perform the systematic neutron and X-ray experiments needed to resolve the discrepancies.

The neutron experiments were scheduled at the CNBC when the NRU reactor was shut down. To continue this research despite the shutdown, the CNBC requested and obtained a one-time 'discretionary' beam time allocation at Oak Ridge National Laboratory (Tennessee, USA). Dr. Kucerka was also awarded beam time at the NIST Center for Neutron Research (Maryland, USA) and participated in X-ray experiments at the Cornell High-Energy Synchrotron Source (New York, USA) to complete the measurements.

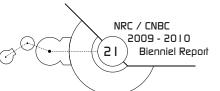
### Exploring Unusual Magnetic Behaviour

Many materials exhibit magnetic ordering at low temperatures, but in cases where competing magnetic states are exquisitely balanced against one another, occasionally none of these states prevail even down to the lowest achievable temperatures. By making small changes to upset the balance using parameters such as composition, pressure or external fields, the system can be "pushed" into any of these magnetic states, which have quite different magnetic properties. Thus, these materials could potentially be used in devices such as sensitive magnetic detectors. But more fundamentally, probing the behaviour of these materials could provide insights into the nature of fundamental interactions inside matter.



(left) Magnetic moments (pink) coordinated on a tetrahedron with moment directions indicated by arrows; the total energy of the system is minimised by an antiparallel arrangement of neighbouring moments, but this cannot be simultaneously satisfied for all four moments, leading to geometric frustration. (right) Arrangement of magnetic Mo<sup>5+</sup> moments in Ba<sub>2</sub>YMoO<sub>6</sub> on a network of edge-sharing tetrahedra.

One such material is  $\mathrm{Ba_2YMoO_6}$ . Several types of measurements have detected the absence of magnetic ordering in this compound down to low temperatures. Recent neutron scattering measurements at Oak Ridge National Laboratory by researchers at McMaster University and the CNBC have revealed evidence for a state that has been hypothesised as the cause of this behaviour in a finely grained powder of  $\mathrm{Ba_2YMoO_6}$ . Follow-up measurements to clarify the nature of this state are in progress.



### INSTRUMENT DEVELOPMENT

### Improving Data Collection on the L3 Stress Scanner

The L3 spectrometer is the CNBC's main instrument for mapping residual stresses in engineering components, and for studying, in situ, the distribution of stress and strain in several texture components of engineering materials during deformation.

To achieve a 2-3 times faster data acquisition rate, an upgrade to a taller detector is in progress. The new design is complete and is being fabricated. The new detector will also increase the spatial resolution of the instrument in some cases.

### Improving Reliability of the L3 Stress Scanner

The air jacks in the L3 monochromator were prone to failure, causing downtime. The air jacks are required to move large steel shielding blocks whenever a different wavelength of neutrons is needed. Further, these jacks were no longer available and replacement while the reactor was operating would cause further loss of beam time. The shutdown period was used to design and install custom replacement airjack assemblies. These replacements were designed so that installation would not require any changes to the control system. This upgrade will improve reliability for L3 and conserve staff resources.

### **Increasing Neutron Flux at C5**

The main C2 reactor gate, part of the reactor itself, is disabled and locked in the open position. Thus, the extended shutdown of the NRU reactor presented a rare opportunity to work safely on components of the monochromator cavity on DUALSPEC (which serves both C2 and C5). The monochromator was upgraded to increase the neutron flux by five times and ensure that users continue to have access to magnetically polarised neutron beams of the highest quality.

The CNBC completed the design, fabrication and installation of a rotary table suitable for the focusing

Heusler-alloy monochromator. Final alignment of the Heusler-alloy blades on the monochromator was performed after the restart of the reactor.

### Upgrades to the Sample Orientation at C5

Motorised specimen rotation stages ("arcs") significantly improve the efficiency of setting up experiments and help minimise radiological exposure to personnel by reducing time spent close to the neutron beams. These arcs are capable of making small adjustments to the angular position of bulky sample chambers that may include large magnets or cryostats. The CNBC originally had three manual arcs. The first unit was motorised a few years ago, but experiments requiring arcs often occur simultaneously and thus, there was a need for a second motorised arc. Because of the NRU shutdown. CNBC was able to allocate personnel time to complete this labour-intensive project, such that users now have access to a second motorised arc with new motor drives, which allow faster driving than the first motorised arc.



### Robot on C2 Automates Routine Sample Changes

A robot was designed and built in-house to automate routine sample changes between experiments, facilitating remote access, saving time and reducing radiation exposure. While some beam facilities use industrial-scale robotics to perform such tasks, this inexpensive alternative is less hazardous.

On C2, many powder samples are held in standard Vanadium cans at room temperature. Using the new robot, up to 22 such sample cans can be programmed to be changed and integrated into the standard control system.

### **Completion of Control System Upgrades**

In 2008, a major upgrade of the L3 electronic control system began, to enhance performance and reliability. As part of this upgrade, new electronics racks and high-density storage units were installed to relieve congestion around the instrument. In 2009, the electronics upgrade was completed—the remaining interface boxes were installed on the spectrometer and additional motor control units were

assembled and installed.

In 2010, a second phase of upgrades was completed, allowing control of up to 32 motors, reducing experimental setup time and improving ease of use and maintenance. The upgrade also gave the CNBC an opportunity to reorganize the layout at the instrument. There is now much more room to work, which is very important when working with large samples, as is typical for industrial components.

Mechanism for orienting and positioning multiple Heusleralloy crystals in a strong, magnetic circuit, to generate a focused, polarised neutron beam of high intensity.



wavelengths (2.37 Å). Since the initial commissioning in 2007, D3 alignment has been based on fiducial marks established during construction, and not against primary reference points, which actually define

> the neutron beams. This alignment convention was due to the fact that some of the primary reference points are

> > inaccessible without causing prolonged disruption to the operation. Therefore, the CNBC took advantage of the NRU shutdown being

the ideal time to perform alignment verification of D3 against the primary references.

**Expanding Capacity for** Study of **Deformation in** Industrial Materials

The CNBC acquired and installed a system capable of detecting tiny sound waves in load-bearing industrial materials.

By observing these materials simultaneously with neutron diffraction, researchers will obtain a greater understanding of the development of deformities that can cause materials to fail, and ultimately, the means of preventing such failures.

Tiny sound waves are generated when energy is liberated as a result of microscopic events that shift the molecules within a material. For example, these waves can be attributed to crack propagation, phase transformations, particle ruptures and twinning. Using both neutrons and these sound waves, researchers will be able to detect the formation of a deformity and monitor its development as the load that the material bears changes.

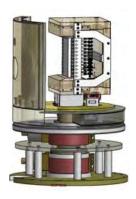




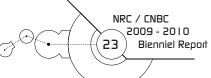
Neutron beam instruments perform best when precisely aligned. Alignment of all the instrument's components to very high precision is a challenge for neutron reflectometry at relatively short neutron

Sample-changing

robot on C2.



Design of the stronger, radiation-resistant rotary table for the Heusler monochromator and additional lead shielding that is required to install and remove the activated monochromator in the C5 monochromator shield.



# Leading-Edge Sample Environment Auxiliary Equipment

A crucial upgrade to the CNBC's infrastructure in support of leading-edge materials science and engineering research is a new servo-hydraulic load frame for in situ experiments, and a corresponding upgrade to the existing specimen rotation stage at L3 to a rotation/translation stage. The electronic control system, hydraulic grips, hydraulic power unit, alignment system, and the

The D3 reflectometer is owned by the University of Western Ontario and was funded through a federal-provincial partnership supported by 12 universities.

Original air jacks (bronze-coloured), replaced with new units (aluminium-coloured) to achieve greater reliability of operation.



### **PUBLICATION LIST**

load frame itself were received in 2010.

The CNBC received notice of the following publications from CNBC staff and users. This list of papers of research conducted at the CNBC, with 43 published in 2009 and 53 in 2010, may not be exhaustive.

In addition, experimental reports from the community of international users are available on the web site of the Canadian Institute for Neutron Scattering:

http://www.cins.ca/expreports.html

The references in the list and the online experimental reports are presented in the language in which they were written.

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