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70 Years of Neutron Scattering in Canada / *70 années de diffusion des neutrons au Canada*

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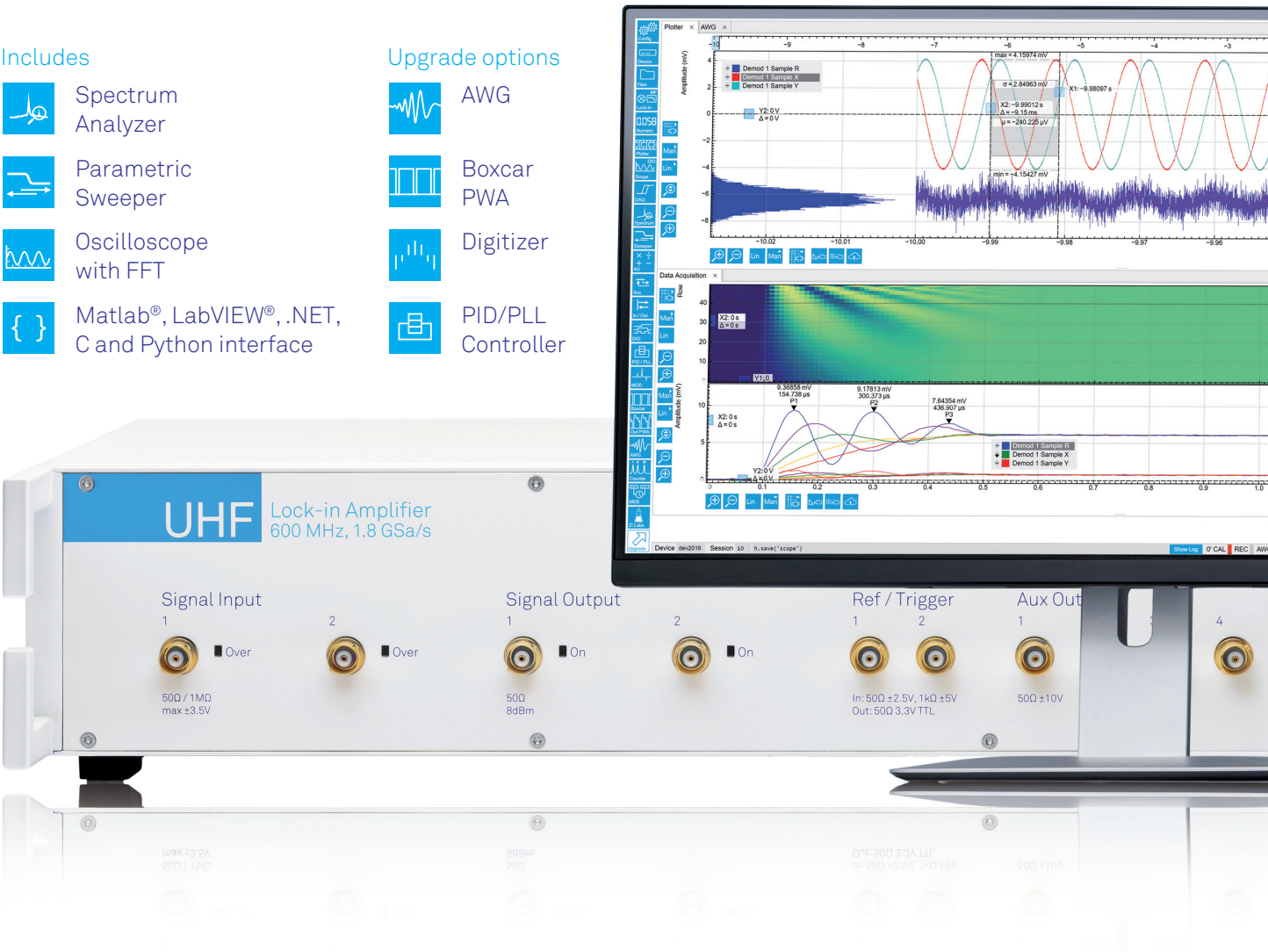

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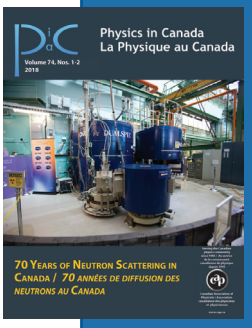

The DUALSPEC instrument (blue) outside the biological shield (light green) of the National Research Universal (NRU) reactor at Chalk River Laboratories is made up of two of the six neutron beamlines for materials research operated by the Canadian Neutron Beam Centre. DUALSPEC was designed and built by Atomic Energy of Canada Ltd, and later transferred to the National Research Council in 1997.

L'instrument DUALSPEC (bleu) du réacteur national de recherche universel des Laboratoires de Chalk River, en dehors de sa protection biologique (vert clair). Il comprend *deux des six lignes de faisceaux de neutrons qu'opère le Centre canadien de faisceaux de neutrons pour la recherche en matériaux. DUALSPEC fut conçu et construit par Énergie atomique du Canada limitée, et plus tard transféré au Conseil national de recherche en 1997.*

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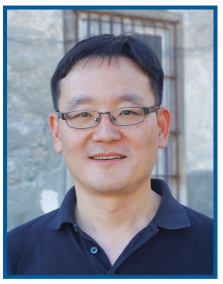
70 Years of Neutron Scattering in Canada



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Canada has been a leader in neutron scattering for 70 years, starting with work at the National Research Experimental (NRX) reactor completed by the National Research Council in 1947, at what was then known as the Chalk River Project. Nobel laureate (physics, 1994) Bertram Brockhouse began his pioneering contributions to the development of neutron scattering at NRX and then continued them at the 10-times more powerful National Research Universal (NRU) reactor, completed in 1957 by Atomic Energy of Canada Ltd. (AECL). In addition to neutron scattering, the NRU reactor was the primary test-bed for developing Canada's fleet of nuclear power stations, which greatly reduces greenhouse gas emissions. The NRU reactor also produced nuclear isotopes for use in medicine, such as molybdenum-99, which have been used to diagnose an estimated 500 million patients around the world over its lifetime.

The neutron scattering user program at the NRU reactor has operated recently as "the Canadian Neutron Beam Centre" (CNBC). Over the last five years, the CNBC has supported about 800 research participants from Canada and around the world, including students and researchers from universities, government labs, and industry. There is an approximately equal 'trade balance' of Canadian researchers who use foreign facilities and foreign researchers who access the CNBC. As a research tool that can solve a diverse array of scientific questions, neutron scattering brings together scientists and engineers from physics, chemistry, life sciences, and materials science in an interdisciplinary fashion. At the CNBC and other neutron facilities, local instrument scientists collaborate with the external user, who is often not an expert in the technique, but brings expertise in the science of the material in question. Reflecting this dynamic in the neutron scattering community, some articles in this issue are written by experts from the facilities, while others are written by users based at universities.

This issue opens with a series of three articles to celebrate key developments in 70 years of neutron scattering: Tom Holden reviews the early development of neutron scattering at Chalk River, including Brockhouse's seminal work. Mechthild Enderle and colleagues summarize the experimental confirmation of the "Haldane gap" in the 1980s, which confirmed the existence of topological phases of matter, and eventually led to Duncan Haldane's 2016 Nobel Prize in physics. Third, John Root provides a programmatic history covering the development of the CNBC and efforts to replace the NRU reactor with a new, modern facility, from 1985 to present.

The NRU reactor is planned to close permanently in March 2018 — probably before you will read this issue. The challenge faced by the neutron scattering community will be exacerbated by the 2018 expiry of Canada's only agreement with a foreign neutron source, under which Canadians get some preferred access to beamlines at the Spallation Neutron Source at Oak Ridge National Laboratory (USA). Thus, Thad Harroun, President of the Canadian Institute for Neutron Scattering, discusses the present crisis and future prospects for the Canadian neutron scattering community via the Canadian Neutron Initiative, which seeks to establish a new framework for neutron scattering for the next decade so that Canada will continue to have a complete 21st century physics toolkit for the study of materials.

The issue then turns to reviews and examples of modern research in the five scientific subject areas that have been enabled by neutron scattering: (1) quantum materials, (2) soft materials and biophysics, (3) materials science and engineering, (4) thin films, and (5) crystallography.

For quantum materials, Zahra Yamani reviews several research highlights arising from the work at the CNBC in superconductivity, and magnetism using triple-axis spectrometers, while Jonathan Gaudet and Bruce Gaulin review highlights from the Canadian participation in the Spallation Neutron Source in investigating geometrically frustrated magnets and superconductors.

For soft materials and biophysics, Maikel Rheinstädter explains why neutron scattering is an indispensable tool for the life sciences, and how it is used in the study of membranes in particular.

For materials science and engineering, Joshua Stroh and Dimitry Sediako demonstrate the power of *in-situ* neutron diffraction in engineering applications, with a study of an

aluminum alloy to inform the development of light-weight alloys for the automotive industry.

For thin films, Kunal Karan and colleagues explore a specific application of neutron reflectometry in polymer-electrolyte-based energy conversion and storage devices, such as fuel cells, while Jamie Noël provides an overview of neutron reflectometry in Canada, illustrated with key examples in electrochemistry and corrosion.

Finally, for crystallography, John Greedan, Chris Wiebe, and Dominic Ryan collaborated to provide an extensive review of powder neutron diffraction for materials chemistry and physics in Canada, from the early days until today, with an emphasis on the past 20 years, including research conducted at Chalk River and Canadian research using foreign sources.

Daniel Banks, Canadian Nuclear Laboratories, and
Young-June Kim, University of Toronto
Guest Editors, *Physics in Canada*

Comments of readers on this Editorial are more than welcome.

70 années de diffusion neutronique au Canada

Le Canada a été un chef de file en diffusion de neutrons depuis 70 ans, en commençant par la recherche au réacteur national de recherche expérimental (NRX) réalisé par le Conseil national de recherches en 1947, dans le cadre de ce qu'on appelait alors le projet Chalk River. Le lauréat du prix Nobel (physique, 1994) Bertram Brockhouse a amorcé au NRX son apport novateur au développement de la diffusion neutronique, le poursuivant au réacteur national de recherche universel (NRU) dix fois plus puissant, mis au point en 1957 par l'Énergie atomique du Canada limitée (EACL). Outre la diffusion de neutrons, le réacteur NRU a été le premier outil d'étalonnage du groupe de centrales nucléaires du Canada, qui réduit énormément les émissions de gaz à effet de serre en Ontario. Le réacteur NRU a aussi produit des isotopes nucléaires pour la médecine tels le molybdène 99, qui a servi à diagnostiquer quelque 500 millions de patients dans le monde entier pendant sa durée de vie utile.

Le programme d'utilisation de la diffusion neutronique au réacteur NRU fonctionnait récemment sous le nom de « Centre canadien de faisceaux de neutrons (CCFN) ». Au fil des cinq dernières années, le CCFN a soutenu quelque 800 participants à la recherche du Canada et du monde entier, dont des étudiants et des chercheurs d'universités, de laboratoires gouvernementaux et de l'industrie. Le nombre de chercheurs canadiens qui utilisent des installations étrangères est à peu près égal à celui des chercheurs étrangers qui recourent au CCFN. À titre d'outil de recherche capable de résoudre diverses questions scientifiques, la diffusion neutronique rassemble des scientifiques et des ingénieurs en physique, chimie, sciences de la vie et science des matériaux en une équipe interdisciplinaire. Au CCFN et dans les autres centres de neutrons, des scientifiques locaux collaborent avec des utilisateurs de l'extérieur qui, souvent, ne sont pas experts dans une technique mais fournissent leur expertise à la science du matériau en question. Certains articles du présent numéro, reflétant cette dynamique dans la collectivité de la diffusion de neutrons, sont signés par des experts des centres de neutrons et d'autres, par des utilisateurs universitaires.

Le présent numéro s'ouvre sur trois articles qui célèbrent les faits marquants de 70 années de diffusion de neutrons : Tom Holden examine la mise au point hâtive de cette diffusion à Chalk River, dont les travaux précurseurs de Brockhouse. Les collègues de Mechthild Enderleand résument la confirmation expérimentale du « gap de Haldane » qui, dans les années 80, a confirmé l'existence de phases topologiques de la matière et a finalement valu à Duncan Haldane le prix Nobel 2016 de physique. Troisièmement, John Root fait un récit pratique du développement du CCFN et des efforts pour remplacer le réacteur NRU par une nouvelle installation moderne de 1985 à nos jours.

Le réacteur NRU est censé fermer en permanence en mars 2018 – probablement avant que vous lisiez le présent numéro. Le défi que devra relever la collectivité de la diffusion de neutrons sera d'autant plus grand que la seule entente du Canada avec une source étrangère de neutrons expirera en 2018, elle qui donne aux Canadiens un accès privilégié aux faisceaux de la source de neutrons Spallation du Oak Ridge National Laboratory (É.-U.). Alors, Thad Harroun, président de l'Institut canadien de la diffusion des neutrons, examine la crise actuelle et les perspectives futures pour la collectivité canadienne de cette diffusion sous l'angle du programme canadien de neutrons qui vise à établir un nouveau cadre de diffusion neutronique pour la prochaine décennie de sorte que le Canada continue d'avoir une boîte à outils complète pour l'étude des matériaux en physique au 21e siècle.

Le présent numéro présente ensuite des revues et des exemples de recherches modernes dans les cinq disciplines scientifiques facilitées par la diffusion neutronique : (1) matériaux quantiques, (2) matériaux mous et biophysique, (3) science des matériaux et ingénierie, (4) couches minces, et (5) cristallographie.

Pour les matériaux quantiques, Zahra Yamani examine plusieurs points marquants de la recherche au CCFN en supraconductivité et magnétisme à l'aide de spectromètres à trois axes, alors que Jonathan Gaudet et Bruce Gaulin dépeignent les grands axes de la participation canadienne à la source de neutrons Spallation par un inventaire géométrique d'aimants frustrés et de supraconducteurs.

Au sujet des matériaux mous et de la biophysique, Maikel Rheinstädter explique pourquoi la diffusion des neutrons est un outil indispensable pour les sciences de la vie et comment on s'en sert pour étudier des membranes en particulier.

Pour la science des matériaux et l'ingénierie, Joshua Stroh et Dimitry Sediako montrent la puissance de la diffraction de neutrons *in-situ* dans des applications d'ingénierie par l'étude d'un alliage d'aluminium pour guider la mise au point d'alliages légers dans le secteur automobile.

Pour les couches minces, Kunal Karan et ses collègues explorent une application particulière de réflectométrie de neutrons dans des dispositifs de conversion et de stockage d'énergie à base d'électrolytes polymériques tels les piles à combustible, alors que Jamie Noël fait un tour d'horizon de la réflectométrie neutronique au Canada, avec des exemples clés en électrochimie et corrosion.

Enfin, en cristallographie, John Greedan, Chris Wiebe et Dominic Ryan ont collaboré pour nous fournir une étude approfondie de la diffraction de neutrons pour la chimie et la physique des matériaux au Canada, de ses débuts jusqu'à aujourd'hui, en mettant l'accent sur les 20 dernières années, incluant les recherches menées à Chalk River et à des installations étrangères par des Canadiens.

Daniel Banks, Canadian Nuclear Laboratories, et
Young-June Kim, Université de Toronto
Rédacteurs honoraires, *La Physique au Canada*

Les commentaires des lecteurs sur cet éditorial sont toujours les bienvenus.

NOTE: Le genre masculin n'a été utilisé que pour alléger le texte.

Editorial note:

It is with great sadness that we witnessed the permanent closure of NRU on March 31st, 2018 with no concrete plan to continue with what Canada has built on the legacy of our great Canadian Nobel Prize Laureate, Bert Brockhouse. Being "old and costly to operate", though highly productive, seems to have formed Canada's choice to terminate one of its most successful scientific ventures without a path forward.

Note de la rédaction :

C'est avec une grande tristesse que nous avons été témoin le 31 mars 2018 de la fermeture permanente du réacteur national de recherche universel (NRU) sans plans concrets pour continuer ce que le Canada a accompli sur la base des travaux de notre grand lauréat du Prix Nobel Bert Brockhouse. L' « âge » du réacteur et son coût élevé d'opération, malgré sa grande productivité, semblent avoir été à la base de la décision du Canada de terminer une de ses meilleures entreprises scientifiques sans plan d'avenir.

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The First Decade of Neutron Scattering at Chalk River: 1949-59

by Thomas M. Holden

The completion of the National Research Experimental Reactor, NRX, at Chalk River in 1947 set the stage for nuclear research in Canada. NRX provided space for in-reactor irradiations as well as external beams of neutrons and γ-rays for experiments outside the biological shielding. The earliest neutron beam experiments were aimed at understanding not only the structure and dynamics of solids liquids and gases but also nuclear structure and fission processes. According to G.C. Hanna in [1], "W.B. Lewis (then director of Chalk River)…left the scientific direction of pure research to the scientists". It appears that the staff scientists were given the initiative to carry out the research that seemed most likely to them to lead to advances in science and technology.

According to A.D.B. (Dave) Woods in a private communication, "There is no doubt in my mind that Don Hurst (then director of the Reactor Research and Development Division) was the inspiration behind the neutron scattering program at Chalk River". In the late 1940s Hurst worked with Norman Z. Alcock and John A. Spiers on neutron scattering from gases and on nuclear physics problems. To augment the program, Hurst hired Bertram N. Brockhouse in 1950 and Dave G. Henshaw in 1951. The goal of measuring the detailed vibrational spectrum of solids by inelastic neutron scattering was formulated in 1950 in study group meetings in Hurst's home between himself, Brockhouse, G. H. (Trudi) Goldschmidt and Noel K. Pope.

The first monochromatic neutron beams were extracted from NRX by diffraction from natural crystals such as NaCl and shortly afterwards a second axis was added to create a diffractometer [2]. The beam had a cross section of 2.5 × 1.25 cm^2 to maximize the intensity and the distance from the monochromator to the sample was 183cm to allow low diffraction angles. The monochromator was surrounded by massive shielding which was required for adequate reduction of unwanted background intensity. With care, the lower and upper limits on neutron energy were 1 meV and 50 eV!

Summary

Contributions from Chalk River Nuclear Laboratories in the first decade, 1949-59, to neutron scattering research in Canada are described.

The first experiment on the scattering of neutrons [3] described diffractometer measurements of pressurized O_2 and CO_2 with 70 meV (1.06 Å) neutrons selected by a NaCl monochromator from the NRX reactor spectrum. The experiment was designed to elucidate the atomic structure of the molecules and the measurements were compared with a calculation based on the scattering of the neutron by systems of two and three point entities assuming no inelastic scattering. The calculation for O_2 matched the variation of the scattered intensity with angle reasonably well, but lay above the experiment for CO_2 at low momentum transfers. It was surmised that, since the CO_2 gas was quite close to the liquid phase, some condensate in the sample chamber might have changed the scattering pattern. The experiments were clearly right at the limit of what could be done at that time and great care had to be taken to avoid systematic errors.

The second experiment reported [4] was on the scattering lengths of the deuteron where the interest was on the impact on the theory of nuclear forces rather than atomic physics. 1.063 Å neutrons from the NRX reactor were selected by reflection from the (100) planes of NaCl. The scattering of slow neutrons by the deuteron of nuclear spin 1 is defined by the two possible spins of the compound nucleus, 3/2 or 1/2. The form of the scattering is a quadratic function of the ratio $\frac{a_{1/2}}{a_{3/2}}$, which had two roots 3.2 ± 0.3 or 0.12 ± 0.04 where $a_{1/2}$ and $a_{3/2}$ are the relevant scattering lengths. As noted in their paper, the remaining ambiguity could only be resolved by experiments with polarized neutrons. The presently accepted values of the scattering lengths [5] of the deuteron are $a_{3/2}$ = 9.53 ± 0.03 fm and $a_{1/2} = 0.975 \pm 0.06$ fm and their ratio $\frac{a_{1/2}}{a_{3/2}}$ is 0.102 ± 0.007. This modern result is within the careful error estimates made by Hurst and Alcock in 1951 for the second of their quoted values. The experiment is a textbook case of considering the sources of systematic and random errors and assigning uncertainties to the measured quantities and carrying these through to the final ratios.

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The first experiment with an impact on solid state physics emerged from measurements of the resonant scattering of slow neutrons by Cd. The one-to-one correspondence between the intensity of neutrons transmitted by Cd near 350 meV and the neutron wavelength led to its use as an analyzer to test the average wavelength of neutrons scattered by Pb, Al and C. The significance of the experiment for the possibility of a measurement of inelastic scattering was recognized by Brockhouse in his Nobel address [6]. The intensity of neutrons scattered by Pb, Al or C was measured for each of ten thicknesses of Cd covering an assembly of six symmetrically arranged BF_3 counters. The actual transmission through Cd showed deviations from the transmission calculated on the basis of elastic scattering alone that correspond to a net increase in neutron energy upon scattering. The deviations increase in the order Pb, Al, C corresponding to larger energy transfers to the neutron as the mass of the scattering nucleus decreases. An Einstein model of the vibrational energy levels of a monatomic solid using reported Einstein temperatures of 65.5, 300.4 and 1740K (5.65, 25.9 and 150.0 meV) for Pb, Al and C, respectively, gave a satisfactory account of the net change in wavelength on scattering from these materials. Significantly, it suggested that the possibility of measuring energy transfers directly was close to being feasible.

The first neutron measurements from Chalk River on the structure of liquid He^4 were reported by Henshaw and Hurst in 1953 [7]. The intensities, corrected for background and the change of effective volume with scattering angle, were accurate to ±7% while double scattering and the effect of resolution were noted to be smaller than the statistical error. The main finding was the position of the first peak in S(Q) at 2.15 ± 0.0.11 $Å^{-1}$ corresponding to a peak in the radial distribution function of atoms, g(r), at 3.6 Å. Further measurements [8] of the intensities normalized by the differential scattering cross section of a free He^4 atom indicated that the coherent scattering, which reveals the liquid structure, was restricted to the peak around 2.057 $Å^{-1}$ and that at greater wave vectors the scattering was essentially free atom scattering. The principal result of the temperature variation of the coherent scattering was that there was no change in the structure of He^4 at the λ-point, where He^4 turns into a superfluid. This was not unexpected since the λ-transition was thought to be essentially a Bose-Einstein condensation in momentum space which would result in a change in the velocity distribution of the atoms but no change in the spatial distribution.

By 1955, large Al single crystals grown by Henshaw had replaced natural single crystals as monochromators providing major improvements in monochromatic beam intensities. The first reports of inelastic neutron scattering using the "crude triple-axis crystal spectrometer", shown in Fig. 1 [6], came in 1955 with the publication of "The scattering of neutrons by phonons in an Al single crystal" [9] by Brockhouse and Alec T.Stewart, which was the culmination of the study group discussions held four years previously. Bragg scattering is far stronger than phonon scattering, but when the single crystal sample is angled to avoid Bragg scattering, the phonons may be observed. When the conditions of wave vector conservation and energy conservation are met simultaneously, a peak may be seen in the scattered intensity plotted as a function of the energy transfer to the crystal. For a monatomic lattice the frequencies are expected to separate into three branches, corresponding in the low frequency limit, to the familiar longitudinal and two transverse sound waves.

In the experiment, neutrons of constant wavelength 1.148 Å (62.2 meV) from a crystal spectrometer fell on an Al sample crystal with [01 $\bar{1}$] axis vertical. Measurements were made with

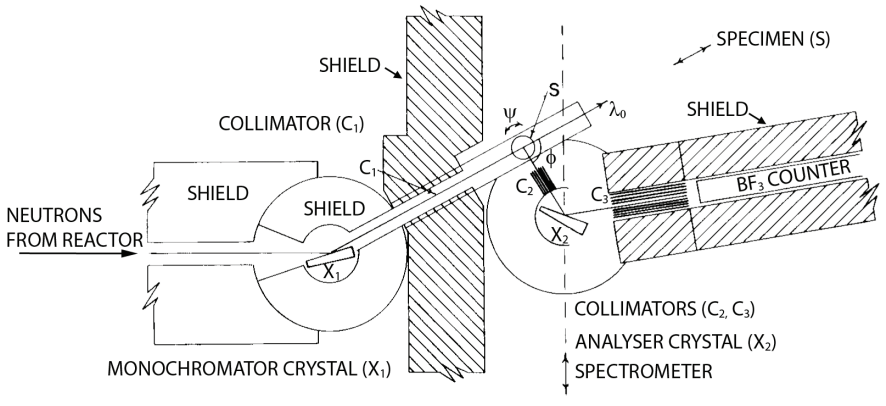

Fig. 1 The first crude version of the triple-axis spectrometer. Monoenergetic neutrons are selected by the large single crystal monochromator (X_1) and impinge on the specimen (S) which is located on a table whose orientation (ψ) with respect to the incident beam can be selected. This table can be moved along the incident beam as desired. The analyzing spectrometer, which employs crystal X_2, is a diffractometer of especially large aperture which can be translated as a unit. The angle, Φ, through which the examined neutrons are scattered, is determined by triangulation. Thick shielding, shown hatched, between X_1 and S, blocks unwanted background neutrons and γ-rays. Thick shielding also surrounds the BF_3 counter. Collimators C_1, C_2 and C_3 determine the precise direction of the neutrons.

the sample crystal angle rotated by increments, δ, from the angle for Bragg scattering for the (333) reflection**.** The energy distribution was measured with a second crystal spectrometer and revealed neutron peaks in both neutron energy loss and gain.

Four points on the TA branch were established and one on the LA branch shown in Fig. 2. The position of the TA phonons matched a sinusoidal curve with an initial linear slope corresponding to the transverse velocity of sound in Al. The authors noted that similar inelastic neutron scattering experiments were being carried out by B. Jacrot in Paris and the group of R.S. Carter, D.J. Hughes, H. Palevsky and R.L. Zimmerman at Brookhaven in the United States.

A more complete series of experiments on the lattice vibrations in Al was reported in the epochal paper [10] in *Reviews of Modern Physics* in 1958. Enormous progress had been made in the intervening four years in obtaining the phonon dispersion relations in three high symmetry directions and checking that the observed results were in agreement with the cross section and selection rules for one-phonon and two-phonon processes. Two different crystals were examined both by crystal and time-of-flight spectrometry. The various processes that give accidental sharp peaks that masquerade as excitations and are usually referred to as "spurions" were identified. Finally, the results were discussed in terms of the existing theories of lattice dynamics and compared with the results of diffuse x-ray experiments. That is, all possible checks were made to establish that the inelastic scattering observed was due to lattice vibrations.

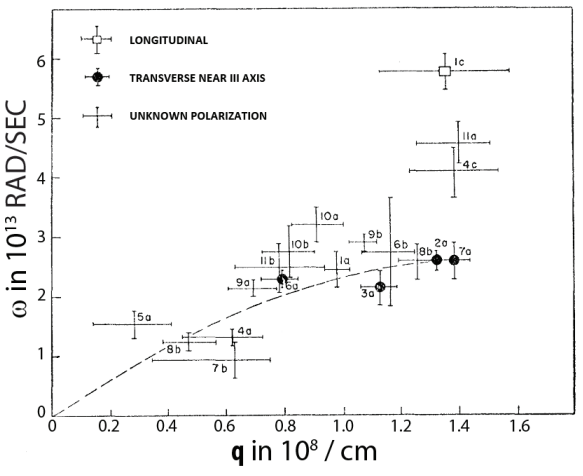

Fig. 2 The relation between the phonon frequency, ω (10^{13} radians/sec) and the phonon wavevector, q (10^8 cm^{-1}), near the [111] direction in aluminium (Al). Positively identified transverse (TA) and longitudinal (LA) modes are indicated by solid and open circles. Phonons of unknown polarization are indicated by dots. The dashed curve is a sine curve whose initial slope corresponds to a velocity of sound of 3080 m/s for Al.

The first measurements of the dispersion relation, $\hbar\omega(q)$, for magnetic excitations in an ordered magnet Fe_3O_4, were reported [11] in 1957. To put the paper in context, it was generally thought that the excitations out of the fully ordered magnetic state were wave-like by analogy with the vibrations of the crystal lattice. However, the only manifestations of the excitations were found from thermodynamic average measurements like magnetization and low temperature specific heat. The sample was a large natural single crystal with about 10% of the Fe sites replaced by vacancies, and impurities such as Ti, Mn, Al, and Si. There are six interpenetrating magnetic sub lattices in Fe_3O_4, and so there is one "acoustic" mode which goes to zero energy at $\mathbf{q} = 0$ and five "optic" branches. In spite of the large coherent phonon scattering and large incoherent scattering from the impurities, the spin-wave dispersion relation was established over an energy range of 16 meV and wave vectors up to 0.04 $Å^{-1}$. Over this small range, it was not possible to decide on the basis of the initial experiments whether the dispersion relation was linear or quadratic. However, a straight line through the data did not correspond to the velocity of sound in magnetite. For a quadratic dispersion relation, J_{AB}, the exchange parameter between the A and B sites was 2.0 meV and with this value, the calculated Curie temperature on a molecular field model was 1050K compared with the actual value of 850K. On this physical basis, it was concluded that a quadratic dispersion relation was more reasonable. In a paper written shortly afterwards, Brockhouse showed that the intensity ratio of the spin wave scattering with and without a magnetic field was 1.42 ± 0.05 compared with the theoretical value of 1.5 thus confirming the magnetic character of the excitations.

Measurements of the energy-momentum relation in liquid He^4 were reported [12] in 1958 by time-of-flight with a rotating crystal spectrometer and the Chalk River filter chopper spectrometer. The results agreed with previous neutron time-of-flight measurements and followed a form consistent with a linear phonon relation at small wave vectors and a roton minimum around 0.7 meV. These experiments marked the beginning of a series of experiments on the inelastic scattering from He^4 over a period of 50 years by Henshaw, Woods, Eric C. Svensson and collaborators.

1957 was an important year for neutron research in Canada since the National Research Universal, NRU, reactor started in November with a power of 200MW and thermal neutron flux of 3×10^{14} neutrons cm^{-2} sec^{-1}, about a factor of 10 higher than NRX. A newly designed triple-axis spectrometer [13] was rapidly deployed. In 1958 A.D.B. Woods was hired by Brockhouse who was embarking on studies of phonons in semiconductors, metals and alkali halides. At this point, measurements of dispersion relations in high symmetry directions had to be made by an iterative process since there was no guarantee that measurements with a fixed incident energy, E, and varying E′ to measure the scattered peak would yield a phonon wave vector on a symmetry direction. Woods, in a private communication, described the discovery of the constant-**Q** method in this way:

> *I remember the Monday morning that Bert came in and announced his idea of the constant-**Q** method of observing phonons. A few weeks earlier R.G. Stedman from Sweden had arrived at Chalk River to work for a year in P.A. Egelstaff's United Kingdom Atomic Energy group on scattering from neutron moderators. Dr. Stedman had explained to us attempts made in Sweden to observe phonons in NaCl on the initial steep branch of the dispersion relation by moving at constant energy transfer across the curve. Bert brilliantly clued into this and realized that if you could control the angle of scattering and the sample crystal orientation along with the energy transfer you could do a scan without changing the momentum transfer [hence constant-**Q**].*

This immediately changed the speed and accuracy of measurements of inelastic scattering in crystals and led to an enormous outpouring of papers on phonons in metals and semiconductors, Kohn anomalies, magnetic excitations, paramagnetic scattering, liquids, crystal fields and an unprecedented understanding of the physics of materials. Brockhouse was awarded the Nobel Prize in Physics in 1994 for his formidable achievements in solid state physics, for the development of the triple axis crystal spectrometer and for the constant-**Q** technique. The measurements made in the first decade at Chalk River led the world in neutron scattering and were remarkable, as in later work, for their ingenuity and rigorous attention to sources of experimental error.

ACKNOWLEDGEMENTS

The author wishes to acknowledge his useful correspondence with Dave Woods.

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Early experimental evidence of a topological quantum state: The signature of the Haldane ground state revealed by scattered neutrons

by Mechthild Enderle, Michel Kenzelmann, and W.J.L. (Bill) Buyers

The quantum behaviour of assemblies of many interacting particles leads to surprising and counter-intuitive new phenomena: superconductivity and superfluidity are well-known examples. Duncan Haldane discovered a new quantum mechanical phenomenon [1]: one-dimensional antiferromagnets (spin chains) have an entirely different quantum ground state depending on whether the individual spins are integers (1,2,3, . . .) or half-odd-integers (1/2, 3/2, . . .). This fundamental distinction is inherently related to the fact that one turn brings an integer spin back to its initial state, while a half-integer spin needs two turns.

Using this peculiar trait of quantum mechanics, Haldane made precise predictions that could directly be tested by neutron scattering experiments (see Haldane ground state section in this article): integer spin chains have a cooperative singlet ground state with only short-range pair correlations. An energy gap (very large for spin 1) separates the ground state from the elementary excitation triplet. In contrast, the singlet ground state of half-integer spin chains features far-reaching spin pair correlations that decay algebraically and the excitation spectrum is gapless. The half-integer spin ground state is therefore fragile with respect to long-range magnetic order in the presence of interchain interactions whereas the integer spin chain ground state is protected by the energy gap. Hence a spin-1/2 antiferromagnetic chain seems closer to the classical antiferromagnetic Néel long-range order than the spin-1 chain. Since quantum effects scale with 1/S, it was generally expected that there is an increasing tendency towards long-range order with increasing spin value. While theorists at the time were working hard to elaborate this puzzle, the new idea was immediately tested experimentally, and early neutron experiments provided "proof" prior to a full theoretical understanding.

Summary

The experimental confirmation of the Haldane gap in 1985 by researchers working at Chalk River was a major contribution toward validating the theoretical ideas of Thouless, Haldane, and Kosterlitz, who won the Nobel Prize in Physics in 2016. This article reviews the signatures of Haldane's predicted topological quantum ground state and their observation in early neutron scattering experiments, which overturned the wisdom of the day.

In real materials, excitation gaps arise for a variety of reasons, amongst which anisotropy and dimerisation were well-known at the time. The first evidence for the Haldane gap was found in the quasi-one dimensional spin-1 compound $CsNiCl_3$ for temperatures above its Néel temperature [2], where magnetic order is absent. The absence of quasi-elastic scattering provided evidence for a singlet ground state, and the observed excitation gap was much larger than what spin anisotropies derived from linear spin-wave theory at low temperature could explain. Polarised neutron experiments provided the first direct proof of the isotropic triplet character of the gapped excitation in $CsNiCl_3$ [3] and excluded anisotropy as origin of the gap. Polarised neutron data also proved Zeeman splitting of the triplet [4] and triplet character along the entire one-dimensional dispersion [5]. For an early theoretical review with a short summary of the early experiments, see e.g., Ref. [6].

The first spin-1 chain discovered that did not order at any temperature was NENP ($Ni(C_2H_8N_2)_2NO_2(ClO_4)$) [7]. Initially, the origin of the excitation gap in NENP was not clear due to the large anisotropy, and dimerisation could not be excluded either. The Zeeman splitting of the three gapped excitations, and the precise ratio between anisotropy and exchange definitely ruled out a trivial anisotropy gap [8,9]. The dispersion of both $CsNiCl_3$ [10] and NENP [9] was found to have a periodicity of $2\pi/d$, reflecting the unbroken translation symmetry by one spin spacing d of the Haldane ground state. In both compounds the elementary triplet excitations were shown to dominate the spectral weight [8,9,11].

Two spin chain materials of identical crystallographic structure, $AgCrP_2S_6$ and $AgVP_2S_6$ with spin 3/2 (Cr) and spin 1 (V), respectively, allowed the first direct comparison of half-integer and integer spin chains [12]. The spin

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3/2 compound showed long-range order and gapless excitations, while long-range order was absent and the excitation spectrum gapped for the isostructural spin-1 compound. Quasi-elastic studies of the correlation length as function of temperature in a series of isostructural ABX_3 compounds resulted in a finite correlation length towards zero temperature for the spin-1 compounds, while the half-integer compounds tended to infinitely long-ranged correlations [13]. The nature of the one dimensional quantum ground state strongly influences even the long-range ordered phases of weakly coupled spin chains: $CsMnI_3$ (S = 5/2), isostructural to $CsNiCl_3$, has standard spinwave excitations and field dependence [14], in contrast to $CsNiCl_3$ where the spectrum in the long-range ordered phase features renormalized Haldane triplets that interact in adjacent chains [15].

Duncan Haldane also pointed out [1] that the one-dimensional quantum spin-1 antiferromagnet at zero temperature is related to the classical two-dimensional planar ferromagnet at finite temperature. According to Kosterlitz and Thouless, the latter has vortex-like topological excitations (skyrmions) that condense into the ground state upon lowering the temperature. The ground state of the quantum spin-1 chain is characterised by a topological string order [16], which is analogous to the topological order responsible for the fractional quantum Hall effect [17]. The main features of the new topological order are sketched below.

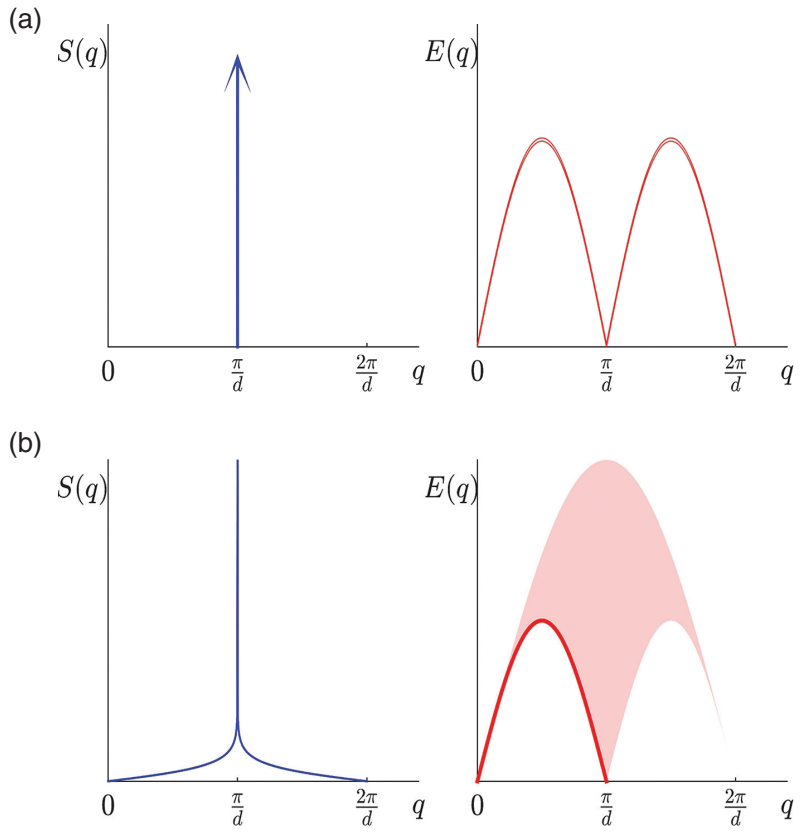

Fig. 2 Diffraction pattern and inelastic scattering of (a) a classical antiferromagnet; and (b) the 1D spin 1/2 antiferromagnet.

THE HALDANE GROUND STATE IN A NUTSHELL (ISOTROPIC CASE)

Consider isotropic magnetic interactions between nearest-neighbour spins that favour antiparallel alignment independent of the spin direction in space (Fig. 1, left). At T = 0, an isotropic classical (i.e., S $\rightarrow\infty$) one-dimensional antiferromagnet is in the Néel state with spontaneously broken translation symmetry (Fig. 1, right).

This strictly periodic pattern of spin states leads to sharp Bragg peaks in neutron diffraction (Fig. 2a). The excitations are doubly degenerate spin waves, small deviations from the ordering direction. Their energy-momentum relation (dispersion) is gapless and has period π/d in q (broken translation symmetry).

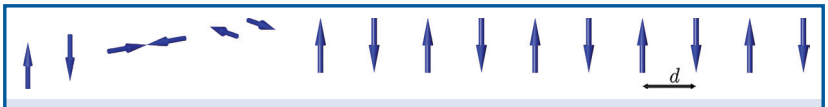

Fig. 1 Isotropic interactions do not prefer any spin direction (left). Long-range order of a classical antiferromagnet (right).

Quantum spins 1/2 form a coherent collective singlet ground state with no local order of the spins. This is not the Néel state, but a snapshot would still show infinitely large regions that look like the classical Néel state. The translation symmetry is unbroken. Since there are no ordered moments there are no Bragg peaks, but the peak intensity diverges in a power-law, i.e., with an infinite correlation length like at a critical point (Fig. 2b). The excitations are pairs of topological (domain-wall like) spinons with a gapless dispersion that repeats with period $2\pi/d$ (unbroken translation symmetry). Even a tiny interchain coupling leads to long-range order in real spin 1/2 materials.

Haldane [1] predicted that integer spin (1,2, 3, . . .) antiferromagnetic chains appear even less ordered, with broad non-diverging peaks in diffraction (Fig. 3). The elementary excitations have a finite minimum energy (Haldane gap), are sharp in energy and triply degenerate. The period $2\pi/d$ of the dispersion reflects the unbroken translation symmetry.

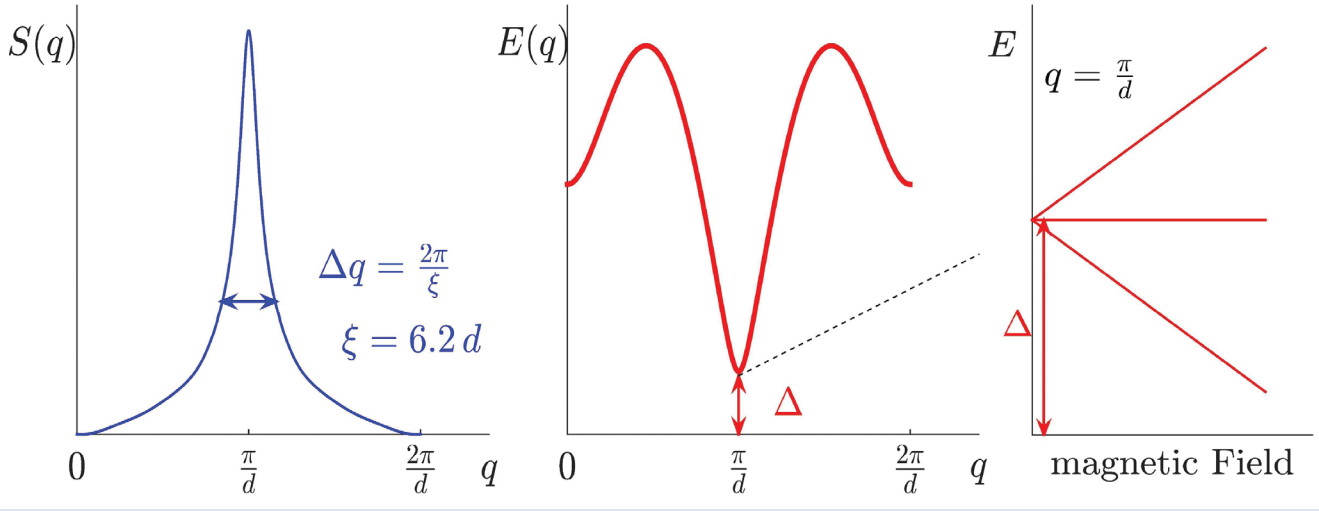

Fig. 3 Diffraction pattern, inelastic scattering, and Zeeman effect of the 1D spin-1 antiferromagnet.

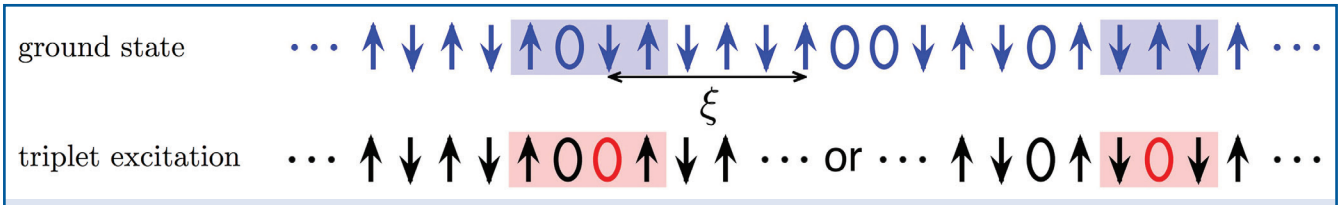

Fig. 4 The non-local order in the Haldane ground state resembles antiferromagnet alignment across any random number of S^z=0 sites. The topological triplet excitations are domain walls with respect to this non-local antiferromagnetic order.

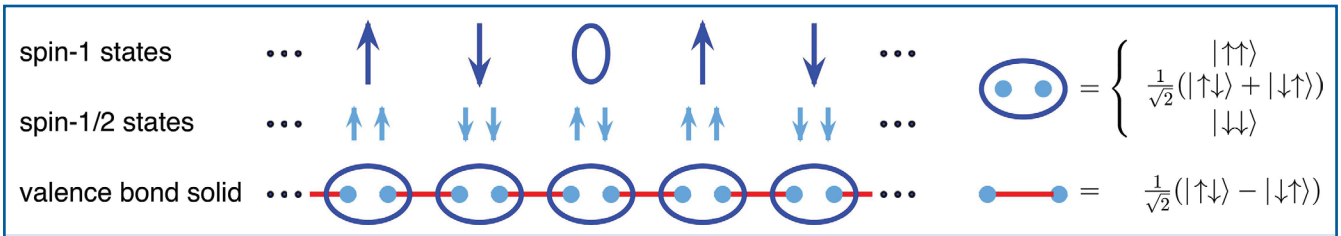

Fig. 5 Non-local antiferromagnetic order of spins 1 (top) is equivalent to a valence bond solid (bottom) of two spins 1/2 per site (middle) that form singlet bonds to neighbouring sites and triplet states on-site.

Half-odd-integer (1/2, 3/2, . . .) antiferromagnetic spin chains should resemble the gapless spin 1/2 case.

For spin 1, the Haldane ground state singlet is characterized by a topological string (i.e., non-local) order (Fig. 4) [16]. This string order can be understood as a dilute antiferromagnetic order: spin up (S^z = 1) needs to be followed by spin down (S^z =−1) or any number of diluting zeros (S^z = 0), and spin down by spin up or any number of zeros. Antiferromagnetic correlations remain short-ranged.

The gapped Haldane triplet excitation ruptures the string order in a topological (domainwall like) manner.

An equivalent picture for the string order is achieved by decomposing each spin 1 into two spins 1/2 [6]. On each site the spins 1/2 are paired symmetrically to a spin 1, between neighbouring sites they form a singlet pair state (antisymmetric pairing, valence bond). This valence bond solid reflects best the unbroken translation symmetry of the Haldane ground state singlet (Fig. 5).

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The Canadian Neutron Beam Centre: 1985 to the Present Day

by John Root and Daniel Banks

From Bertram Brockhouse's pioneering 1950s experiments, Canada's neutron beam capabilities grew organically into the Neutron and Solid State Physics (NSSP) branch of AECL's Physics Division. In the 60s and 70s, university researchers had access by collaborating with AECL scientists. Researchers from McMaster and Guelph established instruments at beams E3 and D3, respectively, but both were decommissioned by the mid-1980s. The high scientific impact of the NSSP branch during these decades is seen in the 2016 Nobel Prize in Physics, awarded to Duncan Haldane and two other American theorists, because AECL's Bill Buyers used neutron scattering to confirm the Haldane gap's existence in 1985, leading to acceptance of the future laureates' theories, which in turn opened the field of topological materials.

The construction of DUALSPEC (1985-1992), at a capital cost of $4M, marked a turning point for general user access to neutron beams at Chalk River. DUALSPEC, including the C5 Polarized Beam Triple-Axis Spectrometer and the C2 High Resolution Powder Diffractometer, was funded 50:50 by AECL and NSERC via McMaster University. Malcolm Collins (McMaster) led 11 university scientists from McMaster, Toronto, Guelph, Laurentian, Queen's and Waterloo on the proposal [1]. Because the two beams are only three feet apart in height, AECL designed a single monochromator shield that would allow both to operate independently.

Neutron scattering researchers established the Canadian Institute for Neutron Scattering (CINS) in 1986 to maximize access to DUALSPEC, evaluate beam time proposals for scientific merit, and represent their collective interests. DUALSPEC's original applicants were joined by others from the University of New Brunswick, St. Francis Xavier, Simon Fraser, and Dalhousie in an NSERC infrastructure grant for $55K/yr, paid via McMaster and matched by

Summary

A program perspective on Canada's primary neutron scattering laboratory as a scientific user facility, and on parallel work to support consideration of replacing the National Research Universal (NRU) reactor.

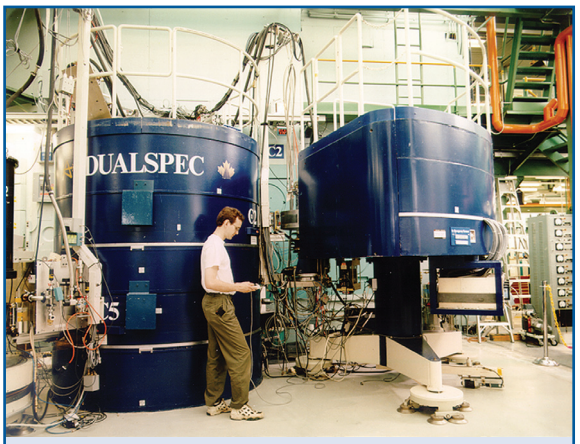

Fig. 1 AECL scientist Ian Swainson adjusting the scattering angle of the C2 powder diffractometer, on the upper beam of DUALSPEC to the right, with the C5 triple-axis spectrometer positioned on the lower beam, to the left.

AECL, for DUALSPEC commissioning and operation starting in 1991. Throughout 1992, DUALSPEC supported 46 users from 9 Canadian universities and 12 foreign institutions, a good beginning for a user-access program [1].

Although the total grant of $110K/yr did not cover DUALSPEC's full costs, AECL increasingly welcomed user access to four of its other spectrometers: three triple-axis spectrometers at E3, L3, and N5, and a prototype low-angle scattering instrument at T3.

While academic access was ramping up, the AECL NSSP branch was developing applications for industry. In 1983, Tom Holden demonstrated stress mapping of intact components of nuclear power reactors on the L3 beamline and established a commercial service, Applied Neutron Diffraction for Industry (ANDI). After the Space Shuttle Challenger disaster in January 1986, ANDI was selected over comparable USA capabilities to examine an as-manufactured section of booster rocket casing. Neutron diffraction showed that the stress distribution was acceptable, pointing the failure investigation to look elsewhere [2]. ANDI became the go-to service for failure analyses for high-profile accidents, such as the Space Shuttle Columbia

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in 2003 and the 2005 train derailment at Lake Wabamun in Alberta, which spilled 800,000 litres of oil. ANDI ran successfully for over 20 years, providing proprietary data to enhance safety and reliability or optimize processes in energy and manufacturing sectors such as air, automotive, rail, and marine transportation, metal production, and oil & gas.

In the early 1990s, the future was bright at AECL's newly renamed Neutron and Condensed-Matter Sciences (NCMS) branch, with the success of ANDI and the growing user-access program. The user community rallied behind a concept for NRU's successor, the Irradiation Research Facility (IRF). This hopeful outlook was validated when Brockhouse shared the 1994 Nobel Prize in Physics with Clifford Shull of Oak Ridge National Lab (USA) for their pioneering contributions to neutron scattering.

Yet clouds of uncertainty began to gather. The McMaster Nuclear Reactor (MNR), which had beamlines for powder diffraction and a Small-Angle Neutron Scattering (SANS), was planned to shut down in 1996 (MNR still operates today). When its SANS detector failed in 1994, there was no funding to continue, and both beamlines were eventually decommissioned. NSERC declined a $3M proposal in 1995 for a new SANS instrument at the vacated D3 beam line at the NRU reactor, to be funded jointly with AECL, as was DUALSPEC [3]. Reportedly, NSERC's decision reflected an understanding that NRU would close in 1998. Meanwhile, the federal government was reducing programs to balance its budget. In mid-1995, it became apparent that AECL's basic research programs were at risk in the federal program review. The neutron user community was mobilized and about 100 support letters for the NCMS branch were secured from eminent Canadian and foreign scientists, directors of foreign neutron laboratories, and representatives of industry.

In spring 1996, AECL's budget was cut deeply, and decisions were made to eliminate many activities in physics, health, and environmental sciences, including the TASCC facility, a leading particle accelerator for heavy-ion nuclear physics. Though AECL continued operating the NRU reactor at ~$20M/yr in direct costs to support its reactor business and generate medical isotopes, it would not continue the expense of $2M/yr to operate the NCMS branch, but allowed a year to find other arrangements. Senior officials at Natural Resources Canada (NRCan, responsible for nuclear matters) and Industry Canada (responsible for science and economic development) agreed that the NCMS's capability should be retained, but it was still in danger of falling between jurisdictional cracks.

Ironically, in early 1997 while NCMS staff awaited news of their fate since they were deemed non-essential for AECL's nuclear business, they were called upon for stress measurements for New Brunswick Power, which was bleeding about $400K per day because of an unplanned shutdown of the Point Lepreau Nuclear Generating Station. A heavy-water leak had been found in one of hundreds of feeder pipes running between the reactor core and the steam generators. About 16 hours after receiving an archived feeder, NCMS staff established that the stress was a worst-case scenario that resulted from the manufacture of the bend. Understanding the problem was key to providing assurance to the regulator, which allowed the reactor to restart. Resolution of this emergency led to a line of research on feeders that saved nuclear plant operations hundreds of millions of dollars over the following years [4].

A deal was struck some weeks later and in April, the NCMS branch was transferred to the National Research Council of Canada (NRC), then under President Arthur Carty, as the Neutron Program for Materials Research (NPMR). Some staff were laid off because of a smaller budget: $1.5M/yr for three years primarily from NRCan with contributions from NSERC and NRC, after which NRC might decide to assume ongoing responsibility for the program. The $110K/yr funding for DUALSPEC operation continued separately.

As NRC now had a direct interest in neutrons, NRC and AECL cooperated on the "Canadian Neutron Facility" (CNF), a new concept for NRU's replacement for nuclear materials testing, neutron scattering, and limited isotope production (excluding Mo-99, which was to be made by the MAPLE reactors under construction). The CNF was approved in principle by a cabinet committee in 1999, and thus was ready to be funded, if funds were found. However, AECL withdrew its support in 2000 to focus resources on developing an Advanced CANDU reactor.

Well supported by NRC and the neutron scattering community, the NPMR emerged strongly from the crisis of the mid-90s. It soon began to grow again, attracting $1M/yr from NSERC's Major Facilities Access (MFA) program in 2001 toward maintaining the entire facility, not just DUALSPEC, in a state of readiness for user access. As CINS president, Bruce Gaulin (McMaster) was the principal applicant to the MFA program, later remodelled as the Major Resource Support (MRS) program, and the funds were paid via McMaster. Excluding the T3 beamline, which had become obsolete, NPMR's five active beamlines averaged 30 users per beamline per year. An international peer review in 2004 reported that only three facilities in world had more users per beamline (ILL, ISIS, and NCNR), observing that "an extraordinarily high fraction (~90%) of the beam time is available to users" compared to 50-66% elsewhere, and the 13% of beam time used by industry as a commercial service "is an extraordinarily high number matched by no other neutron scattering facility." The NPMR "has had productivity per dollar, per instrument, and per staff scientist that competes well with the very top international neutron facilities" concluding that "NPMR is a world-class program run on a shoestring" [5]. Yet the uncertain future about the NRU reactor's lifetime, and a replacement facility, was a challenge, and investment in new equipment or upgrades were not keeping pace with world-leading facilities, for the most part.

In 2004, a CFI award was granted to Western University to build a $2.4M neutron reflectometer at the D3 beam. David Shoesmith and Jamie Noël led the proposal, supported by 12 universities. NRC's Zin Tun provided scientific leadership for the design and D3 opened for user access in 2007. Also in 2004, NSERC's contribution to operate the NPMR was renewed under the leadership of Dominic Ryan (McGill), who served as CINS President until 2014.

Renamed the Canadian Neutron Beam Centre (CNBC) in 2005, the lab reached its peak around 2008, with 6 beamlines highly subscribed by a community of over 700 frequent and occasional research participants of all types: scientists, engineers, and students, from universities, industry, and government labs, from Canada and around the world. The ANDI service had generated about $6M of fee-for-service revenue from over 200 projects. The CNBC had delivered over 1000 beam allocations to users since 2001, and NSERC increased its MRS grant for five years, starting in 2007. The CNBC's $4M/yr operations had achieved a funding balance of 60% from NRC for baseline operations, 30% from NSERC to maintain facilities in a state of readiness for user access, and 10% from commercial services and other R&D income. Numerous beamline upgrades were distinguishing the CNBC in stress scanning, powder diffraction, and polarized triple-axis spectroscopy.

Prospects for a successor to NRU were again looking up, as discussions began anew in 2006 between Industry Canada (IC), Natural Resources Canada (NRCan), AECL, and NRC. These agencies reflected intertwined issues under federal review: Chalk River's role as a national nuclear lab, the structure of AECL, a national nuclear policy, Mo-99 supply, and a framework for investing in major facilities like TRIUMF, the Canadian Light Source, and perhaps a replacement for NRU. The Canadian Neutron Centre (CNC) concept was a flexible, versatile machine that could do whatever Canada might need from a research reactor, including the full range of isotope production, which distinguished the CNC from the earlier CNF, because the MAPLE reactor project was in trouble at the time. CINS published the requirements of neutron beam users in the CNC in 2007 [6]. The Canadian Nuclear Society made a parallel document outlining requirements for reactor-based nuclear science and technology [7], while the Canadian Nuclear Association, which represents companies, helped NRCan to study Canada's needs for nuclear S&T broadly.

Fig. 2 The D3 reflectometer at the time of its opening in 2007, labelled with logos of the funding partners: the Canada Foundation for Innovation, the Ontario Ministry of Research and Innovation, the Ontario Innovation Trust and the National Research Council. Western University was then known as The University of Western Ontario.

The CNC proposal could not retain government attention due to distracting issues such as the divestiture of AECL's commercial business lines to a new company Candu Energy (2009-2011), global shortages of Mo-99 caused by NRU maintenance shutdowns (2007, 2009-2010), and a $1.6B lawsuit from Nordion over cancelling the MAPLE reactors (2008-2013). The government postponed considering the CNC pending AECL's restructuring, and the NRC lost interest after its own restructuring to become more responsive to industry began in 2010. In March 2010, the federal government sent a clear signal to industry and the Ontario government, which owns most of Canada's nuclear power stations, that it was not interested in taking on a new research reactor by itself, calling for "appropriate sharing of costs among the many users and beneficiaries of such a facility" [8]. Although the Saskatchewan government offered $200M in 2009 toward building a dual-purpose reactor for isotopes and neutron beams, that proposal left most of the cost with the federal partner and did not meet the nuclear industry's needs.

Phase two of AECL restructuring began with a February 2012 call for expressions of interest in AECL's Laboratories, which warned "should there be limited or insufficient response, support may be reduced or ended for some or all of the Laboratories' activities beyond radioactive waste and decommissioning obligations." Although CINS and other groups of researchers made submissions, NRCan reportedly didn't recognize a strong constituency for the neutron beam mission, because senior university leaders were not strongly engaged. In February 2013, NRCan announced that the labs would retain a research mission focused on industry and government needs, and that government would assess the business case "for an industry-driven nuclear innovation agenda."

That decision was just in time to preserve the CNBC. Federal austerity measures following the global 2008 recession led to NSERC's moratorium on its MRS program and significant cuts at NRC. The CNBC was at the end of a year of "wind-down" MRS funds when NRC decided to cut CNBC's funding, effective April 1, 2013. However, the CNBC had a role to play for AECL, demonstrating return on investment in NRU and retaining capability that might comprise part of a future nuclear innovation agenda. Therefore, AECL agreed to take responsibility

for operating the CNBC, with the NRC staff seconded to AECL, and assets remaining property of NRC.

From 2009 to 2013, the uncertainty about NRU's future, hiring freezes within NRC, the lack of neutrons for 15-months beginning in 2009, and MRS funding losses presented severe challenges. The CNBC did not recover from losses in soft materials expertise or in the ANDI service's momentum. Yet in other areas, the CNBC bounced back under AECL and its successor organization, Canadian Nuclear Laboratories (CNL). Research participants grew to over 800 over the last five years, compared with over 700 for the five years ending in 2008. Although proprietary research for industry dropped off, the total proportion of beam time for industry remained the same due to a large increase in public domain research involving prominent companies such as GM, Ford, Nemak, Yamaha, StandardAero, Rolls Royce and Schlumberger.

In February 2015, NRU's final closure was announced as March 2018, ironically providing more certainty than in the past 20 years, and enabling productive final years. Now that the NRU reactor is closed, a final year remains in the agreements between NRC, AECL and CNL for continued operation of the CNBC, to wrap up the scientific outcomes of the final neutron beam experiments, and organize future placements for staff and equipment.

This is not the end of Canadian neutron scattering. An enduring truth is that the unique ways neutrons interact with materials enables neutron beams to reveal knowledge that may be difficult or impossible to acquire otherwise. Canadians will still need neutron beams to train and work at the leading edges of science and technology. Companies will still need them to develop new products, to optimize their processes, or to enhance reliability.

The neutron beam community must continue without a domestic high-flux source and without the leadership of the federal agencies that provided stewardship of Canada's neutron-beam capabilities until now. The next article describes the Canadian Neutron Initiative, which seeks to unify all Canadian stakeholders behind a new framework – a new university-led framework that partners with world- leading foreign facilities, fully exploits the medium-flux McMaster Nuclear Reactor, and establishes a trusted voice in the coming deliberations [9] about access to neutrons for the long term.

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The Canadian Neutron Initiative: Planning for the Future of Neutron Scattering in Canada

by Thad Harroun

There's a balance to strike between the federal government's economic responsibilities and the scientific research it funds. Since 2007, and amended in 2014, Canada's federal government has adopted five key Research Priorities, with several additional Focus Areas to assist with it's decision making [1]. The recent release of the report on science funding landscape, Canada's Fundamental Science Review, known generally as the Naylor Report, shows that discovery research across all the granting councils is badly underfunded, and there is an acute need for the funding of major research facilities [2]. Additional calls from Universities Canada have urged the government to establish a dedicated support fund for international research collaboration, and additional support for research infrastructure through the Canada Foundation for Innovation [3].

One common thread running through most of these federal research Focus Areas could be summarized as research in materials. Newly designed materials, and repurposed well known materials, are needed for biomedical technologies, advanced manufacturing, and clean energy systems. The physical characteristics of these materials under varied conditions must be understood to advance the technology and make new discoveries. The grand challenge is to fully characterize their properties at atomic and molecular scales, for which Canadian researchers need a complete 21st century toolkit for probing materials. There are many probes available to the material scientist to study the nano and atomic scales; electrons, X-rays, and neutrons, each with their own physical capabilities, limitations, and overlapping complementarity.

The advancement of our understanding of the materials around us is determined in large part by the capabilities of our scientific equipment. And as discussed in the recent commentary of Charles Day, Editor of *Physics Today*, on the extraordinary advancements of electron microscopy of the last 10 years, advances in scientific equipment are driven by robust funding of the research topics that equipment is used to study [4]. When scientists are properly funded to pursue frontiers of knowledge in particular area, instrumentation designers will rise to the challenge. Advances in instrumentation lead to the discoveries of tomorrow, and eventually, this equipment becomes the necessary routine measurements at the beginning of every new research direction.

Summary

The Canadian Neutron Initiative is a University-led group with a plan to address Canada's looming shortage of neutron beams for materials research when the National Research Universal (NRU) reactor at Chalk River closes in March of 2018.

For many Canadian researchers, a crisis is at hand with the final closure of the venerable NRU reactor at the Chalk River Laboratories in March 2018. NRU has been Canada's primary domestic source for research using neutron beams for six decades. Six research instruments of the Canadian Neutron Beam Centre, used by a community of over 800 researchers and students over the past five years for the understanding of such things as electrolytic corrosion, topological quantum materials, and cell membranes, will be shuttered along with the reactor. Meanwhile, $8 billion has been invested around the world since the year 2000 in new neutron beam instrumentation or new neutron sources. While an, the world is renewing their important scientific tool, Canada is losing it.

The Canadian Institute for Neutron Scattering (CINS) represents researchers using neutron beams for materials research. Research by CINS members touch on every federal science priority. Eighty-two (82) Canadian researchers participated in a recent CINS survey in which one third self-identified as Material Scientists, another third as researchers in Physics, and the rest considered their research to be in the fields of Chemistry, Biology, or Engineering, with 3% choosing 'Other'. All respondents considered neutron scattering as 'very' or 'somewhat important' for advancing their research. The interested reader can find many examples of research advances by CINS members in the other articles in this issue of Physics in Canada, as well as highlights presented at cins.ca/discover.

More importantly, we found that 55% of the planned experiments by CINS members in 2017-2018 will be to the NRU, even in its last year of operation. The Canadian Neutron Beam Centre will continue to welcome over 200

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industrial and academic researchers, graduate and undergraduate students before winding down operations [5]. The demand for neutrons to advance the research of CINS members remains strong. With the closure of the NRU reactor, the research community must act now to prevent the complete loss of an important tool in the researcher's toolbox by establishing a program to ensure that Canadians researchers can effectively use other neutron sources in a world of increasing demand for neutrons.

THE CANADIAN NEUTRON INITIATIVE

The Canadian Neutron Initiative (CNI) is a response to the urgent challenge, aiming to provide continued access for Canadians to this critical scientific tool for the near and medium term. The CNI would establish a new leadership framework of Canada's capacity for materials research with neutron beams, by building on existing national and international resources. The Initiative will ensure Canadians can readily access neutron beams for world-class research and innovation in materials, as well as training students for highly-skilled careers [6].

The CNI is a university-led framework, driven by the University of Saskatchewan and McMaster University, in close collaboration with CINS and the Canadian Nuclear Association. As a pan-Canadian initiative, it is supported by other universities and organizations and presently continues to gather broad support. For the University of Saskatchewan, which has had great success in establishing a large scale user-facility for materials research in the Canadian Light Source synchrotron, the complementary technique of neutron scattering is a value-added proposition to the development of Saskatchewan as a leader in nuclear research for economic benefit. The Sylvia Fedoruk Canadian Centre for Nuclear Innovation at the University of Saskatchewan has already made great investments in the fields of nuclear medicine and nuclear policy research, has invested in materials researchers using neutron beams, and is now contributing its expertise to the CNI.

McMaster University has the largest group of materials researchers in Canada who use neutron beams and hosts the McMaster Nuclear Reactor (MNR), which will be Canada's most powerful multi-purpose research reactor by far at the time of NRU's closing. In the past several years, McMaster has invested heavily in expanding its physics, nuclear, and materials R&D capabilities at the MNR, such as the planned McMaster Intense Positron Beam Facility for materials surface research, and the unique High Level Laboratory Facility for handling large quantities of radioactive specimens.

The MNR is also endeavouring to help meet some of the demand for neutron beams when NRU closes. Through the Brockhouse Institute for Materials Research, construction is well underway for the $9M Canadian Foundation for Innovation and Ontario Innovation Trust funded 'MacSANS', a dedicated small angle neutron scattering beamline in Canada on beam port 4 of the MNR. The MNR has just enough space to operate perhaps two additional diffraction instruments, such as a powder diffractometer and a reflectometer.

University of Saskatchewan and McMaster University are natural leaders for the CNI as a pan-Canadian initiative that will address the loss of NRU for all Canadians across two time horizons. For the next decade, the CNI must focus on coordinating access to leading neutron-beam facilities abroad while fully exploiting domestic, university-based capabilities, including the MNR. By retaining and investing in Canadian capabilities, the CNI will also be able to assist materials researchers to participate in national decision-making processes surrounding large-scale research infrastructure, which could include a new research reactor for 2030 and beyond. Any such new reactor will include contributions from other stakeholders such as the nuclear power, manufacturing and medicine sectors.

Foreign Partnerships

With the loss of NRU, Canadian researchers will immediately need more access to world-leading neutron beam facilities abroad. Currently, over one-third of experiments originating in Canada are conducted in the United States, with a smaller 12% conducted in Europe. There are many hurdles to gain access to these facilities, chief among them is the current over-subscription rates, which can be as high as 4 times for some instruments. Furthermore, although new facilities are being built, the global supply of neutron beam time is shrinking overall because many old facilities have closed or are expected to close in the next 15 years. Another concern is the exclusion of applications from non-contributing countries at European facilities, especially the flagship Institut Laue Langevin (ILL) laboratory in France, and the new European Spallation Source (ESS) now under construction. It's not possible that the global capacity can accommodate an increase demand originating from Canada for neutron beam time without special intervention.

Several of the world's leading neutron scattering laboratories, including the ILL and the facilities in the USA, have expressed a keen interest in establishing a formal partnership with Canada. Funding and managing memberships in foreign facilities are therefore fundamental components of the CNI. Canada's experience with such a partnership consists of a CFI-funded contribution of $15M via McMaster University toward the construction of the SEQUOIA high resolution spectrometer and VULCAN engineering diffractometer at the Spallation Neutron Source at Oak Ridge National Labs (USA), which was exchanged for preferred access by Canadians for a portion of the beam time. However this agreement expires in 2018, and since it represents a significant fraction of the planned trips to the US by Canadian researchers this year, the expiry will add to the stress of finding beam time for experiments originating from Canada.

A new partnership that invests Canadian federal research dollars directly into a foreign laboratory could take several forms, but would certainly result in beam time set-aside specifically for

Canadian applicants on a much wider selection of instruments. This would ease the burden considerably for Canadian researchers, and open the door to others who are neutron scattering novices. In addition, we have identified several other important considerations that must go into an effective partnership agreement, such as travel support, development of ancillary equipment and local instrumentation expertise.

For CINS members, our 2017 survey revealed that the best instrument for their research goals, along with highly knowledgeable local collaborators, were the top concerns when planning a neutron laboratory visit. Reactor and spallation-based neutron sources offer a variety of means of neutron beam delivery; constant or pulsed flux, cold or thermal in energy. Thus, despite the broad overlap in experimental techniques available between facilities, the true strengths within the suite of instruments differ somewhat. As a result, many CINS researchers who use neutron beams frequently have a favorite instrument, with which they are most comfortable and have invested considerable time to understand its capabilities and quirks. For an occasional neutron beam user who may need access once every two or three years, accumulating this knowledge is more difficult. A central coordinating hub can help Canadians at any level of experience to plan, propose, and execute their experiments. The support and knowledge offered by local expertise is invaluable to successfully complete an experiment in the allocated beam time. The coordinating hub will ensure that there are local contacts at the foreign facility that will help guide Canadian visitors through their stay and experiments, and provide training on the data collection, analysis and archiving software.

Most facilities have invested heavily in special ancillary equipment including sample environments, such as cryostats, high magnetic fields, or liquid sample cells. Access to these sample environments is crucial to leverage the unique properties of neutrons to gain knowledge unavailable from other techniques. The neutral charge of the neutron and its weak interaction with many common materials allows the construction of sample chambers with large access windows, greatly simplifying their design compared to any other probe. The neutron's dipole magnetic moment allows for spin and magnetic field dependent measurements. Therefore, development of ancillary equipment that Canadians need would be another important function of the coordinating hub.

Clearly, quality instrumentation and collaboration as keys to a successful experiment were top of mind in our CINS member survey. For experienced users of neutron facilities, the valuable data is worth the time and monetary expense of planning and traveling abroad, as these issues were of lesser concern. However, hearing from the many occasional users of the Canadian Neutron Beam Centre, a trip abroad is prohibitively expensive and risky on tight research budgets. Without some experience, outcomes of a neutron experiments can be a little uncertain, and limited NSERC research money may be better spent at home. Even the tremendous learning experience for students to travel to a foreign laboratory may not be worth the risk. This leads to a vicious cycle, where the next generation of researchers simply do not consider neutron scattering as part of their research program, and while the rest of the world advances with new neutron sources, Canada is left behind. Thus the CNI believes that serious financial travel support is a necessary component to any partnership with a foreign facility.

Expanding Domestic Capabilities

Through the Canadian Neutron Initiative, Canada aims to continue to be good stewards of neutron beam research infrastructure both domestically and abroad. This means proper utilization of the McMaster Nuclear Reactor by expanding its operation schedule to 24/7 and to full power output, capital investment in beamlines and equipment, and critically, an on-going user program to ensure that the Canadian researcher can use these investments most effectively. For CFI funded projects, 87% of project leaders reported that they had both adequate financial and human resources for the operations of management of the infrastructure, primarily through Federal and Institutional grants [7]. This is not really true of MNR today, whose operational budget is limited to what it can recover through commercial revenues from sources such as isotope production and neutron radiography. It has little-to-no operating funding intended to support research presently.

In return for the envisioned investments through CNI, the MNR neutron beams would be available to all Canadian researchers without additional fees. Overall, only about 60% in total of CFI-funded infrastructure is made available to users outside the host institution [7]. The CFI often finds that for equipment it funded underutilization or oversubscription is very rare. However, if adequately supported and operated as a user facility, the MacSANS beamline after its completion in 2019 is expected to draw many polymer and soft material scientists now currently forced to travel abroad. MacSANS is designed to perform optimized neutron diffraction on nanoscale structure in the range from 1 to 100 nm, and could perform up to 40 experiments a year with an improved operating schedule of the MNR.

The CNI also has a priority to add at least two beamlines for routine diffraction experiments, and make user access easier and more convenient. For example, powder diffraction by X-rays is a routine tool for structural characterization of most newly synthesized crystalline materials. Neutron powder diffraction is as well, with the added benefits of being isotope or magnetic lattice sensitive. For stable samples, the flux of MNR is more than sufficient to collect high resolution data. A reflectometer for thin film measurements is also possible on a different beamline.

Paving the Way for the Future

Major investments in new neutron sources worldwide are required even just to keep pace with the closures of old neutron facilities. Canada should be at the discussion table for investing in new international sources and must consider

investing in a new domestic source. Over the next few years, the research community will continue to discuss the questions of how, what kind, and where, establishing itself as a strong constituency in a new research reactor alongside the communities that require isotope production capabilities and in-core testing for nuclear power applications. The focus of the CNI is to preserve and strengthen that community in the absence of a major domestic neutron beam source over the next decade, at least.

Canada has much to learn from experience of Denmark. The DR3 reactor at the Risø National Laboratory was permanently closed in 2000 due to a series of faults with aging infrastructure. This was the last domestic source for neutrons in Denmark, however, the Danish government heeded the needs of the researchers. In the following decade, several instruments were moved to foreign facilities, and the Danish government set up a travel fund so that its community of researchers could continue to collaborate with their European counterparts, and remain on the cutting edge of research.

It wasn't until late 2015 when the European Spallation Source (ESS) project was established by the European Commission as a European Research Infrastructure Consortium. Jointly owned by the governments of Sweden and Denmark, the ESS is currently under construction in Lund, Sweden, an hour by train from Copenhagen. Designed to be the world's most powerful neutron source, the user program for the first few beamlines should be open in 2023 to researchers from Denmark, Sweden, and other financially participating countries. It will have been nearly a quarter century since Danish scientists had direct access to a 'domestic' neutron beam facility, but they continue to use neutrons as a research tool thanks to a government responsive to the needs of its researchers.

In February 2017, King Carl XVI Gustaf of Sweden led a tour of the ESS construction site for the previous Governor General of Canada, David Johnston, and current Canadian Minister of Science, Kirsty Duncan, as part of a four-day Canadian state visit to Sweden. Canadian Nobel Laureate Art McDonald participated in the round table discussion during the February state visit, which focused on cross-disciplinary research as a vital driver for sectors such as life science, clean technology, forestry, and communications technology. McDonald strongly endorses the idea of a financial partnership with Canada and facilities such as the ESS, since `world-class research and innovation require large, national-scale science facilities that are accessible and maintained at the state-of-the-art' [8]. In November 2017, a delegation of CINS members representing quantum materials, engineering, biophysics, and energy research traveled to the ESS to discuss in greater detail possible scientific partnerships. We learned of the plans and needs of this complex facility and fill in details on how Canada can support, and benefit from this powerful laboratory.

Partnerships with world-leading foreign facilities, and expanded use of the MNR, will ultimately bridge the gap to a new Canadian neutron beam laboratory. Hopefully, in the not too distant future, we can reciprocate and bring the world's top researchers to a new neutron source here to Canada.

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Recent Triple-Axis Neutron Scattering Studies of Quantum Materials at the Chalk River NRU Reactor

by Zahra Yamani

Summary

Triple-axis neutron scattering is the technique of choice for studying collective excitations in condensed matter. This technique has been instrumental in unveiling spin excitations in highly correlated electron systems such as high T_c cuprate and the more recent iron-based superconductors and quantum magnets. This article briefly reviews recent research highlights on such materials using the triple-axis facilities at the Chalk River NRU reactor.

The ground-breaking technique of triple-axis neutron spectroscopy was invented [1] by Bertram Brockhouse in the 1950s first at the Chalk River NRX (National Research Experimental) and further developed at the National Research Universal (NRU) reactor. A few years earlier, Clifford Shull at Oak Ridge National Laboratory (ORNL) in Tennessee had already demonstrated the concept of neutron diffraction and the type of information related to the static nuclear structure it provides. In diffraction experiments, a crystal monochromator is used to select a specific and narrow slice of the wavelength distribution from the white neutron beam produced by the fission process in the reactor. The ingenuity of Brockhouse's invention was its simplicity. He added an additional crystal monochromator (called analyzer) after the sample to determine how much energy transfer to and from the sample occurs when monochromated neutrons interact with the sample. Thereby the technique is called triple-axis spectroscopy (TAS) since it requires rotation of three crystals: monochromator, sample, and analyzer. Brockhouse's invention led to a new area in experimental condensed matter physics, allowing determination of lattice (phonon) and spin (magnon) dynamics using neutron scattering technique for the first time. Brockhouse and Shull shared the 1994 Nobel Prize in Physics for their work in neutron scattering.

In 1955, experiments by Brockhouse on an aluminum single crystal in several different orientations led to the successful determination of a phonon dispersion curve for the first time, thus demonstrating convincingly the power of the TAS method. In 1962 Brockhouse relocated to McMaster University where he continued to train young students in using this technique until his retirement in 1984. In the 1960s and the years following young scientists, such as Bill Buyers, Roger Cowley, Eric Svensson, Gerald Dolling, Dave Woods, Brian Powell, Varley Sears and Tom Holden, joined the Chalk River lab and made significant contributions to the study of excitations in solids. These include lattice dynamics and phase transitions [2], crystal field, interatomic exchange and spin-orbit coupling in $KCoF_3$ [3], and later magnetic excitations in the famous hidden order in URu_2Si_2 [4]. Investigations of this mysterious hidden order continues to present day at CNL [5]. Perhaps the most significant experiment from this era was the study of spin excitations in the quasi-1D antiferromagnetic (AF) S=1 spin chain $CsNiCl_3$ in 1986 [6]. The experiments led by Bill Buyers discovered the presence of a gap in its spin spectrum. Duncan Haldane had predicted that a gap in spin excitation spectrum occurs for integer but not half- integer spin chains. Haldane shared the 2016 Nobel Prize in Physics with David Thouless and Michael Kosterlitz for their theories on such topological materials [7].

The condensed matter research program at CNL continues to thrive today, in particular in the area of emergent materials: novel superconductors (SC) and quantum magnets (QM). In this article, several research highlights from the past decade using the TAS C5 (polarized) and N5 spectrometers at NRU are reviewed. The selected examples reflect my personal research interests and do not intend to provide a comprehensive list of all the exciting research performed during this time. The C5 spectrometer was recently upgraded with a vertically focusing Heusler monochromator and thus provides a greater polarized neutron flux: perhaps the greatest of any steady-state neutron source in North America. Polarization analysis is a powerful tool for isolating and elucidating details of elastic and inelastic magnetic scattering cross-sections. This new monochromator together with a new five-coil assembly, to automatically change the orientation of the neutron spin parallel or perpendicular to the scattering vector at the sample position, make the polarized setup at C5 unique, allowing experiments on small samples and a precise determination of the

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sample magnetic moments. The N5 spectrometer was also recently upgraded with a new detector shielding drum, reducing the background to a level that TAS measurements on milligram size samples are now possible.

HIGH T_C SUPERCONDUCTING CUPRATES

Despite numerous experimental and theoretical studies since the discovery of high T_c superconductivity (HTSC) in cuprates in 1986, they still pose an immense challenge [8]. Fundamental questions, such as what is the pairing mechanism and what causes such high T_c, remain unanswered. Meanwhile, it is not hard to imagine the technological revolution that would occur by discovery of room temperature superconductivity. From early days, it became clear that magnetic rather than the electron-ion interactions play an important role in cuprates. Neutron scattering has proven to be a key experimental tool in unraveling both their static and dynamic magnetic properties.

The parent compound $YBa_2Cu_3O_6$ (YBCO6+x with x=0) undergoes a Néel transition to a long range antiferromagnetic (AF) order at T_N~450 K. The ordered phase is characterized by $\mathbf{Q}_{AF}$ = (0.5, 0.5, L) with integer L, where local spins of adjacent Cu sites in the CuO_2 building blocks of the material are antiferromagnetically coupled. The optimally doped YBCO does not show any magnetic long-range order. However, the presence of a resolution-limited excitation (the so-called resonance) peak at $\mathbf{Q}_{AF}$ and energy transfer, E_{res}, indicates magnetism is very much present. The resonance peak is correlated with superconductivity as its intensity increases below T_c and its energy scales roughly with T_c for optimally doped to slightly underdoped YBCO.

Stock *et al.* performed TAS experiments on the C5 spectrometer at NRU on underdoped detwinned YBCO6.5 single crystals with T_c = 59 K [9]. The crystals were prepared by the group of Prof. W. Hardy at University of British Columbia (UBC) who had recognized early the importance of annealing in addition to the oxygen content for the charge transfer to the CuO_2 planes [10]. The high quality of UBC crystals and careful experiments by Stock *et al.* allowed for a complete determination of the magnetic properties of YBCO6.5. They found that the resonance remains almost resolution limited and occurs at a lower energy that is consistent with the doping dependence of the resonance energy for higher doped YBCO. While the intensity of the resonance peak showed a clear increase below T_c, it was found to first appear at temperatures higher than T_c, suggesting it may be related to the pseudogap phase [9].

Li *et al.* performed TAS experiments on the C5 spectrometer at NRU to study lower doped detwinned YBCO6.45 with a lower T_c of 48 K [11]. They found the resonance peak is still correlated with T_c, but is no longer resolution limited. The position of the resonance peak was also found to be lower than the prediction of a linear dependence with T_c from the higher doped region. Based on these results they suggested that the change in the behaviour of the spin dynamics within the SC dome might be related to a fundamental change in the electronic state of the material due to a metal-to-insulator transition (MIT) inside the SC dome [11].

Stock *et al.* later used the C5 spectrometer at NRU to study further lower doped YBCO6.35 (T_c = 18 K) [12,13]. Their results showed that the only prominent feature of spin spectrum is a very broad and weak peak at low energies. They showed that this peak is overdamped and can be fit with a modified Lorentzian. They also found a quasi-elastic and commensurate peak (central mode) at the $\mathbf{Q}_{AF}$ position for this low doped YBCO6.35 which is absent for higher doped YBCO. The central mode intensity was found to gradually grow on cooling with no Néel anomaly. The results were interpreted in terms of a soft mode driving the central mode [12].

Yamani *et al.* performed TAS experiments on the C5 spectrometer at NRU to study YBCO6.33 crystals with exceedingly lower doping yet superconducting with T_c = 8.5 K, less than 1/10 from the optimally doped T_c [14-16]. Similar to YBCO6.35, they found that there is no sign of resonance and that the spin spectrum only consists of a weak and broad excitation at low energies as well as a quasi-elastic peak with much higher intensity (central mode). The lack of a resonance peak at these low doped yet superconducting materials suggest [14] that the resonance peak may not be required for the superconductivity in cuprates. The central mode peak in YBCO6.33 is also commensurate with the lattice and even though still broader than the resolution, it is narrower in YBCO6.33 than YBCO6.35. This indicates that the magnetic correlation lengths increase by reducing doping from YBCO6.35 to YBCO6.33. The fact that for both of these lightly-doped YBCO6.35 and YBCO6.33 only commensurate quasielastic peaks were observed suggests that similar to the resonance peak, the stripes may not be essential for superconductivity in general.

Yamani *et al.* found that in YBCO6.33 the quasi-static correlations also gradually grow on cooling albeit from higher temperatures than YBCO6.35 [14]. Similar experiments under an applied magnetic field revealed no effect on either the static or dynamic correlations while the applied field reduced T_c [14]. This indicates that the lack of a Néel anomaly is not due to the presence of superconductivity and that at this low doping, the spins responsible for AF correlations behave independently from the charges responsible for superconductivity. Since the correlations remain short-range and their temperature dependence does not show any Néel anomaly, a spin-glass state was suggested [14] to coexist with SC.

Although the magnetic excitations measured [14] as a function of **Q** (Fig. 1) revealed no hour-glass dispersion, Yamani *et al.* found that the momentum dependence of the width of the high energy peaks is similar to the spin-wave velocity of the insulating YBCO6.15. From these observations it was suggested [14]

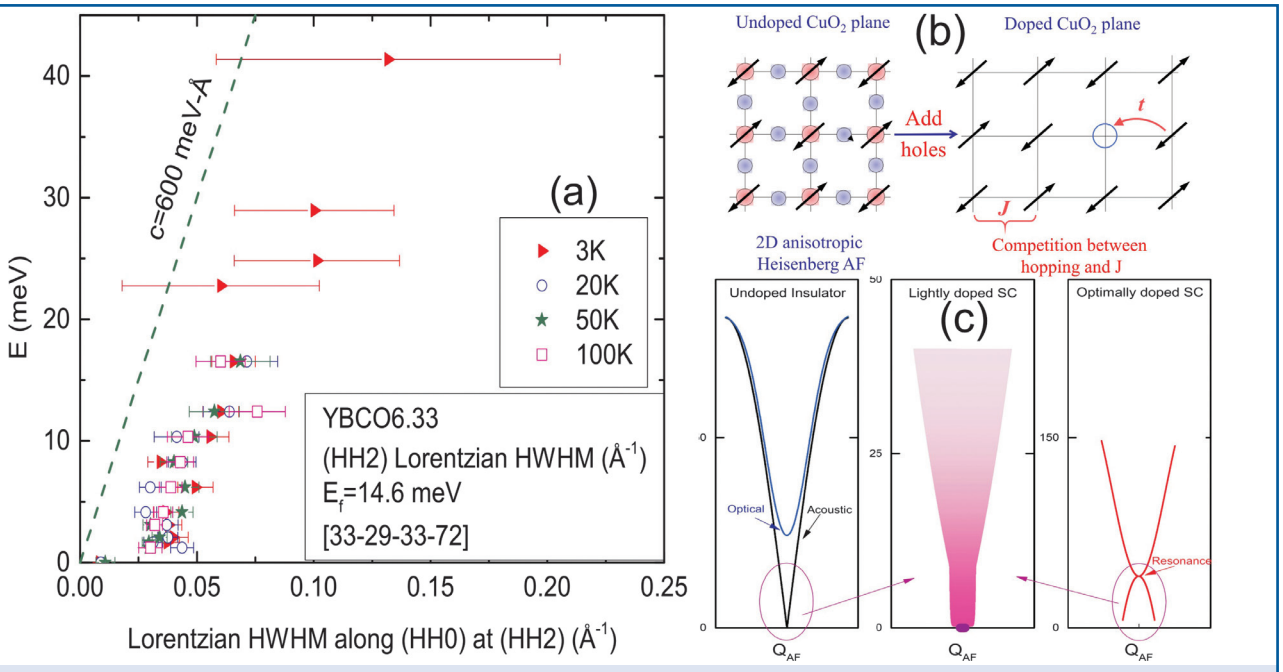

Fig. 1 (a) The resolution-corrected momentum width of the inelastic scattering. (b) The doped holes are effective in destroying long range AF order since each doped hole affects four AF neighbouring bounds. (c) Magnetic excitations in undoped insulator (left), YBCO6.33 (middle), and optimally doped YBCO (right) are schematically depicted. Adapted from Ref. [14].

that the suppression of the low energy excitations, a drastic change upon entering the SC dome, may be the key for inducing superconductivity in cuprates.

IRON-BASED SUPERCONDUCTORS

In 2008, HTSC was discovered in iron pnictides, containing iron ion with strong magnetism, sending shockwaves to the condensed matter community yet again. In conventional superconductors it is well known that addition of a small amount of magnetic impurities significantly reduces T_c. This discovery also revitalized the interest in superconductivity as other materials with T_c beyond the 30 K limit (electron-phonon coupling) than cuprates became available, generating hope that there could be other classes of SC with even higher T_c. Similar to cuprates it was soon established that magnetism plays an important role in pnictides [8]. A tetragonal-to-orthorhombic structural phase transition at T_s was found to be followed by a paramagnetic to AF phase transition at T_N with a collinear magnetic structure. For most pnictides T_s and T_N are identical or very close to one another. Wilson *et al.* used the C5 and N5 spectrometers at NRU to determine the magnetic and structural phase transitions in $BaFe_2As_2$ [17,18]. Later the effects of uniaxial strain on the structural and magnetic phase transitions in $BaFe_2As_2$ [19] and in Co-doped $Ba(Fe_{1-x}Co_x)_2As_2$ [20] were studied. Surprisingly, it was found that relatively small strain fields can change the magnetic order parameter and results in a decoupling between T_s and T_N. The evolution of the anisotropic spin excitations in $BaFe_{2-x}Ni_xAs_2$ was determined by Luo *et al.* by detailed inelastic experiments performed at NRU on the C5 spectrometer [21,22].

From the early days of studies on pnictides, two schools of thought have developed. One is based on itinerant electron physics which appears to be consistent with metallic properties of these materials. The other school of thought is based on the localized electron physics. Song *et al.* performed [23] TAS experiments on the C5 spectrometer at NRU to study the evolution of magnetism in $NaFe_{1-x}Cu_xAs$. For small Cu doping, superconductivity is induced and the static AF order is suppressed (Fig. 2). For doping well below 0.5, the magnetic transition is gradual and spin-glass-like. With increasing Cu doping, the scattering profile becomes narrower and stronger, changing from a broad peak indicative of the short-range magnetic order to an essentially instrument resolution limited peak with long-range magnetic order at x = 0.44. When doping approaches x = 0.5, the transition at T_N becomes more well defined concomitant with appearance of the insulating behaviour. This study showed for the first time that the SC phase can be continuously tuned to the Mott insulating phase, thus providing a direct evidence that the material is more correlated than itinerant [23].

When nearly 50% of Fe ions are replaced by Cu, a real space Fe and Cu ordering occurs which is a structural analogue of the magnetic order in pure NaFeAs. Thus, the use of polarized neutrons is crucial to separate magnetic from nuclear

scattering [23]. By polarizing neutrons (**P**) parallel to **Q**, the spin-flip (SF) scattering is sensitive to the magnetic moment (***m***) components that are perpendicular to **Q** ($\boldsymbol{m}_\perp$) whereas the non-SF (NSF) scattering probes pure nuclear contribution. For neutron polarization perpendicular to **Q** (**P**⊥**Q**), the SF scattering is sensitive to the perpendicular component of the moment that is also perpendicular to the neutron polarization ($\boldsymbol{m}_\perp \perp \mathbf{P}$), while the NSF scattering is sensitive to the perpendicular component of the moment that is parallel to the neutron polarization ($\boldsymbol{m}_\perp \| \mathbf{P}$). The experiments shown in Fig. 2 confirmed [23] the presence of a magnetic scattering at 2 K that disappears at 240 K, in addition to the temperature-independent NSF nuclear super-lattice reflection.

NEW ELECTRONIC STATES IN STRONGLY CORRELATED ELECTRON MATTER

A plethora of new electronic phases have recently been uncovered in a new class of spin-orbit Mott insulators with both strong spin-orbit coupling (SOC) and electron-electron interactions [24]. 5d transition metal oxides, such as $Sr_3Ir_2O_7$, are considered excellent test systems for exploring carrier substitution in spin-orbit Mott materials and for hosting new spin- orbit generated states [24]. Dhital *et al.* used [25] the N5 spectrometer at NRU to study Ru doping in $Sr_3(Ir_{1-x}Ru_x)_2O_7$. The Ir^{4+} ions ($5d^5$) carry the magnetism in pure $Sr_3Ir_2O_7$ with a Néel transition at T_N = 285 K to a G-type AF structure. Dhital

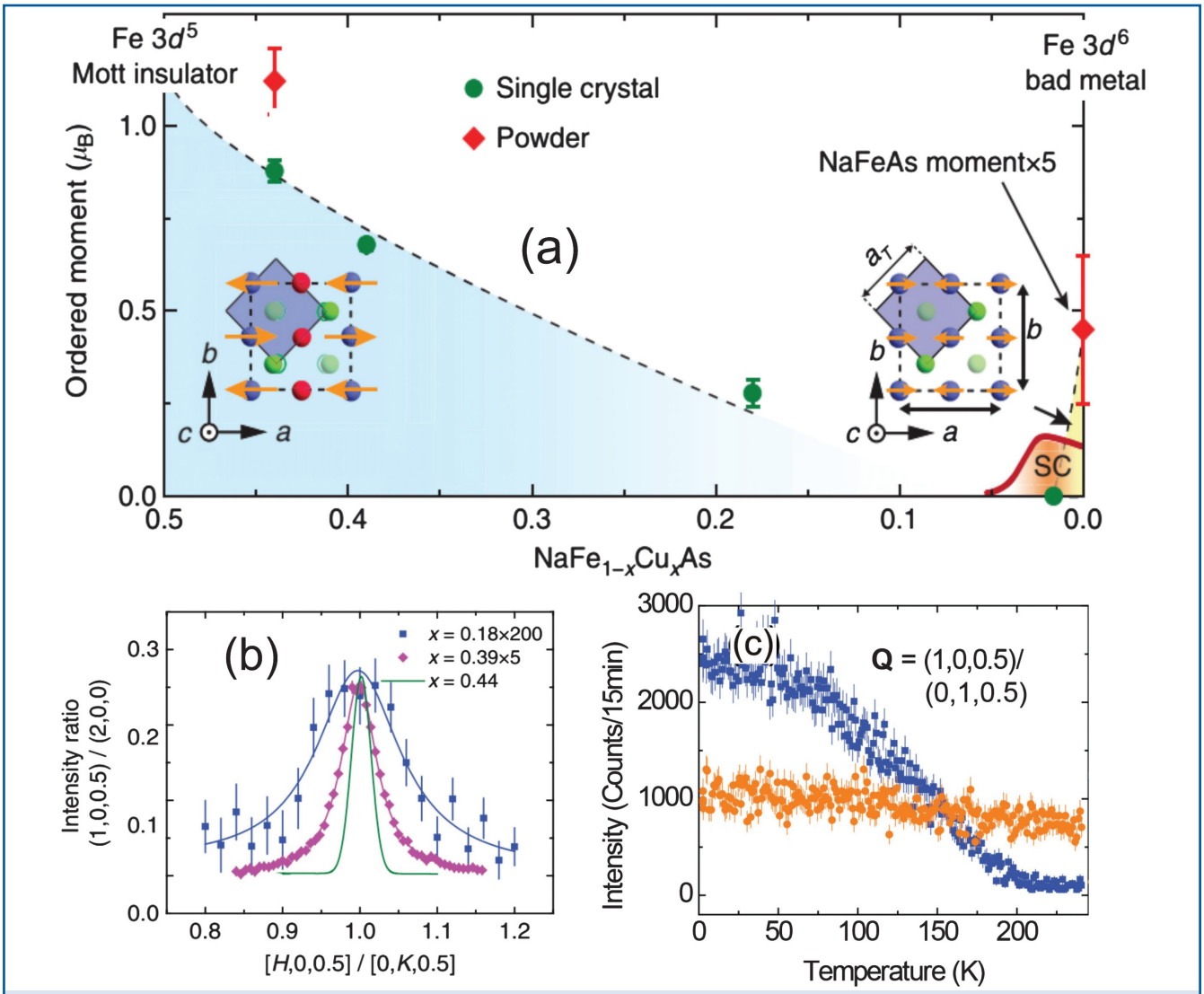

Fig. 2 (a) Magnetic phase diagram of $NaFe_{1-x}Cu_xAs$. (b) Scans along the [H, 0, 0.5]/[0, K, 0.5] direction vs x. (c) Temperature dependence of SF (blue squares) and NSF (orange circles) channels at (1,0,0.5)/(0,1,0.5). Magnetic signal at (0,1,0.5) is seen in the SF channel whereas super-lattice signal coming from (1,0,0.5) is seen in the NSF signal. Adapted from Ref. [23].

et al. showed that the addition of Ru atoms induces charge carriers and weakens the AF order [25]. Initially, the added charges remain in small metallic regions resembling metallic puddles due to the presence of strong correlations. With further increase of the Ru doping, puddles begin to percolate and eventually coalesce to induce a metallic state where charges freely flow. Eventually at a critical doping (x_{cr}), a transition to a metallic regime occurs paralleling the behaviour of Mott insulators. Dhital *et al.* also used polarized neutrons on the C5 spectrometer at NRU to demonstrate that a Bragg peak observed at 300 K (>T_N) in pure $Sr_3Ir_2O_7$ was non-magnetic and due to a nuclear superlattice structure.

Hogan *et al.* later studied [26] the magnetic order in La-doped $(Sr_{1-x}La_x)_3Ir_2O_7$ by means of TAS experiments on the N5 spectrometer (Fig. 3). The results indicated that upon doping electrons, the AF moment is immediately reduced. The reduction in the AF moment under light electron doping was found [26] to largely arise from electronic phase separation of the sample into AF-ordered insulating and paramagnetic metallic regions. An additional structural order parameter develops at T_S which increases with the growth of the volume fraction of the metallic phase upon La-doping. Beyond $x_{cr} = 0.04$, an abrupt, first-order phase boundary is observed where the Néel state is suppressed and a homogenous, correlated, metallic state appears and the system becomes globally metallic. It was suggested [26] that the structural distortion represents a competing instability with the parent spin-orbit Mott state.

Low dimensional spin systems exhibit many exotic magnetic properties. Spin-ladders have been the subject of intense interest recently as they are intermediate objects between 1D and 2D systems [27]. Plumb *et al.* performed [28] TAS experiments on the C5 spectrometer at NRU to study the ground state of the newly discovered quasi-2D spin-ladder $BiCu_2PO_6$. Results confirmed [28] that the $BiCu_2PO_6$ system can be described by weakly interacting two-leg ladders where frustration drives incommensurate dynamic correlations, and showed the importance of strong anisotropic interactions in addition to frustration in this material.

FUNCTIONAL MATERIALS

Functional materials consist of a large class of systems with properties important for technological applications. They are also of significant scientific interest because they possess strong electronic interactions. Multiferroics, exhibiting simultaneous ferroelectricity and magnetism because of cross-coupling between ferroelectric and magnetic order parameters, are among the most sought after functional materials [29]. Neutron scattering again has proven to be an essential tool unveiling their novel properties. Christianson *et al.* used the C5 and N5 spectrometers at NRU to perform polarized and non-polarized neutron scattering experiments under an applied field in the scattering plane of a multiferroic $LuFe_2O_4$ single crystal [30,31], a unique capability at CNL enabled by the M2 horizontal field magnet. They found a 3D Néel order below

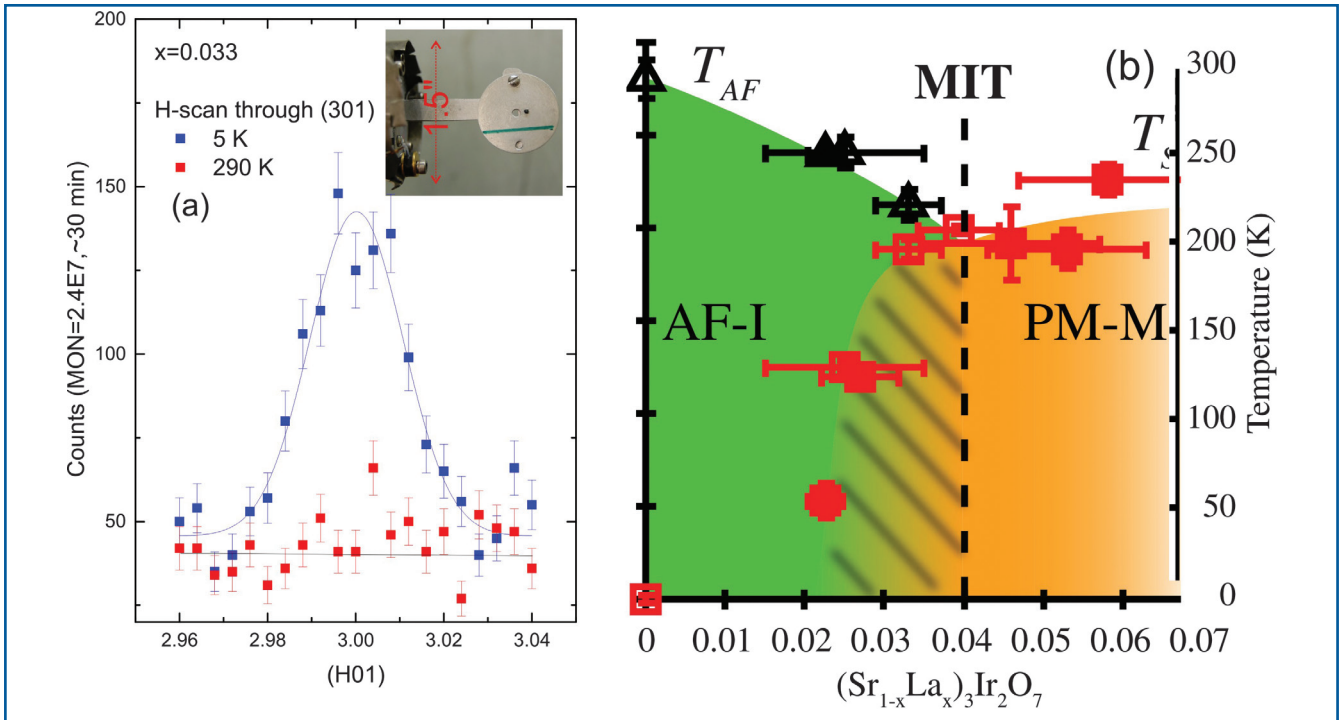

Fig. 3 (a) A representative scan through the magnetic peak (3, 0, 1) for x=0.033 in $(Sr_{1-x}La_x)_3Ir_2O_7$. The inset shows a picture of the milligram-size crystal used in the measurements. (d) Magnetic phase diagram of $(Sr_{1-x}La_x)_3Ir_2O_7$. Adapted from Ref. [26].

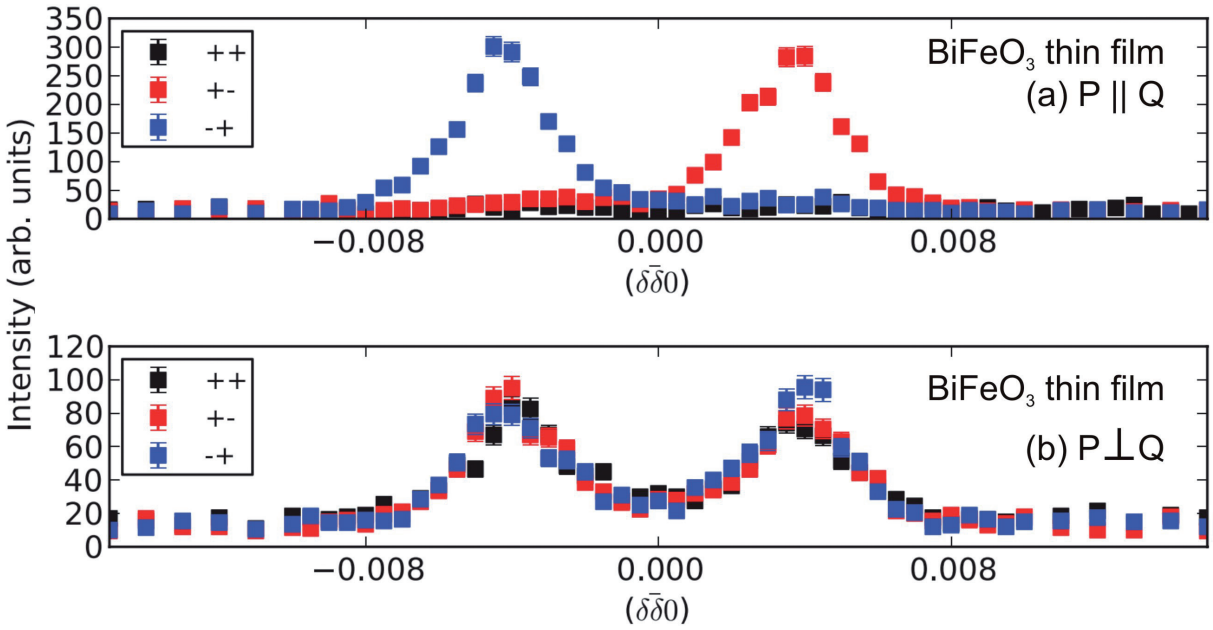

Fig. 4 SF and NSF cross-sections for **P**||**Q** (a) and for **P**⊥**Q** (b) measured close to $\mathbf{Q}_{AF}$ on a $BiFeO_3$ epitaxially grown thin film on $SrTiO_3$ substrate. Adapted from Ref. [32].

T_N = 240 K with a ferrimagnetic spin configuration arising from the charge ordering at 320 K.

$BiFeO_3$ is perhaps the only material that is both magnetic and strongly ferroelectric at room temperature [29]. $BiFeO_3$ undergoes a Néel transition to a G-type like AF order at T_N = 643 K and a ferroelectric Curie transition at T_c = 1103 K. Ratcliff *et al.* performed non-polarized and polarized experiments on the C5 spectrometer at NRU to study the magnetic structure of expitaxially grown $BiFeO_3$ films on $SrTiO_3$ substrates with ferroelectric monodomains [32,33]. The results indicate that close to $\mathbf{Q}_{AF}$=(0.5, 0.5, 0.5) a strong splitting between the I^{+-} and I^{-+} cross sections is observed for **P**||**Q**, whereas for **P**⊥**Q**, they have the same intensity (Fig. 4). The magnetic structure of this $BiFeO_3$ thin film was thus concluded [32] to be markedly different from that of a bulk single crystal since it contains a cycloid with moments spiraling in the plane normal to the polarization. The strain effects were suggested to cause the difference with the bulk [32]. The neutron scattering results provided clear evidence that the application of an electric field changes the AF domain population (concomitant to changes in the ferroelectric domains), thus suggesting a possible new direction for the realization of scalable magnetoelectric $BiFeO_3$-based thin film devices.

CONCLUSION

The thermal triple-axis instruments at the NRU reactor at CNL have been improved to increase neutron flux and to be more versatile with the addition of multi-wire detectors, extreme sample environments and sophisticated polarized setup. The TAS studies of novel superconducting and magnetic materials mentioned here demonstrate that the facilities at NRU can produce information about our world that command international recognition.

The TAS facilities at NRU have also played a tremendously important role in the training of young scientists either through performing experiments as part of graduate theses, hands-on summer schools or three-day courses [34]. Obviously none of these would have been possible without the ground-breaking work of Bertram Brockhouse.

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Neutron Scattering from Quantum Materials with the Spallation Neutron Source

By Jonathan Gaudet and Bruce D. Gaulin

Spallation neutron sources, based on accelerators rather than nuclear reactors, were proposed in the 1960s and then developed in the 1970s. Canadians were at the vanguard of such sources when the Intense Neutron Generator was proposed for Chalk River; unfortunately, it was never funded. Both the Intense Pulsed Neutron Source at Argonne National Laboratory, and the ISIS Pulsed Neutron Source at the Rutherford Appleton Laboratory in the UK ran successful user programs based on spallation neutron sources as early as the 1980s. However, the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory in the USA, which has operated now for just over 10 years, has ushered in a very large expansion in our capabilities to carry out forefront neutron scattering experiments on a wide variety of materials using such a source.

Most of these new measurements are performed using the time-of-flight of the neutron. The neutron is a massive particle (in contrast to photons) so one can measure the energy of a neutron by measuring its speed. New "chopper" inelastic spectrometers are designed to do exactly this, and they are designed to do so while being very efficient with the scattered neutrons. They aim to measure neutrons scattered into a large fraction of 4π steradians of scattered solid angle, and with time, and hence energy, so as to ultimately determine the scattering function, $S(\mathbf{Q},\hbar\omega)$, as comprehensively as possible. $S(\mathbf{Q},\hbar\omega)$ is directly related to the scattered neutron intensity and informs on the correlations between magnetic moments in solids in both space (through $\mathbf{Q}$) and time (through $\hbar\omega$). $\mathbf{Q}$ is the momentum or wavevector transfer of the scattering event, while an amount of energy $\hbar\omega$ is simultaneously transferred from the incident neutron to the sample or vice-versa. A schematic diagram of a chopper inelastic spectrometer is shown in Fig. 1.

Summary

Modern neutron time-of-flight spectroscopy allows a full understanding of complex condensed matter systems. Here, we present several examples related to superconductivity and quantum magnetism.

These advances in neutron instrumentation are almost certain to continue unabated, and even accelerate, as the international community has been very busy building up related neutron capabilities at JPARC in Japan, at the Chinese Spallation Neutron Source (which just turned on) and at the European Spallation Source (scheduled for completion in the early 2020s). Taken together, these international user facilities represent a reinvestment in neutron scattering infrastructure of ~$9B. With new experimental capabilities come new possibilities, and indeed neutron scattering studies are possible today, that would have been unimaginable 10 years ago. The new capabilities can be used in a variety of ways. For example, we can measure weaker signals, smaller crystals, or employ more extreme sample environments, and we can do all of this while obtaining a comprehensive dynamic structure function $S(\mathbf{Q},\hbar\omega)$, even with polarization analysis in favourable conditions.

Several of these issues come to bear in the study of new quantum materials. Quantum materials are often new magnets and superconductors, and sometimes both, where the fundamental degree of freedom in the material is inherently quantum mechanical in nature. The magnetic moments in the new magnetic materials can exhibit strong quantum fluctuations when the quantum numbers describing the moments are small, such as $S = 1/2$. This arises, for example, from the magnetism associated with a single unpaired electron in the d-shell of Cu^{2+}, as occurs in the cuprate-based high Tc superconductors. However it can also arise due to the effects of crystalline electric fields in f-electron rare earth magnets, such as the pyrochlore magnets $Er_2Ti_2O_7$ and $Yb_2Ti_2O_7$. Measurements on both of these types of systems will be described below. What makes such measurements difficult, is that the low quantum numbers tend to produce small magnetic moments in solids, and hence weak signals, as the magnetic neutron scattering cross section goes like the μ^2. To make matters worse, new quantum materials, like almost all new materials, tend to be initially produced as small single crystals. Finally, at least in the case of the high Tc cuprates, the energy scale for the magnetism is very large, and hence the inelastic scattering, which the chopper spectrometers are designed to measure, tends to be distributed over a large dynamic range in energy. Nonetheless, new neutron sources and instrumentation leave us much

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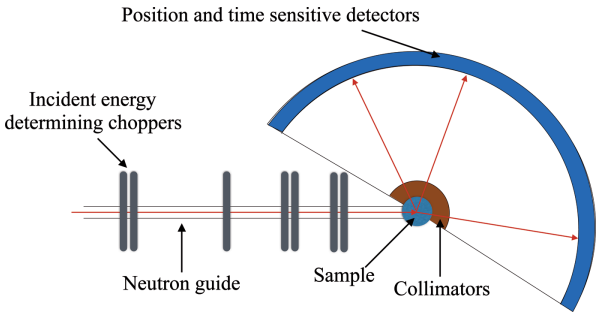

Fig. 1 A schematic diagram of a modern neutron time-of-flight chopper spectrometer is shown. A train of monochromatic neutron pulses is selected by a series of phased choppers, and this incident beam is delivered to the sample. The scattered neutrons are collected as a function of time-of-arrival and position on the detectors banks, allowing the measurement of the dynamic structure function $S(\mathbf{Q}, \hbar\omega)$. The array of position and time sensitive detectors is two dimensional (coming out of the page) so as to provide coverage over as much of 4π steradians in solid angle as possible.

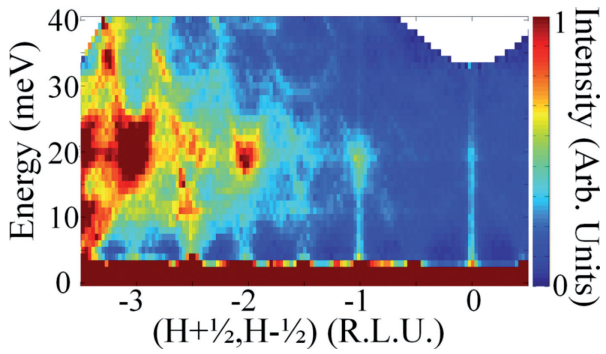

Fig. 2 Inelastic neutron scattering spectra from $La_{(2-x)}Ba_{(x)}CuO_4$ with $x = 0.035$ obtained with the ARCS time-of-flight spectrometer and a neutron incident energy of 60 meV is shown for a temperature of 5 K. Spin wave excitations are most visible at low **Q** and can be seen centered around (1/2 −1/2) and (−1/2 −3/2). Phonon excitations are most visible at high momentum transfer **Q**. Hybridized spin-phonon excitations occur at the crossing of the spin wave excitations and optic phonon excitations, centered around 20 meV.

better "armed" to address these technical challenges, and indeed great progress in the study of new quantum materials with neutrons is being made.

In what follows, we discuss three such recent examples of neutron scattering studies from quantum materials carried out under the auspices of "Canadian Participation at the Spallation Neutron Source". These examples are three of many Canadian experiments carried out at SNS; they are chosen from our own portfolio of results for convenience only. This $15M CFI International Access Fund project was awarded to McMaster University in 2003, and it gave Canadian scientists involvement in the design of two SNS instruments (SEQUOIA and VULCAN), and provided Canadian neutron scatterers enhanced access to these cutting edge capabilities for 10 years. This agreement with SNS concluded at the beginning of 2018. Nonetheless it has been a great success in maintaining Canada at the forefront of neutron expertise, and has had a disproportionate impact on the study of new quantum and frustrated magnets, and these are the subjects of the studies described below.

SPIN AND PHONON EXCITATIONS IN A PROTOTYPICAL HIGH-T_C SUPERCONDUCTOR PARENT COMPOUND

Hole-doped, cuprate-based high temperature superconductors can be thought of as quasi-two-dimensional quantum magnets, based on magnetic moments derived from a single d-level electron in Cu^{2+}, with mobile-hole impurities [1]. In their pristine form, without impurities, materials like $La_{(2-x)}Ba_{(x)}CuO_4$ with $x = 0$, are very strong antiferromagnets with ordered states forming near $T_N \sim 300$ K. However, the mobile impurities break down the commensurate, quasi-two-dimensional antiferromagnetic ordered state very quickly, by $x \sim 0.02$. At the impurity concentrations for which superconductivity is established, $x > 0.05$, the magnetism is incommensurate, consistent with the "stripe" picture of high temperature superconductivity, and it is also highly dispersive, meaning that the spin excitation spectrum is centred on wave vectors such as (1/2,1/2,L), and disperses to high energies, ~200 meV.

As new time-of-flight neutron instrumentation employs large arrays of position sensitive detectors, neutron scattering processes are detected across a large range of three-dimensional momentum space, **Q,** and such measurements give large coverage in reciprocal space. The neutrons' time-of-arrivals at the detectors are also recorded, and this provides the energy transfer of the scattering events, $\hbar\omega$. The data set in Fig. 2, which shows the neutron inelastic spectra of $La_{(2-x)}Ba_{(x)}CuO_4$ with $x = 0.035$, was obtained with the time-of-flight chopper spectrometer ARCS at the SNS using an incident neutrons energy of 60 meV [2]. The total scattering spectra obtained from ARCS gives a 4-dimensional (3 **Q** dimensions and 1 energy dimension) data set. However, it is difficult to analyze or even look at 4-dimensional data sets, and hence the resulting neutron scattering spectra shown in Fig. 2 is the result of two different integrations within reciprocal space of this 4 dimensional data set. For this particular example, integrations along the [H,−H,0] and the [0,0,L] directions in reciprocal space have been performed, revealing inelastic scattering as a function of energy, plotted along the [−H,−H,−4 < L < 4] direction in reciprocal space.

Figure 2 illustrates the approximate separation of the inelastic signal, with spin excitations at relatively low **Q**, and phonon or lattice vibration scattering at relatively large **Q**. The spin excitations are identified as the very dispersive, almost vertical rods of inelastic scattering, emanating out of the (1/2, −1/2, −4 < *L* < 4) and (−1/2,−3/2,−4 < *L* < 4) positions in reciprocal space. In contrast the phonons give much stronger intensity at larger **Q**, and their dispersion is more complex. This approximate separation of spin and phonon scattering, according to low and high **Q**, is due to the fact that neutron scattering from phonons goes like $\mathbf{Q}^2$, while the magnetic neutron scattering cross section goes like the square of the magnetic form factor, which falls off at high **Q**. For this reason, the phonons can be inferred from Fig. 2 and correspond to features whose intensity grows as a function of **Q**, such as the acoustic phonons centred at (−1,−2, −4 < *L* < 4). Multiple optic phonon branches are also observed and correspond, for example, to the non-dispersive excitations centred around 20 and 30 meV.

Since both phonon and spin-wave excitations can be simultaneously measured and analyzed from scattering spectra such as the one shown in Fig. 2, one can also infer the existence of more exotic excitations. For $La_{(2-x)}Ba_{(x)}CuO_4$, an intriguing feature in these experiments is the very large enhancement of scattered intensity (or resonance-like scattering) observed at the crossing of the highly dispersive or "vertical" spin wave dispersions originating from wave vectors such as (1/2, −1/2, −4 < *L* < 4) and (−1/2, −3/2, −4 < *L* < 4), and the ~ "horizontal" optic phonons centred at 20 meV. Such an enhancement is attributed to a hybridized spin-phonon excitation as it occurs at their crossing in **Q** and $\hbar\omega$ space. Density functional theory for the phonons in $La_{(2-x)}Ba_{(x)}CuO_4$ reveals that the particular optic phonon involved in this process, near 20 meV, corresponds to vibrations of the oxygen ions localized between the Cu^{2+} ions. The magnetic exchange interaction strength in $La_{(2-x)}Ba_{(x)}CuO_4$ comes from strong super-exchange between neighbouring Cu^{2+} ions, mediated by the O^{2-} ions. Flexing this Cu^{2+}- O^{2-}-Cu^{2+} bond, through this optic phonon, is expected to couple directly to the magnetism in this system. Thus a strong magneto-elastic coupling is perhaps not unexpected. Nonetheless, observing such a subtle effect requires rather comprehensive $S(\mathbf{Q},\hbar\omega)$ information and new time-of-flight chopper spectrometers are very well suited to providing such data on systems of interest. Our measurements have shown that such coupling between the spin excitation spectrum and the phonons in $La_{(2-x)}Ba_{(x)}CuO_4$ extends across x to at least $x = 0.11$, and it is therefore a general physical characteristic of this important family of quantum materials [3].

THE SPIN GLASS GROUND STATE IN THE RANDOM BILAYER QUANTUM ANTIFERROMAGNET $LuCoGaO_4$

The comprehensive nature for which $S(\mathbf{Q}, \hbar\omega)$ can be measured using chopper spectrometers and a spallation source really comes into its own for the study of disordered materials. In the case of magnets with disordered ground states, such as spin glass states, comprehensive coverage of $S(\mathbf{Q}, \hbar\omega)$ is very important as the magnetic scattering is itself distributed in **Q** and $\hbar\omega$, rather than organized into sharp, three dimensional Bragg peaks, and spin excitations with well-defined energies and momenta, as occurs in ordered magnets. A spin glass ground state is typically stabilized by the combination of structural disorder and competing interactions, such that a frozen, disordered magnetic state results at low temperatures. This is illustrated below for the random-bilayer spin-glass $LuCoGaO_4$, using the SEQUOIA chopper spectrometer at the SNS [4].

$LuCoGaO_4$ possesses a hexagonal crystal structure with magnetic Co^{2+} ions and nonmagnetic Ga^{3+} ions randomly occupying triangular bilayers in a 1:1 ratio. The single ion ground state of the Co^{2+} ions gives rise to an effective quantum spin-1/2 moment that interacts antiferromagnetically with its random two-dimensional network of neighbouring Co^{2+} ions. This material therefore has the key ingredients necessary to stabilize a spin glass ground state − frustrated antiferromagnetic interactions on triangular lattices and structural randomness.

While the spin glass ground state lacks long range order, it does possess frozen, short range order at low temperatures. The elastic magnetic neutron scattering shown in Fig. 3 illustrates how this appears in such a spin glass state. In both Fig. 3(a) and (b), $S(\mathbf{Q}, \hbar\omega)$, integrated in energy from −1 to 1 meV in order to isolate the elastic scattering, is shown. In (a), an additional integration have been performed along the [0,0,*L*] direction (from −2.75 to 2.75 in reciprocal lattice units) so as to reveal the static spin correlations occurring within the triangular bilayers occupied by the Co^{2+} and Ga^{3+} ions. Examination of these data sets for $LuCoGaO_4$ obtained at different temperatures reveals that the static spin correlations build up near **Q** = (1/3,1/3,0) and equivalent wave vectors, starting at temperatures as high as $T \sim 120$K, which corresponds to the Curie-Weiss temperature of this system. The **Q** = (1/3,1/3,0) wave vector indicates a local magnetic structure. A long range ordered version of this magnetic structure is known to exist, for example, in $YbFe_2O_4$ in the absence of structural disorder. The width of these "quasi-Bragg peaks" are indicative of the short range order of the $LuCoGaO_4$ ground state. The correlation length within the **a-b** plane (the plane of the bilayers) is related to the inverse of the width of these quasi-Bragg peaks. Analysis reveals that the correlation length, ξ, increases from about 2-3 Å at 120K to 6.5-7.5 Å by ~19K, which corresponds to the spin-glass transition in $LuCoGaO_4$. On further lowering the temperature from 19K to 1.8K, the correlation length saturates at this small value, consistent with the spin freezing of this system. Finally, Fig. 3(a)) shows that the width of each quasi-Bragg peak is independent of the direction of **Q** within the [*H*,*H*,0]/[*H*,*H*,0] plane, and therefore ξ is isotropic within the triangular bilayers of $LuCoGaO_4$.

In Fig. 3(b), $S(\mathbf{Q},\hbar\omega)$ for $LuCoGaO_4$ is once again shown with an integration in energy from −1 meV to 1 meV, hence picking

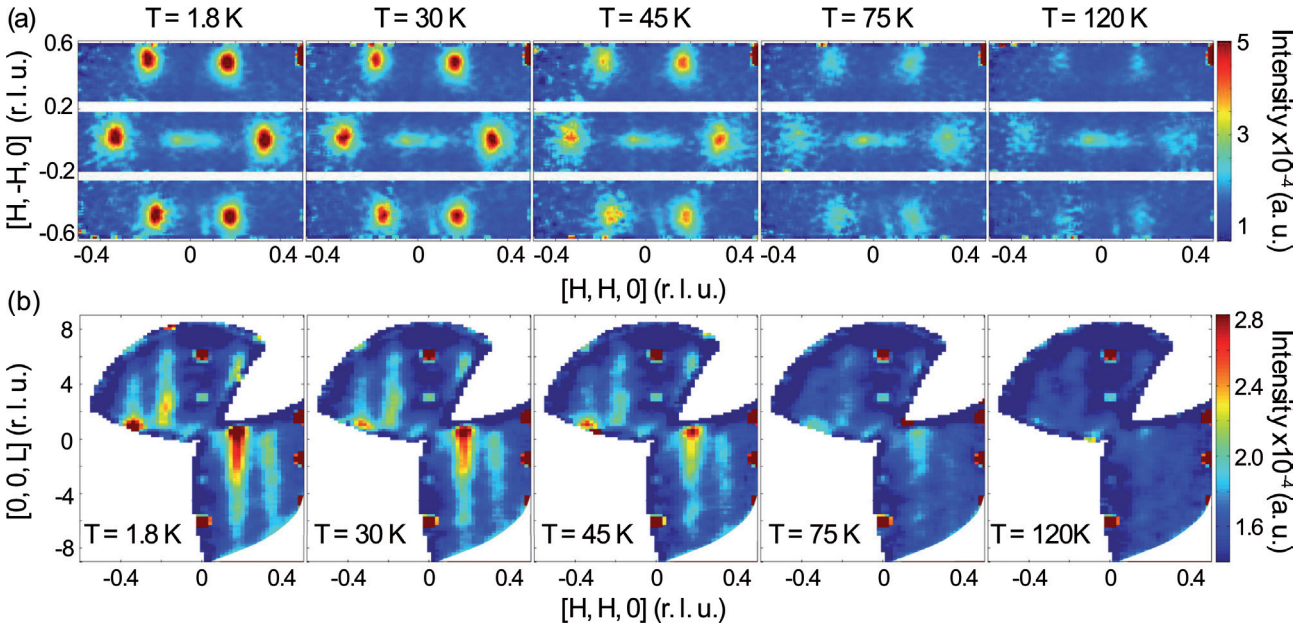

Fig. 3 (a) shows the elastic neutron scattering spectra from LuCoGaO4 within the $[H,-H,0]$-$[H,H,0]$ plane. (b) reveals the scattering spectra within the $[H,H,0]$-$[0,0,L]$ plane. The appearance of "rods" of scattering along $[0,0,L]$ are indicative of two dimensional correlations. Both data sets are presented for temperatures ranging from 1.8K to 120K, both above and below the spin freezing temperature of LuCoGaO4 (~19K), and up to the ~Curie-Weiss temperature of this system (~100K).

up elastic scattering only, but now with a **Q** integration along the $[H,-H,0]$ direction. This particular plane of the four-dimensional $S(\mathbf{Q},\hbar\omega)$ shows elastic scattering within the $[H,H,0]/[0,0,L]$ plane of reciprocal space, and therefore informs on static spin correlations arising between the bilayers. The scattering spectra shown in Fig. 3(b) for $LuCoGaO_4$ at 1.8K reveals rods of scattering along $(0,0,L)$ that are centered at $\mathbf{Q} = (1/3,1/3,L)$. The rod-like shape of these features is typical of the two-dimensional nature of the spin correlations, indicating that little or no correlations exist between the different Co/Ga bilayers, even at the lowest temperatures measured. We thus conclude that the spin glass state in $LuCoGaO_4$ is intrinsically two dimensional in nature.

SPIN ANISOTROPY AND S_{EFF} = 1/2 QUANTUM MOMENTS IN RARE EARTH PYROCHLORE MAGNETS

While triple-axis spectroscopy is still widely used to study excitations in solids, inelastic neutron scattering with triple axis instruments at high energy transfers, say above 30 meV, is relatively challenging. However, such measurements are routinely performed using time-of-flight techniques and instrumentation, such as the SEQUOIA chopper spectrometer at the SNS. The combination of a forefront spallation neutron source and a forefront chopper spectrometer such as SEQUOIA allows routine neutron spectroscopic measurements with energy transfers in the 100s of meV regime, and up to the 2-3 eV regime if required. This "high energy physics" is vital in condensed matter physics as it informs on the single-ion properties of the atoms and ions that constitute a specific material. For example, it is known that the single-ion properties of the magnetic ions in the frustrated rare-earth (RE) pyrochlore magnets $RE_2M_2O_7$ strongly influence the magnetic ground states of these systems, as these properties determine both the spin anisotropy and the moment at the magnetic RE site.

Within the cubic pyrochlore structure, both the RE and M sublattices correspond to a network of corner-sharing tetrahedra. Due to the triangular motif that forms each tetrahedron, the pyrochlore lattice is the archetype example of geometrical frustration in three dimensions. This geometrical frustration makes pyrochlore magnets amenable for the realization of new exotic magnetic ground states [5]. For this reason, they have attracted intense and sustained interest in the condensed matter community. A key ingredient for the stabilization of the different observed magnetic states is the local spin anisotropy of the rare-earth moments that results from their single-ion physics. In pyrochlore magnets, as shown in Fig. 4a, the rare-earth moments sit at the centre of a distorted cube of O^{2-} ions and the spin anisotropy is defined locally using the axis that connects the centres of two adjacent tetrahedra. Ising or unidirectional anisotropy is stabilized if the spins can only point into or out of the centre of the tetrahedra on which a spin resides (e.g., the red spin in Fig. 4(a)). XY or planar anisotropy results from spins constrained to lie within a plane perpendicular to the Ising axis

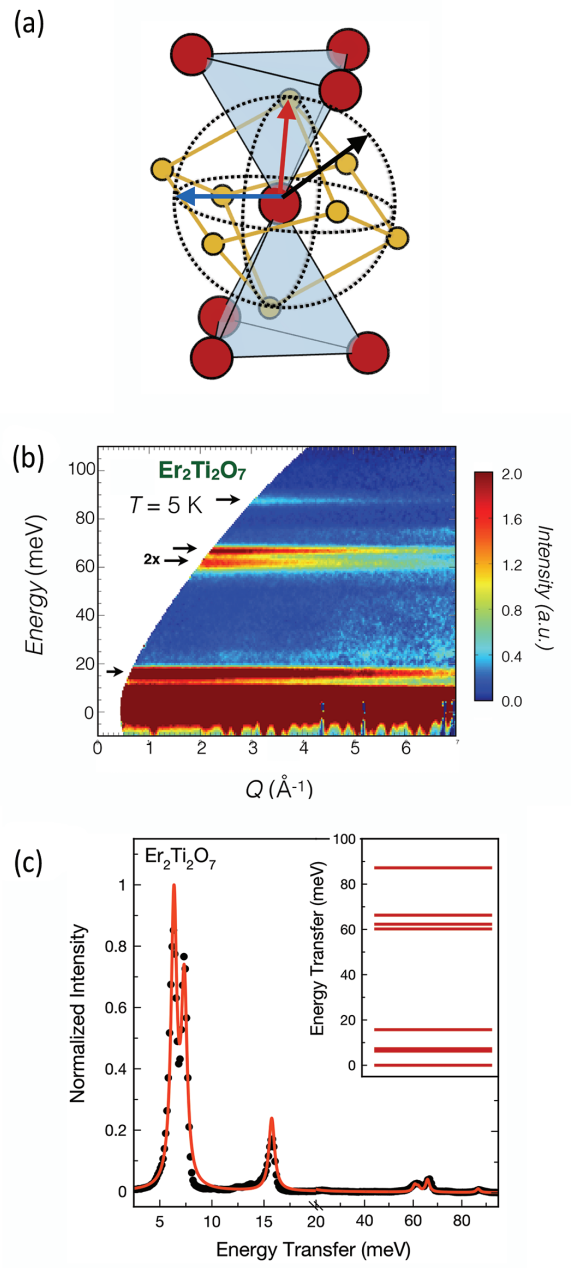

Fig. 4 (a) The local environment of the rare-earth ions within the pyrochlore magnet. The yellows dots correspond to the oxygen ions arranged on a distorted cube and the red dots correspond to the rare-earth ions. The red spin displays typical Ising anisotropy, while the blue spin is indicative of XY anisotropy and the black spin is typical of a Heisenberg system. (b) shows the neutron inelastic spectra of $Er_2Ti_2O_7$ obtained using the SEQUOIA time-of-flight spectrometer with incident neutrons of energy 150 meV. (c) shows the resulting CEF fit to the inelastic scattering from $Er_2Ti_2O_7$ and the excellent agreement between the calculation (red line) and the experimental data (black dots). The inset to (c) shows the CEF energy scheme for Er^{3+} in $Er_2Ti_2O_7$.

(e.g., the blue spin in Fig. 4(a)). If the spins are isotropic, that is if they lack anisotropy, such a system is referred to as Heisenberg in nature and its spins are free to point anywhere in three dimensional space (e.g., the black spin in Fig. 4(a)). Which spin anisotropy a given rare earth pyrochlore magnet displays depends on the exact details of the degeneracy breaking of the (2J+1) manifold of its spin-orbit ground state. The lifting of this degeneracy occurs due to interaction between the magnetic ion and the crystalline electric field originating from its local environment of neighbouring ions. A determination of the exact crystal electric field (CEF) Hamiltonian is possible using inelastic neutron scattering via a detailed analysis of the transition energies between different CEF levels, as well as their respective scattered intensities. As the strength of the CEFs in the rare earth pyrochlores is on the order of 50-100 meV, the determination of the spin anisotropy through the detailed characterization of the CEF Hamiltonian of rare earth pyrochlore magnets is perfectly suited for the time-of-flight SEQUOIA spectrometer at SNS.

To illustrate the analysis of neutron spectroscopy that leads to the determination of the local spin anisotropy, and the size of the magnetic moment within the CEF ground state, we focus on the particular case of $Er_2Ti_2O_7$ [6]. In this material, the magnetic erbium ions have a 3^+ oxidation state with an electronic configuration corresponding to $[Xe]4f^{11}$. Following Hund's rules, the spin-orbit ground state then has total angular momentum J = 15/2 with $L = 3$ and $S = 2$ and is $(2J+1) = 16$ fold degenerate. Kramer's theorem stipulates that each CEF level should be at least doubly degenerate, which implies that a maximum of 8 different CEF states can be obtained. The exact symmetry of the CEF Hamiltonian appropriate for this Er^{3+} site predicts that the complete degeneracy of the 8 CEF states should be lifted. Thus, at a temperature that is sufficiently low to only thermally populate the CEF ground state, 7 inelastic transitions from the CEF ground state to CEF excited states should be observed, and these will fully determine the entire CEF manifold.

The inelastic spectra of $Er_2Ti_2O_7$ is shown in Fig. 4(b) for a neutron incident energy of 150 meV and a temperature of 5K. The first excited CEF doublet of $Er_2Ti_2O_7$ is located at around 6 meV (~70K) which implies that the inelastic spectra shown in Fig. 4(b) should only involve CEF transitions originating from the CEF ground state. The magnetic CEF excitations can be identified by analyzing the **Q** dependence of the inelastic features appearing in Fig. 4(b). Indeed, the intensity of a magnetic excitation, as compared to phonons, should decrease in intensity as a function of the momentum transfer **Q**. From Fig. 4(b), it is clear that the features around 15, 65, 70 and 90 meV correspond to CEF excitations. For this specific analysis, inelastic spectra using 25 meV and 90 meV incident neutron energy have also been collected and revealed that the feature around 15 meV in Fig. 4(b) corresponds to three different CEF levels. Furthermore, the feature around 60 meV in Fig. 4(b) is in fact, two closely space CEF excitations. These five CEF excitations, along with the CEF excitations observed in Fig. 4(b) around 70 meV and 90 meV reveal the energies of all of the excited

CEF levels, and a robust CEF Hamiltonian can be determined for $Er_2Ti_2O_7$.

The CEF Hamiltonian (H_{cef}) for $Er_2Ti_2O_7$ can be derived using the Stevens formalism [7]. This formalism consists of writing the Coulomb potential of the CEF in terms of Stevens operators (O_{nm}) made up from J_z, J_+ and J_- operators. For the pyrochlore structure, the point-group symmetry of the Er^{3+} site is D_{3d}, and the CEF Hamiltonian consists of six Stevens operators: O_{20}, O_{40}, O_{43}, O_{60}, O_{63} and O_{66} (e.g., $O_{20} = 3J_z^2 - J(J+1)$). Each Stevens operator is unit-less, but is multiplied by a CEF parameter B_{nm} ($H_{cef} = \sum B_{nm} O_{nm}$). The energy distribution of the CEF levels, as well as the composition of each CEF eigenvector, depends on the B_{nm} parameters. Fitting of the CEF parameters B_{nm} can be performed using the energies of the CEF transitions observed via neutron spectroscopy as shown in Fig. 4(b). Further constraints are provided by the relative intensity of each of the CEF transitions. The result of the fitting procedure is shown in Fig. 4(c) where this CEF calculation is reproduced along with the experimentally-derived inelastic neutron scattering spectra for $Er_2Ti_2O_7$ at low temperature. Excellent agreement between the calculation and the neutron scattering experiment is obtained, validating the determination of the CEF Hamiltonian for $Er_2Ti_2O_7$.

With the CEF Hamiltonian for $Er_2Ti_2O_7$ in hand, it is possible to calculate the strength of the local g-tensor, parallel ($g_{\|}$) and perpendicular (g) to the Ising axis, and this will determine the local anisotropy of the Er^{3+} moment. As we are interested in the ground state properties of this material, the g-tensor anisotropy can be computed solely using the composition of the CEF ground state doublet. This procedure leads to $g_{\|} = 3.9$ and $g = 6.3$, implying that the CEF ground state doublet of $Er_2Ti_2O_7$ has XY anisotropy, and its spins have a preference to lie within a plane perpendicular to the local Ising axis. It also allows us to conclude that the eigenfunction making up the CEF ground state doublet is mostly made up of $m_J = 1/2$, and hence the moments in $Er_2Ti_2O_7$ correspond to quantum degrees of freedom. This XY or planar anisotropy helps stabilize antiferromagnetic long-range magnetic order in $Er_2Ti_2O_7$ with the Er^{3+} spins pointing within the XY local plane. The ground state selection of this particular XY spin structure is proposed to originate from a novel order-by-disorder mechanism [8], which selects a particular ordered magnetic structure due to it's propensity to fluctuate, as opposed to the usual propensity to lower its energy. This entropic selection is rare in nature, but is possible in $Er_2Ti_2O_7$ due to a well isolated CEF ground state doublet with an effective spin 1/2, XY anisotropy and the high symmetry of the pyrochlore structure.

CONCLUSION

Neutron scattering techniques are of fundamental importance to the study of condensed matter physics, as they measure $S(\mathbf{Q},\hbar\omega)$ across entire Brillouin zones and over energies of relevance to elementary excitations in solids. New quantum materials present challenges for neutron scattering, as their quantum degrees of freedom often correspond to small magnetic moments originating from low quantum numbers. New spallation neutron sources and new instrumentation based on the time-of-flight of the neutron have vastly expanded our capabilities to perform meaningful neutron experiments on such systems. We illustrated this with three recent examples taken from Canadian work at the Spallation Neutron Source at Oak Ridge National Laboratory. These examples focused on quantum magnetism and its interactions with phonons in a prototypical high temperature superconducting parent material; on a disordered quasi-two dimensional spin glass; and on the use of high energy neutron spectroscopy to determine the local spin anisotropy and moment size in a rare earth-based pyrochlore magnet.

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Neutrons and Biology

by Maikel C. Rheinstädter

Neutron and x-ray scattering are indispensable tools in the life sciences. Their main impact is probably the determination of high-resolution protein structures using dedicated and high-throughput protein crystallography beamlines, where scattering of minuscule protein crystals is detected and analyzed to determine the structure of proteins and complexes to tell us for instance how receptors and enzymes work. While a large percentage of protein structures is still done by scattering techniques, nuclear magnetic resonance (NMR) and cryogenic electron microscopy (cryo-TEM) are catching up. While our current techniques often suffer from the fact that the corresponding structures are determined under non-physiological conditions, there is a strong effort to develop techniques to study protein structures in more physiological environments, such as in solution or in contact or embedded in membranes. These disordered and highly-dynamic structures pose particular challenges for the application of scattering techniques, which have been developed for the application in well-ordered and periodic systems. This challenge is being addressed by the development of new instrumentation and analysis techniques to get the most amount of structural information of this biological state of matter. The new Small Angle Neutron Scattering (SANS) for Nanostructured Materials instrument, which is currently being constructed at the McMaster Nuclear Reactor, is a good example for an instrument that will address this challenge.

Neutron and x-ray scattering are still one of our best microscopes for the determination of small structures and the global investment in neutron reactors and spallation sources and synchrotron facilities has reached an all-time high with far more than $20B spent in recent years. While there is a global network of these facilities, which provide access to users world-wide, the availability of local, national facilities, such as the Canadian Neutron Beam Centre at Chalk River Laboratories, the McMaster Nuclear Reactor and the Canadian Light Source, is a prerequisite for successful research programs and economic impact, and indispensable for the training of highly qualified personnels.

Summary

Neutron beams are indispensable tools to determine molecular structure and dynamics of proteins and membranes. We review properties and their use to investigate membrane rafts.

As distances between molecules are typically much larger than atomic distances in crystals, the corresponding scattering signals occur at small scattering angles ($\lambda/d = 2\sin(\theta)$, with λ the wavelength of neutrons or x-rays, d the molecular spacing and θ the scattering angle). Neutron beams can be optimized for large scale structures by preparing so-called cold neutrons with velocities between 100 and 2,000 m/s, only, and corresponding long de-Broglie wavelengths ($\lambda = h/(m \cdot v)$) of 2-40 Å. In combination with long flight tubes, which allow the measurements of signals at very small scattering angles, these instruments are optimized to detect molecular distances of up to 10,000 Å.

Because of their relatively low speed, neutron beams can also be used to determine dynamical processes. By measuring the velocity of neutrons before and after the scattering process, their energy transfer during the scattering process can be calculated. The corresponding dynamical processes are related to well-defined excitation frequencies of rotations and vibrations of molecules, or protein or lipid diffusion. Energy transfers of as small as nano electron Volts can be measured, approaching slow, almost microsecond time scales. Changes in energy are detected at different values of the scattering vector, Q. In contrast to other spectroscopic techniques, inelastic neutron scattering thus results in wave vector resolved access to molecular dynamics. A typical dynamic scattering experiment measures $(Q,\hbar\omega)$ pairs, resulting in a frequency along with a corresponding length scale, and possibly a corresponding direction such as parallel or perpendicular to a protein's axis. This additional information is of paramount importance when it comes to relating dynamical information to structure. In short, the suite of inelastic instruments used to study soft and biologically relevant materials comprises of time-of-flight, backscattering, triple-axis and spin-echo spectrometers.

As shown in Fig. 1, neutron spectroscopy fills an important gap in the suite of spectroscopic techniques [1]. The relevant length scale for dielectric spectroscopy is in the order of an elementary molecular electric dipole, which

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can be estimated by the bond length of a C--O bond (about 140 picometers), and frequencies from kiloHertz to GigaHertz can be measured.

Because the wavelength of the probe is usually around λ = 500 nm, light scattering techniques are limited to small momentum transfers of about 10^{-4} Å^{-1} to 10^{-3} Å^{-1}, and corresponding to a length scale of about 100 nanometers. Inelastic neutron and x-ray scattering access length scales from smaller than Angstrom to more than 100 nanometres, and time scales from picoseconds to almost one microsecond. High speed AFM has combined a high spatial resolution of about 5 Å with a time resolution of milliseconds, just outside the time range in the figure. Molecular Dynamics computer simulations have become an invaluable tool in developing models for molecular structure and dynamics in membranes and proteins. Because of the ever-increasing computing power and optimized algorithms, large complex systems (i.e., hundred thousands of molecules) and long simulation times of µs can now routinely be addressed. The dashed rectangle in Figure 1 marks the dynamic range currently accessed by computer simulations – the elementary time scale for simulations is in the order of femtoseconds.

SELECTIVE DEUTERATION

While x-rays are electromagnetic waves and scattered by the electrons in the electron shell, neutrons scatter off the nuclei of atoms. The peculiarity of neutrons is that they may scatter incoherently or coherently, and give access to local or collective dynamics (see [2] and references therein). The scattering length, b, depends on the spin of the nucleus-neutron system. If the spin of the nucleus is I, then every nucleus with non-zero spin has two values of b, namely for $I+½$ and $I-½$, depending on the orientation of neutron and nucleus spin. The scattering length is thus not simply a monotonic function of the atomic number, as it is for x-rays, but depends on the spin configurations of the nuclei. In addition, different isotopes of the same element can have different scattering lengths as they have nuclei with the same number of protons (the same atomic number) but different numbers of neutrons and also different nuclear spins. So while for x-rays, all atoms of the same element look the same, they may look different for neutrons because of (1) different orientations of the nuclear spin, and (2) different isotopes (nuclides). The most pronounced difference between the x-ray and the neutron probe is, therefore, that x-ray scattering is always coherent, while neutron scattering may contain contributions from coherent and incoherent scattering.

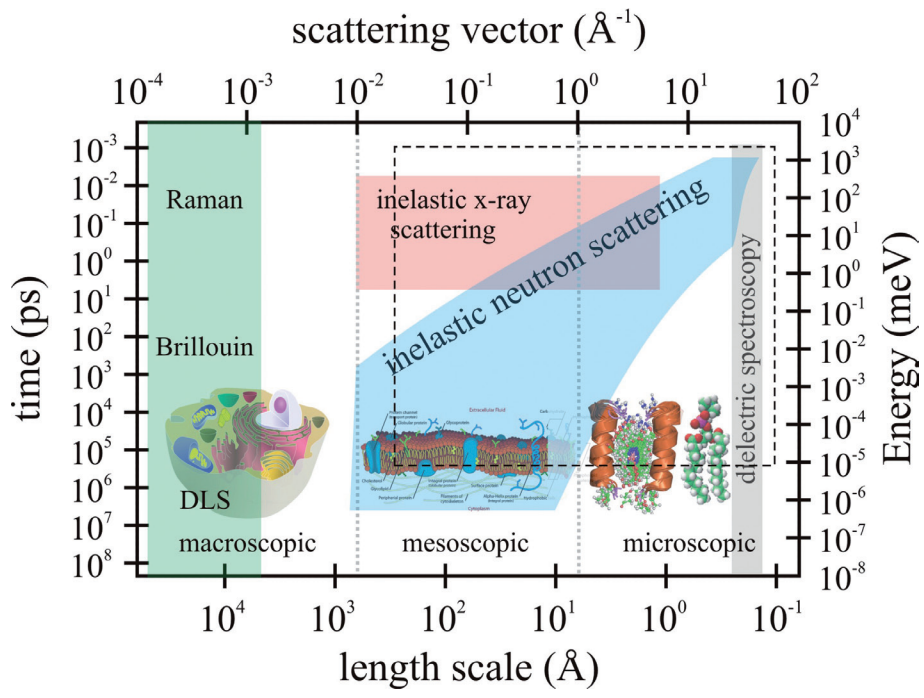

Fig. 1 Accessible length and time scales, and corresponding energy and momentum transfer, for some spectroscopic techniques covering microscopic to macroscopic dynamics. Light scattering techniques include Raman, Brillouin, and Dynamic Light Scattering (DLS). Inelastic x-ray and neutron scattering access dynamics on Angstrom and nanometer length scales. Dielectric spectroscopy probes the length scale of an elementary molecular electric dipole, which can be estimated by the bond length of a C—O bond (about 140 picometers). The area marked by the dashed box is the dynamical range accessible by Molecular Dynamics simulations (Adapted from [1]).

The coherent and incoherent neutron cross sections of an element can be illustrated by two extreme cases. If all the nuclei in a sample have different cross sections, there can be no interference between the waves scattered by different atoms. This incoherent scattering can only depend on the correlation between the positions of the same nucleus at different times and measures the auto or self-correlation function and diffusive processes. If all scattering lengths are the same, i.e., all nuclei are identical for the neutron probe, the coherent scattering still depends on the correlation between the positions of the same nucleus at different times, but more so on the correlation between the positions of different nuclei at different times. It therefore gives interference effects and allows measuring collective dynamics and interaction forces.

The fraction of coherent and incoherent scattering depends on the atomic composition and the respective scattering lengths. Substitution of certain elements in

a compound by their isotopes may increase contributions of certain molecules or functional groups to the coherent or incoherent scattering contribution. Because the incoherent cross section of hydrogen atoms is about 40 times larger than that of deuterium and of all other atoms present in biological macromolecules, hydrogen atoms dominate the incoherent scattering signal. The hydrogen atoms reflect the movements of larger groups to which they are attached, such as amino acid side chains. Deuteration, i.e., the substitution of protons by deuterium (^{2}H), is often used to suppress the incoherent scattering contribution of certain functional groups to the total scattering or increase their coherent contribution.

The effect of deuteration labeling is sketched in Fig. 2. While in protonated samples the incoherent scattering is usually dominant and the time self-correlation function of individual scatterers is accessible, (partial) deuteration emphasizes the coherent scattering and gives access to collective motions by probing the pair correlation function. In a membrane sample with protonated proteins, the experiments would be sensitive to the diffusive motions of the proteins. Deuteration of the proteins increases the coherent scattering and allows measuring the interaction forces between the embedded proteins. In Fig. 2(a), self-correlated, diffusive motions of membranes and embedded proteins can be accessed when the membrane-protein system is labeled, and deuterated solvent is used. Diffusive dynamics of the proteins is highlighted when solvent and membrane are deuterated, and hydrogenated proteins are used. The effect of protein insertion on membrane dynamics can be studied in Fig. 2(c), with deuterated solvent and proteins. Note that at the same time, the interfaces between protonated and deuterated areas scatter coherently. The preparation in Fig. 2(b) can therefore be used to study possible protein-protein interactions. Selective deuteration is in particular very powerful for the investigation of functional domains in membranes, so-called rafts.

THE RAFT CONCEPT

Biological membranes are the most important biological interface. Composed mainly of lipid molecules and proteins, they serve a number of functions, which include acting as a barrier to the external environment for the contents of the cell. Over 20-30% of genes encode membrane embedded proteins, and these proteins play important roles in cell signalling and cell adhesion. The cellular plasma membrane contains over 100 lipid species. Lipids are amphiphilic molecules with a hydrophilic head group and hydrophobic lipid tails. Lipid membranes are bilayers of lipid molecules, which form to minimize water contact with the lipid tails. This bilayer may then wrap to form a closed surface and a passive barrier. In early research of membranes and membrane embedded proteins, lipid molecules were not considered active participants in membrane processes. In 1972, shortly after it was determined that proteins may embed within the lipid membrane, Singer and Nicholson published their "Fluid Mosaic Model" of lipid membranes. In this model, the membrane serves as a passive, unstructured, two-dimensional liquid within which embedded proteins float and the lipid molecules act as a solvent. The model quickly became popular as it allowed for the lateral diffusion of protein molecules, as well as the transverse diffusion of small molecules, such as oxygen or carbon dioxide.

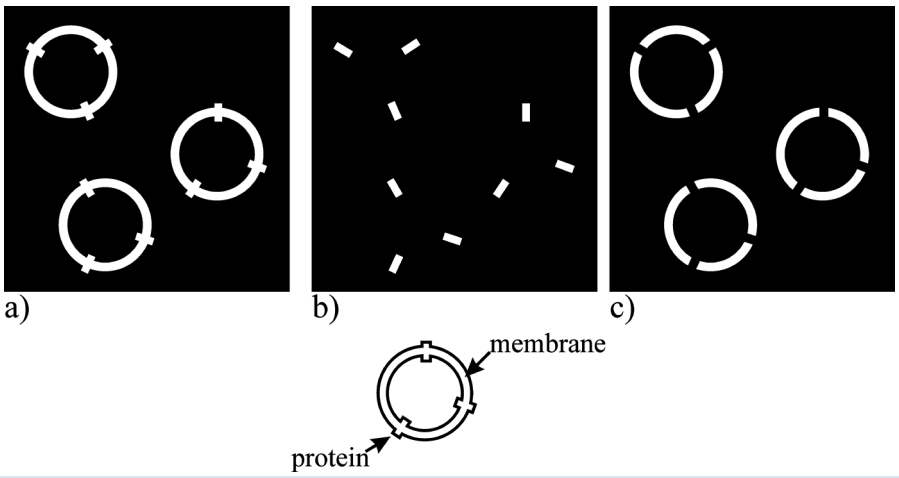

Fig. 2 Selective deuteration can be used to highlight molecules or functional groups in neutron scattering experiments. Depicted are vesicles with embedded proteins in a solvent: (a) membrane and embedded proteins are visible in incoherent scattering experiments for neutrons when the solvent is deuterated. (b) When solvent and membrane are deuterated, local dynamics of the embedded proteins can be investigated. (c) Deuterated proteins allow investigating membrane dynamics (Adapted from [2]).

In order to increase the amount of structural information, scattering experiments in membranes are often performed on oriented, stacked bilayers applied on a substrate. The membranes are typically prepared by dissolving the component molecules in solvent, then depositing the solution on flat, hydrophobic silicon wafers. Stacked bilayers are formed upon solvent drying and subsequent annealing in high humidity and temperature. The structure of the membrane perpendicular to the flat substrate (the out-of-plane axis, q_z) can then be determined independently of the lateral structure (in-plane axis, $q_{||}$), as shown in Fig. 3.

As research on membranes progressed it appeared that not all membranes are created equal

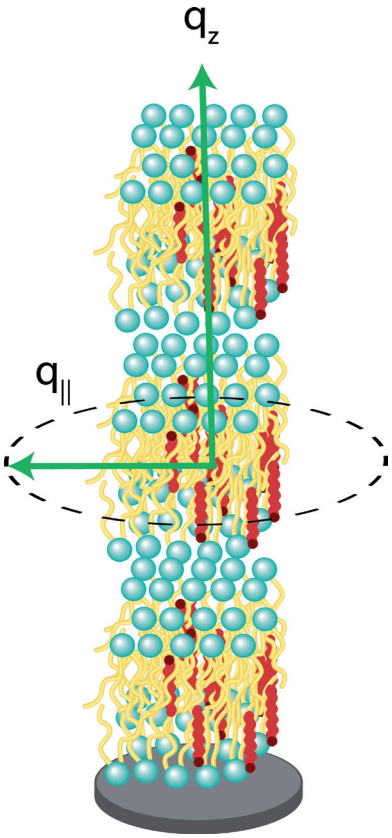

Fig. 3 Schematic of oriented, stacked lipid bilayers, which defines the principle axis used in scattering analysis. The q_z axis describes scattering along the direction of the oriented stack, while the $q_{||}$ axis describes scattering from the in-plane organization of membrane molecules (From [3]).

(see [3] and references therein). The preferential sorting of proteins in the plasma membrane was attributed to local differences in composition. Experiments on plasma membranes found that certain fractions were resistant to detergents, and that certain proteins are found in the detergent resistant fractions. In addition, the proteins in these detergent resistant fractions were often observed to be organized in specific membrane locations. The evidence led to in the proposal of "lipid rafts": isolated membrane fractions enriched in cholesterol and saturated lipids, which serve as membrane compartments, as pictured in Fig. 4. Proteins may interact with the raft region or non-raft regions, depending on hydrophobic thickness or specific lipid/cholesterol interactions. In the raft model, the lipids are no longer a passive solvent. Instead, their physico-chemical properties impact the structure and function of specific proteins. With rafts most likely being small and transient structures, understanding their structure, function, and even proving their existence is an experimental challenge.

There are two properties of neutrons scattering experiments, which make them amenable to identifying rafts. By selectively deuterating lipids, the experiment can be made primarily sensitive to lipid organization while cholesterol molecules are basically invisible or vice-versa (see [4] and references therein). Lipid structure can be determined unambiguously and independently from cholesterol structure. The second important property of neutrons is the ability to increase the experiment's sensitivity to smaller structures by controlling the (longitudinal) coherence length of neutron beams in situ. The coherence length ξ of the neutron is the spatial extent of the neutron particle and is given by the neutron wavelength, λ, and the uncertainty in the wavelength of the particle, $\Delta\lambda$, by $\xi = \lambda^2/\Delta\lambda$. In a scattering experiment, the structure of a domain smaller than the coherence length of the neutron will be

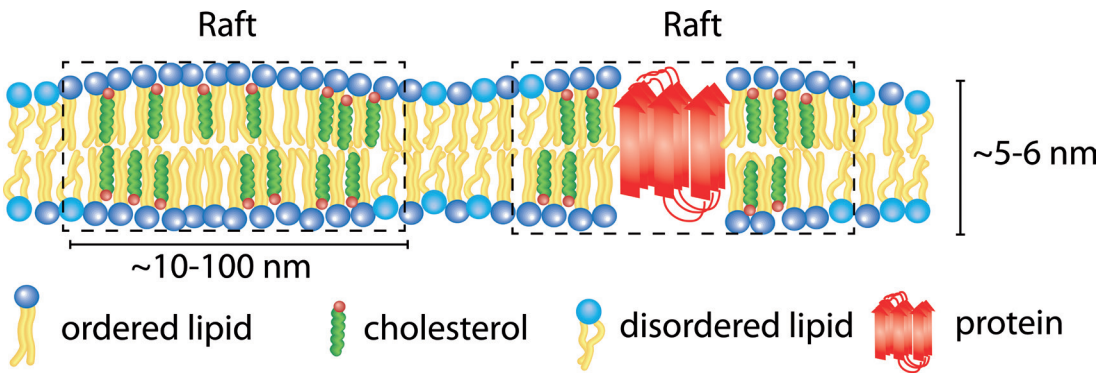

Fig. 4 Schematic of rafts in a lipid membrane. The raft region contains high concentrations of ordered lipids and cholesterol. Lipid motions are constrained in the presence of cholesterol and lipid molecules are found as well-ordered as in the gel state but with lateral and rotational diffusion similar to that of the fluid phase; in that respect, rafts are a manifestation of the liquid-ordered, l_o, phase. These rafts have different material properties, such as decreased elasticity and permeability, and may serve as anchor points for certain proteins (From [3]).

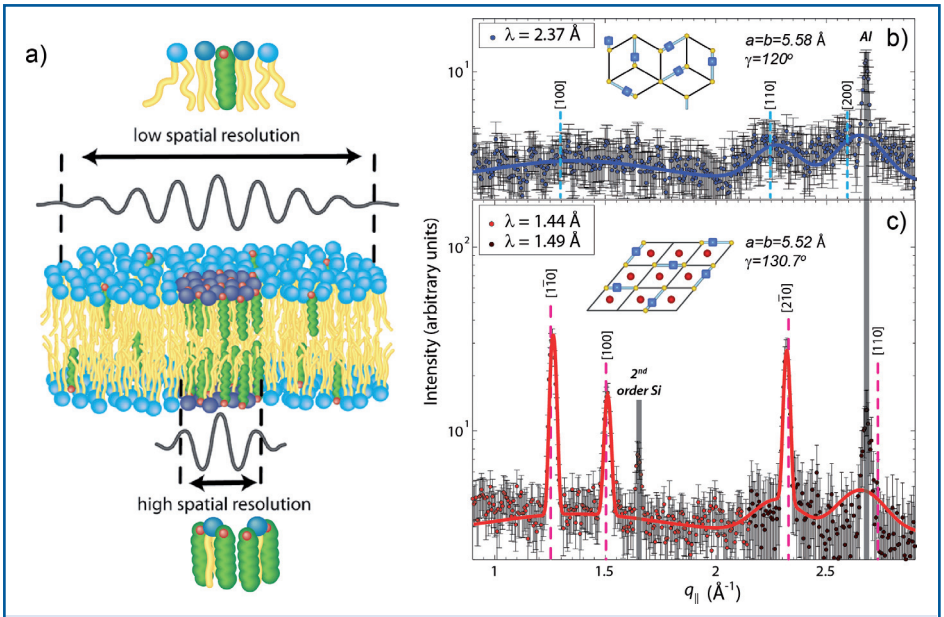

Fig. 5 Neutron diffraction of a deuterated lipid bilayer with 32.5 mol% (protonated) cholesterol. a) The "spatial resolution" of neutrons can be altered. At high spatial resolution, small scale structures are more visible in the diffraction signal. b) An in-plane measurement at low spatial resolution. Only disordered membrane features are observed. c) At high spatial resolution, sharper peaks are observed which are indicative of a more ordered, small scale structure (Adapted from [4]).

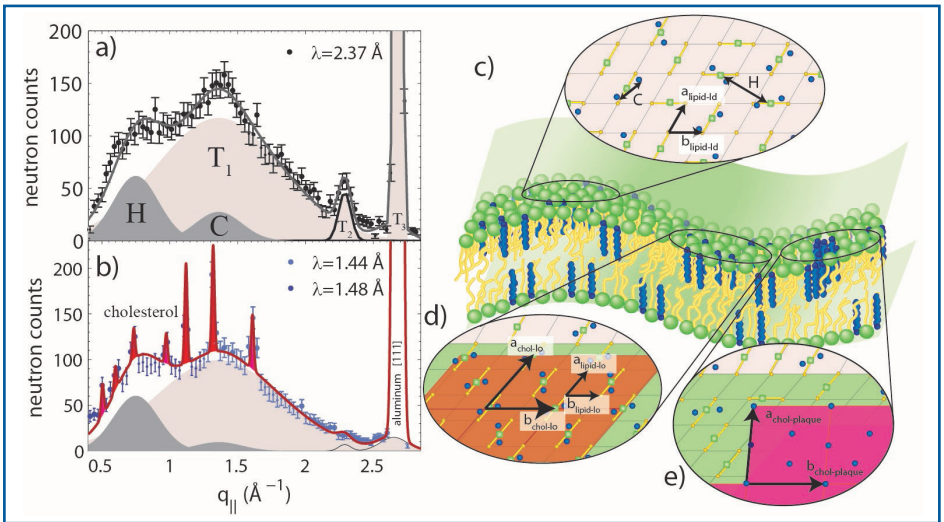

Fig. 6 Neutron diffraction of a protonated lipid membrane with 32.5 mol% deuterated cholesterol. This experiment is sensitive to the structure of cholesterol. a) A diffraction measurement at low spatial resolution, revealing a disordered membrane structure. Features describe scattering from lipid head-head interactions, tail-tail interactions, as well as direct cholesterol-cholesterol interactions. b) In addition to the broad peaks appearing in a), additional sharper peaks appear which describe small scale, ordered structures. c) A depiction of the disordered structures observed in the scattering. d) A monoclinic cholesterol lattice appears which agrees well with the structure observed in Fig. 5. e) Cholesterol plaques consisting of bilayers of cholesterol molecules (Adapted from [5]).

averaged with the surrounding membrane. In a membrane, raft regions will be averaged with the more abundant non-raft regions and the signal will be lost. However, by shrinking the coherence length of the probe, the scattering signal becomes an incoherent sum of many smaller coherent averages, giving more weight to the smaller scale structure, as depicted in Fig. 5. At high coherence length, non-raft regions dominate in a diffraction measurement. At low coherence length, both raft and non-raft regions are visible indicated by the well-developed scattering signals.

The results for (protonated) membranes containing 32.5 mol% deuterated cholesterol are shown in Fig. 6 [5]. At low spatial resolution, a diffraction pattern corresponding to a disordered structure was observed (Fig. 6(a)). The observed scattering is a result of lipid tail and head group scattering as well as cholesterol-cholesterol scattering (although the lipids were not deuterated, they still have some scattering power). These correlations are short ranged. At high spatial resolution, peaks appear to be significantly sharper (Fig. 6(b)). These peaks can be described by three different structures: Broad peaks correspond to a fluid membrane phase, where cholesterol molecules form complexes with lipids according to the umbrella model. Sharper peaks can be indexed by small, well-ordered lipid patches, where lipid and cholesterol molecules form l_o domains (rafts). The third set of peaks agrees well with cholesterol plaques, bilayers made entirely of cholesterol molecules, which have been observed at high cholesterol concentrations. By combining selective deuteration and the ability to control the neutrons' coherence length, these neutron diffraction experiments unambiguously identify the

presence of highly ordered, fluctuating domains in binary lipid cholesterol mixtures.

CONCLUSION

For decades, elastic and inelastic neutron scattering have provided essential information for the life sciences, such as molecular biology, biochemistry and molecular medicine and in particular computational biology. The neutron probe allows the determination of molecular structure and dynamics in biological systems, such as proteins and membranes, in a window of length and time scales not easily accessible by other techniques. By selective deuteration, different components of complex, multi-component systems can be highlighted and their structure, dynamics and interactions can be studied unambiguously and independently. The next generation of neutron instrumentation at the latest and most powerful neutron sources will likely give unprecedented insight into molecular processes to address important questions, such as infectious diseases and novel antibiotics, Alzheimer's disease and cancer.

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Microstructure and *In-Situ* Solidification Analysis of Al-Ce-Mg Alloy

by Joshua Stroh and Dimitry Sediako

The constant need to improve engine performance and fuel economy has led the automotive and aerospace industries to maximize the use of lightweight alloys. Aluminum (Al) alloys are becoming increasingly popular because of their high strength to density ratio and their great casting properties. Al alloys have become one of the most widely used alloys for the manufacturing of powertrain component such as engine heads, pistons and turbochargers [1-4].

Recently, the effects of rare earth (RE) additions, such as cerium (Ce), on Al alloys have been a focus because these additions tend to increase strength and produce higher temperature resistance, and these improvements have demonstrated in pistons and turbochargers, specifically.

Notably, a large increase in yield strength, up to 77%, and creep resistance at temperatures exceeding 300 °C was observed for an Al-Ce-Mg alloy in comparison to an Al-Cu based industrial alloy A206 [5-8].

Why Ce has such positive effects in Al-Ce-Mg is a subject of on-going research. One study indicates that part of the answer may be in the formation of secondary phases (e.g., $Al_{11}Ce_3$, or Al-Ce-Mg) [7], but much is still unknown about the microstructural characteristics (i.e., the effects of the phases present as well as the solidification kinetics) – knowledge needed for further developing high strength Al alloys.

Studying the microstructural characteristics of alloys is challenging because all methods have significant limitations, as many are only useful to study the surface. X-ray diffraction, for example, is limited to characterization of surface properties, which may be different from the bulk. Neutron beams, however, are highly penetrating in aluminum: 10% of the beam will penetrate as deeply as 30 cm. This penetrating power enables the design of experiments to observe changes to microstructural properties *in situ*. Sediako *et al.* [9-13] have demonstrated *in situ* neutron diffraction (ND) can analyze the characteristics of Al alloy systems during solidification. These studies indicate that *in-situ* ND is precise and reproducible, and is advantageous over thermal analysis because it characterizes the solid growth of each phase in multiple crystallographic planes.

Summary

Higher performing or more efficient cars and planes challenge conventional approaches to understand and improve alloys. *In-situ* neutron diffraction reveals critical insights into alloys' microstructural evolution.

In this article, we illustrate the application of *in-situ* ND to Al alloys with current research to characterize the kinetics of solidification, phase evolution and fraction solid of several phases of Al-8%wt.%Ce-10wt.%Mg alloy. To obtain a fuller picture, ND is complemented with Optical Microscopy (OM), Scanning Electron Microscopy (SEM), and an equilibrium model FactSage™ simulation.

MICROSCOPY

To prepare for optical and electron microscopy, circular samples with an approximate diameter of 19 mm and a thickness of 12.5 mm were cut from a larger as-cast Al-Ce-Mg specimen, ground and polished and then submersed in Keller's etchant [14] for 30 seconds. Images were captured with the optical microscope at 100×, 200× and 500× magnification.

OM revealed six phases present in varying quantity throughout the continuous Al matrix, with approximate grains sizes from 50-200µm. SEM was then conducted to characterize the composition of each phase. Figure 1 illustrates several different phases that were further characterized with SEM techniques such as X-ray Energy Dispersive Spectroscopy (EDS) point analysis as well as secondary electron (SE) imaging. The SEM data obtained and the binary Al-Mg phase diagram suggest that the continuous matrix (location A in Fig. 1) is the α-aluminum containing dissolved magnesium, as well as Al-Mg phases (mostly Al_7Mg and $Al_{140}Mg_{89}$ [15-17]) phases with combined Mg concentration of approximately 13at.% (+/−2%).

Within the matrix was a "fish bone" secondary phase (location B) that ranged in size from 10-600 µm. This phase was determined to be composed of Al, Ce and Mg. The composition of a square or "X" (location C) shaped

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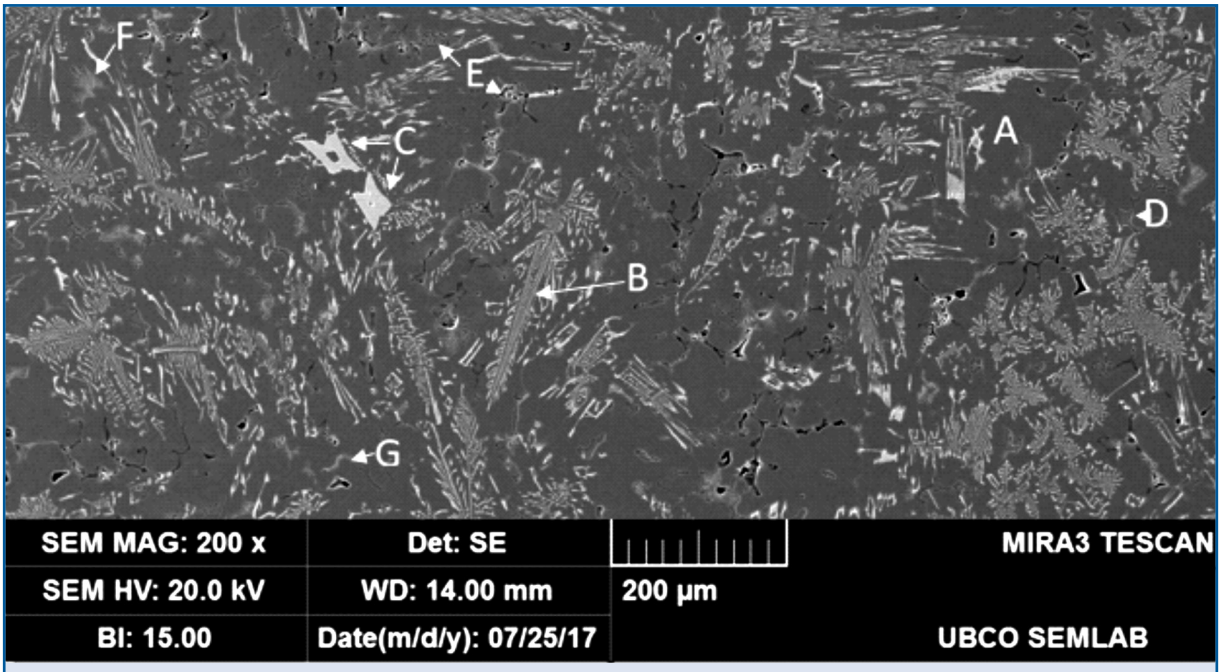

Fig. 1 SEM image illustrating the seven phases present in the Al-Ce-Mg alloy.

intermetallic was found to be similar to the $Al_{11}Ce_3$ phase of the Al-Ce-Mg alloy. A smaller, dark Chinese script phase (location E) as well as three different irregular shaped phases (locations D, F and G) were also present, but they appeared in lower quantity as compared to the fish bone phase.

NEUTRON DIFFRACTION

The *in-situ* ND experiments were performed at the C2 powder diffractometer at theCanadian Neutron Beam Centre (CNBC) in Chalk River, Ontario. To monitor temperature, ahole for a thermocouple was drilled in one end of a 10.5 mm diameter, 40 mm cylinder sample of the Al-Ce-Mg alloy. The sample was mounted into a graphite crucible and aligned within the furnace sample chamber to the neutron beam. Argon gas was used to minimise oxidation during the experiment. The methodology of the experiment is explained in more detail in [9-12].

To determine the range of temperature needed for the experiment, a FactSage™ simulation was used to predict the approximate liquidus, nucleation and solidification temperatures. The sample was elevated above the predicted liquidus temperature by ~25 °C to ensure the entire sample was completely molten. The temperature was then lowered stepwise and neutron diffraction data were collected for 1 hour at each step, using a monochromatic incident neutron beam with a wavelength of 2.37 Å, and a wide span detector collected neutron counts over a diffraction angle (2θ) range of 35° to 115°. The collection time represents a balance between the total beam time spent and the statistical quality of low intensity peaks for the semi-solid metal at high temperatures. Applying Bragg's law for diffraction, as shown in Eq. (1), where n indicates the order of reflection, λ is the wavelength, and θ is the diffraction angle, the interplanar spacing d for various phases can be calculated [2,16],

$$n\lambda = 2d\sin\theta \quad (1)$$

Seven peaks were obtained from the ND data and analysed with application of the Inorganic Crystal Structures Database [18] based on the collected diffraction angles and corresponding d-values for the Al-Ce-Mg alloy. It was determined that three α-Al peaks, Al ({111}, {200} and {220}), three $Al_{11}Ce_3$ peaks ({103}, {112}, and {200}), and one Al-Ce-Mg peak were present.

As the metal is completely liquid at 610 °C, no noticeable peak is present at the first temperature step in Fig. 2. The next temperatures illustrate evolution of peak intensity. Figure 2 also illustrates a new phenomenon where the Bragg's peaks initially shift towards the left (i.e., smaller angles, larger d-spacing of the *hkl*-planes) until the temperature drops to ~530 °C, indicating an expansion in interplanar spacing, rather than a decrease as would be expected from thermal contraction and described by Lombardi *et al.* [4]. The reason for this unexpected shifthas yet to be determined, but may be due to the secondary Al-Ce-Mg phase forming quite rapidly below approximately 570 °C (shown in Fig. 2), which takes place simultaneously with evolution of a-aluminum, and the atomic planes of the intermetallic phase may be affecting the *hkl* spacing of the aluminum matrix. Another possible reason for the angle shift is the rapid

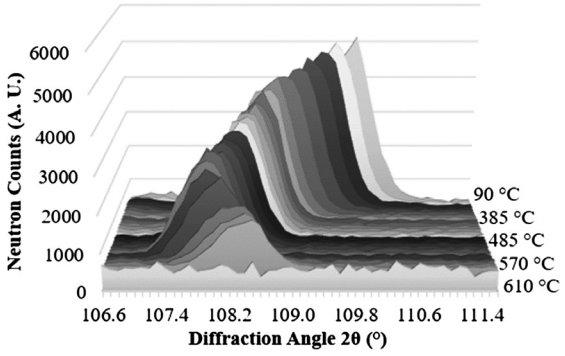

Fig. 2 Neutron diffraction peaks of the Al {220} plane in the Al-Ce-Mg alloy.

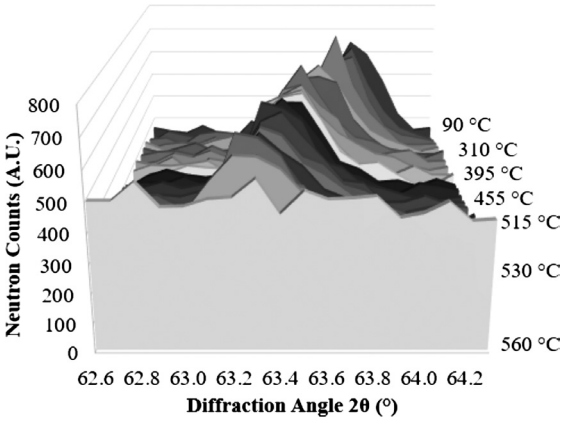

Fig. 3 Neutron diffraction peak of the "Fish bone" Al-Ce-Mg phase in the Al-Ce-Mg alloy.

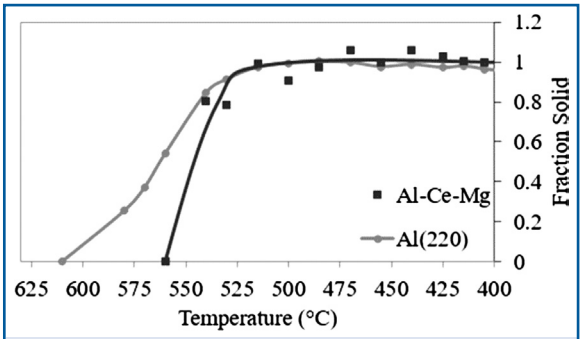

Fig. 4 Solidification curve of the Al (220) plane and the Al-Ce-Mg fish bone phase in the Al-Ce- Mg alloy (undetermined crystallographic plane).

increase in the amount of Mg dissolved in face centered cubic Al (FCC_Al) phase.

According to the FactSage™ simulation, the Mg begins precipitating out of FCC_Al at approximately 410 °C. This Mg precipitation contributes to the formation of the new Al-Ce-Mg phase, and further complicates the analysis. It especially complicates the Debye-Waller normalization, which is supposed to be temperature-dependant only [4]. Nonetheless, the simultaneous evolution of the Al-Ce-Mg, $Al_{11}Ce_3$, and the Al phases could increase the distance between adjacent lattice planes in the matrix and therefore cause the unexpected angular shift.

Figure 3 shows the peak corresponding to the low intensity Al-Ce-Mg secondary "fish bone" phase. The diffraction pattern for this phase is weak, with 13% of the intensity of the Al{220} plane, and no peak is clearly detectable until 530 °C, before which either the metal is fully liquid, which causes a relatively high background neutron count, or the phase has a very low volume fraction. In contrast, solid phases are visible in the data for $Al_{11}Ce_3$ at the highest temperature, 610 °C, even though the FactSage™ simulation predicted $Al_{11}Ce_3$ phase nucleation at ~560 °C. Thus, although FactSage™ properly predicted the primary the kinetics for α-Al phase, it misrepresented the evolution of $Al_{11}Ce_3$ phase.

While the location of the peaks corresponds to the interplanar spacing for a phase, the intensity of the peak is related to the fraction of the phase in the alloy, relative to the maximum amount of the phase (100%) at the completion of phase evolution. Integrating the peak intensities over the angular interval at the specific temperatures allows one to calculate the solidification kinetics for each of these phases. This calculation requires removing the background neutron scattering due to the graphite crucible or thermocouple materials, followed by normalizing against the peak intensity from liquidus to solidus.

Solidification curves similar to the representative trends shown in Fig. 4 were produced for each peak. The point at which a fraction solid of 1.0 is first reached was determined to be the end of evolution for that phase. For the Al-Ce-Mg alloy, the nucleation of the primary α-Al phase begins at temperatures above 580 °C and the phase continues to solidify until approximately 515 °C. Although the ND data indicated that the $Al_{11}Ce_3$ phase was still partially solid at the highest recorded temperature and therefore the exact nucleation temperature could not be determined, the end of solidification of this phase was found to be ~515 °C. The fraction solid curve of the new Al-Ce-Mg phase in Fig. 4 suggests that this phase begins nucleation at 560 °C and completes its solidification at 515 °C.

CONCLUSIONS

In-situ ND during the solidification of an Al-Ce-Mg alloy, complemented by microscopy analysis, provided a more comprehensive understanding of phase nucleation and evolution on multiple crystallographic planes. Though FactSage™ has been a reliable tool to get an understanding of the solidification path and primary and secondary phase evolution for systems, such as Mg-Al, Mg-Zn, Al-Cu, and Al-Si [2-4,11], it did not properly

predict the kinetics of phase evolution or the composition of the secondary phases in our Al-Ce-Mg alloy. This experiment provided data on evolution kinetics of Al-Ce and Al-Ce-Mg intermetallic phases that contribute to high yield strength at elevated temperatures, information that could lead to optimizing the composition and casting process for maximum strength. *In-situ* ND is therefore a powerful tool for the development of advanced alloys of interest to automotive and aerospace applications.

ACKNOWLEDGEMENTS

The authors gratefully acknowledge contribution of the sample material and expert support received from Dr. David Weiss of Eck Industries, Manitowoc, WI. We are also grateful to Canadian Nuclear Laboratories for neutron beam time. We acknowledge Dr. Daniel Banks of the Canadian Neutron Beam Centre for editing of the manuscript.

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The 75th CAP Annual Congress
75e Congrès annuel de l'ACP

June 3-7 juin, 2019, SFU, Burnaby BC

Preliminary Information

Programme préliminaire

https://www.cap.ca/congress/2019 https://www.cap.ca/congres/2019

Mark your calendar
Marquez votre calendrier

Monday, June 3 / lundi, le 3 juin - 08h45

Opening Plenary Lecturer
Conférencière plénière d'ouverture

Dr. Donna Strickland
University of Waterloo

https://uwaterloo.ca/physics-astronomy/people-profiles/donna-strickland

Monday, June 3 / lundi, le 3 juin - 19h30

Herzberg Public Lecturer
Conférencier publique Herzberg

Dr. Manu Prakash
Stanford University

http://web.stanford.edu/group/prakash-lab/cgi-bin/labsite/

Congratulations to 2018 Nobel Prize recipient Donna Strickland

The 2018 Nobel Prize in Physics was awarded “for groundbreaking inventions in the field of laser physics”, with one half to Arthur Ashkin (US) and the other half jointly to Gérard Mourou (France) and Donna Strickland (Canada).

Dr. Ashkin is recognized for his development of “optical tweezers” which have allowed tiny organisms to be handled with light beams. Drs. Mourou and Strickland share their prize for “their method of generating high-intensity, ultra-short optical pulses”.

Canadian physicist Dr. Strickland (University of Waterloo) was recognized for her research on laser beam amplification and compression undertaken while a PhD student working with Dr. Mourou.

Her work on developing very short, very intense laser pulses, referred to as the Chirped Pulse Amplification (CPA) technique, has transformed the world of laser physics, and has opened this field of research to many others around the world. It has led to improvements in eye surgery and machining applications, among other applications.

More information about the 2018 Nobel Prize in Physics can be found on the Nobel Prize website at https://www.nobelprize.org/nobel_prizes/

Le Prix Nobel de physique 2018 a été décerné « pour inventions novatrices dans le domaine de la physique des lasers », avec une moitié à Arthur Ashkin (États-Unis) et l’autre moitié conjointement à Gérard Mourou (France) et Donna Strickland Canada).

Le Dr Ashkin est reconnu pour sa mise au point des « pinces optiques », faisceaux lumineux qui permettent de manipuler de minuscules organismes. Les Drs Mourou et Strickland partagent le prix pour « leur méthode de production d’impulsions optiques ultracourtes de forte intensité ».

La Dre Strickland, physicienne canadienne (Université de Waterloo), a été reconnue pour ses recherches sur l’amplification et la compression de faisceaux laser, entreprises lors de ses études doctorales avec le Dr Mourou.

Ses travaux de mise au point d’impulsions laser ultracourtes de forte intensité, appelés méthode d’amplification d’impulsions compressées (CPA), ont transformé le monde de la physique des lasers et ouvert ce domaine de recherche à nombre d’autres chercheurs du monde entier. Ils ont mené à des progrès en chirurgie oculaire et à des applications d’usinage, entre autres.

Pour plus de renseignements à propos du Prix Nobel de physique 2018, prière de consulter le site Web du Prix Nobel à https://www.nobelprize.org/nobel_prizes/

Félicitations à Donna Strickland, Lauréate du Prix Nobel 2018

https://www.cap.ca/publications/cap-news https://www.cap.ca/fr/publications/nouvelles

Congrès de l'ACP 2019 CAP Congress, June 2-7, Simon Fraser Univ., Burnaby BC

PRELIMINARY OUTLINE (subject to change) - **PROGRAMME PRÉLIMINAIRE** (sous réserve de modifications) — Updated/Mise-à-jour : 2018 Oct. 26

Time	Sunday, June 2	Monday, June 3	Tuesday, June 4	Wednesday, June 5	Thursday, June 6	Friday, June 7
	Pre-Congress Meetings	NOTE: One of the plenaries during the week will focus on equity, diversity and inclusion	Exhibitors	Exhibitors		Post-Congress Meetings
7:30	Schedule of Division Meetings Monday 12:30: DASP DNP DPMB DPP Wednesday 12:30: DAPI DCMMP DPE PPD Thursday 12:30: CEWIP DHP DTP			Science Policy Cmte Meeting (w/food) / PIC Editorial Board Meeting (w/food)	CNILC Meeting (w/food) / CINP Board Meeting (w/food)	
7:45		Registration Opens				
8:00						CAPF AGM (w/food)
8:15						
8:30		Formal Opening	THEME 1 / THEME 2 / THEME 3 / THEME 4 / THEME 5 / THEME 6 / THEME 7 / Parallel Sessions T1	Wed AM Plenary Talk Speaker: tba	Thur AM Plenary Talk Speaker: tba	
8:45		Monday Plenary Talk Speaker: Donna Strickland, U.Waterloo 2018 Nobel Prize recipient				
9:00						
9:15		Monday AM Plenary Talk Speakers: tba		CAP Herzberg Medal Talk	CAP-TRIUMF Vogt Talk / Medal	
9:30						
9:45				CAP Brockhouse Talk	CAP-CRM Prize Talk / CAP Industrial and Applied Medal	
10:00						
10:15		Health Break	Health Break	Health Break	Health Break	
10:30						
10:45		Parallel Sessions M1 (90 Minutes)	THEME 1 / THEME 2 / THEME 3 / THEME 4 / THEME 5 / THEME 6 / THEME 7 / parallel Sessions T2	Parallel Sessions W1 (90 Minutes)	Parallel Sessions R1 (90 Minutes)	
11:00						
11:15						
11:30						
11:45						
12:00	CAP Advisory Council Mtg (old & new) (w/lunch) Followed by meeting of Council, Friends, others to discuss membership campaigns					
12:15		Past Pres. Dinner and Meeting / Canadian Light Source Users Consult. / New Faculty Lunch with NSERC / CAP Division Business Meetings	Lunch	CAP Outreach Cmte mtg / Student Seminar: tbd / Science Policy Workshop: tbd / CAP Division Business Meetings	Comms Cmte Meeting / Student Seminar: tbd / CEWIP Bus Mtg & Recep / CAP Division Business Meetings	
12:30						
12:45						
13:00						
13:15						
13:30		Parallel Sessions M2 (90 Minutes)	THEME 1 / THEME 2 / THEME 3 / THEME 4 / THEME 5 / THEME 6 / THEME 7 / parallel Sessions T3	Parallel Sessions W2 (90 Minutes)	Parallel Sessions R2 (90 Minutes)	
13:45						
14:00						
14:15						
14:30						
14:45						
15:00		Health Break	Health Break	Health Break	Health Break	
15:15						
15:30		CAP Teaching Medal Talk	THEME 1 / THEME 2 / THEME 3 / THEME 4 / THEME 5 / THEME 6 / THEME 7 / parallel Sessions T4	Wednesday PM Plenary Talk Speaker: tbd	Finals: Best Student Oral Competition (BSOC)	
15:45		CAP Lifetime Achievement Medal Talk				
16:00						
16:15		NSERC Report NSERC EG Chair Report CAP-NSERC LC Report		Parallel Sessions W3 (90 Minutes)		
16:30						
16:45						
17:00			Poster Session & Finals: Poster competition			
17:15						
17:30	Dept Leaders Dinner and meeting (this is a tentative date and is subject to change. Alternate possibility is Tuesday evening from 18:45-21:15)			CAP President's Report	Thursday PM Plenary Talk Speaker: tbd / Judges Meeting	
17:45						
18:00		Welcome Reception (BBQ)		CAP AGM	Student Awards Ceremony	
18:15						
18:30					Close of Congress and Formal thanks to LOC	
18:45			Students: PD / Industry liaison / Friends of CAP Dinner and Meeting			
19:00					Meeting of LOCs / CJP Editorial Board Dinner	
19:15						
19:30		Herzberg Public Lecture Speaker: Manu Prakash, Stanford U.		CAP Medallists Awards Banquet @ ?? 19h30 - 21h00 (sit down dinner) - Limited seating. Tickets will not be sold at the door.		
19:45						
20:00					CAP Board-Institutional Partners dinner meeting (20h00-21h30)	
20:15						
20:30						
20:45						
21:00		Reception following lecture (light refreshments served)				
21:15						
21:30						

High School / Cégep Teachers' Day Workshop

CAP Board (old & new) (w/food)

IPP Annual General Meeting

IPP Science Council Meeting (w/food)

IPP Institutional and Board Meetings

CINP+IPP Joint Session

CINP AGM

CAPF Board Meeting

Neutron Reflectometry Investigation of Near Ionomer/Catalyst Interface Structure in Polymer Electrolyte Based Energy Devices

by Kunal Karan, Udit N. Shrivastava, and Helmut Fritzsche

Concerns of effects of climate change on human life [1] and of urban air pollution on human mortality [2] is pushing the transition to low-carbon energy systems, as seen by a rapid growth in renewable energy sources such as wind and solar. However, the intermittency of renewables has created a critical need for affordable, robust and application-matched electrical energy conversion and storage (ECS) systems [3]. Of particular interest are polymer electrolytes (PE) based ECS devices such as fuel cells, batteries, electrolyzers and artificial photosynthesis. Canada is a world leader in PE-based fuel cells (PEFC) and electrolyzers for generating hydrogen from water. Automotive Fuel Cells Cooperation (Burnaby) is developing PEFC stacks for vehicles. Ballard Power Systems (Burnaby) is developing them for a variety of other applications in transportation (bus, rail), materials handling (forklifts), defence, and backup power. Hydrogenics Corporation (Mississauga) is the world leader in PE electrolyzers and also develops PEFC stacks. These companies aim to develop ECS systems that are highly efficient, low-cost and durable. Development of new materials to support engineering of devices is critical to meeting these goals.

PE-BASED ECS DEVICES

In PE-based ECS devices, the PE is an ion-conducting polymeric membrane that separates the two electrodes. In the porous electrodes of these devices, charge is transferred from sub-micron thin films of ion-conducting polymer (the "ionomer") to an electron-conducting material, which in the case of a PEFC is an electrocatalyst, such as Pt, or in the case of PE supercapacitors, carbon. The total active interfacial area controls the amount of electrical current, while the composition of the electrochemical interface controls the efficiency of the charge-transfer process. Thus, the physical and chemical characteristics of the electrochemical interface is a topic of intense research. While our discussion focuses on the ionomer-catalyst interface in a PEFC, the scientific aspects are pertinent to electrochemical interfaces in all PE-based devices.

Summary

The neutrons' ability to non-destructively probe structures of polymer films shines new light on the platinum-ionomer electrochemical interfaces in energy conversion and storage devices.

In a PEFC, illustrated in Fig. 1a, hydrogen and oxygen/air are supplied to the anode and cathode, respectively. These reactant gases diffuse from the respective flow channel through a porous carbon layer (~300 μm) called the gas diffusion layer (GDL) to a-few-microns-thick catalyst layer (CL); this is depicted for the cathode side in Fig. 1b. The CL is comprised of aggregates of ~30 nm carbon supporting 2-5 nm Pt nanoparticles covered by 3-10 nm thin ionomer films. For the occurrence of oxygen reduction reaction (ORR) at the PEFC cathode, the reactants – electrons, protons and oxygen gas – must arrive simultaneously via Pt/Carbon, hydrophilic channels of the ionomer, and pores, respectively to the Pt/ionomer interface. The product water generated on the Pt surface must exit through or around the ionomer film.

RESEARCH QUESTIONS

Understanding the hot bed of activity around the Pt-ionomer interface, especially with respect to water distribution is critical to designing high performance PE-based devices. Proton conduction in these ionomers occurs via a connected network of water-filled hydrophilic domains distributed within a hydrophobic matrix. Nafion, a DuPont product, is the most commonly used ionomer and belongs to the perfluorosulfonated acid (PFSA) class of materials. In bulk membranes of Nafion, SAXS data indicate the characteristic dimension of the proton- conducting hydrophilic domains as 2-4 nm [4-5]. Recent TEM images indicate that ionomers in PEFC catalyst layers are of comparable thickness, 3-10 nm [6], raising the question, can hydrophilic domains exist in ultra-thin ionomer films in PEFC's? If not, how do protons conduct in such thin films?

Furthermore, when confined to thicknesses below 50 nm, ionomers exhibit remarkably different properties (such as proton conductivity, water uptake, swelling, and possibly oxygen diffusion) compared to bulk membranes [7-8].

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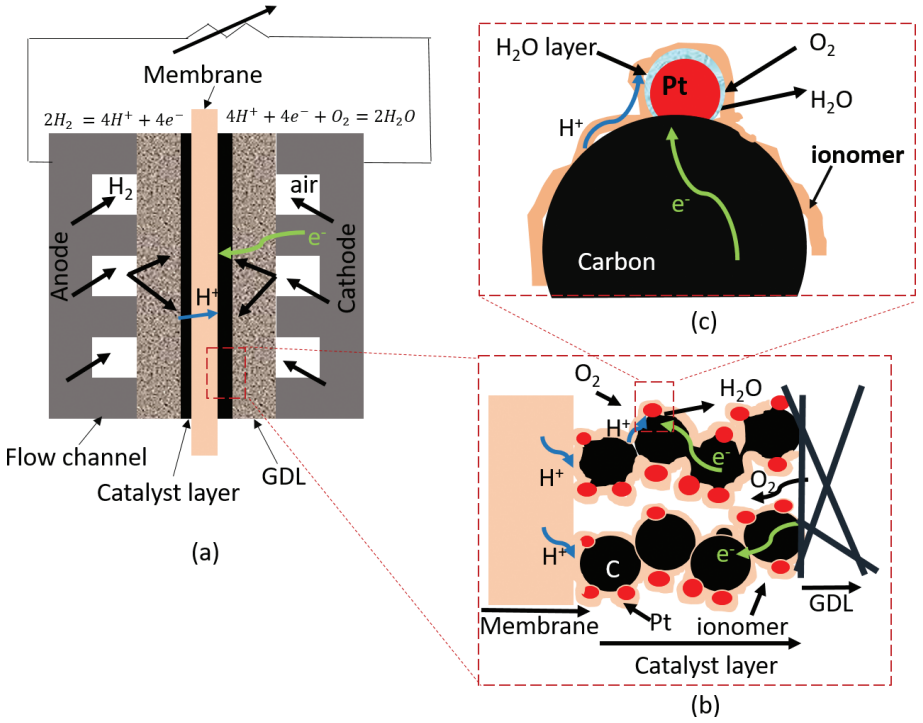

Fig. 1 (a) Schematic representation of a polymer electrolyte fuel cell (PEFC), (b) Structure of and transport in the PEFC catalyst layer, (c) Local structure and transport near the Pt-C-ionomer interface.

The density of ionomers may increase near the Pt-ionomer interface [9]. There is evidence that the hydrophilic sulfonic groups of Nafion are coordinated with the Pt [10-11]. However, it is not known how such interactions affect the formation of hydrophilic domains responsible for water-mediated proton transport. Is there interfacial water at the ionomer-catalyst interface? And, does it contribute to interfacial proton transport?

NEUTRON REFLECTOMETRY (NR) INVESTIGATIONS OF IONOMER THIN FILMS

NR is an ideal tool for probing the interfacial and bulk structures of polymer thin films [12]. The sensitivity of neutrons to light elements and the ability to penetrate most materials enables the in-situ investigation of water at the buried Pt-ionomer interface as well as in the ionomer film. The weak interaction of neutrons with matter do not change the sample under investigation, unlike x-rays and electrons, and there is no need to keep the sample in a vacuum.

Principle of NR: The scattering geometry for a typical reflectometry experiment is shown in Fig. 2. An incoming neutron beam, with wave-like properties, hits the surface of a specimen at a grazing angle θ_i and is partly reflected specularly at an angle θ_r and partly transmitted (refracted) into the specimen at an angle θ_t with respect to the sample surface.

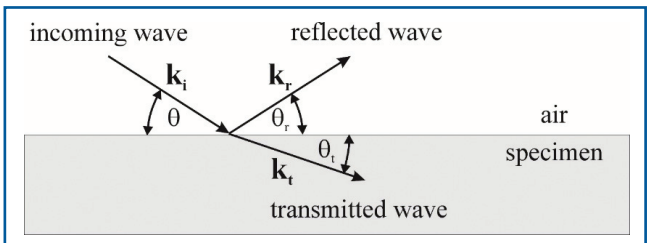

Fig. 2 Scattering geometry of a typical neutron reflectometry set-up.

The intensity of the reflected and transmitted wave can be described with an index of refraction n, identical to classical optics: $n = k_t/k_i$, with the wavevector $k_i = 2\pi / \lambda$ in air, the wavevector k_t in the specimen, and the neutron wavelength λ, respectively. The wavelength is calculated from the de Broglie relationship. The index of refraction can be written as

$$n = \sqrt{1 - \frac{\lambda^2}{\pi} Nb} \qquad (1)$$

with N being the atomic density and b being the nuclear scattering length. The product $N \times b$ is called scattering length density (SLD), which varies randomly from element to element and isotope to isotope but their values are well known [13].

NR is highly sensitive to water uptake because the SLDs of water and dry Nafion differ in sign and magnitude, -0.56×10^{-6} Å^{-2} and 4×10^{-6} Å^{-2} respectively; the slightest water uptake leads to a decrease in the net SLD.

The neutron refractive index and the Fresnel reflectivity arising at interfaces can be calculated based on the Parratt recursion algorithm and Eq. (1) [14]. In a typical NR experiment, the reflectivity, which is the specularly reflected intensity divided by the incident intensity, is obtained as a function of incidence angle (θ), and is commonly presented as a function of the scattering vector (Q), where Q is given by $Q = 4\pi/\lambda \cdot sin\theta$. For thin films, reflectivity is fit to a layered model where the SLD, layer thickness, and, if needed, interface roughness of each layer are variables [15].

Pioneering work on NR of ionomer thin films have been carried out by Dura and co-workers at NIST, USA. Their study examined 60 nm Nafion thin films on gold or SiO_2 substrates under high relative humidity (RH) [16] conditions. For SiO_2, they observed a multi-lamellar structure near the interface, comprising of alternating 3 nm thick water-rich and water-lean layers but for Au, only a single polymer layer was observed with a water rich layer at the interface. Wood *et al.* performed an NR study at Los Alamos on ~60 nm Nafion films on Pt, PtO, and hydrophilic glass carbon (GC) substrates at room temperature and 97% RH [17]. The interfacial layer for films on Pt was water lean but for PtO and GC was water-rich compared to bulk ionomer layers. Upon hydrophizing the SiO_2 substrate, Page *et al.* [18] at NIST observed the multi-lamellar structure of the ionomer change to a single bulk layer containing water. Recently, Kalisvaart *et al.* applied NR at Canadian Nuclear Laboratories to study the hysteresis effect of temperature from 25 °C to 60 °C and RH up to 97% for a 15 nm Nafion film on SiO_2 [19]. The films showed increased water absorption and hygro-expansion with temperature, but after cooling to the original temperature at 97% RH, the film demonstrated hysteresis by retaining some of the water.

OUR NR STUDIES OF THE IONOMER-PT INTERFACE

We are investigating ultra-thin ionomer films (50 nm and less) on a Pt substrate. Interpretation of NR data requires a careful choice of a layer model [20]. Instead of relying on statistical measures only, we employ complementary techniques such as quartz crystal microbalance (for water mass uptake) and ellipsometry (for swelling) to cross-correlate or constrain the NR model. The substrate is characterized by x-ray reflectometry and atomic force microscopy.

Preliminary Experiments: Here, we discuss NR for a 17 nm film of Nafion (EW1100) ionomer spin-coated on a 10 nm Pt film with a 4 nm Cr buffer layer sputter-coated on a Si wafer (with native oxide). NR measurements were carried out in dry (8% RH) and humid (97% RH) conditions at 30 °C using a humidity and temperature controlled cell [21]. The reflectivity measured over 12 hours from Q = 0.006 Å^{-1} to 0.14 Å^{-1} is shown in Fig. 3a. The fit using a three-layer model — an interfacial layer at the Pt-ionomer interface, a bulk ionomer layer, and a roughness

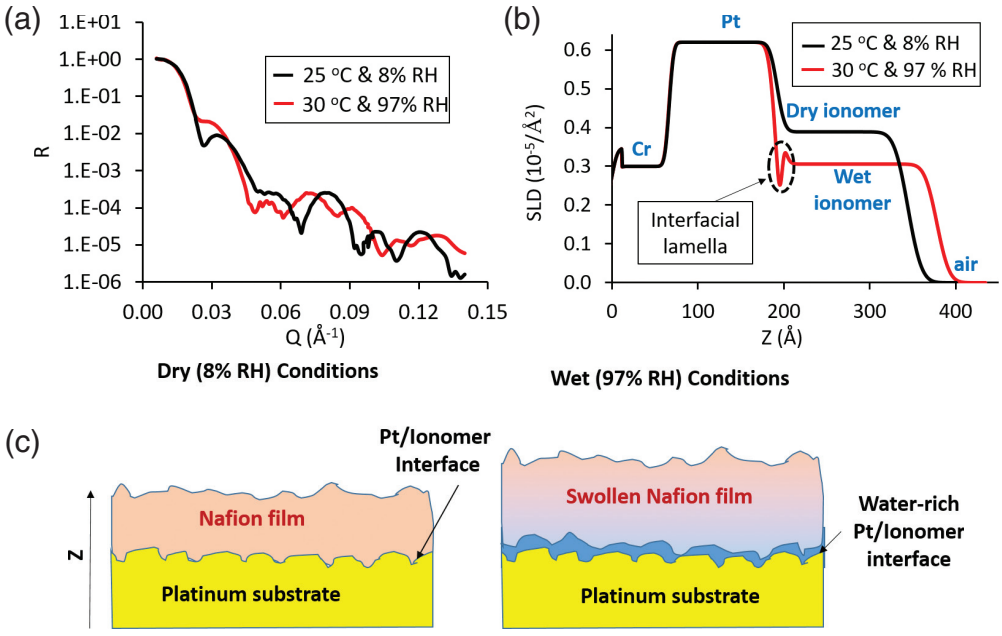

Fig. 3 (a) Reflectivity data of a 17 nm Nafion film on Pt-Cr-SiO_2. (b) Corresponding SLD profiles at 25 °C, 8%RH and 30 °C, 97% RH. (c) Depiction of the near ionomer-Pt structure deduced from the SLD profiles of (b).

layer — is depicted in Fig. 3b in terms of the SLD profiles. The dip in SLD at the Pt-ionomer interface corresponds to a 6 Å thick, 90% water interfacial layer, which was critical in the fit of all the NR data at high RH. Dura's previous work on ionomer-metal film presents similar findings [16]. The water uptake (λ = number of water molecules per SO_3^- group) determined from the SLD using Dura's approach was found to be 8.9 and a swelling ($\Delta L/L$) of 23% is consistent with ellipsometry data.

OUTLOOK

NR is a critical and powerful tool for studying the physical structure of the ionomer-catalyst interface for PE-based ECS devices. NR allows a quantitative assessment of the distribution of water *at* the electrochemical active ionomer-catalyst interface and *within* the ionomer films covering the catalytic surface. NR is unique in its ability to provide nm-scale resolution on spatial distribution of water at this critical interface of ECS devices. As the nature of this interfacial region is poorly understood, there is a tremendous opportunity to explore the unknowns for this system using NR, to detemine the effect of ionomer architecture or molecular structure on near ionomer-Pt interface structure, to investigate ionomer films of thickness relevant to fuel cell electrodes (4-10 nm), and to study the structure under operational conditions of electrical potential. Although NR relies on a model, experiments can be designed to remove artifacts by characterizing substrates separately, exchanging D_2O for H_2O, and cross- correlating with data obtained from other techniques.

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Canadian Research Combining Neutron Reflectometry and Electrochemistry

by James J. Noël

Summary

I overview Canadian neutron reflectometry, with a focus on applications in electrochemical and corrosion science research.

Neutron reflectometry (NR) is a powerful technique for probing surface layers, because it is sensitive to isotopic makeup and has excellent depth resolution, typically 0.5-1 nm, for layers in the range 0.5-300 nm thick. It is non-destructive and often amenable to in-situ observations. Its applications are well described [1-3]. Canadian NR capabilities have yielded key data on a variety of experimental systems: polymers [4-10], adsorbed layers [11,12], hydrogen storage materials [13-19], electrochemical capacitors [20], and corroding metals [21-26].

NR is based on specular reflection of neutrons from a planar surface, or from a series of layered interfaces. As does optical reflectivity technique, NR yields information on the differences between the refractive indices of the materials on either side of the interface in the form of a profile in the direction normal to the interface. The neutron refractive index of a material is related to its scattering length density (SLD), the weighted average of ρb of all the material's components, where ρ is the number density of atomic nuclei and b is their coherent neutron scattering length, an intrinsic and isotope-specific property of the atomic nucleus. NR can reveal a compositional depth profile of the interfacial layers to about 1 at.%, and its isotopic sensitivity is useful for isotopic labelling experiments or contrast matching [1]. When the surface contains multiple layers, a portion of the incident coherent neutron beam reflects from each interface, creating an interference pattern at the detector, which is related to the thickness of each of the surface layers by Bragg's law.

THE HISTORY OF NR IN CANADA

The earliest NR experiments [1] were reported in the 1980s, and NR became available in Canada in 1992 at the NRU reactor at Chalk River. The first experiments at NRU were conducted on a system of giant magnetoresistance (GMR) multilayers [27,28], for which beam scientist Zin Tun configured the C5 triple axis neutron spectrometer as a part-time reflectometer, since C5 already had the components required for reflectometry: monochromator; rotatable sample table; neutron detectors for signal counting and beam monitoring (in lieu of a reference beam); collimating slits; computer for instrument control and data acquisition; and radiation shielding (see schematic in Fig. 1). Only high-precision collimating slits had to be added for NR, and further success with studies of magnetism [28], polymer surfaces [7,8], and corrosion [22-26] facilitated formation of a user community that supported the construction of the CFI-funded custom-built neutron reflectometer at the D3 beam (Fig. 2) to improve quality of data and ease of operation. The D3 reflectometer, which was completed in 2007 and described by Fritzsche [10], was designed to balance competing issues, such as functionality, complexity and cost; high neutron flux versus low background; and resolution versus dynamic range [9]. Amongst its optimizations are: a very tall focusing monochromator to maximize neutron flux on the sample, a limiting parameter that determines resolution or time required for data collection; a correspondingly tall 32-wire detector for simultaneous measurement of specular and off-specular reflections; and supermirror polarizers for measurements involving magnetism. It was designed with the capacity to use cold neutrons, so that it could later be relocated to a reactor with a cold neutron source.

SOLID-LIQUID ELECTROCHEMICAL SETUP

Difficulties in passing neutrons through the electrolyte solution, or in obtaining large, flat interfaces in a solid electrolyte cell, make NR challenging for electrochemistry at liquid-liquid or solid-solid interfaces, respectively, but the solid-liquid electrochemical NR setup is often amenable for in-situ NR, even at elevated temperatures and pressures. The solid-liquid case uses some of neutrons' unique properties, including high penetrating power in most solids. They can be directed through the substrate, instead of through hydrogenous solutions, as is often done with electromagnetic probes, because hydrogen has high neutron cross-sections for absorption and inelastic scattering. Typically, a very thin, uniform layer of the electrode material, deposited on a substrate, is mounted in an

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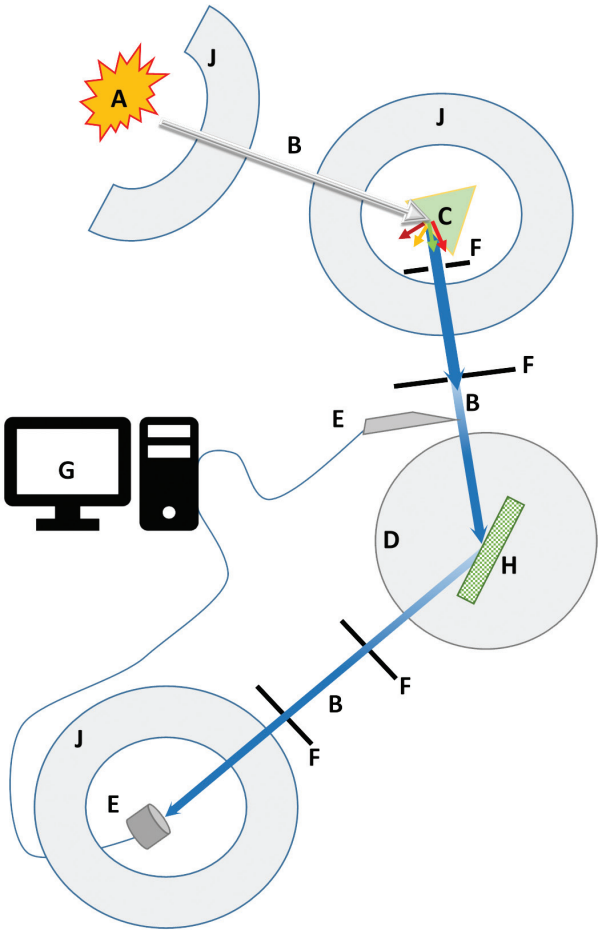

Fig. 1 Schematic layout of a neutron reflectometer, showing: **A**-neutron source; **B**-neutron beam; **C**-monochromator; **D**-rotatable sample table; **E**-neutron detectors for signal counting and beam monitoring (in lieu of reference beam); **F**-collimating slits; **G**-computer for instrument control and data acquisition; **H**-sample; and **J**-massive radiation shielding.

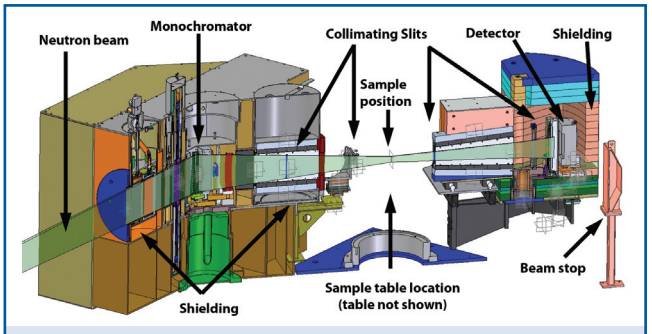

Fig. 2 Cut-away diagram of the D3 reflectometer at Chalk River Laboratories, with key features highlighted.

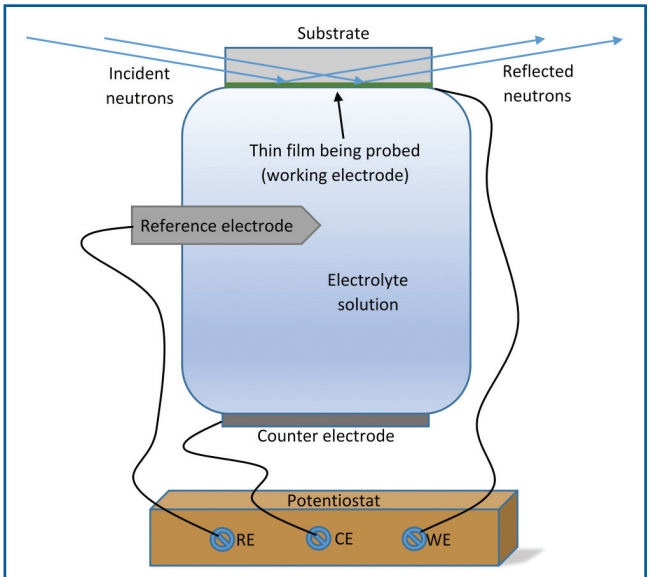

Fig. 3 Schematic illustration of electrochemical setup showing the path of neutrons through the substrate. The substrate, coated with the material under study, may be made to reside at the top, bottom or sidewall of the electrochemical cell, affording flexibility for work at a reflectometer with either vertical or horizontal beam orientation and with systems affected by the gravitational field.

electrochemical cell that allows neutrons to pass through the "back" of the electrode and reflect from the electrode-solution interface, continuing then to travel through the underlying substrate toward the detector (Fig. 3). Only neutrons that have reflected before crossing the outermost layer of the electrode-solution interface are detected. Thus, the electrochemistry in the solution does not interfere with the NR measurement. The surface can be configured either horizontally or vertically to suit the orientation of the reflectometer, but practical considerations, such as removal of evolved gas bubbles, or buoyancy or hydrophilicity effects on adsorbates, may favour one or the other orientation.

NR requires a very large, single-crystal substrate of a neutron-transparent material, such as silicon, quartz, or sapphire, which must be polished nearly atomically flat. Single crystal substrates avoid undesired scattering from grain boundaries. Neutron-transparency is needed since neutrons may travel through the full length of the substrate at the glancing incidence angles (<5°) required for reflection.

Similarly, the deposited electrode layer must also be thin, flat, and uniform over several square centimetres. Thinness minimizes incoherent and inelastic scattering. The large surface area is required for two reasons: (1) the low neutron flux, which is much lower than flux in analogous optical techniques, requires a larger beam, and (2) even with a narrow ribbon-shaped beam, the beam footprint is large at the glancing

incidence angles (<5°) required for reflection. That is, there is a wide separation between where the front of the beam hits the interface and the point where the back of the beam encounters it (Fig. 3). Since the maxima and minima in the reflected neutron interference pattern are related via Bragg's law to the thicknesses in a system of layers, flatness and uniformity of the electrode are essential to distinguish layers as thin as 1 nm from the surface roughness. Electrode preparation is not as daunting as it may sound. For example, the author has used 10 cm diameter single-crystal Si slabs of 6 mm thickness as substrates [21-26], with measured intensity losses of only about 15% over the 10 cm path that the neutrons travel through the Si.

CORROSION STUDIES

Much in-situ electrochemical NR research at Chalk River has been on corrosion of metals, particularly Ti [21-26], Zr [25,26], and Zr-2.5Nb alloy [24], because of their importance to the Canadian nuclear industry: Zr and Zr-Nb alloys are used in reactor fuel channels and fuel sheathing, and Ti was a candidate material for fabrication of nuclear fuel waste disposal containers, though it has been displaced for this purpose by copper-coated steel [29]. These metals are well suited for in-situ electrochemistry NR experiments, first, because they can be prepared by magnetron sputtering deposition. Second, their spontaneously-formed passive oxide films exhibit no roughening due to localized corrosion and they have very low corrosion rates, which enables stability over the 8-24 h periods required to collect clean, low noise NR data. Third, they tend to absorb atomic hydrogen, a common by-product of corrosion, and in situ NR has a rare ability to quantify hydrogen in metals non-destructively. Thus, we could simultaneously measure the metal and oxide layer thickness and composition, including hydrogen content, observing oxide film growth or hydrogen absorption as a function of electrochemical potential.

Titanium

On Ti, NR revealed that the air-formed passive oxide was a single layer with composition and density corresponding to that of the rutile polymorph. Neither the oxide layer nor the underlying metal changed when exposed to deaerated, near-neutral pH aqueous NaCl at the open-circuit potential [22,23]. However, applying anodic polarization thickened the oxide layer at the expense of the metal layer, and the metal absorbed a small amount of oxygen. The anodization ratio (potential-driven thickening), Pilling-Bedworth (volume expansion) ratio, and ionic transport numbers determined by NR were consistent with reported values determined by other means. Unlike the air-formed oxide, the anodic oxide consisted of two layers, an inner "dry" TiO_2 and an outer hydrated oxide with high OH content. Subsequent cathodic polarization changed the composition, but not the thickness of the oxide film. At more negative potentials, the film absorbed hydrogen progressively from the outer surface, increasing the outer hydrated oxide region's hydrogen content, converting the "dry" inner oxide (possibly reducing it to TiO(OH)), and penetrating into the underlying Ti metal. At a potential of −1.4 V vs the saturated calomel electrode (SCE), the inner "dry" oxide appeared to be almost fully hydrogenated, and at the next step of the polarization, −1.6 V(SCE), the electrode was destroyed by rapid hydrogen ingress into the metal and formation of gaseous hydrogen bubbles at the Si/Ti interface. Blisters and tattered remnants of burst metallic bubbles were visible on the electrode surface after the experiment [22,23].

More detailed studies to determine a threshold potential for hydrogen entry into Ti [21] were conducted in heavy water (D_2O) to create a higher contrast when hydrogen is absorbed in Ti. While natural abundance Ti and ^1H have negative SLD, deuterium's SLD is positive. Electrochemical impedance spectroscopy (EIS) measurements were made simultaneously with NR to link hydrogen absorption with changes in the oxide film's electronic properties. This approach allowed us to reconcile conflicting reports of the threshold potential for hydrogen entry into Ti: −0.37 V(SCE) and −0.6 V(SCE). At –0.37 V(SCE), significant changes in current density, oxide resistivity and capacitance, and the SLD of the Ti indicated the onset of oxide conductivity, D atom adsorption, and D ingress through electronically conductive, physically defective pathways in the oxide. At −0.6 V(SCE), both the current density and the D content in the Ti film increased substantially, and this potential was recognized as the threshold for reducing the protective oxide from the original TiO_2 to a less-protective TiOOD (i.e., TiOOH) and rendering it ineffective as a barrier to hydrogen ingress.

Zirconium and Zr-2.5Nb Alloy

On Zr in near-neutral Na_2SO_4 solution, the anodization ratio determined using NR was 3.4 $nm \cdot V^{-1}$, somewhat higher than the generally accepted anodization ratio for Zr (2.8 $nm \cdot V^{-1}$) determined by coulometry. The Pilling-Bedworth ratio was in good agreement with the value calculated from bulk densities or crystal lattice parameters [25,26]. Surprisingly, the oxide film growth continued beyond the expected logarithmic growth, albeit at a very low rate, for upwards of 12 h. EIS detected cracking in the oxide film at potentials above 1 V(SCE) when its thickness exceeded ~12 nm, evident in the sudden decrease of oxide film resistance and loss of passivation. Water in the cracks lowered the oxide layer SLD, and corrosion at the base of the cracks resulted in hydrogen absorption in the metallic Zr layer, a surprising observation, as cathodic polarization is normally required for hydrogen absorption. Neither the anodization ratio nor the Pilling-Bedworth ratio showed any discontinuity at the time of oxide cracking, and the EIS retained its single time constant response. These observations were taken as evidence that the cracks and intact regions of the electrode were behaving nearly independently, as parallel electrodes. In situ EIS measurements [26] were used to determine the oxide film capacitance and resistance. Since NR provided

an independent measure of the oxide layer thickness, it was possible to calculate the dc dielectric constant and resistivity of the oxide film according to ε = Cd/A ε°, where ε isthe dc dielectric constant, C the capacitance, d the oxide film thickness, A the surface area, and ε° the permittivity of free space, and to r = RA/d, where r is resistivity, and R resistance. The dc dielectric constant was at the lower end of the range of published values (25-56), and remained constant over the potential range −0.17 V(SCE) to 3 V(SCE), showing no deviation when the oxide film cracked. The resistivity was constant over the polarization range from −0.17 V(SCE) to 1 V(SCE) up to the point of oxide cracking.

Under cathodic polarization, NR showed that no hydrogen absorption into either the oxide or the metal, nor layer thickness changes, occurred, down to a potential of −2.5 V(SCE) [25,26]. EIS, however, detected significant changes. Immediately after the polarity reversal from 3 V(SCE) to −1 V(SCE), the oxide film resistance increased by more than an order of magnitude, due to repassivation of the metal at the base of the cracks in the oxide (not detected by NR due to small surface coverage by cracks). As the potential was decreased stepwise to −3 V(SCE), both the resistance and capacitance of the oxide layer decreased because of increased conductivity due to band bending in the semiconducting oxide (wide bandgap = 5.7 V) and possibly hydrogen doping at levels too low to detect by NR (i.e., <1 at.%).

The alloy Zr-2.5Nb, which is used to fabricate pressure tubes in CANDU® reactors, behaved much like pure Zr in that the oxide film thickened anodically and cracked at potentials above 1 V(SCE), with water filling the cracks, leading to hydrogen absorption into the underlying alloy [24]. The Pilling-Bedworth ratio was very similar to that of the pure Zr, but the anodization ratio was different, assuming two values, 1.74 nm·V^{-1} between –0.2 and 0.7 V(SCE) and 4.85 nm·V^{-1} between 0.7 and 2.0 V(SCE). Under cathodic polarization, NR observed no changes to either the oxide layer or the underlying metal, just as for pure Zr.

Co_3O_4

The spinel-structure oxide Co_3O_4 is a redox-active semiconductor material (bandgap ~1.1 V) that is of interest for supercapacitor applications, due to its large electrochemical pseudocapacitance. In situ NR using contrast-matched mixtures of H_2O and D_2O, combined with EIS, was used to probe the extent and reversibility of chemical changes occurring during activation of its pseudocapacitative properties [20]. Immersed in water, the oxide layer swelled from 44 nm to 54 nm thick and about 40% converted to CoOOH, distributed uniformly through the layer. Increasing the pH changed the open circuit potential and the EIS response, due to chemical or electronic property changes in a very thin layer, below detection by NR, at the oxide-substrate interface. Anodic polarization to 1 V(SCE) resulted in further conversion of the oxide to CoOOH (65%), which spontaneously reversed after the anodic polarization was removed.

ADSORPTION-DESORPTION OF SURFACTANT MOLECULES AT THE METAL-AQUEOUS SOLUTION INTERFACE

The final electrochemistry-NR experiments summarized here were performed by Canadians in collaboration with instrument scientists on the NG-7 reflectometer at the NIST Center for Neutron Research (USA), because NG-7 operates in the horizontal configuration, an orientation not available in Canada. The horizontal configuration was important to control for gravitational effects such as buoyancy and preference of surfactant molecules for the air-solution interface. In these experiments, a thin film of gold, deposited onto a quartz substrate with a chromium adhesion layer on its surface, was used as the electrode, and the electrochemical potential-driven adsorption and desorption of a surfactant was monitored simultaneously by electrochemical and NR methods. The surfactants studied included mixtures of dimyristoylphosphatidylcholine (DMPC) with cholesterol [30,31], 4-Pentadecyl-pyridine (C15-4Py) [32,33], n-octadecanol [34], sodium dodecyl sulfate (SDS) [35-37], N-dodecyl-N,N-dimethyl-3-ammonio-1-propanesulfonate (DDAPS) [36], and N-decyl-N,N,N-trimethylammonium triflate (DeTATf) [36].

By controlling the potential, the charge density at the metal surface can be varied from about −30 μC/cm^2 to about 40 μC/cm^2, which, over the very short distances relevant to the electric double layer at the electrode-electrolyte interface, generates fields on the order of 10^{10} V/m. Such a field strongly influences the energetics of interactions between the metal surface and polar molecules at the interface [35]. Because the field can be varied enormously, surfactant molecules can be made to adsorb, desorb, or change orientation during NR. The authors used NR to monitor the thickness and density of surfactant layers under controlled conditions and, by employing H_2O-D_2O mixtures in the electrolyte solution, determine the water content of the surfactant films. Together with independently obtained spectroscopic information from techniques like polarization modulation infrared reflection-absorption spectroscopy (PM-IRRAS), NR measurements allowed them to determine: the surfactant layer thickness; whether they had formed monolayer or bilayer films; the orientation of the molecules on the surface; and the amount of water incorporated into or under the films. They found that the electrochemical potential-driven desorption process sometimes led to formation of partially desorbed hemi-micelle structures with water trapped between gold and surfactant aggregates, or individual micelles [31-37].

FUTURE DIRECTIONS

With the permanent shutdown and decommissioning of Chalk River's NRU reactor, Canadian scientists will have to rely on

access to foreign neutron laboratories for performing their NR experiments, at least in the short term. Reflectometers, each with unique capabilities, are available at NIST Centre for Neutron Research (USA), Oak Ridge National Laboratory (USA), the Institut Laue Langevin (France), the OPAL Reactor (Australia), the ISIS Neutron and Muon Source (UK) and others. In the medium term, a reflectometer could be made to function at the McMaster Nuclear Reactor in Hamilton, ON. Two reflectometers are planned at the extremely intense European Spallation Source, which is under construction and is expected to have its first beamlines available to users in 2023. In the long term, the only satisfactory outcome will be for Canada to construct its own domestic neutron source.

Future improvements in NR experiments will come from new, higher flux sources that offer better resolution for a given experiment time or quicker experiments for a given resolution. NR is limited by the need for very large samples (normally several cm in at least one direction) due to the compromise between the neutron flux and the beam footprint geometry. Higher flux will enable NR on some materials that are now very difficult or impossible for NR.

Improvements to record and thoroughly analyze off-specular and grazing incidence scattering to probe in-plane structures and correlation phenomena are under development. The D3 reflectometer, with its 32-wire detector for simultaneous capture of specular and off-specular reflectivity, represents initial progress.

Time-resolved NR to capture system kinetics is an exciting new area. Until recently, most NR experiments have examined systems at steady-state or those with very slow kinetics to compensate for the very long data acquisition times. Time-resolved NR is now being put into practice by time-stamping every neutron count at the detector to deconvolute the spatial and compositional information from its time dependence [38-40].

Another promising area is in coupling NR with other analytical techniques, such as spectroscopic and scanning probe methods that add other simultaneous dimensions of exploration; e.g., in the X-Y plane or in chemical reactivity or composition, including EIS, as described in this paper, and FTIR.

Undoubtedly, NR will prove to be at its greatest advantage when employed in combination with one or more other advanced methods.

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POWDER NEUTRON DIFFRACTION AND MATERIALS CHEMISTRY/PHYSICS RESEARCH IN CANADA (1949-2017)

BY JOHN E. GREEDAN, CHRISTOPHER R. WIEBE, AND DOMINIC H. RYAN

SUMMARY

We present a review of power neutron diffraction research in Canada from 1949-2017.

INTRODUCTION: THE EARLY DAYS OF DIFFRACTION AT CHALK RIVER (1949-1969)

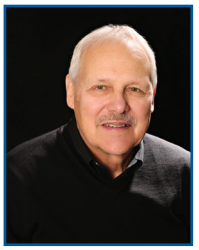
The story of powder neutron diffraction at Chalk River is inextricably linked to the history of neutron science at Chalk River itself. Canada's interest in nuclear research grew out of our involvement in World War II and the race to harness the power of the atom. In 1942, a joint Canadian-British laboratory was built in Montreal to assist in the war effort under the leadership of the National Research Council of Canada (NRC) [1]. There were many Europeans working in Canada at the time, including the UK's John Cockcroft and France's Lew Kowarski and Hans von Halban. Kowarski and von Halban were physicists that had recently escaped Nazi occupied Germany with 200 kg of heavy water (the largest supply in the world at the time) [2]. This formed the impetus for the design of a heavy water moderated reactor with the initial goal of producing plutonium for the Manhattan project. In 1944, the Montreal research group moved to a newly built laboratory at Chalk River, Ontario, where the first reactors in Canada were being built. In 1949, the National Research Universal reactor (NRU) project began, which was a Canadian design and would form the basis for the future for Canadian neutron beam research [3]. The 135 MW reactor is a significant Canadian success story, providing not only intense neutron beams for materials research, but also medical isotopes for over 20 million people in 80 countries, and a testing ground for innovative reactor and fuel rod design projects [4].

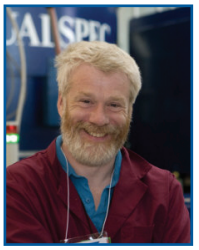
In the 1950s, the neutron beams at the NRU reactor were being used predominantly for condensed matter physics experiments by eminent scientists such as Bertram Brockhouse, a Nobel Laureate and pioneer of the triple axis spectroscopy method [5]. Powder neutron diffraction (PND) studies of materials was not developed as a broader technique outside of solid state physics until much later. In PND, the entire contents of reciprocal space are mapped onto one dimension, the Bragg angle, 2θ (or the momentum transfer, $Q = 4\pi\sin\theta/\lambda$). Prior to 1970 or so, PND was restricted to very high symmetry materials, say cubic or perhaps tetragonal, due to severe Bragg peak overlap since early instruments had at best moderate $\Delta d/d$ resolution and experiments were time consuming due to the use of "single" or point detectors. One notable interdisciplinary pioneer of PND at NRU was Professor Osvald Knop of Dalhousie University (chemistry) [6]. Osvald, a consummate crystallographer (partially trained under Linus Pauling), completed many experiments at Chalk River throughout the 1960s, in particular the first PND study of an oxide pyrochlore material, $Er_2Ti_2O_7$. Pyrochlore oxides have been of great interest to many in the Canadian physics community up to the present time [6]. The real breakthrough in neutron powder diffraction came in the late 1960s as the Rietveld method was developed along with more sophisticated computational techniques and technology [7].

THE RIETVELD REVOLUTION: 1969-1991

Hugo Rietveld (1932-2016) was a Dutch crystallographer and pioneer of neutron powder diffraction [7]. Although born in the Netherlands, he later studied physics at the University of Western Australia in Perth, obtaining his PhD in 1964. His thesis was the first single crystal neutron diffraction study in Australia (completed at the nuclear reactor HIFAR in Sydney). He then became a research officer at the Netherlands Energy Research Foundation ECN in Petten where his interest in powder diffraction was piqued during studies of uranates and other ceramics. In 1967 he finished an early version of his refinement method, and published the results in 1969 [8]. The Rietveld refinement method was born.

It took many years for the Rietveld revolution to change neutron powder diffraction. Computing facilities were rudimentary at many national laboratories, and the method required high quality neutron diffraction data with good





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resolution. However, the method has now completely changed how scientists obtain and analyze structural data in materials, and is now the gold standard in the materials science community. Rietveld's revolutionary data analysis technique — fitting of the entire diffraction profile rather than individual Bragg peaks — permitted extraction of the maximum amount of structural information from a PND pattern. In many cases, the results were comparable to those from single crystal x-ray data [9]. The importance of this technique is not to be underestimated, especially in the materials chemistry community where it can be difficult if not impossible in some cases to obtain large, high quality single crystals. The Rietveld technique changed everything, from how modern neutron scatterers take data, design instruments, and develop analysis software. For example, in the late 1970s, the construction of higher resolution or higher throughput diffractometers to take advantage of Rietveld method was made a priority by many neutron research groups and laboratories. Wide angle, multi-wire, and multi-tube detectors were rapidly designed throughout the 1980s. Another key development was the establishment of user-centred programs on a peer reviewed proposal basis to increase access to PND data. This greatly expanded the use of the technique by non-specialists and built a large user base, especially in Europe at the ILL (Institute Laue Langevin).

Compared to this rapid progress in Europe, Canada and USA were relatively late to the game with respect to powder neutron diffraction, except for the IPNS (Intense Pulsed Neutron Source) at ANL (Argonne National Laboratory). The building of a suite of powder diffractometers at the ILL started soon after the reactor was commissioned in 1967, and in the UK, ISIS (1985) also quickly adapted and advanced modern neutron diffraction techniques [10,11]. The IPNS, in comparison, began operation in 1981. Canada's first modern powder neutron diffractometer (PNDiff) was built at the McMaster Nuclear Reactor (MNR) adapting a design from the University of Missouri's neutron research group (MURI) by M.F. Collins, J.R.D. Copley, C.V. Stager, J. Couper, K. Lushington and J.E. Greedan and became fully operational in 1986 [12]. The central feature was a position sensitive detector (PSD) with a 2θ range ~ 25°/setting which travelled on the diffraction circle built originally by Brockhouse in the 1960s. Due to the low MNR power at 2MW, the dataset collection time was approximately 2 days/sample for $5° < 2\theta < 130°$, $\lambda = 1.39$ Å: [0.394 Å$^{-1} < Q < 8.19$ Å^{-1}] at a single temperature. Although somewhat impractical as a true user facility, nonetheless, ~50 papers with ~1500 citations included data from this diffractometer from 1984-1998. Highlights included the solution of the correct structure of $YBa_2Cu_3O_7$ in March 1987 (effectively tied for first with a group using the IPNS) [13]. PND was particularly useful in locating the oxygen atomic positions and in avoiding the problem of heavily twinned crystals which plagued early x-ray studies.

In the late 1980s, a proposal was put forward to upgrade the powder diffraction facilities at Chalk River by Chalk River and NSERC: the DUALSPEC suite of instruments. The initial cost estimate was $3.5 M [14]. DUALSPEC completely changed the diffraction landscape in Canada, and arguably all of North America, as it housed one of the most powerful diffractometers — the C2 instrument.

THE DUALSPEC ERA: 1991-2017

With the commissioning of DUALSPEC at NRU in 1991, a true user facility existed in Canada for the first time. Two instruments were built, C2 (PNDiff) and C5 (inelastic triple-axis spectroscopy). C2 is equipped with an 800 element multi-wire detector, with a 2θ range of 80°/per setting. With a neutron wavelength of $\lambda = 1.33$ Å – 2.37 Å, the angular range of $3° < 2\theta < 120°$ covered an impressive Q-range [0.14 Å$^{-1} < Q < 8.18$ Å^{-1}]. Other wavelengths such as 4 Å with a Be filter could also be used. For comparison, in 1992 at NIST (National Institute of Standards and Technology) a 32-element detector was built! Thus, by 1991, C2 was the most efficient PNDiff at a reactor source in North America. The success of C2 spawned highly successful Canadian Powder Diffraction Workshops across Canada that ran for many years. While comparisons with spallation source instruments are difficult, C2 was probably more efficient than GPPD (General Purpose Powder Diffractometer) or SEPD (Special Environment Powder Diffractometer) at IPNS. Unfortunately, the IPNS ceased to function in 2008 due to budget cuts to the Department of Energy. A comparable next generation diffractometer, POWGEN at the SNS (Spallation Neutron Source), was commissioned in 2011-2012. Thus, for approximately 20 years (1991-2011), C2 was likely the most efficient PNDiff in North American (this is certainly true if only reactor source instruments are considered). The wide range of ancillary equipment, cryostats to 3.5 K and atmosphere-controlled furnaces with a range up to 1800 °C rendered C2 a highly versatile instrument [14]. Datasets were also typically gathered in less time that other comparable diffractometers.

Having said all of the above, C2 exists now more or less as it was built in 1991. No significant improvements, such as installation of focusing monochromators, which had the potential to increase the flux on sample by large factors were ever implemented, in spite of significant efforts. Starting in 2007, initial design and testing of focusing monochromators was carried out. The large-area mosaics of deformed germanium crystals were expected to deliver a factor of 10 increase in flux-on-sample at both 1.33 Å and 2.37 Å. A similar improvement in detector efficiency was planned by moving from a relatively short BF_3 detector to a taller ^{3}He-based detector like the ones on the two powder instruments at OPAL, the Australian research reactor. The 15 month shutdown of NRU from technical difficulties and Chalk River scientist Lachlan Cranswick's untimely passing in 2010 were setbacks to the planned C2 improvements. Lachlan spent a considerable amount of effort making upgrades to C2 a priority. While the low-Q limit of 0.14 Å^{-1} has made C2 invaluable for studies of magnetic materials where long-period magnetic modulations are common, one major design flaw — that the maximum scattering angle is limited to ~120° (2θ) — cannot be

changed as it is set by the large monochromator drum that C2 shares with C5, the inelastic instrument that forms the other half of DUALSPEC. The main consequence of this was that the maximum $Q \sim 8.2$ Å^{-1} ($d_{min} = 0.76$ Å) placed C2 at a disadvantage compared to spallation instruments, such as POWGEN, where $d_{min} \sim 0.4$ Å ($Q_{max} \sim 15$ Å^{-1} for resolving structures). However, C2 is still a workhorse for many research groups for medium resolution applications.

Although the basic hardware remains essentially as it was built, there has been an ongoing process of upgrades to the instrument operation and sample environments. A system of macros and encoded slits combined with an ILL-designed neutron camera permit precise, and often remote, alignment of samples. It should also be noted that very important improvements in ancillary equipment were implemented fairly recently. Perhaps the two most significant were the building of a very short path length sample cell permitting studies of materials containing extremely high absorption cross section elements, such as Sm, Eu and Gd [15] and the addition of a ^{3}He (Heliox) sample cell which allows data collection to ~340 mK. Concerning the former, C2 is one of a very few PNDiff at which experiments on highly absorbing samples can be done more or less routinely without resorting to a hot source. Credit here is due to the efforts of Dominic Ryan, Ian Swainson and Lachlan Cranswick.

Taking all of the above into account, C2 will be very difficult to replace as a Canadian asset for the foreseeable future.

RESEARCH AT CHALK RIVER (C2)

The great strengths of powder neutron diffraction vis à vis x-ray diffraction are: (1) the ability to detect and refine accurately the positions of light (low atomic number) atoms such as hydrogen, lithium and oxygen 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, among many others, (3) the ability to solve and refine magnetic structures including the quantitative measurement of magnetic moments, (4) the ease of use of sample environments such as furnaces and cryostats for the study of phase transitions and in situ transformations. In the following section, highlights of some Canadian research activities using C2 will be presented.

A survey of published results using C2 over the past ~20 years or so suggests that the research output fits into the following categories:

(a) Minerals, molecular solids, and related systems – hydrogen bonding in hydrates.
(b) Crystal and magnetic structures of intermetallic compounds and Fe-based superconductors. Included are Gd, Sm and Eu – based materials and mK studies.
(c) Crystal and magnetic structures of transition metal oxides. Li battery materials, low dimensional and geometrically frustrated oxides, magnetism and the Mott transition, potential multi-ferroics.
(d) Studies of hydrogen containing materials and hydrogen storage materials.

It should also be noted that Ian. P. Swainson carried out structural studies of hybrid inorganic/organic perovskites long before this became a trendy area of research.

Selected examples from each category will be described briefly.

Minerals, molecular solids and related systems

Prior to the commissioning of C2 as a part of DUALSPEC there existed a very active program in neutron powder diffraction at the Chalk River laboratory involving Brian Powell, Bruce Torrie (Univ. of Waterloo) and other collaborators. The focus was on molecular organic crystals, initially, such as acetonitrile (CH_3CN), methanol (CH_3OH) or formaldehyde (CH_2O). Inorganic solids with molecular cations and anions, their structures and phase transitions were also studied by Robin Armstrong (Univ. of Toronto) and Julian Brown (Queen's Univ.) Materials of interest included fluorite and anti-fluorites such as $(NH_4)_2PbCl_6$ and scheelite structures such as $KReO_4$. These studies were done on triple axis instruments run in double axis mode with single counters. Later, a 30 element position sensitive detector was used but still on instruments not dedicated to powder diffraction. These studies continued after the C2 commissioning and benefitted from the greatly enhanced efficiency of the 800 element C2 detector. Several substituted halo-carbons $CH_x(F,Cl,Br,I)_{4-x}$ were studied along with more complex inorganic materials such as zeolites and related porous solids in collaboration with the Tony Cheetham group at Oxford University.

The positions of H atoms and their participation in hydrogen bonding is a perennial issue in hydrated minerals. R.C. Peterson

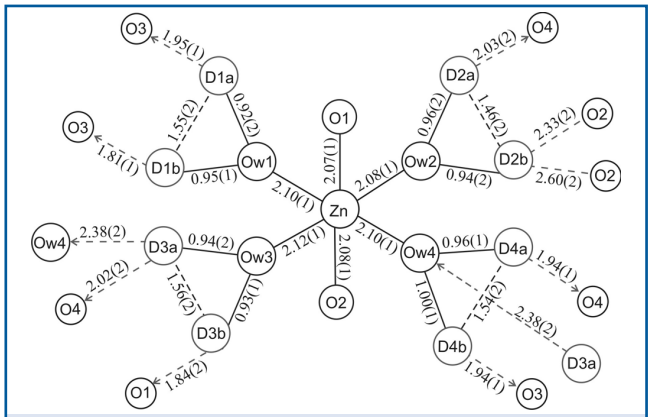

Fig. 1 The hydrogen bond network in $ZnSO_4{\cdot}4D_2O$ [22].

(Geology and Geological Engineering – 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 $MnSO_4 \cdot 4H_2O$ [22]. In these materials, the $Zn^{2+}$and Mn^{2+} ions are in octahedral coordination which are connected by a hydrogen bonding network. While hydrogen positions derived from single crystal x-ray data were available, it was possible to obtain much more accurate and precise positions from the neutron powder data which is much more sensitive due to the cross-section of neutron-proton scattering. The results for $ZnSO_4 \cdot 4D_2O$ are shown in Fig. 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, D2b and D3a in Fig. 1, a single D-ion forms a "bifurcated" hydrogen bond involving one short and two long bonds.

Crystal and magnetic structures of intermetallic compounds and Fe-based superconductors

Among the most interesting examples is very recent work on the half-Heusler intermetallic, GdBiPt, which is a candidate antiferromagnetic topological insulator [23]. These collaborators from the Univ. de Montreal, McGill and McMaster were able to solve the magnetic structure using the data in Fig. 2 to show that below T_N = 9K, 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 – small by traditional neutron scattering standards.

The availability of the Heliox sample cell enabled a study of the complex magnetic structures of $Er_3Cu_4Ge_4$. There are two Er sites (2d) and (4e) which order at different temperatures, 8K and 3.5K, respectively. While Er (2d) shows a commensurate order and a nearly full moment of 8.9(2)μ_B, (g_J = 9 for Er^{3+}) the Er(4e) ions order incommensurately with about half of the free ion moment at 1.5K. With the Heliox insert and cell, data were taken to 0.34K as shown in Fig. 3 and it was shown that the Er (4e) moments now order in a nearly commensurate manner but still with a much reduced moment. A strong diffuse component, even at 0.34K, indicates that much of the (4e) magnetic scattering is due to short range ($\xi \sim 10$ Å) spin correlations [24].

The high temperature furnace available at C2 also plays an essential role in the study of magnetic materials, especially when the effects of magnetism and chemical disorder are intertwined. In Mn_xGa ($1 < x < 2$) [25], a potential medium-cost/medium-performance hard magnet, the excess manganese substitutes on the gallium site and also carries a magnetic moment, so in the ordered state the total scattering includes comparable contributions from Mn-Ga disorder and Mn magnetism.[b] Mn and Ga are sufficiently similar in atomic number that PND provides much better contrast than x-ray powder diffraction (b_{Mn} = –3.75 fm; b_{Ga} = +7.29 fm). Diffraction data taken at 500 °C, well above T_c, established the crystal structure (confirmed by density functional theory (DFT) calculations of substitution energies). With the structure constrained, the manganese moments on both the Mn site and the substitutional (Ga) site could be determined with confidence, Fig. 4. These moments and the antiparallel coupling between them were fully consistent with DFT results, and this steady improvement in calculation accuracy combined with validation by neutron

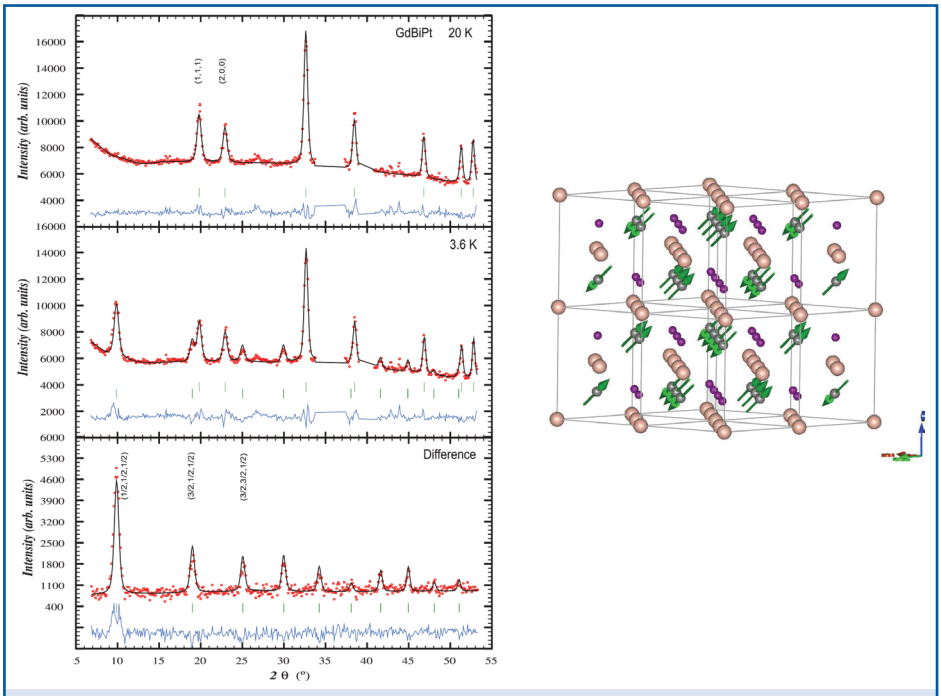

Fig. 2 (Left) C2 diffraction patterns for GdBiPt at 20K and 3.6K and the difference plot showing the magnetic peaks indexed on $\boldsymbol{k}$ = (1/2 1/2 1/2). (Right) The magnetic structure of GdBiPt. The Gd atoms are shown in gray, the Bi in pink, and the Pt in purple. The spins on the Gd atoms are oriented in ferromagnetic planes which are stacked antiferromagnetically along the magnetic propagation vector [23].

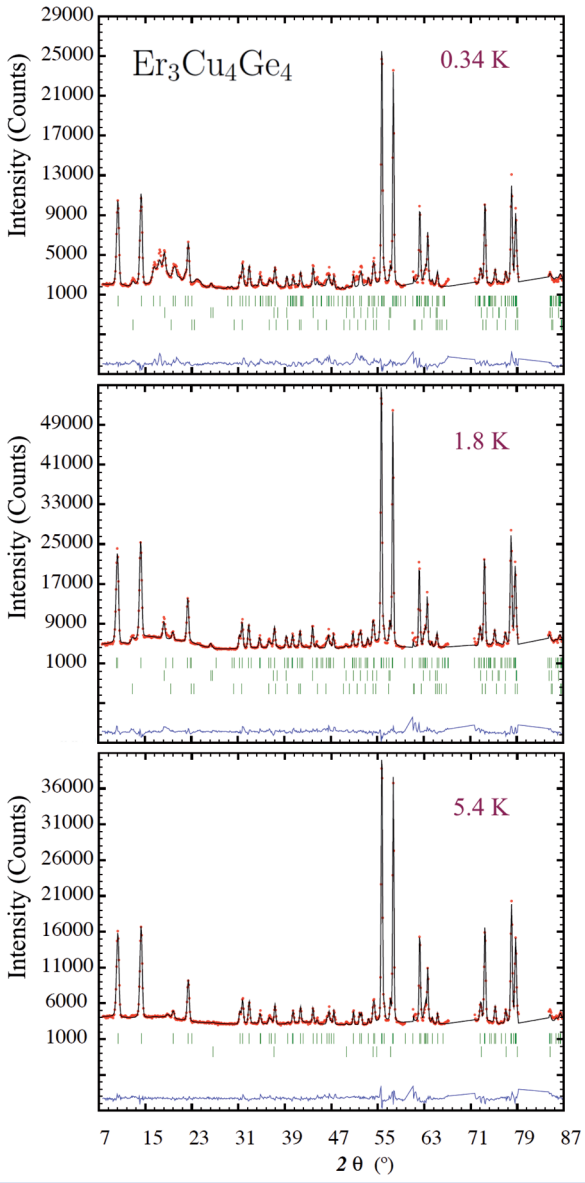

Fig. 3 C2 data for $Er_3Cu_4Ge_4$ taken with the Heliox sample cell at 0.34K (TOP), 1.8K (MIDDLE) and 5.4K (BOTTOM) [24].

scattering opens the possibility of *designing* new magnetic materials rather than blindly searching for them.

Crystal and magnetic structures of transition metal oxides

C2 has also seen extensive use to aid in the unraveling of quite complex magnetic structures in several oxide materials. In the dugganite material, $Pb_3TeCo_3V_2O_{14}$, the magnetic Co^{2+} ions form an unusual set of trimers which in turn form a hexagonal net, Fig. 5, introducing geometric frustration. There are two magnetic phase transitions occurring at T_{N1} = 8.6K and T_{N2} = 6.0K. Below T_{N1} the Co spins appeared to order according to an incommensurate wave vector, $\boldsymbol{k}$ = (0.752 0 1/2). A commensurate, but very odd $\boldsymbol{k}$ = (5/6 5/6 1/2) appeared to describe the magnetic structure below T_{N2}, implying a magnetic cell which 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 ISIS, in combination with C2 data, it was possible to solve the magnetic structures associated with both transitions as shown in Figs. 6a and b with propagation vectors **k** = (1/2 0 – 1/2) for T_{N1} and **k** = (1/2 1/2 – 1/2) for T_{N2}, the directions of which are indicated by the thick arrows. In the new unit cell, the Co-trimers form isosceles triangles rather than equilateral triangles [26].

In a collaboration with S. Derakhshan (Univ. Calif. 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 consisting of corner-sharing FeO_5 square planar units and FeO_6 octahedral units, Fig. 7 [27].

Again, there are two apparent magnetic phase transitions T_{N1}= 47K and T_{N2} = 36K. C2 data were used to solve the magnetic structures in both regimes. In the range 36K < T < 48K, a commensurate, $\boldsymbol{k}$ = (0 0 1/3) structure was found, best described as a spin density wave (SDW) with moments fixed along the b-axis. Below 36K, an incommensurate $\boldsymbol{k}$ = (0 0 0.35) structure is found, best described as a cycloid with the moments now in the bc plane, Fig. 8.

Studies of hydrogen containing materials, and hydrogen storage materials

Huot *et al.* have exploited the relative ease of performing in situ PND experiments in the study of the important hydrogen storage material $Mg_2FeH(D)_6$ [28]. Structural and phase changes associated with both hydrogenation and de-hydrogenation were carried out in a specially designed sample cell. The effects of the presence of both H and D were also assessed using phase contrast (the different scattering cross-sections allows to distinguish between the two isotopes). A typical result is shown in Fig. 9 below.

CANADIAN RESEARCH AT FOREIGN SOURCES

The high quality data from the C2 powder diffractometer over the years have been complemented by Canadian research at foreign sources using techniques such as polarized neutron diffraction and nPDF methods (pair distribution function). Polarized neutron diffraction takes advantage of the spin of the neutron (s = 1/2) and the capability of polarizing the incoming neutron beam to

separate out the nuclear, magnetic, and spin incoherent contributions (using the XYZ technique). Canadians have mostly utilized the D7 instrument at the ILL over the last few decades, but new beamlines such as the DNS (Diffuse scattering Neutron time of flight Spectrometer) in Jülich are seeing more prominence.

One example of recent work at D7 by Canadians is on the highly correlated spin ice $Ho_2Ge_2O_7$. These materials are prepared at high pressure, and the sample size used in the polarized experiments was only 200 mg. Nonetheless, with the large Ho^{3+} moment (~ $10\boldsymbol{\mu}_B$), the magnetic scattering can clearly be seen on D7 after a few minutes of counting time (even after the XYZ analysis), illustrating the power of modern neutron sources.

The diffuse neutron scattering can be tracked as a function of temperature, and with modern methods of Reverse Monte Carlo (RMC) modeling of the data, the development of the 2-in, 2-out Ho^{3+} spin ice structure can be determined (Fig. 10). This is crucial for investigating claims of "monopole" formation, that are effectively defects within the 2-in, 2-out short range ordered structure.

With modern RMC methods (and new software developments such as Spinvert), fits of polarized neutron diffraction data can now be used to extrapolate to single crystal data. Figure 11 illustrates the RMC fits to three different spin ices measured at D7 ($Dy_2Ti_2O_7$, $Ho_2Ti_2O_7$, and $Ho_2Ge_2O_7$ in the left panels). The corresponding magnetic scattering can be then calculated for single crystal data (right panels), and compared to each other. While single crystal polarized data is preferred over powder data, there are many compounds of interest in which single crystal growth is challenging at best (such as the high pressure pyrochlores $A_2Ge_2O_7$, A = rare earth) [29].

Neutron pair distribution function (nPDF) analysis has been used increasingly by chemists and materials scientists to study disorder in complex crystalline materials, i.e., to determine not only the average but also the local structure. This approach is often dubbed "total scattering". Data are taken to $Q > 30$ Å^{-1}, typically, and normalized by the total scattering cross section of the sample to yield the total scattering structure factor S(Q) from which the pair distribution function G(r) can then be obtained through a Fourier transform. Such experiments are not possible at C2 and specialized

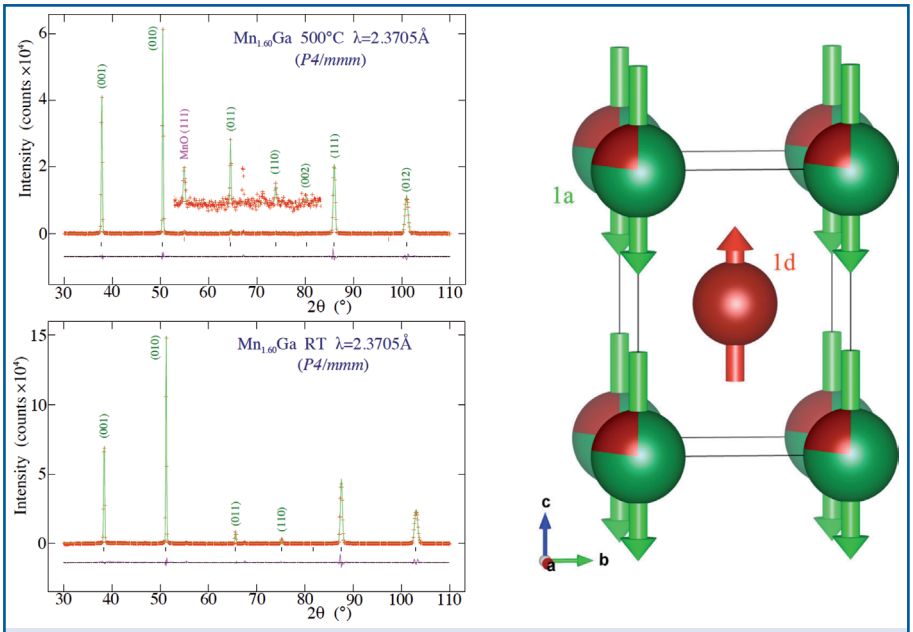

Fig. 4 (Left panels) PND patterns for $Mn_{1.60}Ga$ taken (top) at 500° C, well above T_c, to establish the crystal structure and (bottom) room temperature where the system is magnetically ordered. Note the small intensity changes at most of the peaks, especially the (011) and 110). (Right panel) The magnetic structure of $Mn_{1.60}Ga$. The Mn moment on the 1d site, ($2.45\mu_B$) fully occupied by Mn, is antiparallel to that on the 1a site (~$3\mu_B$) where Mn substitutes for Ga [25].

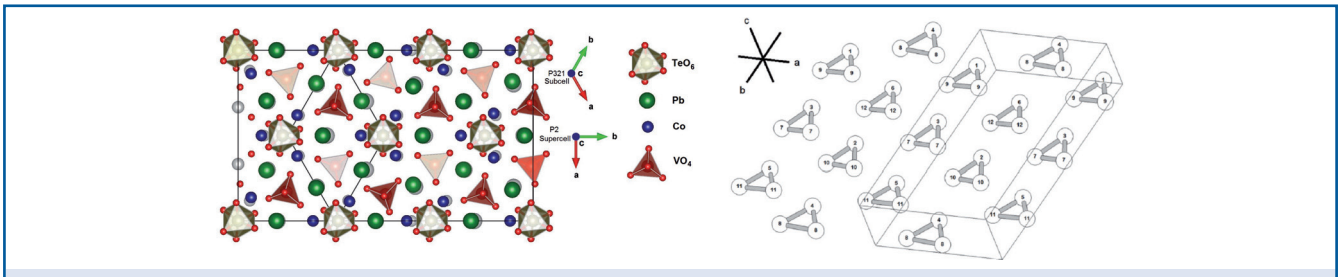

Fig. 5 (LHS) The crystal structure of $Pb_3TeCo_3V_2O_{14}$ showing the relationship between the idealized P321 cell and the distorted P2 cell of six times the volume. (RHS) The Co^{2+} trimers, now isosceles triangles in P2 [26].

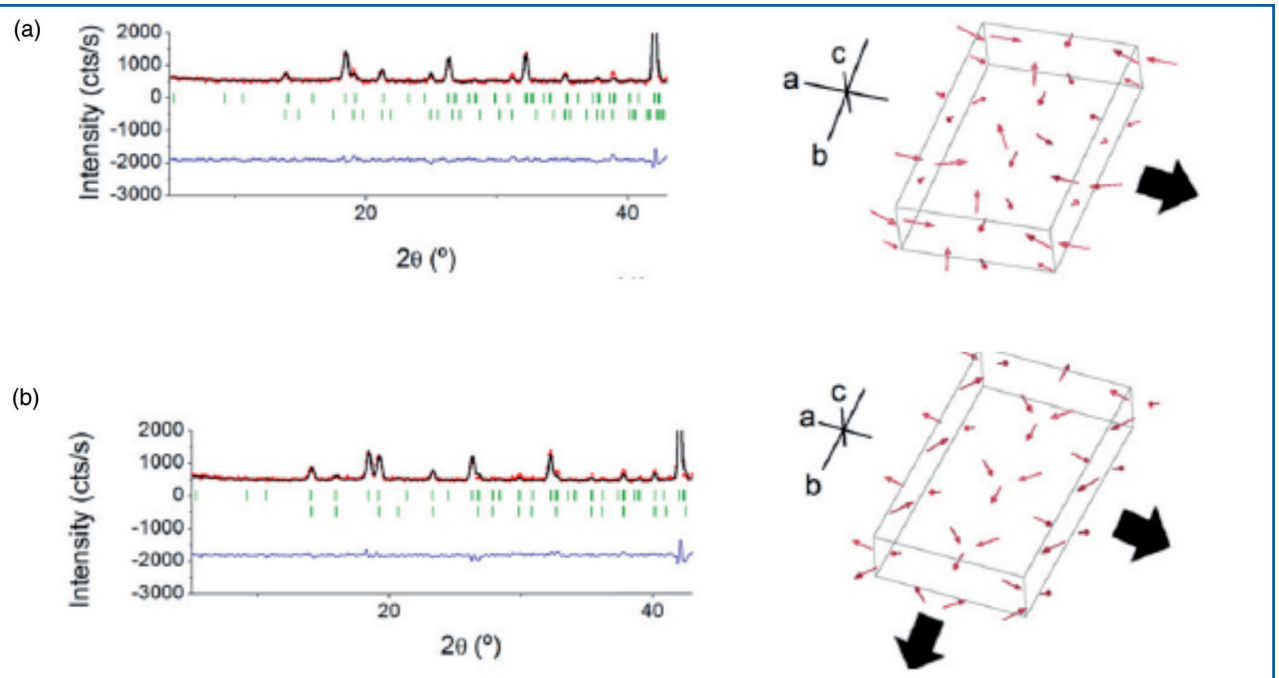

Fig. 6 (a) Refined magnetic structure below 8K for $Pb_3TeCo_3V_2O_{14}$. $\boldsymbol{k}$ = (1/2 0 − 1/2) [20]. (b) Refined magnetic structure below 6K for $Pb_3TeCo_3V_2O_{14}$. $\boldsymbol{k}$ = (1/2 1/2 − 1/2) [26].

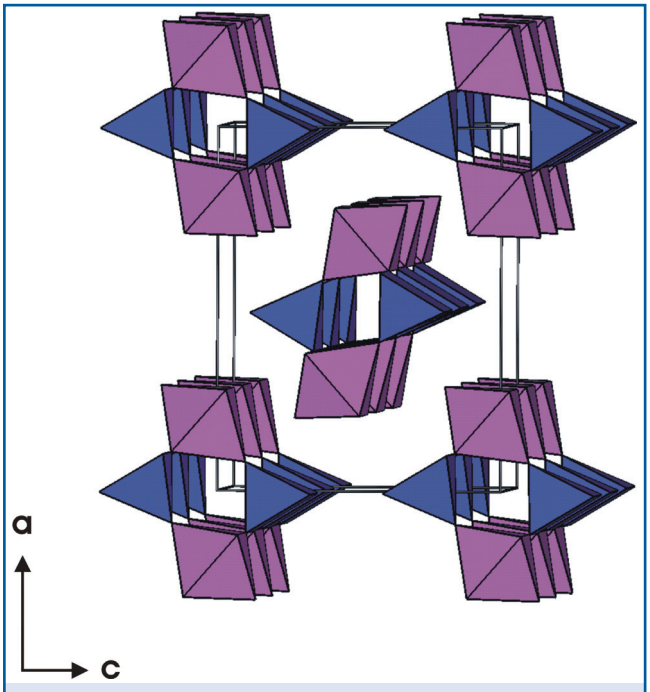

Fig. 7 View of the crystal structure of $BaYFeO_4$ along the b-axis showing columns of edge-sharing FeO_6 octahedra (magenta) linked by corner-sharing FeO_5 square pyramids (blue) [27].

instruments such as NPDF at the M. Lujan Jr. Center for Neutron Scattering at Los Alamos have been used in the past by Canadians on a wide variety of materials. With the recent highly unfortunate closure of the Lujan Center, it is not clear where Canadians will be able to travel for high quality nPDF data. While NOMAD at SNS and GEM at ISIS can be used for nPDF data collection, these instruments are not a direct substitute for NPDF. The planned DISCOVER diffractometer at SNS will likely become the best nPDF instrument in the world but it is several years from operation.

An example of the use of nPDF concerns the highly disordered material Sr_2FeMnO_5 which appears to be a cubic perovskite, Fig. 12, but with a 17% vacancy concentration on the O-site [25]. One would normally expect the vacancies to order giving the brownmillerite structure, also Fig. 12. Data from NPDF (Lujan) for this material are shown in Fig. 13. In Fig. 13a the S(Q) data to Q = 30 Å^{-1} are shown. The sharp Bragg peaks are consistent with the cubic Pm-3m cell. The inset shows that the background consists of much broader features and here is where the information on the local structure resides. The derived G(r) is given in Fig. 13b. Two fits to the nearest neighbour region, 1.5 Å-5 Å are shown in Fig. 13c (cubic perovskite – Pm-3m) and Fig. 13d (brownmillerite – Pmna). Clearly, the local structure is better modeled by brownmillerite than by the cubic average structure.

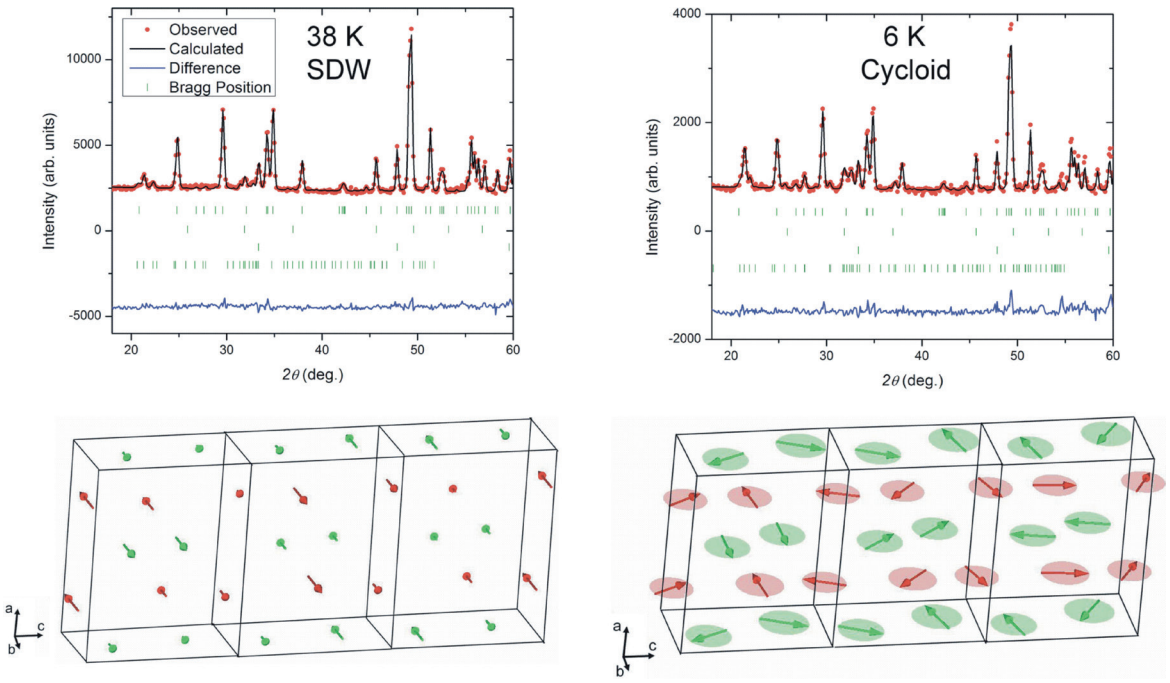

Fig. 8 Magnetic structures for $BaYFeO_4$: (LHS) the refined C2 data (TOP) and the derived SDW structure (BOTTOM) at 38K. (RHS) the refined C2 data (TOP) and the derived cycloid structure at 6K (BOTTOM).

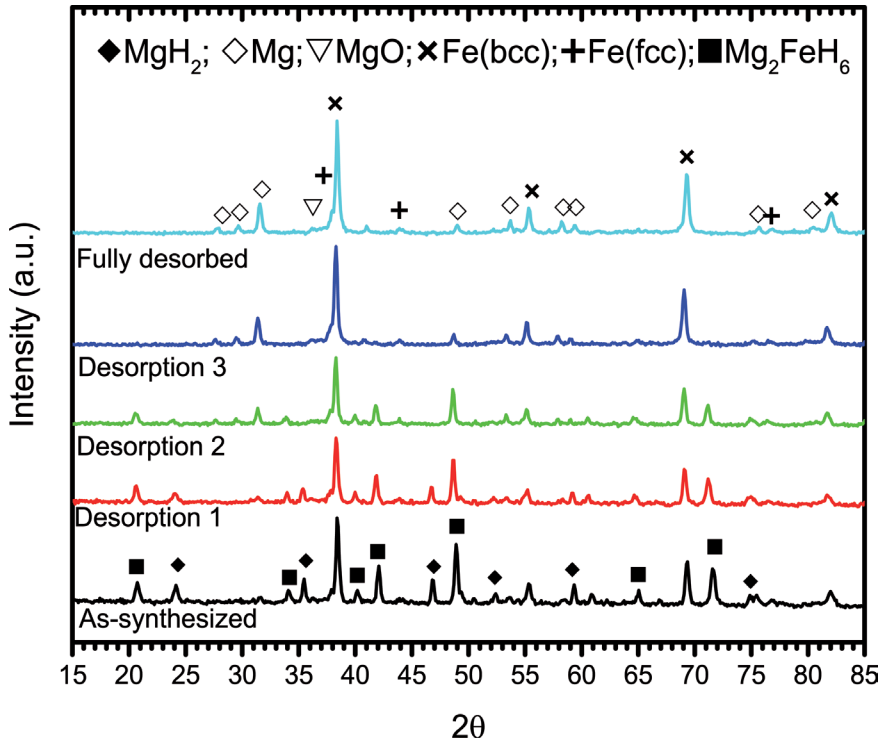

Fig. 9 PND patterns of $Mg_2Fe(D,H)_6$ at various stages of dehydrogenation. Desorption 1 is a 473K, desorption 2 at 493K and desorption 3 at 523K [28].

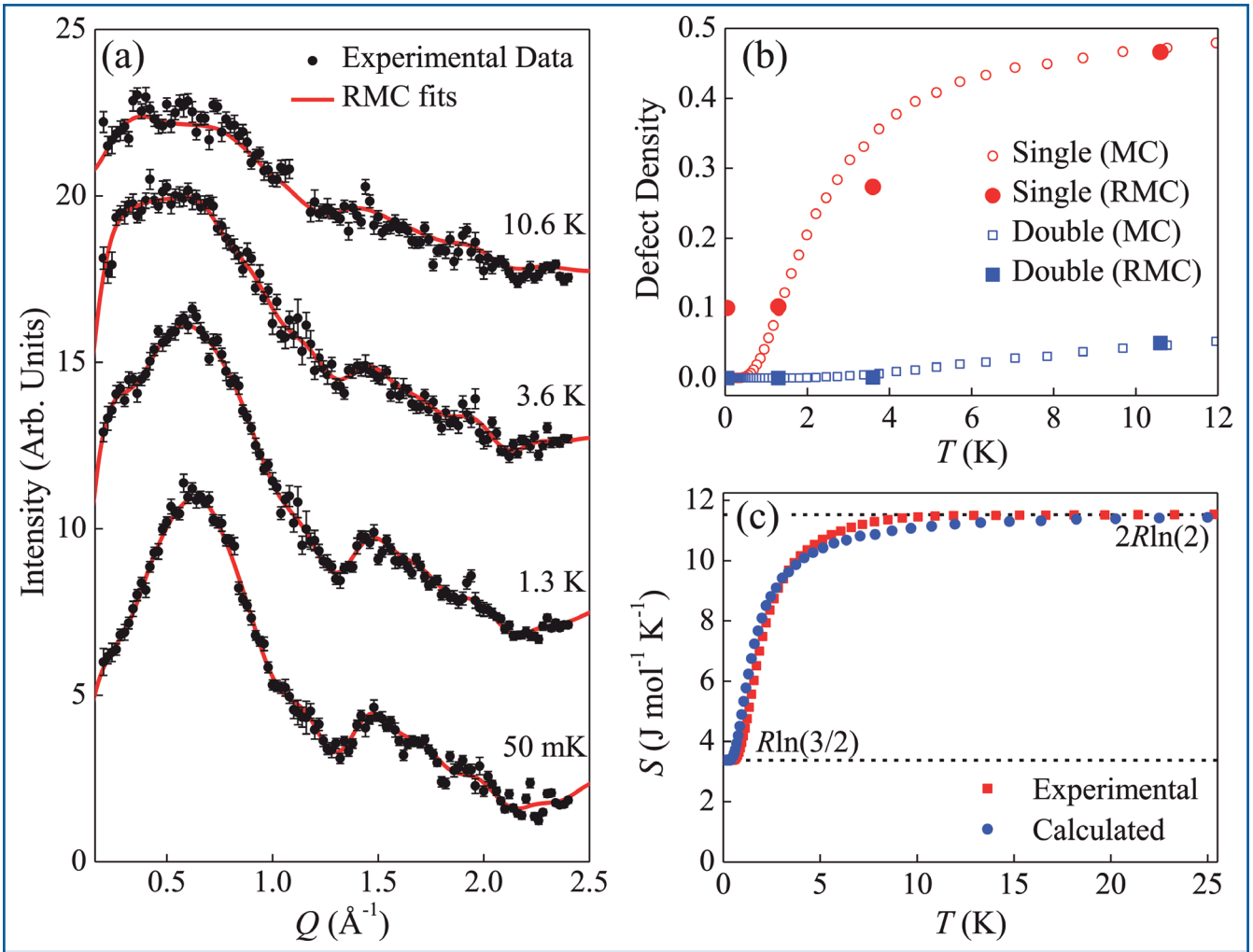

Fig. 10 (a) Temperature variation in the magnetic diffuse scattering of $Ho_2Ge_2O_7$ with RMC fits. (b) Density of ice-rules defects as a function of temperature for $Ho_2Ge_2O_7$. (c) Comparison of theoretical magnetic entropy for $Ho_2Ge_2O_7$ with experimental results [29].

SUMMARY AND FUTURE OUTLOOK

Chalk River laboratories has had a long and fruitful history of neutron powder diffraction research over the last five decades. The development of DUALSPEC and in particular of the C2 diffractometer brought Canada into the upper echelons of materials research. In a relatively short period of time, hundreds of papers were published using C2 with thousands of citations on a wide variety of materials. With the future of Chalk River and neutron scattering in Canada uncertain, it is unclear how Canadian scientists will proceed in powder diffraction research. One proposal is to resurrect PNDiff at the McMaster Nuclear Reactor. This would involve a single PSD covering 120°-150° in 2θ. With a proposed power increase to 5MW and the use of focusing monochromators, the new powder diffractometer might approximate the capabilities of C2. Even with this possibility, it is clear that for neutron scattering to survive as a discipline in Canada, there will have to be involvement in other foreign neutron sources at least in the short term. With the new Canadian Neutron Initiative (CNI), this may take place in the form of instrument development at foreign sources (such as DISCOVER at Oak Ridge National Laboratory) [32], membership in European neutron sources (such as the ILL and ESS – the European Spallation Source), or some combination that would enable Canadians to succeed. It would be unfortunate if we, as a community, could not promote our legacy in powder neutron diffraction and maintain our strengths on the world stage.

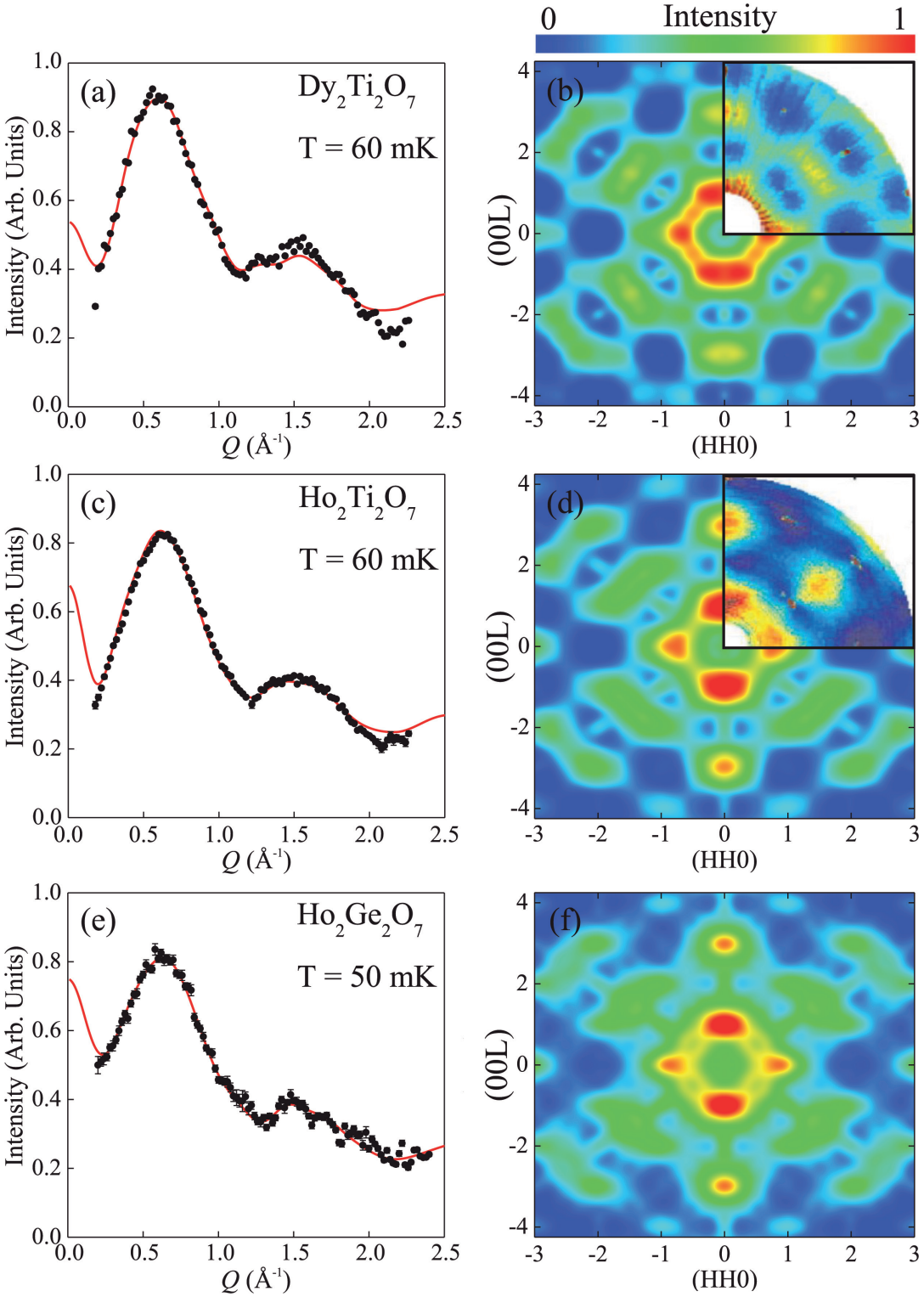

Fig. 11 Left: Fits to experimental powder magnetic data for the spin ice materials (a) $Dy_2Ti_2O_7$ (c) $Ho_2Ti_2O_7$ and (e) $Ho_2Ge_2O_7$. Fits are shown for an average of 64 independent refinements. Right: Single-crystal magnetic scattering predicted from RMC configurations for (b) $Dy_2Ti_2O_7$, (d) $Ho_2Ti_2O_7$, (f) $Ho_2Ge_2O_7$. The insets to figures (b) and (d) show one quadrant of magnetic scattering from single crystalline $Dy_2Ti_2O_7$ and $Ho_2Ti_2O_7$, respectively [29].

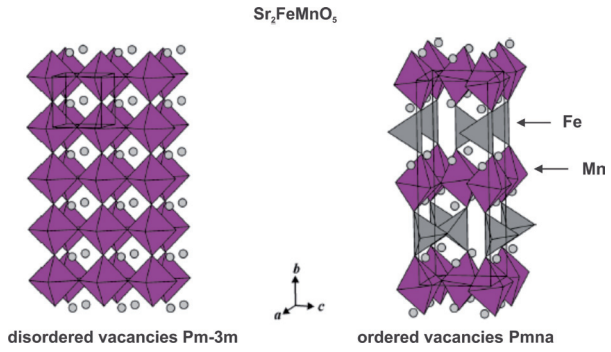

Fig. 12 (left) The cubic disordered perovskite structure (Pm-3m) for Sr_2FeMnO_5. At the centres of the violet octahedra reside the disordered Fe/Mn ions with oxygen ions at the vertices. 17% of these vertex sites will be randomly vacant. (right) An ordered brownmillerite structure (Pmna) in which the oxide vacancies, Fe and Mn ions all order resulting in layers of alternating corner sharing octahedral layers (Mn) and corner sharing tetrahedral chains (Fe). The Ca ions are shown as grey spheres. The unit cells for both cases are outlined.

ACKNOWLEDGEMENTS

This work builds upon a previous review of neutron powder diffraction at Chalk River by J.E. Greedan [33]. The authors would like to acknowledge financial support for their research programs from NSERC. This work would also not be possible without the many researchers that have worked at Chalk River over the years, including technicians, instrument scientists, graduate students, and post-doctoral fellows. C.R.W. is also grateful for past support from the NSF, CFI, the CRC program (Tier II) and the ACS Petroleum Fund.

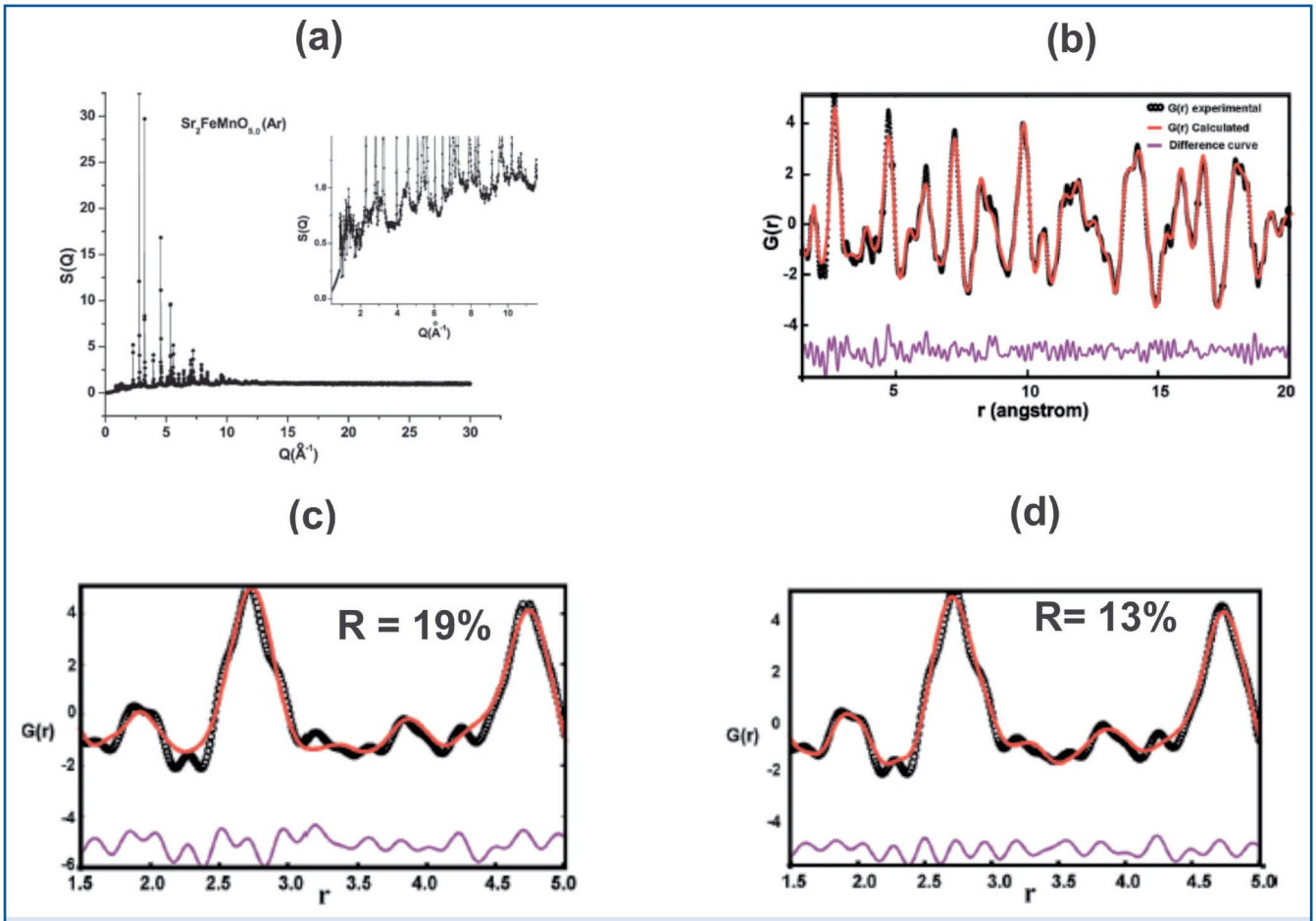

Fig. 13 (a) The S(Q) out to 30Å^{-1}. The inset shows broad features of the background upon which sharp Bragg peaks, consistent with Pm-3m symmetry, are superimposed. (b) The G(r) obtained by Fourier transform of S(Q). (c) Fit of the G(r) to a cubic local model. (d) Fit of the G(r) to a brownmillerite local model.

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Join the Fun
Joignez l'amusement

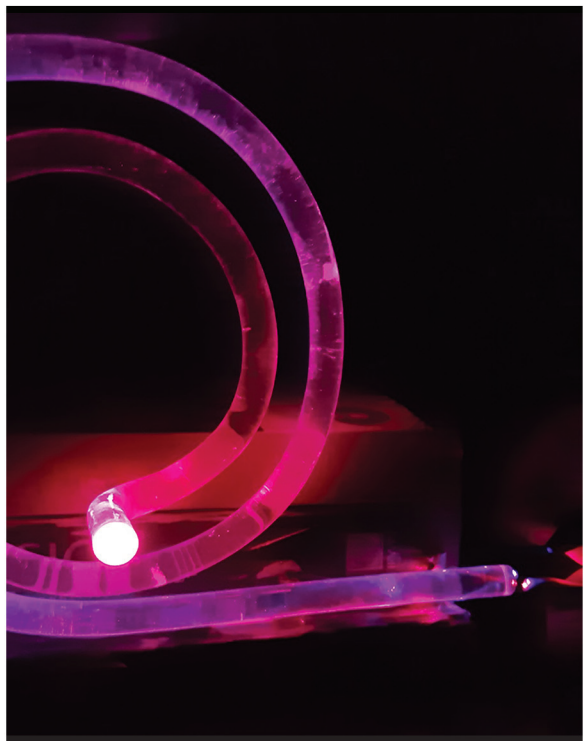
Art of Physics Competition

You are invited to enter the competition (open or high school categories) by capturing in a photograph a beautiful or unusual physics phenomenon and explaining it in less than 200 words in terms that everyone can understand.

The emphasis of this contest is not so much on having a high level of physics comprehension as it is on being able to explain the general principle behind the photograph submitted. Individual (open and high school) and high school class entries are invited up until April 15 each year (see http://www.cap.ca/en/activities/art-physics for entry form and rules). Please note that all entries must be original artwork produced by the participant.

Winning entries will form part of our Art of Physics exhibition which may be on display at the Canada Science and Technology Museum, and may appear as a cover on our publication, *Physics in Canada*. They will also be posted on our Art of Physics website at http://www.cap.ca.

We hope you will take advantage of this opportunity to explore the art of physics by submitting entries for the next competition.



"Total Internal Reflection and Colour Therapy""

First place - 2018 Competition High School/Cégep Individual Category

by Eduard Radut, Victoria Park Collegiate Institute, North York,ON

Concours l'Art de la physique

Vous êtes invité(e)s à participer (aux catégories ouverte ou école secondaire) en photographiant un phénomène physique magnifique, ou particulier, et en rédigeant un court texte explicatif de moins de 200 mots, en termes simples et à la portée de tous.

L'accent de ce concours est de pouvoir expliquer le principe général de la photo soumise plutôt que de démontrer un niveau élevé de compréhension de la physique. L'échéance pour les inscriptions individuelles (ouverte et école secondaire) et projets scolaires (voir le formulaire d'inscription et les règlements à http://www.cap.ca/fr/activites/lart-de-physique) est fixée au 15 avril chaque année. Notez bien que toutes les inscriptions doivent être des oeuvres originales du participant ou de la participante.

Les soumissions gagnantes feront partie de notre exposition L'Art de la physique au Musée des sciences et de la technologie du Canada et auront une chance de paraître sur la couverture d'un numéro de *La Physique au Canada*. Elles seront également affichées sous la rubrique L'Art de la physique du site web de l'ACP à l'adresse suivante: http://www.cap.ca.

Nous espérons que vous profiterez de cette occasion d'explorer l'art de la physique en soumettant une oeuvre pour la prochaine compétition.

CAP Award + Physics Teachers = ∞ Possibilities

Opinion piece for CAP Newsletter

Lisa Cole

I was honoured to be the recipient of the 2017 CAP Excellence in High School Physics Teaching Award and be recognized by my peers, former students, parents and the Canadian Association of Physicists for my work in Physics Education in Ontario. I was also thrilled to be selected to attend the Teacher Workshop at CERN in July 2017 as a result of the award! Thank you CAP and Perimeter Institute!

I have spent the past 18 years committed to developing and providing active learning experiences for students, teachers and the public through a variety of roles – classroom teacher, Science Department Head, Science & Technology & STEM Program Facilitator at the Durham District School Board, President of the Ontario Association of Physics Teachers (www.oapt.ca) and Eastern Ontario Teacher Network Coordinator for Perimeter Institute Outreach (www.perimeterinstitute.ca). My passion and dedication to physics education is a result of the inspiring educators I have had the privilege to meet and collaborate with and the students who continue to ask questions and push my own thinking about my role as an educator today. I feel it is important to foster curiosity and provide opportunities for all students by creating inclusive learning environments that support achievement. Educators play a critical role – we help students realize their potential and imagine possibilities for their future! We support students as they discover who they want to become! As a first generation immigrant, I have faced my share of obstacles in my personal life and in my own educational journey. However, I have been very fortunate to have encountered amazing educators who inspired, guided and supported me to become the physics and STEM educator I am today. Educators have the power to impact people's lives!

Over the past 18 years, I have learned to work with secondary students and build a physics program that fosters curiosity that engages students to learn and view the world through a physics and mathematics lens. The language of science and mathematics allows humanity to be innovative problem solvers, designers, creators, and explorers. My students may claim that I "taught" them a lot about physics, but truly, they have taught me about what it means to be an educator that mentors, advocates, facilitates and learns alongside my students. I have also developed a great appreciation for my colleagues and the opportunities to network with professionals. My active participation within the Ontario Association of Physics Teachers community and the Physics Teacher Network with the Perimeter Institute for Theoretical Physics stretches my own thinking around physics education. I think about the importance of scientific literacy and numeracy in today's dynamic global society.

During my time as the Program Facilitator for Science and Technology (K-12) for the Durham District School Board, I was able to collaborate with exemplary educators to co-create a system STEM (Science, Technology, Engineering and Mathematics) Plan and provide supports as elementary and secondary schools implemented strategies and programs. I have dedicated my professional career to working alongside educators to create and inspire our educators to support student achievement in science. Physics continues to struggle with societal stereotypes and although K-12 Science Curriculum in Ontario is rich in physics concepts, these stereotypes continue to create anxiety amongst our students and educators. My work with educators focuses on breaking down barriers in physics education. I am always thinking about how I engage with audiences to break down these stereotypes and consider different perspectives in physics education to provide diverse opportunities for all people. I believe that by supporting educators, we will be able to reach more students.

One of the most memorable moments of by career will be the trip to CERN in July 2017. During this trip I was able to network with physics educators from around the world and CERN scientists and engineers. As a result of this

Images they plan on including:
Lisa Cole @llimcole
https://www.linkedin.com/in/lisa-limcole

opportunity, we collaborated in co-creating and co-delivering the Cultural Collisions by Origin-Canada program inspired by art@CMS-CERN. The program was a unique collaboration between international scientific research institutions (Origin), the System Planning, Research and Innovation Division at the Ontario Ministry of Education and the Ontario Science Centre. #Cultural_Collisions @OriginPhysics. It is quite amazing that one conversation with Dr. Michael Hoch art@CMS-CERN, resulted in a project that connected high school art, science and physics students with professional artists, musicians and physicists from across Canada and around the world!

I encourage the physics community to network and collaborate with educators! It is critical that we start to support our youth by working together to create moments that engages our students learn and create opportunities for them to wonder, question, explore and discover the fascinating mysteries that still puzzle physicists today! It truly is an exciting time in science with a wealth of opportunity! Let's inspire students together! We are truly better together! Let's Connect!

I am currently on secondment to the Ministry of Education as an Education Officer on the Innovation Design & Implementation (IDI) Team.

Take Action for Gender-Balanced and Diverse Scientific Meetings

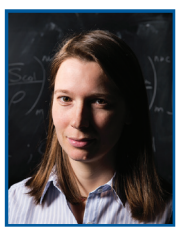
We are writing to suggest action to enhance "equity, diversity, and inclusion" [1] in physics, particularly representation of women, as well as other under-represented groups ("visible minorities, Indigenous peoples, people with diverse gender identities and people with disabilities" [1]), as invited and keynote speakers at conferences.

At a recent international conference we attended involving 200 participants from around the world, there were 5 keynote and 12 invited speakers. None of the keynote speakers were women, and only 1 of the 12 invited speakers was a woman. At the same time, the conference featured excellent proffered (not invited or keynote) presentations by women at all career stages, as well as men. The lack of women on the keynote and invited speakers list was striking and discouraging, as was the fact that there were few women on the conference organizing committee. This is certainly not the first conference in recent years to exhibit such disparities in representation amongst invited and keynote speakers.

There are plenty of reasons to take action to ensure scientific meetings are both gender-balanced and diverse. In parallel with the three broad "Merit Indicators" considered in NSERC's Discovery Grant evaluation, consider the following three reasons for seeking gender balance and diversity at meetings.

i) *To enrich development of highly qualified personnel (HQP)*: Making connections is at the heart of scientific meetings, and interactions between trainees and younger investigators may come more easily when there are senior/established researchers that the trainees or younger investigators can relate to. Gender balance and diversity are important for establishing good interactions and connections between generations of researchers. It also provides role models for young women physicists and others from under-represented groups, thereby encouraging them to stay in the field.

ii) *To enhance researcher career progression:* Not including or under-representing women and individuals from other under-represented groups as keynote and invited speakers hinders the careers of these scientists. In the highly competitive environment for grants and jobs, an invited or keynote speaker entry on a CV is an indication of respect amongst peers and recognition of research excellence and innovation. If one or more groups within the population is under-represented, then the corresponding/associated scientists are also at a disadvantage when it comes to applications for jobs, grants, research chairs, promotions, and so on. If there are unconscious or implicit biases in play resulting in groups not being invited, then these are (hidden) barriers.



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iii) *To advance research*: Diversity at meetings enhances interactions, leading to innovative approaches to solving problems as well as new and sometimes unexpected directions in research. Collaboration is at the heart of many new discoveries, and scientific meetings play important roles in initiating, nurturing, and fostering collaborations.

It is clear that action on gender-balanced and diverse scientific meetings aligns with NSERC's framework [1] and 2017 statement on equity, diversity and excellence in natural sciences and engineering research [2]. However, there are no clear guidelines or best practices for action towards achieving gender balance and diversity at scientific meetings. Some major international conferences have actively taken steps to achieve gender balance and diversity with great success [3]: it's time for best practices to be developed and adopted by CAP for the annual meeting and the lecture tour, and put into to practice for advancing Canadian science, leading the way for all scientific meetings.

Practices to achieve more diversity include: collecting data on gender balance and diversity in conferences/meetings and reporting the data; developing a speaker policy regarding this issue (e.g., speaker gender/diversity balance must reflect audience or profession) and making it visible; ensuring organizing committees are balanced and informed; building databases of speakers; providing support for speakers and families [4,5].

Relatively simple actions have substantially enhanced diversity at recent meetings of other societies [6]. Martin [4] has proposed and discussed the following 10 rules to achieve conference speaker gender balance:

1. Collect the data
2. Develop a speaker policy
3. Make the policy visible
4. Establish a balanced and informed program committee
5. Report the data
6. Build and use databases (of potential women speakers)
7. Respond to resistance
8. Support women at meetings (child care)
9. Be Family-friendly (at larger conferences especially)
10. Take the pledge (*i.e.,* proactively check on speaker policy before accepting an invitation to speak)

While Martin's rules focus on gender balance, they may be extended to generally encompass inclusion of individuals from other traditionally under-represented groups, and thus promote diversity within Canadian scientific meetings.

By training the next generation of physicists/scientists, by providing opportunities for demonstrating excellence, and by developing new directions in research, we all win with gender balance and diversity at meetings: "diversity leads to better science." [7]

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7. M.W. Nielsen, S. Alegria, L. Börjeson, H. Etzkowitzd, H.J. Falk-Krzesinski, A. Joshi, E. Leahey, L. Smith-Doerrj, A. Williams Woolley, and L. Schiebinger, "Gender diversity leads to better science." *Proc. Nat. Acad. Sci.* **114**, 1740-1742 (2017).

Eric Carl Svensson, PhD, FRSC, FAPS, FInstPhys (1940-2018)

Eric Svensson, a leader in the Canadian physics community, passed away peacefully in Ottawa, Ontario on May 16, 2018 following a brief battle with cancer.

Eric was born on August 13, 1940 in the small hamlet of Hampstead, New Brunswick, on the banks of the beautiful St. John River. Starting from a home that was full of love, but lacked both electricity and running water at the time, he traced an amazing arc through life. His formative years were spent exploring the woods and streams around Hampstead, where he developed his lifelong love of the outdoors, while his grade 1-8 education took place in the proverbial one-room school house to which he "walked 5 miles, uphill in both directions." His academic abilities were recognized early, with Eric often acting as a tutor to his fellow students, both younger and older. As a result, he was taken in by the family of the local physician, Dr. W.M. Jenkins, in order to complete high school approximately 25 km away in Gagetown, New Brunswick. From there, scholarships from General Motors and the Canadian Mathematical Congress enabled Eric to attend the University of New Brunswick in Fredericton, where he earned his B.Sc. in Physics in 1962. Studentships and Bursaries from the National Research Council then took Eric to McMaster University in Hamilton, Ontario, where he joined a unique cohort of young researchers and completed his Ph.D. in Physics in 1967 under the supervision of (future) Nobel Laureate Bertram Brockhouse.

In 1966, even before completing his Ph.D., Eric was hired as a research scientist at the Chalk River Nuclear Laboratories in Chalk River, Ontario. With the exception of sabbatical years at Atomenergi in Studsvik, Sweden (1972-1973) and Brookhaven National Laboratory in the United States (1981-1982), he spent his entire scientific career in Chalk River, first with Atomic Energy of Canada Ltd. and subsequently with the National Research Council of Canada. He was a leader in the experimental condensed matter physics community, applying the techniques of neutron scattering to study the static and dynamic properties of matter under a wide range of conditions. He made fundamental contributions to understanding the various amorphous and crystalline phases of water ice that occur at low temperatures and high pressures and was widely acclaimed for his pioneering experiments that demonstrated the existence of a Bose-Einstein condensate in the superfluid phase of liquid helium-4 and measured the associated condensate fraction as a function of temperature.

A recognized world leader in the science of liquid helium, Dr. Henry Glyde (Unidel Professor Emeritus, Physics and Astronomy, University of Delaware), characterizes Eric's contributions as follows: "Bose-Einstein condensation (BEC) was first observed in liquid ^{4}He — at the Canadian Nuclear Laboratories using reactor source neutrons in the 1960s. Subsequently, in the 1970s and 1980s, Eric Svensson made precise measurements and with Varley Sears developed new methods of data analysis that provided reliable and accurate values of BEC. Their values [1,2] and those of Herbert Mook at Oak Ridge National Laboratory, obtained using their CNL methods of data analysis, stood as the world standard for many years. Particularly, their data were an integral part of the development of our understanding of BEC and its temperature dependence. Similarly Eric made highly accurate measurements [3] of the less well known static structure factor of liquid ^{4}He that still stand today as the most accurate available. These data provide a bench mark that any formulation of quantum liquids must meet. Eric's data are a critical part of our current knowledge and understanding of liquid ^{4}He."

Eric was an encouraging mentor and great source of technical ideas for the large cohort of graduate students working at CNL through the 1980s and 90s. Many of these informal discussions took place in Eric's large vehicle as he gave us a ride back to Deep River following a long day at the lab. And for one of us (BDG), these developed into a successful ongoing collaboration and our 1st PhD student's (Ron Rogge) thesis related to phonons and "spinodal ordering" in Cu3Au.

Eric's many fundamental research contributions were recognized internationally and he was elected a Fellow of the American Physical Society (1987), a Fellow of the Royal Society of Canada (1996), and a Fellow of the Institute of Physics (1998). He remained actively engaged in research following his retirement and was named a National Research Council Researcher Emeritus in 2006.

In addition to his own research, Eric was passionate about the advancement of physics in Canada in general and he was actively engaged in the operations of the Canadian Association of Physicists (CAP) over a period of more than 20 years. His many contributions to the physics community include: the CAP Committee to Encourage Women in Physics (1988-2006), Editorial Advisory Board of the Canadian Journal of Physics (1992-2002), CAP Division of Condensed Matter Physics, Secretary-Treasurer (1979-1981), Vice-Chair (1992-1993), and Chair (1993-1994), CAP Science Policy Committee (1993-2006), CAP Councillor at Large (1994-1995), Vice-President Elect (1995-1996), Vice-President (1996-1997), President (1997-1998), and Past President (1998-1999),

Co-ordinator of the joint CAP, APS, SMF meeting CAM97 (1995-1997), Chair of the Program Committee for the CAP Congress (1996-1997), CAP-NSERC Physics Liaison Committee (1997-1998), International Advisor to the Council of the American Physical Society (1996-1999), Canadian National IUPAP Liaison Committee (1996-2002), Member of the Canadian delegation to the IUPAP General Assembly (1999) and International Conference on Women in Physics (2002), Director of International Affairs for the CAP (1999-2002), member of the Board of Trustees of the CAP Educational Trust Fund (1999-2002), and Chair (2000-2001), Friend of the CAP for the Chalk River Laboratories (2000-2006) and Chair of the CAP Science Policy Committee (2003-2006). In 2003, Eric received a Special Merit Award from the CAP in recognition of exceptional contributions to the management of the Association.

One of Eric's colleagues in leadership of the Canadian physics community, Marie D'Iorio has served as Executive Director of the National Institute for Nanotechnology (NINT), as Director General of the NRC Institute for Microstructural Sciences, and as President of the Canadian Association of Physicists (1999-2000). She characterizes Eric's leadership as follows: "I first met Eric at CAP meetings, and at a CAP congress in the early nineties he convinced me to attend the DCMP business meeting. There, he said "… you should be the co-chair next year — there is really nothing to it — just watch me!" What was almost terrifying in prospect became almost easy with his example. Eventually this led to following in his footsteps as President of the CAP, and pitching persuasion of my own. I am thankful for his dedication to the physics community and his calm and sensible approach, and will cherish the memory of his smiling eyes and his funny recounting of many anecdotes."

Eric's gentle nature, his wry smile, and the sparkle in his eyes, whether he was working in the laboratory or meeting room, enjoying a fine bottle of wine at the dinner table, or paddling his canoe through Algonquin Park, will be deeply missed by all who knew him.

Bruce Gaulin, Director of the Brockhouse Institute for Materials Research, McMaster University and President of the Canadian Association of Physicists

John Root, Director of the Canadian Neutron Beam Centre, National Research Council of Canada

Carl Svensson, Professor and Canada Research Chair in Gamma-Ray Spectroscopy and Rare Isotope Physics, University of Guelph

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2. E.C. Svensson and V.F. Sears, *Progress in Low temperature Physics*, Vol. 11, Chap. 4, p. 186 (1987).
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Announcing the creation of the Eric C. Svensson Memorial Graduate Scholarship

In recognition of his many years of exceptional service to the Canadian physics community, as well as the important role that scholarships played in his own education and career, the Canadian Association of Physicists, in cooperation with the family of Dr. Svensson, is establishing an endowment fund for the "Eric C. Svensson Memorial Graduate Scholarship". Charitable donations to this fund can be made, and further details regarding the scholarship can be found, at:

https://www.cap.ca/programs/medals-and-awards/prizes-students/svensson

Annonce de la création de la Bourse commémorative d'études supérieures Eric C. Svensson

En reconnaissance des nombreuses années de service exceptionnel à la collectivité canadienne de la physique ainsi que du rôle important que les bourses ont joué dans sa formation et sa carrière personnelles du Dr Svensson, l'Association canadienne des physiciens et physiciennes crée un fonds de dotation pour la « Bourse commémorative d'études supérieures Eric C. Svensson » de concert avec la famille du Dr Svensson. Des dons de bienfaisance peuvent être faits à ce fonds et l'on peut trouver de plus amples détails concernant la bourse à cette adresse :

https://www.cap.ca/fr/activites/medailles-bourses/prix-etudiants/svensson/

Akira Hirose, PhD, DSc, FAPS, FIEEE, FRSC (1941-2017)

It is with great sadness that I write words of tribute in memory of Dr. Akira Hirose, emeritus professor of Physics & Engineering Physics at the University of Saskatchewan.

Dr. Hirose completed his BSc and MSc at Yokohama National University, and his PhD at University of Tennessee followed by a research scientist position at Oakridge National lab. He joined the University of Saskatchewan Physics Department in 1971 as research scientist, faculty in 1977, professor in 1979, and led the Plasma Physics Laboratory since 1994. He served as Department Head of Physics & Engineering Physics from 1998-2001 and held a Canada Research Chair from 2001 until his retirement in 2015.

Dr. Hirose made pioneering theoretical and experimental contributions to the basic understanding of waves and instabilities in plasmas and their effects on diffusion and heating of plasmas. Dr. Hirose was responsible for building the first Canadian tokamak (STOR-1M): a magnetic plasma containment device for studying controlled nuclear fusion. He also led the construction of its successor (STOR-M) which continues to be the only active tokamak in Canada. These tokamaks were used to demonstrate alternating current operation of a tokamak for the first time, an operation mode later adopted by the Joint European tokamak. Dr. Hirose has also carried out groundbreaking work with STOR-M on the development of compact torus injection fueling technology to meet the needs of future large tokamak reactors.

Akira's research accomplishments are incredible in their scope and impact: over 330 publications, including books, and book chapters. His accomplishments were recognized with numerous national and international honours including: Fellow of the Academy of Science of the Royal Society of Canada; Fellow of European Academy of Science; Fellow of the Institute of Electrical and Electronics Engineers (IEEE); Fellow of the American Physical Society; IEEE Nuclear and Plasma Sciences Society Merit Award and Plasma Science and Applications Award; Saskatchewan Centennial Medal; University of Saskatchewan Distinguished Researcher Award and earned D.Sc. His award citations state, "For pioneering contributions to the understanding of linear waves, instabilities, and turbulent heating in plasmas and confinement studies in tokamaks"; and, "for outstanding contributions to theoretical/experimental work on basic and fusion related plasma science including studies on waves, turbulent heating, quasi-steady state operation and anomalous transport in tokamaks."

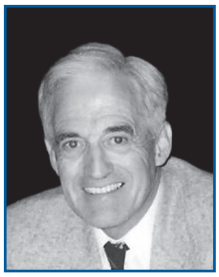
Dr. Hirose was also a distinguished teacher, a legendary instructor of an advanced EM theory graduate course. Dr. Hirose supervised more than 30 MSc/PhD theses and supervised many postdoctoral fellows and research associates, helping ensure continued progress in science and engineering for the benefit of humanity.

Dr. Hirose was active in the Canadian Association of Physicists: a member since 1975 (and sustaining member for many years), and Chair of the Division of Plasma Physics in 1980 and in 1994. His work was honoured during a special session at the 2015 Canadian Association of Physicists congress. He was an Associate Editor for the Canadian Journal of Physics (2008-2010) and a member of the Editorial Board (2010-).

In his personal life Akira enjoyed playing tennis and Go, and also enjoyed classical music. Akira will be lovingly remembered by his wife, Kimiko Hirose; son, Tad Hirose; daughter, Kyoko Hirose; and grandchildren, Vanessa, Patrick and Lovely Rose. He will be dearly missed by his many friends and colleagues.

Dr. Tom Steele
Professor and Head
Department of Physics and Engineering Physics
University of Saskatchewan

John Arthur Davies (1927-2016)



John Davies died on July 25, 2016, in Deep River, Ontario, Canada, his home for 60 years. He was a towering figure in the field of the interaction of energetic ions with matter.

His many awards include Fellow of the Royal Society of Canada and the Danish Academy of Sciences and Letters, the W B Lewis Medal of the Canadian Nuclear Society and others. In 2003, in Brazil, the Radiation Effects in Matter conference (REM3) was organized to honor John Davies for "his many and important contributions in the field of the ion beam interactions with matter, in particular, for his pioneering work regarding the channeling technique." To those of us in the field he was the epitome of an excellent experimentalist, constantly active, always involved and a wealth of knowledge and good science.

John was born 1927 in Wales and studied physical chemistry in England and Canada, where his family moved after World War II. He earned a PhD in electrochemistry from the University of Toronto and spent two years as a post-doctoral fellow at the University of Leeds in the UK before joining the Chemistry Division of Chalk River Nuclear Labs in 1956. He was also a Professor at McMaster University in Hamilton, Canada until his retirement in 1991. John maintained a strong Catholic faith throughout his life, and also was active in the community, serving on the local hospital board from 1974 to 1984, and on the local school board for a lesser time.

At Chalk River John's first task was to develop a technique to measure ranges of keV ions penetrating solids, so as to enable physicists to determine the energies of nuclear reaction products. The Davies ingenious solution was implantation of radioactive ions into a solid and layer-by-layer removal of the target material via electrochemical stripping, employing his chemistry expertise. This was the first demonstration of depth profiling, a prime task in micro-and nanotechnology, surface science and environmental science.

An intriguing feature in early measurements of ion range distributions was the occurrence of exponential tails of deeply penetrating ions, rather than the expected Gaussian distribution. This phenomenon found a surprising solution in a dialogue with Mark Robinson and Ordean Oen from Oak Ridge National Laboratory. In binary-collision simulations of ion penetration in single crystals, they found a pronounced dependence of nuclear stopping rates on the incident direction of the beam with respect to major crystalline symmetry directions. In a famous 1963 paper, Piercy, Brown, Davies and McCargo reported the application of the stripping technique to ions incident on a single crystal; thus the first experimental demonstration of channeling!

John had a special relationship with Scandinavia, particularly with leading groups in Stockholm, Sweden and Aarhus, Denmark. In 1964 he was appointed a visiting professor at Aarhus University, the home of the leading ion beam theorist, Jens Lindhard, who became interested in these single crystal results. In Lindhard's picture, the fundamental event was not the modified stopping power and range but the ion trajectory formed from the correlated scattering from a string of atoms, rather than a random array of single atoms. This led to the prediction of a drastic dip in the yield of nuclear reactions and other "close" (nuclear dimensions) collisions when the beam was incident along major crystalline direction. In a classic 1964 paper Bøgh, Davies and Nielsen demonstrated this for a p-Υ reaction in silicon.

In his contribution to a Festschrift for Jens Lindhard's 60th birthday John called 1964 the year of the channeling explosion. He writes: "From an Aarhus perspective, probably the most important event was that I had brought with me from CRNL the preprint of Geoff Dearnaley's pioneering experiment, confirming channeling for MeV proton energies; I had also brought a pocketful of W and Al single crystals." However, this is far too modest. John became a leading figure in the legendary 'Aarhus Saturday meetings' where experiments on channeling were critically discussed, and he became a mentor for a group of young physicists in Aarhus. In the following years young scientists from the physics institute in Aarhus and other laboratories active in channeling were invited to Chalk River, and the collaboration with John and the warm hospitality of the whole Davies family, in particular his wife Flo, led to lifelong friendships.

John recognized the power of the channeling technique for analyzing the structure of a crystal and its defects. A major breakthrough occurred on the formation of a collaboration with James W. Mayer, a pioneer in semiconductor materials and detectors. Together with Lennart Eriksson, a visiting scientist from Stockholm, this team developed channeling as a tool to determine lattice locations of impurities as well as damage profiles in semiconductor crystals. Thus John was a founding father of ion implantation and ion beam analysis of materials. This research led to a breakthrough in semiconductor science and technology. These ion beam processes have become essential components enabling the Si revolution.

John played an important role in almost all aspects of channeling, including the study of surface relaxation with Peter Norton at CRNL and measurements of very short nuclear lifetimes with Walt Gibson and others. He was a critical member

of numerous international collaborations that studied many basic and applied aspects of channeling. He also participated in studies of the channeling of very energetic heavy ions at the accelerator facility at CRNL and even in studies of positron channeling. Deservedly, he is internationally recognized as the leading figure in the development of channeling, from the pioneering range studies to a very broad field with important applications.

Beyond channeling John had a hand in almost every "ion beam interaction" innovation. These varied from new ways of doing materials analysis such as energy recoil spectroscopy to anomalies in ranges and "strange" sputtering in complex insulators. The latter work produced new insights into much discussed ion beam phenomena such as thermal spikes. In our field he knew his trade better than anybody (and he let us know it too). He was a walking library and a vocal and critical presence at conferences, workshops and in casual conversation.

Those of us in the ion beam community enjoy a special relationship. This has been fostered by many inter-laboratory visits, long and short, by attendance at family-involved Gordon conferences where we watched the kids grow and numerous personal involvements. John set the style for this. John and Flo generously opened their cottage first at Smoke Lake and later at Lyell Lake to our families. By way of the celebration of life's events, some sad, we became family. John's and Flo's warm hospitality, ability to engage colleagues, keen personal interest and friendship have kept our atomic collision physics community together and vibrant for over sixty years.

Jens Ulrik Andersen, Leonard Feldman, Frans Saris, Peter Sigmund, and Bruce Winterbon

The Editorial Board welcomes articles from readers suitable for, and understandable to, any practising or student physicist. Review papers and contributions of general interest of up to four journal pages in length are particularly welcome. Suggestions for theme topics and guest editors are also welcome and should be sent to bjoos@uottawa.ca.

Le comité de rédaction invite les lecteurs à soumettre des articles qui intéresseraient et seraient compris par tout physicien, ou physicienne, et étudiant ou étudiante en physique. Les articles de synthèse d'une longueur d'au plus quatre pages de revue sont en particular bienvenus. Des suggestions de sujets pour des revues à thème sont aussi bienvenues et peuvent être envoyées à bjoos@uottawa.ca.

PhD Physics Degrees Awarded in Canadian Universities*
Doctorats en physique décernés par les universités canadiennes*

December 2016 to December 2017 / Décembre 2016 à décembre 2017

Brock University

PRZEBORSKI, M., "Nonlinear dynamics of granular assemblies", (T. Harroun), October 2017, now pursuing a Postdoctoral Fellowship at the University of Waterloo, Waterloo, ON, Canada.

Carleton University

CREE, G., "Direct Measurement of the Higgs Boson Mass, Natural Width, and Cross Section Times Branching Ratio to Four Leptons Using a Per-Event Line shape in the Higgs to ZZ to Four Lepton Decay Channel with the ATLAS Detector", (T. Koffas), June 2017.

HUNTER, C., "A Study of the Prevalence of Patient Body Motion and Its Subsequent Correction by Projection Consistency Conditions", (R. deKemp), June 2017.

Concordia University

HASSANPOUR, A., "Controlled Hydrothermal Growth of ZnO Nanorods Arrays: Selective Growth and Cation Doping", (P. Bianucci), May 2017, now pursuing a MITACS Elevate Postdoctoral Fellowship at Institut National de la Recherche Scientifique in Québec, QC, Canada.

Dalhousie University

NELSON, K., "Studies of the Effects of High Voltage on the Performance and Impedance of Lithium-Ion Batteries", (J. Dahn), September 2017, now pursuing a Postdoctoral Fellowship at Dalhousie University, Halifax, NS, Canada.

PARSONS, D., "Volume of Interest Imaging for Image Guided Radiotherapy", (J. Robar), September 2017, now completing a 3-year residency training program in radiation oncology medical physics at the University of Texas Southwestern Medical Center, Dallas, Texas, USA.

PERRO, C., "Satellite Retrievals of Total Column Water Vapor and Surface Emissivity During Artic Winter", (T. Duck), September 2017, now pursuing a Postdoctoral Fellowship at Dalhousie University, Halifax, NS, Canada.

POEHLS, J., "Ultralow Thermal Conductivity and Novel Thermoelectric Materials", (M.A. White), September 2017, now pursuing a Postdoctoral Fellowship at the University of Alberta, Edmonton, AB, Canada.

SUN, J.P., "Organic Photovoltaics: Integrating Non-Fullerene Acceptors into Solution-Processed Devices", (I. Hill), September 2017, now pursuing a Postdoctoral Fellowship at Duke University, Durham, North Carolina, USA.

*This list includes all information submitted to the CAP office up to 21 January, 2018.

**La liste comprend l'information reçue au bureau de l'ACP jusqu'au 21 janvier 2018.*

École Polytechnique de Montréal

BLANCHAND-DIONNE, A.-P., "Propriétés optiques de nano-trous périodiques dans une couche mince métallique: modélisation, fabrication et application comme biocapteur", (M. Meunier), October 2017, now a Research Associate at Laboratoire de MicroFabrication (LMF), Polytechnique Montréal, Montréal, QC, Canada.

DUBOIS, M.-A., "Simulation intrusive dynamique d'imagerie à effet tunnel", (A. Rochefort, X. Bouju), June 2017, now a senior software developer at CaSa Appareils connectés, Béloeil, QC, Canada.

HIDOUCHE, Akila, "Étude des écoulements critiques (bloqués) pour des fluides aux états sous et sur critiques", (A. Teyssedoy), December 2017, now searching for employment.

HOUSSEINEY MILANY, S. R., "Development of a Hybrid Deterministic - Stochastic Method for full Core Neutronics", (G. Marleau), May 2017, now an Engineer Analyst at AmecFW, Toronto, ON, Canada.

LAJOIE, M.-A., "Développement d'un schéma de calcul prismatique généralisé parallèle en transport déterministe hétérogène 3-D", (G. Marleau, F. Fevotte), September 2017, now a Data scientist at National Bank of Canada, Toronto, ON, Canada.

LAPOINTE, J., "Fonctionnalisation des écrans de téléphones mobiles: des premiers dispositifs invisibles à l'amélioration de l'écriture par laser", (R. Kashyap), October 2017, now a Scientific Coordinator at Sentinel North and a Research Scientist at Centre d'optique, photonique et laser (COPL), at Université Laval, Québec, QC, Canada.

LI, J., "Hollow Core Photonic Bragg Fibers for Industrial Sensing Applications", (M.A. Skorobogatiy), March 2017, now pursuing a Postdoctoral Fellowship at Electrical and Computer Engineering Department at the University of British Columbia, Vancouver, BC, Canada.

LOQUAI, S., "Durable Thermochromic V02 Films Deposited by Hipims", (L. Martinu, J. Klemberg-Sapieha), April 2017, now pursuing a Postdoctoral Fellowship at Polytechnique Montréal, Montréal, QC, Canada.

MA, T., "Practical Terahertz Waveguides for Advances Light Management", (M.A. Skorobogatiy), April 2017.

MENG, X., "Electrolyte-Gated Tungsten Oxide Transistors: Fabrication, Working Mechanism, Device Performance", (C. Santato), September 2017, now searching for employment.

MUKHERJEE, S., "Isotope Engineering and Lattice Disorder in Group IV Nanoscale and Quantum Semiconductors", (O. Moutanabbir), September 2017, now pursuing a Postdoctoral Fellowship at Polytechnique Montréal, Montréal, QC, Canada.

RAOUAFI, H., "Simulation de mécanismes de contrôle de la réactivité inclinés du réacteur SCWR-canadien en utilisant les codes DRAGON5 et DONJON3", (G. Marleau), May 2017, now searching for employment.

ROOHI NOOZADI, A.A., "Forward and Inverse Modelling of Magnetic Induction Tomography (MIT) for Biomedical Application", (A. Yelon, D. Ménard), June 2017, now pursuing an Industrial Postdoctoral Fellowship at Ubisoft, Montréal, QC, Canada.

McGill University

AL TAMIMI, W., "Collinear laser spectroscopy on exotic isotopes of rubidium and gallium", (F. Buchinger, J. Crawford), May 2017, now a Full-time Lecturer at University of Jordan, Amman, Jordan.

ALONSO ORTIZ, E., "Gradient echo-based quantitative myelin water imaging", (I. Levesque, G. Pike), May 2017, now a Medical Physics Resident at The Ottawa Hospital, Ottawa, ON, Canada.

ARCHIBALD, R., "X-ray timing of young pulsars", (V. Kaspi), October 2017, now pursuing a Postdoctoral Fellowship at University of Toronto, Toronto, ON, Canada.

BAZRAFSHAN MOGHADDAM, H., "Reheating in early universe cosmology", (R. Brandenberger), October 2017, now pursuing a Postdoctoral Fellowship at Institute for Research in Fundamental Sciences (IPM), Tehran, Iran.

BOHLOUL, S., "First-principles quantum transport and linear response modeling of nano-devices and materials", (H. Guo), October 2017, now a Research Scientist/Scientific Software Developer at NanoAcademic Technologies, Brossard, QC, Canada.

BONAVENTURA, N., "A multiwavelength exploration of unexpected star formation activity in SpARCS brightest cluster galaxies", (T. Webb), October 2017, now a James Webb Space Telescope (JWST) Postdoctoral Researcher at Cosmis Dawn Center (DAWN), Niels Bohr Institute, University of Copenhagen, Copenhagen, Denmark.

BORCHMANN, J., "Entanglement and disorder in gapped and gapless topological states", (T. Pereg-Barnea), February 2017, now a Data Scientist at Capital1, Toronto, ON, Canada.

CÉSAR, M., "Ab initio study of disordered nanoelectronic devices: copper interconnects and group-III nitrides", (H. Guo), October 2017, now pursuing a Postdoctoral Fellowship at French Alternative Energies and Atomic Energy Commission (CEA), Saclay, France.

D'ANJOU, B., "Optimization of real-world qubit measurements", (W. Coish), October 2017, now pursuing a Postdoctoral Fellowship at University of Konstanz, Konstanz, Baden-Württemberg, Germany.

DUPUIS, G., "Model-dependent collider signatures of particle dark matter", (J. Cline), February 2017.

GOUVÊA MAURICIO FERREIRA, E., "Early universe cosmology and dark energy: from the Big Bang to the late expansion of the universe", (R. Brandenberger), October 2017, now a Research Associate at McGill University, Montreal, QC, Canada.

MANTIFEL, R., "Measurement of the production cross section of jets in association with a Z boson in 8 TeV proton-proton collisions with the ATLAS detector", (F. Corriveau), May 2017.

MARKEL, D., "Simultaneous registration and segmentation coupling using the Jensen Rényi divergence for adaptive radiotherapy", (I. El Naqa), February 2017, now a Physics Resident at Princess Margaret Hospital, Toronto, ON, Canada.

MCDONOUGH, E., "High energy physics and the early universe", (R. Brandenberger, K. Dasgupta), October 2017, now pursuing a Postdoctoral Research Fellowship at Brown University, Providence, Rhode Island, USA.

PATER, P., "Numerical Models for radiation-induced DNA damage", (J. Seuntjens, I. El Naqa), February 2017, now a Medical Physicist at Cedar's Cancer Center - McGill University Health Center, Montreal, QC, Canada.

RENAUD, J., "On the development of absorbed dose calorimeter systems for absolute clinical dosimetry", (J. Seuntjens, A. Sarfehnia), February 2017, now pursuing a Postdoctoral Fellowship at McGill University, Montreal, QC, Canada.

ROEBBER, E., "Characterizing the nanohertz gravitational wave background produced by a cosmological population of binary supermassive black holes", (G. Holder, V. Kaspi), October 2017, now pursuing a Postdoctoral Prize Fellowship at Institute of Gravitational Wave Astronomy, University of Birmingham, Birmingham, United Kingdom.

ROY-GOBEIL, A., "Single-electron charging using atomic force microscopy", (P. Grütter), February 2017, now pursuing a Postdoctoral Fellowship at McGill University, Montreal, QC, Canada.

SCHOLZ, P., "Single-electron charging using atomic force microscopy Observations of magnetars: from outburst to quiescence Single-electron charging using atomic force microscopy", (V. Kaspi), February 2017, now pursuing a Postdoctoral Fellowship at National Research Council, Penticton, British Columbia, Canada.

YU, V., "Breakdown of the quantum hall effect in InGaAs/InP quantum wells", (M. Hilke, D. Austing), October 2017.

ZHANG, Y., "Nanofluidic coupled membrane devices for single molecule sensing and imaging", (W. Reisner), October 2017, now pursuing a Postdoctoral Fellowship at McGill University, Montreal, QC, Canada.

McMaster University

ALSOP, R., "Pharmaceuticals and Physics: Studies of Drug-Membrane Interactions Using Advanced X-ray and Neutron Scattering Techniques", (M. Rheinstadter), August 2017, now an Analyst at PwC, Toronto, ON, Canada.

CRIDLAND, A., "Connecting the Chemical Composition of Planetary Atmospheres with Planet Formation", (R. Pudritz), August 2017, now pursuing a Postdoctoral Fellowship at the Leiden University, Leiden, Netherlands.

EADIE, G., "Lights in Dark Places: Inferring the Milky Way Mass Profile using Galactic Satellites and Hierarchical Bayes", (W. Harris), July 2017, now pursuing a Postdoctoral Fellow at the University of Washington, Seattle, Washing, USA.

HALLAS, A., "Application of Chemical Pressure to Magnetically Frustrated Pyrochlores", (G. Luke), August 2017, now pursuing a Postdoctoral Fellowship at the Rice University, Houston, Texas, USA.

HOWARD, C., "The Effects of Radiative Feedback on Star Cluster Formation and the Galactic Interstellar Medium", (R. Pudritz, W. Harris), August 2017, now pursuing a Postdoctoral Fellowship at McMaster University, Hamilton, ON, Canada.

JOSHI, G., "Mass Loss and Preprocessing of Galaxies Traversing Group Environments", (L. Parker, J. Wadsley), September 2017, now pursuing a Postdoctoral Fellowship at the Max Planck Institute for Astronomy, Heidelberg, Germany.

KELLER, B., "Super bubble Feedback in Galaxy Formation & Evolution", (J. Wadsley), January 2017, now pursuing a Postdoctoral Fellowship at the Gastronomists Rechen-Institut, Heidelberg, Germany.

LUNTS, R., "Low Energy Behavior of the Antiferromagnetic Quantum Critical Metal", (S. Lee), August 2017, now pursuing a Postdoctoral Fellowship at Flatiron Institute, New York, NY, USA.

MILADINOVIC, N., "The Abraham-Minkowski Controversy and the He-McKellar-Wilkens Phase", (D. O'Dell), December 2016, now a Programmer at Preteckt, Memphis, Tennessee, USA.

MOK, A., "The Effects of Environment on the Atomic and Molecular Gas Properties of Star-Forming Galaxies", (C. Wilson), July 2017, now pursuing a Postdoctoral Fellowship at the University of Toledo, Toledo, Ohio, USA.

MUMFORD, J., "Singularities in a BEC in a Double Well Potential", (D. O'Dell), May 2017, now pursuing a Postdoctoral Fellowship at Jagiellonian University, Krakow, Poland.

MUNSIE, T., "Synthesis and Characterization of Constrained Magnetism in Niobates", (G. Luke), June 2017, now a Scientist at the National Defence, Edmonton, AB, Canada.

Memorial University

LeBLANC, M., "Magnetic Order in the FCC Kagome Antiferromagnet", (J. Whitehead, M. Plumer), June 2017, now a Part-Time Research Assistant at the Department of Physics and Physical Oceanography, Memorial University, St. John's, NL, Canada.

LeMORZADEC, K., "Scaling Issues in Glaciology: Addressing Subgrid Topography", (L. Tarasov), June 2017, now a Project Manager with Open Groupe, France.

ZHANG, Y., "Waves and Eddies on a ß Plane: Experiments with Altimetry", (I. Afanassiev), June 2017, now an Assistant Professor at Guangdong Ocean University, China.

Queen's University

ALTAL, F., "Scanning Optical Imaging and Stress Tests of Polymer Light-Emitting Electrochemical Cells", (J. Gao), April 2017, now pursuing a

Postdoctoral Fellowship at Queen's University, Kingston, ON, Canada.

AMOLE, C., "The Pico-2L Program: A Giant Leap Towards Background-Free Matter Direct Detection Using Bubble Chamber", (A.J. Noble), November 2017, now pursuing a Postdoctoral Fellowship at the University of Zurich, Zurich, Switzerland.

BOBBARA, S., "Effect of Encapsulation and Light-soak on Charge Transport Properties of Organic Semiconductor-based Diodes", (J.-M. Nunzi), November 2017, now pursuing a Postdoctoral Fellowship at Queen's University, Kingston, ON, Canada.

GIAMPA, P., "Identification and Reduction of the Alpha Background, From 238U and 232Th Decay Chains, in the DEAP-3600 Experiment", (M.G. Boulay), November 2017, now a Physicist at TRIUMF, Vancouver, BC, Canada.

MANN, N., "Theoretical and computational studies of disorder-induced scattering and nonlinear optical interactions in slow-light photonic crystal waveguide", (S. Hughes), April 2017, now a Data Scientist at automotiveMastermind Inc. New York, NY, USA.

OUELLETTE, N., "The SHIVir Survey: A Dynamical Catalogue of Virgo Cluster Galaxies and their Scaling Relations", (S. Courteau), April 2017, now an Education and Outreach Officer at the Canadian Particle Astrophysics Research Centre, Queen's University, Kingston, ON, Canada.

SIMPSON, E., "CMOS-Integrated Transducer Arrays for High-Frequency Ultrasonic Imaging", (M.M. Dignam, J. Brown), November 2017, now a Senior Research Engineer at Siemens Healthineers, Seattle, WA, USA.

Royal Military College of Canada

EARL, MICHAEL A., "Photometric Analyses and Preliminary Attitude Estimation of Inactive Box-Wing Geosynchronous Satellites", (G.A. Wade), June 2018, now a research associate at the University of Saskatchewan, Saskatoon, SK, Canada.

Ryerson University

DA SILVA, E., "A Hydroxyapatite Phantom Material for the Calibration of In Vivo X-Ray Fluorescence Systems of Bone Strontium and Lead Quantification", (A. Pejovic-Milic), June 2017, now an Assistant Professor at the Department of Physics, Ryerson University, Toronto, ON, Canada and a Medical Physics Resident at Odette Cancer Centre - Sunnybrook Hospital, Toronto, ON, Canada.

DAVLETSHIN, Y., "A Computational Analysis of Nanoparticle-Mediated Optical Breakdown", (C. Kumaradas), June 2017, now pursuing a Postdoctoral Fellowship at Studio1Labs, Toronto, ON, Canada.

JAKUBOVIC, R., "Feasibility of Radiation Dose Planning Guided Surgical Resection in Spinal Tumors", (V. Yang, A. Pejovic-Milic), October 2017, now a Medical Physics Resident at Northwell Health, New York, New York, USA.

LIAO, L., "Mathematical Models of Influenza A Virus Infections In Vitro: Investigating Defective Interfering Particles and Virus Release", (C. Beauchemin), October 2017, now a Postdoctoral Research Associate at Los Alamos National Laboratory, Los Alamos, New Mexico, USA.

Simon Fraser University

CHU, R., "Design and Fabrication of Nanoscale Bismuth Hall Probes", (D. Broun), December 2016.

DARBANDI, A., "Growth, characterization, and fabrication of GaAs core/shell and axial nanowire devices", (S. Watkins), December 2016.

GAVRILOV, M., "Experiments on the thermodynamics of information processing", (J. Bechhoefer), December 2016.

REZAEI, N., "Mechanical Studies of Single Collagen Molecules Using Imaging and Force Spectroscopy", (N. Forde), December 2016.

TRUNCIK, C., "Precision microwave spectroscopy of the heavy fermion superconductor CeCoIn5", (D. Broun), December 2016.

MOHAMMADBEIGI, F., "Optical characterization of doped zinc oxide nanowires", (S. Watkins), April 2017.

VAN NIEUWKOOP, K., "Evidence for the Production of the Standard Model Higgs Boson Produced via Vector Boson Fusion in the WW* Channel at the ATLAS Detector", (B. Stelzer), April 2017.

Université de Montréal

AL MAKDESSI, G., "Formation de poudres carbonées dans un plasma de haute fréquence produit à très basse pression dans des mélanges actylène-argon", (J. Margot), septembre 2017, maintenant un Physicien médical à CUSM-Glen, Montréal, QC, Canada.

LAURIN, M., "Recherche de la matière sombre à l'aide de détecteurs à liquides surchauffés dans le cadre de l'expérience PICO/Picasso", (V. Zacek), mars 2017, maintenant un Agent de recherche pour l'Université de Montréal, avec le groupe PICO, Montréal, QC, Canada.

LEVASSEUR, O., "Étude de la dynamique de croissance de revêtements nanostructurés multifonctionnels sur le bois par plasmas froids à la pression atmosphérique", (L. Stafford, N. Gherardi), mars 2017, maintenant un Professeur au CEGEP Édouard-Montpetit, Longueuil, QC, Canada.

PROFILI, J., "Dépôt de couches minces nanocomposites par nébulisation d'une suspension colloïdale dans une décharge de Townsend à la pression atmosphérique", (L. Stafford, N. Gherardi), mars 2017, maintenant suit une bourse Postdoctorale à l'Université de Montréal, Montréal, QC, Canada.

SHOALEH SAADI, D., "Search for Heavy Gluons from Composite Higgs Model through Vector-Like Top Quark Decay Topologies with the Atlas Experiment", (C. Leroy), September 2017, now a Research and Development Engineer at Big Data - Analytics - AI, Activeeon, Paris, France and Montréal, QC, Canada.

SIMARD, C., "Détermination des coefficients de transport turbulent et analyse des cycles magnétiques produits dans un modèle dynamo en champ moyen avec et sans rétroaction magnétique", (P. Charbonneau), septembre 2017, maintenant une Spécialiste Science Physique en Production radar opérationnelle chez Environnement Canada et Changement Climatique, Dorval, QC, Canada

Université de Sherbrooke

DAUPHINAIS, G., "La correction d'erreur pour les ayons non abéliens", (D. Poulin), avril 2017, maintenant suis une bourse Postdoctorale à l'Université Complutense de Madrid, Espagne.

DION, M., "Interface p-n à base de cuprates supraconducteurs", (P. Fournier), septembre 2017, maintenant un Professionnel de recherche à l'Institut Quantique, Sherbrooke, QC, Canada.

MÉNARD, M., "Applications du groupe de renormalisation aux conducteurs unidimensionnels dimérisés", (C. Bourbonnais), mai 2017, maintenant en recherche d'emploi.

PETROV, B., "Études des matériaux photoconducteurs ultra rapides à faible gap et leurs applications dans les dispositifs et systèmes THz", (D. Morris), juin 2017, maintenant un Scientifique à Qube 4D Ventures Inc., Montréal, QC, Canada.

SHAHBAZI, M., "Application du Groupe de Renormalisation à la théorie du transport et de l'état supraconducteur sous champs magnétique dans les conducteurs organiques", (C. Bourbonnais), mars 2017, maintenant complète un diplôme en mathématiques financières au HEC de à l'Université de Montréal, Montréal, QC, Canada.

Université Laval

ALARIE-VÉZINA, L., "Les superpolynômes de Jack et le modèle Calogero-Moser-Sutherland N=2", (P. Mathieu), novembre 2017, maintenant Stagiaire postdoctoral, Université Laval, Québec, QC, Canada.

COLLINS-FEKETE, C.-A., "On particle imaging with application to particle radiotherapy", (L. Beaulieu), October 2017, now pursuing a postdoctoral fellowship at the University College London - National Physics Laboratory, London, United Kingdom.

DALLAIRE, X., "Miniaturisation de caméras grand angle", (S. Thibault)), décembre 2017, maintenant Concepteur Optique chez Immersion, Montréal, QC, Canada.

ESPAGNET, R., "Mise au point d'un compteur sanguin pour l'imagerie moléculaire quantitative", (P. Després), juillet 2017, maintenant Stagiaire postdoctoral à l'Université de Sherbrooke, Sherbrooke, QC, Canada.

FORTIN, M., "Les faisceaux optiques avec trajectoires courbées", (M. Piché), février 2017, maintenant Enseignant au CEGEP Sainte-Foy, Québec, QC, Canada.

KAFANDO, I., "Analyse spectroscopique et photométrique d'un échantillon d'étoiles de la branche horizontale", (C. Robert), novembre 2017.

MATENINE, D., "Conception et évaluation d'un nouvel algorithme de reconstruction itérative en tomodensitométrie à faisceau conique implanté sur matériel graphique", (P. Després), novembre 2017, maintenant Stagiaire postdoctoral, ETS - Centre de recherche du CHUM, Montréal, QC, Canada.

MUGNES, J.-M., "Développement d'une méthode d'analyse bayésienne simultanée et multiparamétrique des spectres stellaires et son application aux spectres d'étoiles massives", (C. Robert), mars 2017.

PARADIS, G., "Étude du mécanisme de croissance du filament bactérien", (S. Rainville), novembre 2017, now a R&D Optical Designer, JGR Optics Inc., Ottawa, ON, Canada.

ROUSSEAU-NEPTON, L., "Étude des régions de formation stellaire dans les galaxies spirales avec SpIOMM", (C. Robert), janvier 2017, maintenant Stagiaire postdoctorale à l'Université de Hawaii à Hilo & Télescope Canada-France-Hawaii, Hawaii, USA.

VAHANIAN, E., "Développement de couches antireflets à base de nanoparticules de silice pour des systèmes photovoltaïques à haute concentration", (T. Galstian), décembre 2017.

University of Alberta

ALEMIE, W., "Time-Lapse Full Waveform Inversion Methods", (M. Sacchi), November 2017.

ANWAR, T., "Study of the Chinese Loess and Siberian Flood Basalts: New Global Scale Insights to the Paleoclimate and Geomagnetic Field Changes", (V. Kravchinsky), June 2017.

BISWAS, T., "Fabrication, Characterization and Applications of Nanomechanical Resonators", (J. Davis), November 2017.

CHENG, J., "Gradient Projection Methods with Applications to Simultaneous Source Seismic Data Processing", (M. Sacchi), November 2017.

EBUFEGHA, V., "Anisotropy of Mudrocks: Quantifying Controls and Fabric Implications in the Horn River Basin", (D. Potter), June 2017.

FANI SANI, F., "Torque Magnetometry for Concurrent Acquisitions of Magnetostatics and Spin-Dynamics", (M. Freeman), November 2017.

JABBAR, S., "Search for the Minimal Supersymmetric Standard Model Neutral Higgs Bosons (A/H) Decaying to tau+tau- in pp Collisions at sqrt{s}=13 TeV with the ATLAS Detector", (R. Moore), June 2017.

KAZEMI NOJADEH, N., "Efficient Algorithms for Least Squares Wave Equation Migration and Source Signature Estimation", (M. Sacchi), November 2017.

LI, Z., "Rotational Seismology and Its Applications in Microseismic Event Localization", (M. van der Baan, M. Dumberry), November 2017.

MALEHMIR, M., "Reflectivity Analysis from the Low Symmetric Anisotropic Media", (D. Schmitt), November 2017.

MILES, D., "Advances in Fluxgate Magnetometry for Space Physics", (I. Mann, M. Unsworth), June 2017.

MOHAMMED HOSSEINI DOKHT, R., "Imaging Upper Mantle Discontinuities Using Long Period Seismic Data", (Y. Gu), June 2017.

STANTON, K., "Vector Interpolation and Regularized Elastic Imaging of Multicomponent", (M. Sacchi), November 2017.

TZOUNIS, C., "Radiation from Particles Revolving Around a Magnetized Schwarzschild Black Hole", (V. Frolov), June 2017.

WU, L., "Apparent Polar Wandering and Its Implications for Past Plate Motions", (V. Kravchinsky, D. Potter), June 2017.

University of British Columbia

CHEN, H., "Validation and optimization of myelin water imaging in a preclinical model of spinal cord injury", (P. Kozlowski), January 2017.

CLARK, H., "Assessment of spatially inhomogeneous intra-organ radiation dose response in salivary glands", (S. Thomas), April 2017.

CRUZ, S., "Single particle structure of exotic strontium isotopes", (R. Kruecken), June 2017.

ESQUINAS FERNANDEZ, P., "Quantitative measurements of Rhenium-188 for radionuclide therapies", (A. Celler), June 2017.

GIGNAC, M., "Searches for Supersymmetry in events with one-lepton, jets and missing transverse momentum with the ATLAS detector", (C. Gay), August 2017.

KHADEMI, A., "Tuning Graphene's Electronic and Transport Properties via Adatom Deposition", (J. Folk), August 2017.

KIM, N., "Holographic gauge/gravity duality and symmetry breaking in semimetals", (G. Semenoff), February 2017.

KLYUZHIN, I., "Deformable motion correction and spatial image analysis in positron emission tomography", (V. Sossi), January 2017.

MÖLLER, M., "Temperature-driven spectral weight transfer in doped magnetic insulators", (M. Berciu), January 2017.

MIRSADEGHI, S., "A silicon photonic circuit for optical trapping and characterization of single nanoparticle", (J. Young), April 2017.

NIELSEN, C., "Constraining the flux and cross section models using carbon and oxygen targets in the off-axis near detector for the 2016 joint oscillation analysis at T2K", (S. Oser), March 2017.

OMID, H., "2+1d quantum field theories in large N limit", (G. Semenoff), January 2017.

PARK, J., "Decay spectroscopy of N ~ Z nuclei in the vicinity of 100Sn", (R. Kruecken), March 2017.

ROSSOKHATY, O., "Non-equilibrium transport in electron solids", (J. Folk), January 2017.

SABOURI, S., "A new multiparametric MRI protocol for diagnosis of prostate cancer", (P. Kozlowski), August 2017.

SAMANI NASAB, M., "Local probe of electronic states in high mobility quantum Hall samples", (J. Folk), September 2017.

SCHELEW, E., "Nonlinear optical response of triple-mode silicon photonic crystal microcavities coupled to single channel input and output waveguides", (J. Young), October 2017.

SCHULZ-WEILING, M., "Ultracold molecular plasma", (E. Grant), August 2017.

SHI, Z., "Conductance of junctions of multiple interacting quantum wires and long Aharonov-Bohm-Kondo rings", (I. Affleck), July 2017.

SULLIVAN, T., "A high-precision measurement of the pion branching ratio", (D. Bryman), April 2017.

SUZUKI, F., "Quantum Mechanics of Composite Objects with Internal Entanglement", (T. Momose), August 2017.

TANIMURA, H., "Probing the Large-Scale Structure of the Universe with the Sunyaev-Zel'dovich Effect", (G. Hinshaw), September 2017.

TOBAYAMA, S., "An analysis of the oscillation of atmospheric neutrinos", (H. Tanaka), January 2017.

TROESTER, T., "Weak gravitational lensing cross-correlations", (L. Van Waerbeke), August 2017.

VINCART-EMARD, A., "Numerical investigation of spatial inhomogeneities in gravity and quantum field theory", (M. Rozali), August 2017.

ZAKARIAEE KOUCHAKSAR, R., "Localized bladder dose accumulation in multi-fraction cervical cancer brachytherapy", (A. MacKay), January 2017.

University of Calgary

ARCHER, W.E., "Birkeland Current Boundary Flows", (D. Knudsen), June 2017.

CONROY, L. A., "Respiratory and breath hold motion in contemporary breast irradiation: dosimetric impact and management techniques", (W. Smith), June 2017.

GHAHREMANINEZHADGHARELAR, R., "Study of Dimethyl sulfide, sulfate aerosol and ice nucleation particles in the Arctic summer", (A.-L. Norman), June 2017.

KOGER, B. M., "Radiation dosimetry in the presence of gold nanoparticles", (C. Kirkby), June 2017.

LAU, H. W., "Nonlinear dynamics of mathematical models and proposed implementations in ultracold atoms", (C. Simon), June 2017.

SANG-NOURPOUR, N., "Characterization of surface-plasmon polaritons and electromagnetic waveguides with positive, negative and near-zero permittivity and permeability", (B. Sanders), November 2017.

University of Guelph

VAN BOMMEL, S., "Expanding the Capability of the Alpha Particle X-ray Spectrometer Including Quantification of Fine-Scale Chemistry and Atmospheric Monitoring", (R. Gellert), October 2017, now currently pursuing a Postdoctoral Fellowship at the University of Guelph, Guelph, ON, Canada.

ILLES, E., "Properties of the alpha-T3 Model", (E. Nicol), August 2017, now working for the Federal Government - security – Canada.

MILLER, J., "Selected Problems in Computational Gravity", (E. Poisson, E. Schnetter), July 2017, now working for the Federal Government, USA.

LANDRY, P., "Tidal Response of a Rotating Neutron Star in General Relativity", (E. Poisson), July 2017.

KLASSEN, J., "Existence and Uniqueness in the Quantum Marginal Problem", (B. Zeng, Y. Shen), June 2017.

MALCOLM, J., "The role of pseudospin in the optical and electronic properties of relativistic materials", (E. Nicol), March 2017, now a Quantitative Analyst at a Pension Fund in Toronto, ON, Canada.

University of Lethbridge

BOSSO, P., "Generalized Uncertainty Principle & Quantum Gravity Phenomenology", (S. Das), August 2017, now searching for employment.

University of Manitoba

HEUSEN, M., "Analytical and Numerical Investigation of Energetic Particles Interacting with Turbulent Magnetic Fields, (A. Shalchi), February 2017, now a Data Scientist at XE.com Inc, Newmarket, ON, Canada.

MCCREA, M., "Parity Violation and Cold Neutron Capture: A Study of the Detailed Interaction Between Hadrons", (M. Gericke, J. Martin), February 2017, Pursuing a Postdoctoral Fellowship at the University of Kentucky, Lexington, Kentucky, USA.

TEO, P.T.T., "Autonomous Lung Tumor and Critical Structure Tracking Using Optical Flow Computation and Neural Network Prediction", (S. Pistorius), February 2017, Now a Medical Physics Resident at the University of Pittsburgh Cancer Institute / UPMC Cancer Centre, Pittsburgh, PA, USA.

ZHANG, Z., "Spin-Dependent Electrical and Thermal Transport in Magnetic Tunnel Junctions", (C-M. Hu), February 2017, now pursuing a Postdoctoral Fellowship at Northeastern University, Department of Electrical & Computer Engineering, Boston, Massachusetts, USA.

SKOROPATA, E., "The Origin of the Magnetism of Maghemite (Y-Fe203) Based Core/Shell Nanoparticles", (J. van Lierop), October 2017, now pursuing a Postdoctoral Fellowship at Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA.

TEIGELHOFER, A., "Isotope Shift and Hyperfine Structure Measurements on Silver, Actinium and Astatine by In-Source Resonant Ionization Laser Spectroscopy", (J. Lassen, G. Gwinner), October 2017, now pursuing a Postdoctoral Fellowship at TRIUMF, Vancouver, BC, Canada.

WEI, P-S., "New Methods for Optimizing Parallel Transmit / Receive Array Coils to Small Field - of - View Excitation for Breast and Cardiac MRI", (S. King, C. Bidinosti), October 2017.

University of New Brunswick, Fredericton

ATHIENO, R, "Empirical model in the characterization of Hi Frequency propagation in the Artic region", (P.T. Jayachandran), May 2017.

MEZAOUI, H, "Characterization of Ionospheric Scintillation at High Latitudes", (P.T. Jayachandran, A. Hamza), October 2017.

University of Ottawa

BAGHERI, M., "A Minimal Model for Disordered Proteins", (J. Harden, B. Joos), October 2017, now pursuing a Postdoctoral Fellowship at the University of Ottawa, Ottawa, ON, Canada.

SEAN-FORTIN, D. S., "Highly Driven Polymer Translocation in the Presence of External Constraints: Simulations and Theory", (G. Slater), May 2017, now pursuing a Postdoctoral Fellowship at the Institute for Computational Physics, Universität Stuttgart, Stuttgart, Germany.

VAN DER KOLK, J. N., "Theory of Image Formation in Non-linear Optical Microscopy", (L. Rammuno), October 2017, now pursuing a Postdoctoral Fellowship at the University of Ottawa, Ottawa, ON, Canada.

XU, Y., "Fiber random grating and its applications", (X. Bao), October 2017, now an Optical Systems Engineer at Ciena Inc., Ottawa, ON, Canada.

University of Regina

LI, W, "Exclusive Backward-Angle Omega Meson Electroproduction", (G. Huber), October 2017, now pursuing a Postdoctoral Fellowship at the College of William & Mary, Williamsburg, VA, USA.

PAUDYAL, D, "Spin Polarizability of a Proton Using Polarized Photon Beam and Polarized Butanol Target at Mainz Microtron", (G. Huber), August 2017, now pursuing a Postdoctoral Fellowship at the University of Regina, Regina, SK, Canada.

University of Saskatchewan

ALIBAZI, R. B., "Enhancement of charged particle emission from a plasma focus device", (C. Xiao), August 2017, now pursuing a Postdoctoral Fellowship at the University of Denver, Denver, Colorado, USA.

BASSEY, B., "Development of a Multiple Energy Synchrotron Biomedical Imaging System", (D. Chapman), November 2017, now Self Employed, Saskatoon, SK, Canada.

MARTINSON, M., "Bent Laue X-ray Beam Expander", (D. Chapman, P. Babyn), February 2017, now an Experimental Floor Coordinator at Canadian Light Source, Saskatoon, SK, Canada.

ROHOLLAHI, A., "Experimental Studies using compact Torus Injector", (A. Hirose, C. Xiao), November 2017, now a Scientist at General Fusion, Burnaby, BC, Canada.

TOLHURST, T., "Soft X-ray Spectroscopy of Metal Nitrides and Oxides: Uncovering Structure-property University Relationships in Phosphorus for pd-LEDs", (A. Moewes), April 2017, now an Analyst at MDA Corporation, Vancouver, BC, Canada.

University of Toronto

BLACKPORT, R., "The atmospheric response to arctic sea ice loss in the coupled climate system, (P.J. Kushner), March 2017, now pursuing a Post Doctoral Fellowship at the University of Exeter, Exeter, UK.

CHAU, C. C., "Measurement of di-photon induced production of W-boson pairs and limits on anomalous quartic gauge couplings", (W. Trischuk), June 2017.

DIAMOND, M., "Search for dark gauge bosons decaying into displaced lepton-jets in proton-proton collisions at √s=13 TeV with the ATLAS detector", (W. Trischuk), June 2017, now an Experimental Research Associate at SLAC National Accelerator Laboratory, Melo Park, CA, USA.

EDGE, G., "Imaging fermionic atoms in a quantum gas microscope", (J.H. Thywissen), June 2017, now a Data Scientist at JW player, New York City, NY, USA.

FOSTER, S., "Applications of photonic crystals to photovoltaic devices", (S. John), November 2017.

GODIN, P., "Laboratory spectroscopy for atmospheric physics, (K. Strong), November 2017, now pursuing a Post Doctoral Fellowship at York University, Toronto, ON, Canada.

GRIFFIN, D., "Investigation of tropospheric pollutants and stratospheric ozone using infrared Fourier transform spectrometers from the ground, space, and balloons", (K.A. Walker), June 2017.

HICKEY, C., "Novel phases from the interplay of topology and strong interactions", (A. Paramekanti), November 2017, now pursuing a Post Doctoral Fellowship at the Institute for Theoretical Physics, University of Cologne, Cologne, Germany.

INMAN, D., "Nonlinear dynamics of the cosmic neutrino background", (U.-L. Pen), November 2017, now pursuing a Post Doctoral Fellowship at New York University, Cosmology, New York, NY, USA.

JARDINE, I., "Deformed D1D5 CFT: a holographic probe of quantum gravity", (A.W. Peet), November 2017, now pursuing a Post Doctoral Fellowship at the University of Toronto, ON, Canada.

KONTENIS, L., "Experimental nonlinear polarimetric microscopy", (V. Barzda), November 2017, now a Research and Development Engineer at Light Conversion, Vilnius, Lithuania.

LUCIUK, C., "Non-equilibrium dynamics of strongly interacting fermions", (J.H. Thywissen), November 2017.

MARSHALL, K., "Hybrid methods in quantum information", (D.F.V. James), November 2017.

MCGOLDRICK, G., "Measurement of tt-bar polarization with the ATLAS detector", (W. Trischuk), June 2017.

MENDONCA, J., "Improving the retrievals of greenhouse gases from ground-based absorption spectra", (K. Strong), June 2017.

RATZLAFF, M., "Phenomenology of heavy lepton and heavy higgs decays at the lhc", (B. Holdom), November 2017.

ROY, K., "High quality constraints on the glacial isostatic adjustment process over North America: the ICE-7G_NA (VM7) model", (W.R. Peltier), June 2017, now pursuing a Post Doctoral Fellowship at the National Technical University of Singapore, Singapore.

SAHOTA, J., "Quantum-enhanced phase estimation in optical interferometry", (D.F.V. James), November 2017.

SALEHIPOUR, H., "Stratified turbulence and ocean mixing", (W.R. Peltier), November 2017, now pursuing a Talent-Edge Post Doctoral Fellowship at the University of Toronto, ON, Canada.

SEARS, J., "Structure and magnetism of a-RuC13", (Y.J. Kim), November 2017, now a Scientist at DESY in Hamburg, Germany.

SWIECICKI, S., "Response of periodic systems to electromagnetic fields: multipole expansion, microscopic charge - current density, polarization and magnetization", (J.E. Sipe), November 2017, now a Manager at Market Risk Measurement at Scotiabank, Toronto, ON, Canada.

TIAN, D., "Pressure induced quantum phase transitions", (S.R. Julian), November 2017.

TRIM, S., "The dynamic interaction of mantle compositional heterogeneities at the surface and the core mantle boundary", (J.P. Lowman), November 2017.

Vernon, Z., "Micro resonators for nonlinear quantum optics", (J.E. Sipe), November 2017.

YIGE, C., "Topological phases in perovskite iridates with strong spin - orbit coupling", (H.Y. Kee), November 2017.

YU, J., "Ground state properties of strongly correlated electron systems in high magnetic field", (S.R. Julian), November 2017, now a Data Scientist at Capital One, Toronto, ON, Canada.

ZHANG, Z., "Single molecule spectroscopy of disordered states and dynamics in proteins", (C.C. Gradinaru), June 2017.

ZHAO, X., "Studies of atmospheric ozone and related constituents in the Arctic and midlatitudes", (K. Strong), June 2017, now pursuing a Visiting Fellowship at Natural Sciences and Engineering Research Council of Canada (NSERC), Toronto, ON, Canada.

UNIVERSITY OF VICTORIA

DE JONG, S., "Study of Thermal Neutron Flux from SuperKEKB in the Belle II Commissioning Detector", (J.M. Roney), November 2017, now a Research Assistant at University of Victoria, Victoria, BC, Canada.

ELLIOT, A., "Search for Dark Matter in Association with a Leptonically Decaying Z Boson in the ATLAS Detector at the Large Hadron Collider", (R. Keeler, R. McPherson), November 2017, now a Research Assistant at University of Victoria, Victoria, BC, Canada.

FATTAHI SAVADJANI, A., "The Local Group and its Dwarf Galaxy Members within the Standard Model of Cosmology", (J. Navarro), November 2017, now pursuing a Postdoctoral Fellowship at Durham University, Durham, UK.

FRADETTE, A., "From Gas and Dust to Protostars: Addressing the Initial Stages of Star Formation Using Observations of Nearby Molecular Clouds", (M. Pospelov), December 2017, now a Consultant at the Boston Consulting Group, Montreal, QC, Canada.

HILL, E., "Search for direct scalar top pair production in final states with two tau leptons in pp collisions at √S=8 TeV at the ATLAS Detector at the Large Hadron Collider", (R. Kowalewski, I. Trigger), September 2017, now searching for employment.

KOLTHAMMER, J., "Chirality control and magnetization dynamics in a dual vortex spin valve nanopillar", (B.C. Choi), May 2017, now searching for employment.

KWAN, T., "Measurements of Neutral Current Drell-Yan Production at 8 TeV with the ATLAS Detector", (R. Keeler), November 2017, now a Research Assistant at University of Victoria, Victoria, BC, Canada.

LAMB, M., "On the Calibration and Use of Adaptive Optics Systems: RAVEN Observations of Metal-Poor Stars in the Galactic Bulge and the Application of Focal Plane Wavefront Sensing Techniques", (K. Venn, D. Andersen), November 2017, now pursuing a Postdoctoral Fellowship at the Dunlap Institute, Toronto, ON, Canada.

LE DALL, M., "Portal Interactions Within Leptogenesis and Precision Observables and Quantum Theory of Orbitally-Degenerate Impurities in Superconductors", (A. Ritz, R. de Sousa), November 2017, now pursuing a Postdoctoral Fellowship at the University of Victoria, Victoria, BC, Canada.

LEBLANC, M., "Characterising the Decays of High-pT Top Quarks and Addressing Naturalness with Jet Substructure in ATLAS Runs I and II", (R. McPherson), May 2017, now pursuing a Postdoctoral Fellowship at University of Arizona, Tucson, Arizona, USA.

LLOYD, S., "Measurement and Monte Carlo simulation of electron fields for modulated electron radiation therapy", (A. Jirasek, I. Gagne), May 2017, now a Medical Physics Resident at University of California at San Diego, CA, USA.

MAIRS, S., "From Gas and Dust to Protostars: Addressing the Initial Stages of Star Formation Using Observations of Nearby Molecular Clouds", (D. Johnstong, F. Herwig), December 2017, now a Support Astronomer at East Asian Observatory (James Clerk Maxwell Telescope), Hilo, Hawaii, USA.

MORTON, D., "Quantitative Techniques for Permanent Breast Seed Implant Brachytherapy",

(A. Jirasek, W. Beckham), September 2017, now a Medical Physics Resident at BC Cancer, Abbotsford, BC, Canada.

OMAN, K., "An Explanation for the Unexpected Diversity of Dwarf Galaxy Rotation Curves", (J. Navarro), November 2017, now pursuing a Postdoctoral Fellowship at University of Groningen, Netherlands.

RITTER, C., "Nucleosynthesis in stellar models across initial masses and metallicities and implications for chemical evolution", (F. Herwig), May 2017, now a Research Associate at Keele University, Staffordshire, UK.

SHANKMAN, C., "On the Characteristics and Evolution of Dynamically Excited Trans-Neptunian Objects", (J.J. Kavelaars, F. Herwig), November 2017, now a Toronto Urban Fellow Research Associate at the City of Toronto, Toronto, ON, Canada.

TASNEEM, N., "Search for the Lepton Flavour Violating Decay in Y(3S)→e^± μ^∓", (J.M. Roney), November 2017, now an Academic Instructor, Engineering Department at Saint Francis Xavier University, Antigonish, NS, Canada.

TURRI, P., "Advancing Next Generation Adaptive Optics in Astronomy: From the Lab to the Sky", (D. Andersen, K. Venn), November 2017, now pursuing a Postdoctoral Fellowship at University of California at Berkeley, CA, USA.

University of Waterloo

AGNE, S., "Exploration of Higher-Order Quantum Interference Landscapes", (T. Jennewein), August 2017, now pursuing a Postdoctoral Fellowship at The Rockfellar University, New York, NY, USA.

AHMADZADEGAN, A., "Probing the Unruh and Hawking effects using Unruh-DeWitt detectors", (R. Mann, D. Terno), October 2017, now pursuing a Postdoctoral Fellowship at the University of Waterloo, Waterloo, ON, Canada.

BANBURSKI, A., "Towards vertex renormalization in 4d Spin Foams", (L. Smolin, L. Freidel), July 2017, now pursuing a Postdoctoral Fellowship at MIT, Cambridge, MA, USA.

CHEN, L., "Amplitudes in the Spin Foam Approach to Quantum Gravity", (L. Smolin, L. Freidel), July 2017, now pursuing a Postdoctoral Fellowship at the Okinawa Institute for Science and Technology, Okinawa, Japan.

CORONA UGALDE, P., "Experimental Prospects for Detecting the Quantum Nature of Spacetime", (R. Mann), September 2017, now pursuing a Postdoctoral Fellowship at the University of Waterloo, Waterloo, ON, Canada.

GOULD, Elizabeth, "New Views on the Cosmological Big Bang", (N. Afshordi), September 2017, now pursuing a Postdoctoral Fellowship at Southampton University, Southampton, UK.

GRAYDON, M., "Conical Designs and Categorical Jordan Algebraic Post-Quantum Theories", (R. Spekkens), January 2017, now pursuing a Postdoctoral Fellowship at the University of Hong Kong, Hong Kong.

HOLLOWAY, G., "Electron transport in semiconducting nanowires and quantum dots", (J. Baugh), January 2017, now an Electron Beam Lithography Scientist at the Institute for Quantum Computing, Waterloo, ON Canada.

KOUCHEKZADEH YAZDI, Y., "Entanglement Entropy of Scalar Fields in Causal Set Theory", (N. Afshordi, R. Sorkin), August 2017, now pursuing a Postdoctoral Fellowship in the Department of Physics at the University of Alberta, Edmonton, AB, Canada.

LAN, T., "A Classification of (2+1) D Topological Phases with Symmetries", (X.-G. Wen, R. Melko), September 2017, now pursuing a Postdoctoral Fellowship at the Institute for Quantum Computing at the University of Waterloo, Waterloo, ON, Canada.

MASON, J., "RF-QPC Charge Detector and S-T+ Qubit in a Lateral Double Quantum Dot Device", (J. Kycia), January 2017, now pursuing a Postdoctoral Fellowship in the Department of Physics and Astronomy at the University of Waterloo, Waterloo, ON, Canada.

MAZAC, D., "Explorations in the Conformal Bootstrap", (D. Gaiotto, F. Cachazo), July 2017, now pursuing a Postdoctoral Fellowship at C.N. Yang Institute for Theoretical Physics in Stoney Brook, NW, USA.

NSOFINI, J., "Quantum Information Enabled Neutron Interferometry", (D. Cory), June 2017, now pursuing a Postdoctoral Fellowship at the Institute for Quantum Computing at the University of Waterloo, Waterloo, ON, Canada.

PANFILOV, I., "Topology and interactions in Weyl metals and quantum Hall systems", (A. Burkov), May 2017, seeking employment.

PUGH, C., "Free Space Quantum Key Distribution to Moving Platforms", (T. Jennewein), August 2017, now an Assistant Professor in the Department of Physics and Astronomy at Brandon University, Brandon, MB, Canada.

REMPEL, T., "An Exploration of Locality, Conservation Laws, and Spin", (L. Freidel, L. Smolin), January 2017, now employed at Aperio, New York, NY, USA.

SHALABY, M., "Cosmological bean plasma instabilities", (A. Broderick, N. Afshordi), August 2017, now a Teaching Assistant of Physics at Cairo University, Cairo, Egypt.

SIERENS, L., "Simulating quantum matter through lattice field theories", (R. Melko), May 2017, now a PSI Fellow at Perimeter Institute for Theoretical Physics, Waterloo, ON, Canada.

SIERENS, T., "Quantum critical responses via holographic models and conformal perturbation theory", (R. Myers), June 2017, now employed as a Data Science Consultant at QuantaVerse, Wayne, PA, USA.

SMITH, A., "Detectors, Reference Frames, and Time", (R. Mann, M. Piani, D. Terno), November 2017, now employed as a Junior Fellow at Dartmouth College, Hanover, New Hampshire, USA.

TAN, B., "Evaluation and Correlation of Morphological, Blood Flow and Physiological Retinal Changes in a Rat Model of Glaucoma with a Combined Optical Coherence tomography and Electroretinography System", (K. Bizheva), August 2017, now pursuing a Postdoctoral Fellowship in the Department of Physics and Astronomy at the University of Waterloo, Waterloo, ON, Canada.

TOEWS, W., "An investigation of low energy quasiparticle excitations via thermal transport measurements", (R. Hill), June 2017, now seeking employment.

VON KONIGSLOW, K., "An off-lattice derivation and thermodynamic consistency consideration for the Sanchez-Lacombe equation of state", (R. Thompson, C. Park), November 2017, now a Professor of Mathematics at Humber College, Etobicoke, ON, Canada.

WALES, B., "Ultrafast Imaging of Molecular Processes in Small Molecules Using Coulomb Explosion Imaging", (J. Sanderson), September 2017, now employed at Thalmic Labs, Kitchener, ON, Canada.

ZHANG, Q., "A Novel Combination Therapy of Cisplatin with a Molecular Promoter for Cancer Treatment", (Q.-B. Lu), January 2017, now pursuing a Postdoctoral Fellowship at UC-Berkeley, USA.

ZWANE, N., "Cosmological Tests of Causal Set Phenomenology", (R. Sorkin, N. Afshordi), September 2017, now employed as a lecturer in the Physics Department at the University of Swaziland, Kwaluseni, Swaziland.

University of Western Ontario

EZUGWU, S., "Nanoscale thermal and electronic properties of thin films of graphene and organic polyradicals", (G. Fanchini), December 2016, now a First Year Labs Demonstrator at Western University, London, ON, Canada.

HAGHSHENASFARD, Z., "Linear and Nonlinear Dynamics of Spin Waves in Ferromagnetic Nanowires", (M.G. Cottam), April 2017, now a Research Assistant at Western University, London, ON, Canada.

HUSSAIN, B., "Methods for Improved Estimation of Low Blood Velocities using Vector Doppler Ultrasound", (T. Poepping, J. Lacefield), April 2017, now a Visiting Researcher at Western University, London, ON, Canada.

KAZEMIAN, S., "Modelling the thermal conductivity of layered materials from photothermal measurements", (G. Fanchini), August 2017, now currently unemployed and searching for work.

LIU, Y., "Three Experiments on Complex Fluids", (J. de Bruyn), December 2017, now currently unemployed and searching for work.

SUBASINGHE, D., "Physical properties of faint meteors through high-resolution observations", (M. Campbell-Brown), December 2017, now a pursuing a Postdoctoral fellowship at Western University, London, ON, Canada.

TABESHIAN, M., "Detection and Characterization of Extrasolar Planets through Planet-Disk Dynamical Interactions", (P. Wiegert), April 2017, now a First Year Lab Assistant and Sessional Instructor at Western University, London, ON, Canada.

KELLOGG, K., "Investigating Brown Dwarf Atmospheres: Gravity, Dust Content, Cloud Structure and Metallicity", (S. Metchev), July 2017, now searching for work.

University of Windsor

DILORETO, C., "Quantum Control of Open Systems and Dense Atomic Ensembles", (C. Rangan), June 2017, now pursuing a Postdoctoral Fellow at University of Windsor, Windsor, ON, Canada.

Book Review Policy

Books may be requested from the Book Review Editor, Richard Marchand, by using the online book request form at http://www.cap.ca. You must be a residing in Canada to request a book.

CAP members are given the first opportunity to request books. For non-members, only those residing in Canada may request a book. Requests from non-members will only be considered one month after the distribution date of the issue of *Physics in Canada* in which the book was published as being available.

The Book Review Editor reserves the right to limit the number of books provided to reviewers each year. He also reserves the right to modify any submitted review for style and clarity. When rewording is required, the Book Review Editor will endeavour to preserve the intended meaning and, in so doing, may find it necessary to consult the reviewer. Reviewers submit a 300-500 word review for publication in PiC and posting on the website; however, they can choose to submit a longer review for the website together with the shorter one for PiC.

La Politique Pour la Critique De Livres

Si vous voulez faire l'évaluation critique d'un ouvrage, veuillez entrer en contact avec le responsable de la critique de livres, Richard Marchand, en utilisant le formulaire de demande électronique à http://www.cap.ca.

Les membres de l'ACP auront priorité pour les demandes de livres. Ceux qui ne sont pas membres et qui résident au Canada peuvent faire une demande de livres. Les demandes des non-membres ne seront examinées qu'un mois après la date de distribution du numéro de la Physique au Canada dans lequel le livre aura été déclaré disponible.

Le Directeur de la critique de livres se réserve le droit de limiter le nombre de livres confiés chaque année aux examinateurs. Il se réserve, en outre, le droit de modifier toute critique présentée afin d'en améliorer le style et la clarté. S'il lui faut reformuler une critique, il s'efforcera de conserver le sens voulu par l'auteur de la critique et, à cette fin, il pourra juger nécessaire de le consulter. Les critiques pour publication dans la PaC doivent être de 300 à 500 mots. Ces critiques seront aussi affichées sur le web; s'ils le désirent les examinateurs peuvent soumettre une plus longue version pour le web.

Books Received / *Livres Reçus*

The following titles are a sampling of books that have recently been received for review. Readers are invited to write reviews, in English or French, of books of interest to them. Unless otherwise indicated, all prices are in Canadian dollars.

Lists of all books available for review, books out for review and book reviews published since 2011 are available on-line at www.cap.ca (Publications).

In addition to books listed here, readers are invited to consider writing reviews of recent publications, or comparative reviews on books in topics of interest to the physics community. This could include for example, books used for teaching and learning physics, or technical references aimed at professional researchers.

Les titres suivants sont une sélection des livres reçus récemment aux fins de critique. Nous invitons nos lecteurs à nous soumettre une critique en anglais ou en français, sur les sujets de leur choix. Sauf indication contraire, tous les prix sont en dollars canadiens.

Les listes de tous les livres disponibles pour critique, ceux en voie de révision, ainsi que des critiques publiées depuis 2011 sont disponibles sur : www.cap.ca (Publications).

En plus des titres mentionnés ci-dessous, les lecteurs sont invités à soumettre des revues sur des ouvrages récents, ou des revues thématiques comparées sur des sujets particuliers. Celles-ci pourraient par exemple porter sur des ouvrages de nature pédagogique, ou des textes de référence destinés à des professionnels.

GENERAL LEVEL

Brave New Arctic: The Untold Story of the Melting North [v], Mark C. Serreze, Princeton University Press, 2018; pp. 264; ISBN: 9780691173993; Price: 31.95.

Essays on the Frontiers of Modern Astrophysics and Cosmology, Santhosh Mathew, Springer, 2014; pp. 2016; ISBN: 978-3319018867; Price: 37.77.

Our Cosmic Habitat [v], Martin Rees, Princeton University Press, 2017; pp. 224; ISBN: 9780691178097; Price: 21.95.

Particle Physics Brick by Brick: Atomic and Subatomic Physics Explained... in LEGO, Dr. Ben Still, Firefly Books, 2018; pp. 176; ISBN: 978-0228100126.0; Price: 24.70.

Quantum Information Theory: Mathematical Foundation, Masahito Hayashi, Springer, 2016; pp. 636; ISBN: 978-3662497234; Price: 140.43.

Solar System Astrophysics: Planetary Atmospheres and the Outer Solar System, Eugene F. Milone & William J.F. Wilson, Springer, 2014; pp. 480; ISBN: 978-1493939060; Price: 144.04. (Live: 0)

The Milky Way: An Insider's Guide (V), William H. Waller, Princeton University Press, 2017; pp. 336; ISBN: 9780691178356; Price: 24.95.

The New Science of Strong Materials: Or Why You Don't Fall through the Floor [v], J. E. Gordon, Princeton University Press, 2018; pp. 328; ISBN: 9780691180984; Price: 20.32.

The Oceans: A Deep History [v], Eelco J. Rohling, Princeton University Press, 2017; pp. 272; ISBN: 9780691168913; Price: 37.95.

The Philosophy of Cosmology, Editors: Khalil Chamcham, Joseph Silk, John D. Barrow, and Simon Saunders, Cambridge University Press, 2017; pp. 526; ISBN: 978-1107145399; Price: 62.81.

The Secret Life of Science: How It Really Works and Why It Matters [v], Jeremy J. Baumberg, Princeton University Press, 2018; pp. 248; ISBN: 9780691174358; Price: 33.15.

The Semiclassical Way to Dynamics and Spectroscopy [v], Eric J. Heller, Princeton University Press, 2018; pp. 472; ISBN: 9780691163734; Price: 113.86.

The Strength in Numbers: The New Science of Team Science [v], Barry Bozeman & Jan Youtie, Princeton University Press, 2017; pp. 248; ISBN: 9780691174068; Price: 43.95.

The Travel Diaries of Albert Einstein: The Far East, Palestine, and Spain, 1922 - 1923 [v], Albert Einstein, Princeton University Press, 2018; pp. 384; ISBN: 9780691174419; Price: 36.78.

Time Machine Tales: The Science Fiction Adventures and Philosophical Puzzles of Time Travel, Paul J. Nahin, Springer, 2017; pp. 383; ISBN: 978-3319488622; Price: 25.32.

Timefulness: How Thinking Like a Geologist Can Help Save the World [v], Marcia Bjornerud, Princeton University Press, 2018; pp. 224; ISBN: 9780691181202; Price: 31.99.

UNDERGRADUATE LEVEL

A Student's Guide to Python for Physical Modeling Updated Edition [v], Jesse M. Kinder & Philip Nelson, Princeton University Press, 2018; pp. 168; ISBN: 9781400889426; Price: 31.95.

An Introduction to Complex Systems: Society, Ecology, and Nonlinear Dynamics, Paul Fieguth, Springer, 2016; pp. 346; ISBN: 978-3319446059; Price: 78.56.

An Introduction to Quantum Theory, Jeff Greensite, 2017, 0; pp. 560; ISBN: 978-0750311687; Price: 182.19.

Charles W. Misner, Kip S. Thorne & John Archibald Wheeler, Gravitation [v], Priceton University Press, 2017; pp. 1336; ISBN: 9780691177793; Price: 74.95.

Classical Field Theory, Joel Franklin, Cambridge University Press, 2017; pp. 216; ISBN: 978-1107189614; Price: 59.40.

Cosmology and the Early Universe [v], Pasquale Di Bari, CRC Press, 2018; pp. 243; ISBN: 9781498761703; Price: 118.75.

Mathematical Foundations of Quantum Mechanics (new edition) [v], John von Neumann [v], Princeton University Press, 2018; pp. 464; ISBN: 9780691178578; Price: 125.00.

Picturing Quantum Processes: A First Course in Quantum Theory and Diagrammatic Reasoning, Bob Coecke and Aleks Kissinger, Cambridge University Press, 2017; pp. 844; ISBN: 978-1107104228; Price: 97.95.

Picturing Quantum Processes: A First Course in Quantum Theory and Diagrammatic Reasoning (2nd Copy), Bob Coecke & Aleks Kissinger, Cambridge University Press, 2017; pp. 844; ISBN: 978-1107104228; Price: 97.95.

The Physics of Cancer, Caterina A. M. La Porta and Stefano Zapperi, Cambridge University Press , 2017; pp. 184; ISBN: 978-1107109599; Price: 68.95.

SENIOR LEVEL

Advanced Quantum Mechanics: Materials and Photons, Rainer Dick, Springer, 2016; pp. 692; ISBN: 978-3319256740; Price: 87.76.

Algèbre linéaire et applications (5° Éd.) (Manuel + MonLab xL), Lay David, Lay Steven R., Macdonald Judi J., Pearson, 2017; pp. 530; ISBN: 9782761376525; Price: 109.95.

Chiral Nanophotonics: Chiral Optical Properties of Plasmonic Systems, Martin Schäferling, Springer, 2017; pp. 159; ISBN: 978-3319422633; Price: 112.35.

Foundations of Nuclear and Particle Physics, T. William Donnelly, Joseph A. Formaggio, Barry R. Holstein, Richard G. M, Cambridge University Press, 2017; pp. 658; ISBN: 978-0521765114; Price: 74.82.

Hemo-Dynamics, Mair Zamir, Springer, 2016; pp. 407; ISBN: 978-3319241012; Price: 200.66.

High-Energy Atomic Physics, Evgeny G. Drukarev & A.I. Mikhailov, Springer, 2016; pp. 384; ISBN: 978-3319327341; Price: 112.32.

Introduction to Plasma Physics and Controlled Fusion (Third Edition), Francis F. Chen, Springer, 2015; pp. 490; ISBN: 978-3319223087; Price: 90.90.

Lectures on General Relativity, Cosmology and Quantum Black Holes, Badis Dr Ydri, Iop Publishing Ltd, 2017; pp. 351; ISBN: 978-0750314763; Price: 153.13.

Lectures on the Infrared Structure of Gravity and Gauge Theory [v], Michael Mayerfeld Bell, Princeton University Press, 2018; pp. 200; ISBN: 9780691179735; Price: 113.04.

L'effet Science: comment la démarche Scientifique a changé notre vision du monde, Louis Marchildon, Éditions MultiMondes, 2018; pp. 180; ISBN: 9782897730789; Price: 22.95.

Medical and Biomedical Applications of Shock Waves, Achim M. Loske, Springer, 2017; pp. 378; ISBN: 978-3319475684; Price: .

Microwave and RF Vacuum Electronic Power Sources, Richard G. Carter, Cambridge University Press, 2018; pp. 838; ISBN: 978-0521198622; Price: 201.24.

Molecular Machines: A Materials Science Approach [v], Giovanni Zocchi, Princeton University Press, 2018; pp. 192; ISBN: 9780691173863; Price: 81.99.

Monte Carlo Methods for Radiation Transport: Fundamentals and Advanced Topics, Oleg N. Vassiliev, Springer, 2016; pp. 281; ISBN: 978-3319441405; Price: 138.50.

Neutron Scattering and Other Nuclear Techniques for Hydrogen in Materials, Editors: Helmut Fritzsche, Jacques Huot & Daniel Fruchart, Springer, 2016; pp. 413; ISBN: 978-3319227917; Price: 181.01.

On Gravity: A Brief Tour of a Weighty Subject [v], A. Zee, Princeton University Press, 2018; pp. 192; ISBN: 9780691174389; Price: 24.61.

Practical Bayesian Inference: A Primer for Physical Scientists, Coryn A. L. Bailer-Jones, Cambridge University Press, 2017; pp. 320; ISBN: 978-1316642214; Price: 35.40.

Precision Cosmology: The First Half Million Years, Bernard J. T. Jones, Cambridge University Press, 2017; pp. 774; ISBN: 978-0521554336; Price: 106.20.

Quantum Measurement, Paul Busch, Pekka J Lahti, Juha-Pekka Pellonpää, Kari Ylinen, Springer, 2016; pp. 542; ISBN: 978-3319433875; Price: 160.03.

Quantum Metrology, Imaging, and Communication, David S. Simon, Gregg Jaeger & Alexander V. Sergienko, Springer, 2016; pp. 273; ISBN: 978-3319465494; Price: 114.49.

Quantum Plasmonics, Editors: Sergey I. Bozhevolnyi, Luis Martin-Moreno & Francisco Garcia-Vidal, Springer, 2016; pp. 327; ISBN: 978-3319458199; Price: 160.45.

Quantum Scaling in Many-Body Systems: An Approach to Quantum Phase Transitions, Mucio Continentino, Cambridge University Press, 2017; pp. 246; ISBN: 978-1107150256; Price: 79.95.

Spectroscopic Analysis of Optoelectronic Semiconductors, Juan Jimenez & Jens W. Tomm, Springer, 2016; pp. 307; ISBN: 978-3319423470; Price: 172.80.

The Quantum Handshake: Entanglement, Nonlocality and Transactions, John G. Cramer, Springer, 2015; pp. 218; ISBN: 978-3319246406; Price: 63.05.

Theory of Low-Temperature Plasma Physics, Shi Nguyen-Kuok, Springer, 2017; pp. 495; ISBN: 978-3319437194; Price: 228.79.

Ultrasonic Spectroscopy: Applications in Condensed Matter Physics and Materials Science, Robert G. Leisure, Cambridge University Press, 2017; pp. 254; ISBN: 978-1107154131; Price: 102.95.

Understanding Stellar Evolution, Henny J.G.L.M. Lamers & Emily Levesque, Iop Publishing Ltd, 2017; pp. 342; ISBN: 978-0750312790; Price: 184.44.

Universal Themes of Bose-Einstein Condensation, Editors: Nick P. Proukakis, David W. Snoke & Peter B. Littlewood, Cambridge University Press, 2017; pp. 660; ISBN: 978-1107085695; Price: 114.95.

Book Reviews / *Critiques de livres*

Book reviews for the following books have been received and posted to the *Physics in Canada* section of the CAP's website: http://www.cap.ca.

Des revues critiques ont été reçues pour les livres suivants et ont été affichées dans la section "La Physique au Canada" de la page web de l'ACP:http://www.cap.ca.

Approximating Perfection: A Mathematician's Journey into the World of Mechanics, Leonid P. Lebedev and Michael J. Cloud, Princeton University Press, 2004, pp. 225, ISBN 9780691168265, price: 32.81.

Ce livre traite de la mécanique en tenant compte du point de vue d'un mathématicien. Bien que l'auteur mentionne dans le résumé que l'apport mathématique est réduit au minimum et que le livre peut donc plaire à un large public, je crois plutôt que quelques cours de mathématiques universitaires sont essentiels pour bien en comprendre tout le contenu. Par exemple, on y parle de tenseurs, un sujet souvent couvert dans les cours plus avancés. De plus, il ne s'agit pas d'un livre pédagogique puisqu'il ne contient aucun exemple résolu et aucun exercice. Il est toutefois vrai que l'auteur discute parfois de certains sujets en minimisant le nombre d'équations et explique parfois en détails la façon de penser particulière des mathématiciens afin de ne pas déstabiliser les lecteurs non mathématiciens. Il y a aussi parfois, de brefs passages historiques. Par contre, comme physicien, je préfère nettement un livre plus classique de physique avec une approche plus traditionnelle.

Le livre est divisé en quatre chapitres. Chaque chapitre est divisé en plusieurs sections (26 pour le chapitre 2!) et il n'est donc pas toujours facile de s'y retrouver. Le premier chapitre porte sur les outils de calculs. On y traite, entre autres, de l'infini, des nombres irrationnels, des limites, des séries, de la continuité des fonctions, des dérivées, des intégrales, des équations différentielles, de l'optimisation et des variables complexes. Au deuxième chapitre, on s'intéresse à plusieurs sujets de mécanique. Le chapitre débute avec une question: « Pourquoi les bateaux flottent-ils? ». On traite ensuite de la force, de la loi de Hooke et de résistance des matériaux (en traitant du tenseur de contrainte et du tenseur de déformation). On discute aussi des problèmes aux limites. On insère les concepts de travail et d'énergie. Vers la fin du chapitre, l'hydrodynamique entre en jeu.

Le troisième chapitre débute avec une explication de la loi de Hooke plus traditionnelle et moins mathématique en montrant les courbes contrainte-déformation obtenues lors d'expérience. On revient toutefois assez rapidement à des outils mathématiques complexes, comme les tenseurs. On discute ensuite du transfert de chaleur, de la dilatation thermique, de thermodynamique et de la stabilité. Le dernier chapitre porte sur les questions surgissant lors de la modélisation de phénomènes en sciences.

En conclusion, le titre du livre a sa raison d'être. On aborde la mécanique, mais d'un point de vue mathématique. Je préfère personnellement une approche plus physique. La lecture du livre demande au minimum quelques cours de mathématiques universitaires (équations différentielles, tenseurs). L'absence de problèmes ou d'exercices résolus empêche aussi de s'assurer de notre compréhension si on aborde les concepts pour la première fois.

Léo Barriault
Professeur de cégep

Beauty of Physics: Patterns, Principles, and Perspectives, by A.R.P. Rau, Oxford University Press, 2014, pp:219, ISBN 978-0-19-8700991-6, price 63.00.

The Beauty of Physics covers eight themes (in eight chapters) that reoccur throughout physics. The first theme is how a problem often becomes solvable by adding a dimension to it. The author, Rau, goes through various examples giving you a feel for what is happening, without you getting bogged down in details. In each case, the extra dimension appears as a clever mathematical trick but as it keeps showing up, clearly something is behind this. Rau then covers the themes of representations and saddles discussing along the way, notation, and global/local descriptions. In the fourth chapter Rau explores in-depth and beautifully the metaphor of a coin in both classical and quantum systems, highlighting clearly the fundamental differences of quantum description. Next Rau reviews the concept of symmetry not just as a powerful problem-solving tool but also as something that lets us peek into the deep nature of reality. In the sixth chapter Rau takes us into the wonder of the interaction of mathematics and physics. Rau next asks if the concept of time is even necessary for physical descriptions and makes the case that is a representational choice. In the final chapter, Rau explores levels of phenomena, and how at each level new notions arise, such as those of "collective" properties. As I got deeper in the book, the various themes began to play on each other, and I found myself not just nodding in agreement but thinking, 'I never really thought about that in this way before.

In all of these themes, Rau looks at some everyday examples, then a classical physics understanding, and then plunges into quantum and relativistic descriptions. This book is not meant to really teach you the details of the nitty gritty of the physics, although as Rau highlights, the differences between different descriptions, the understanding he brings, I believe, would certainly help folks as they plunge into new areas of physics such as quantum mechanics. Rau does an amazing job of highlighting how the different concepts change as we go through this process. When Rau mentions various physicists and their contribution, there are often footnotes which give interesting details on that physicist's life. If you want to go back reread a concept, the book has a surprisingly complete index, that I found useful.

Clearly, physicists at undergraduate or higher levels will get the greatest value from this book, but there is plenty here for the person just interested in the philosophical side of physics. The book is so clearly written that the general public should be able to read and appreciate its contents, and gain real insight in the subject matter. All this is done without complex proofs or derivations to follow through. In short, this book is a gem for physicists and the general public alike.

Collin Carbno, retired

Can the Laws of Physics Be Unified?, by Paul Langacker, Princeton University Press (2017), pp: xi + 271, ISBN 9780691167794, price 43.95.

La collection « Princeton Frontiers in Physics » publie, depuis 2010, une série d'ouvrages concis de physique et d'astrophysique, s'adressant aux étudiants de premier cycle en physique ou aux scientifiques de domaines connexes qui souhaitent se familiariser avec la recherche de pointe sur un sujet. Paul Langacker a fort bien réussi à présenter à cet auditoire le modèle standard des particules.

Après avoir rappelé que les interrogations sur les constituants fondamentaux de la matière remontent aux atomistes grecs, l'auteur choisit d'introduire son sujet de manière progressive. Un survol historique présente, au chapitre 2, une période d'exploration jusqu'aux années 60, suivie de l'élaboration du modèle standard et, enfin, des questions actuelles qui vont au-delà de celui-ci. Le chapitre suivant introduit les protagonistes du modèle, c'est-à-dire les particules et les interactions fondamentales. L'auteur présente également une chronologie succincte de l'évolution de l'univers, signalant les liens entre la cosmologie et les propriétés des particules.

Le chapitre 4 constitue le cœur de l'ouvrage. Certes, la présentation rapide des diagrammes de Feynman ne permettra pas au lecteur d'effectuer des calculs concrets. Mais la discussion des différents termes de couplage donne une idée générale de la manière dont les calculs sont faits. Ici encore l'auteur avance progressivement : l'électrodynamique quantique d'abord, ensuite la chromodynamique quantique, le mécanisme de Higgs et la théorie électrofaible. Le lecteur ne peut que rester impressionné par l'ensemble des prédictions du modèle standard et par l'accord remarquable de la théorie avec l'expérience.

Les deux chapitres suivants nous emmènent au-delà du modèle standard. Comme la plupart des chercheurs, Langacker estime que, malgré tous ses succès, le modèle est fondamentalement incomplet. On n›a aucune idée d›où viennent les valeurs de tous les paramètres numériques (près de 30) qu›il contient, d›autant plus que certaines valeurs sont beaucoup plus petites que ce à quoi on s›attendrait. On comprend mal la prédominance de la matière sur l›antimatière, l›origine de la matière sombre ou la stabilité du proton. L›auteur indique différentes pistes pour répondre à ces interrogations, comme la supersymétrie, la grande unification ou les dimensions additionnelles. Il signale également les nouvelles installations qu›on pourrait construire au cours des prochaines décennies. L›ouvrage se clôt sur un lexique détaillé d›une vingtaine de pages, une bibliographie et un index.

Proposé il y a plus de 40 ans, le modèle standard a toujours un énorme succès, beaucoup plus grand sans doute que ce à quoi on s›attendait au début. Langacker a bien mis en lumière la richesse des travaux auxquels il a conduit et, en même temps, le mystère sur lequel il s›ouvre.

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Do We Really Understand Quantum Mechanics, by Franck Laloe, Cambridge University Press, 2012, pp. 406, ISBN 9781107025011, price 70.95.

Quantum mechanics, first formulated by Werner Heisenberg in 1925 (Nobel prize in 1932 'for the creation of quantum mechanics') and further developed soon after by Erwin Schroedinger, Niels Bohr and others, is undoubtedly one of the most successful theories of science. It has provided a complete and incredibly-accurate description of the observed physical phenomena in the microscopic world of atoms, electrons, and other subatomic particles. It is responsible for the origin of nanoscale physics, transistors (thereby today's computers), lasers, information technology, some aspects of chemistry, biology, and discovery of a whole host of novel materials with remarkable quantum properties. Interestingly, modern nanoscale devices have directly confirmed some of the theoretical foundations of quantum mechanics. Most notably, the quantum dots (the so-called 'artificial atoms') can be made to display the discrete energy levels of a quantum system, or the quantum corrals that allow a direct visualization of electronic wave functions.

This impressive success of quantum mechanics notwithstanding, we still do not fully understand the basic foundations of the theory. Most of the laws of quantum mechanics defy our common intuition. One therefore relies on various 'interpretations' to describe the measurements on quantum systems. The breathtaking progress of our understanding of the properties of quantum systems is largely due to, what is commonly known as the 'shut up and calculate' approach. However, it is essential to understand the conceptual issues underpinning this theory, that is actually crucial for, at the very least, most of the developments of modern-day technology. This is the subject of Frank Laloe's book. In eleven chapters and eleven appendices, the author provides us with a balanced view of the subject and in-depth analysis of the conceptual problems that it entails. The book begins with a brief historical overview of the subject with a description of the status of the state vector. Chapter two deals head on with the conceptual difficulties of quantum mechanics, that includes a clear description of Schroedinger's cat, and Wigner's friend. Chapter three describes the "EPR paradox" with the analogy of Gregor Mendel's peas, and the ensuing discussions by Bohr, Heisenberg and others. The author then proceeds to describe Bell's theorem and the nonlocality. Quantum entanglement, cryptography, Bose condensate and many other topics are discussed in the chapter titled 'Experiments'. The final section of the book deals with various interpretations of quantum mechanics, including the hidden variables, a detailed discussion of the Bohmian theory and various other topics.

Despite its title, it is not a popular science book. It is a detailed, highly technical book that often delves into heavy mathematical details to make its case. This book is a valuable addition to the literature on quantum mechanics. As for the answer to the question posed in the title; *Do We Really Understand Quantum Mechanics*, my answer has to be a resounding 'No'. It is an interesting book for the practitioners of quantum mechanics and for others who are involved with the foundations of quantum mechanics.

Professor Tapash Chakraborty
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Gravitation, by Misner, Thorne, and Wheeler, Princeton University Press, 2017 (reprint from 1973 edition), pp. 1336, ISBN 9780691177793, price 74.95.

The Misner-Thorne-Wheeler (known colloquially as MTW) textbook *Gravitation* is a well-loved classic on the topic of general relativity. Originally published in 1973, this 2017 reissue remains largely unchanged; the preface highlights outdated chapters and subjects (e.g., gravitational wave detection) as well as providing a brief summary of concepts which the modern reader should peruse in lieu of updating the actual content of the textbook. MTW is nearly 1300 pages long with 44 chapters divided into 10 parts. The book notably features two "tracks," interwoven throughout, the first examining introductory material and the second delving into more mathematically intensive topics. Intended for graduate study and above, this book was challenging but not impenetrable for me as a first year graduate student. Too often reading physics feels like reading a laundry list of equations with little conceptual framework; I found *Gravitation*'s detailed written explanations refreshing.

Initially, the "tracks" separating introductory and advanced material struck me as superfluous. Why not just place more advanced material in later chapters, as most textbooks do? As I continued reading, however, I began to see the benefit of keeping related material grouped together. Tracks allow the reader to pick and choose which topics to consider deeply and which to skim without skipping entire chapters of content. Some reviewers of the original MTW claim this makes the book difficult to read sequentially, but I did not find this to be the case.

I am on the fence about this textbook's use of "boxes." Allegedly, the boxes cover material which might otherwise be taught in a lecture setting. In some cases I felt this worked well; setting aside certain topics from the main text makes sense. In other cases I felt confused as to why a box was used, e.g., in chapter 31, the Eddington-Finkelstein coordinate system is given a box, but other coordinate systems are described in the body of the chapter. MTW also uses summarizing comments in the margin of its chapters, which I found to be immensely helpful--with the most important concepts set aside, this textbook practically takes notes for you.

MTW is famous for its lengthy written explanations and copious use of figures. For the mathematically gifted who detest reading, this textbook may not be for you; for the rest of us, it is a godsend. Though I have taken a GR course before, the figures in this textbook deepened my conceptual understanding of the topic considerably. Some figures seem needlessly complicated, e.g., figure 1.7 describes a device with walls of lucite and mesh pockets to catch steel balls--why are the pockets necessary? Why do we need to know the kind of material the walls are made of? I am the first to appreciate detailed writing, but there are some cases where brevity is preferable. Figure captions is one of those cases--a good figure should speak for itself! Though I found myself raising my eyebrows on more than one occasion at captions over a half a page long, the majority of figures are well constructed with captions of appropriate length.

Most exercises in MTW are grouped at the end of each chapter (as is to be expected), but there are a notable minority interspersed throughout the chapters. I cannot recall having seen this in a textbook before. Placing an exercise or two at the end of each section encourages the student to work through the problem immediately after reading the relevant material, which I think is a very smart move. By the time I get to the end of a long chapter, I've forgotten what's at the beginning; exercises at the end of each section act as checkpoints of understanding. More textbooks should do this!

Flaws notwithstanding, the MTW textbook is the only physics textbook I can recall being a pleasure to read. Where dry, jargon-laden writing seems to be the norm, MTW use a conversational tone easily accessible to graduate (and some bright undergraduate) students. If you have a complete conceptual understanding of general relativity and only want a textbook which regurgitates the relevant mathematics, MTW is a bad choice. Otherwise, I cannot recommend this book enough.

Charlee Amason
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Flow, Deformation and Fracture: Lectures on Fluid Mechanics and the Mechanics of Deformable Solids for Mathematicians and Physicists, by G.I. Barenblatt, Cambridge University Press, 2014, pp. 255, ISBN 978-0-521-71538-6, price 122.54.

Professeur Emerite de la mécanique des fluides à l'Université de Cambridge et à l'Université de Californie, ainsi que scientifique principal à l'institut d'océanologie de l'académie des sciences de Russie, Grigory Isaakovich Barenblatt, mathématicien russe octogénaire, présente dans ce livre plus de 40 ans d'expérience d'enseignement.

Le but de ce livre est de présenter concepts et méthodes fondamentales, ainsi que des résultats particuliers, de la théorie mathématique unifiée intermédiaire asymptotique (unified intermediate asymptotic mathematical theory) de l'écoulement, déformation et fracture des fluides et les solides déformables. Cette théorie est une approche où les matériaux sont remplacés par un medium continu, souvent appelé mécanique du continu. Elle généralise et unifie les disciplines de la dynamique des fluides, dynamique des gaz, théorie de l'élasticité, théorie de la plasticité, etc.

Pour débuter, à l'aide d'un milieu continu idéalisé tridimensionnel, l'auteur développe l'équation de continuité et celle de la conservation de la quantité de mouvement. On se retrouve donc avec quatre équations et treize inconnues, le système est alors non fermé. En négligeant la variation de la densité avec le temps et la variation spatiale du tenseur de contraintes, on obtient un système fermé. Ce modèle est alors appelé un fluide idéal incompressible. On peut, par la suite, faire ressortir l'équation du tourbillon et l'équation intégrale de Bernoulli. Une application de la portance d'une aile d'avion termine alors le quatrième chapitre.

Après avoir développé ce modèle, l'auteur présente, l'étude de l'analyse dimensionnelle et la théorie de la similitude physique, utilisée tout au long du livre.

Dans la poursuite de la mécanique du continu, l'auteur présente la théorie mathématique de l'élasticité et développe celle-ci jusqu'à l'obtention de l'approximation linéaire d'un corps élastique et l'équation dynamique de la théorie de l'élasticité. On résout, à l'aide de la théorie, le cas d'un corps bidimensionnel. Ce chapitre a pour but de nous amener à l'étude de la résistance des matériaux, plus spécifiquement aux notions de fissure, de fracture et de fatigue.

Au septième chapitre, l'auteur construit le système d'équations fermées pour un fluide newtonien visqueux incompressible à densité constante, à l'aide de l'équation de Navier-Stokes et de l'équation de continuité. Le chapitre inclue aussi quelques exemples d'application. De manière plus spécifique, au chapitre suivant, à l'aide de l'équation pour la couche limite, il sera possible cette fois de déterminer un terme de traînée d'une aile d'avion, jusque-là impossible avec uniquement avec le modèle d'un fluide idéal incompressible. Des références sont données aux travaux d'origine des diverses équations et leurs développements historiques; le texte devient d'autant plus intéressant.

Le neuvième chapitre, lequel porte sur les méthodes de « complète » et « incomplète similarité » fait référence au livre « Scaling » du même auteur, publié en 2003. Plusieurs phénomènes naturels présentent la propriété d'auto-similarité (self similarity) et dans ces cas, les modèles mathématiques pourront être correctement formulés, comme par exemple les fractals. Par contre, il existe une classe plus générale de phénomènes physiques présentant une similarité incomplète ou un manque de similarité. Dans de tels cas, l'analyse dimensionnelle n'est pas suffisante et on utilisera une loi d'échelle (scaling), l'ajout d'un exposant, une approximation asymptotique ou carrément une solution numérique pour obtenir une solution. On utilise ces notions par la suite, pour résoudre le problème de la formation d'une onde de choc dans un gaz compressible.

L'auteur traite ensuite des notions générales de la turbulence pour mettre l'accent tout particulièrement sur l'écoulement à grand nombre de Reynold dans un long tube cylindrique (pipe). L'auteur conclue que la loi logarithmique de Karman-Prandtl, pour la région intermédiaire du tube, devrait être abandonnée au profit d'une loi à puissance pour la distribution de la vitesse d'écoulement dans le cas turbulent. Dans le chapitre suivant, on démontre l'équation de la quantité de mouvement et de l'énergie pour ce cas.

Près de deux-cents références sont citées à la fin du volume, mais je constate qu'à l'exception du chapitre sur la turbulence, les références mentionnées dans le livre datent des années 60. Les chapitres portant sur la théorie de l'élasticité et l'étude de la résistance des matériaux étaient ceux qui m'intéressaient avant la lecture de l'ouvrage; une lecture intégrale m'a cependant permis de faire une bonne rétrospective.

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Learning the Art of Electronics: A Hands-On Lab Course, by T.C. Hayes and P. Horowitz, Cambridge University Press, 2016, pp: 1150, ISBN 978-0-521-17723-8, price 91.95.

Approximately 40 years ago Paul Horowitz started an electronics course at Harvard from which the infamous book **The Art of Electronics** (AoE) by Horowitz and Hill was born. For the past 25 years, Hayes has been teaching this course with Horowitz. The book **Learning the Art of Electronics: A Hands-On Lab Course** is the based on this course with a large emphasis on practical circuit design, construction, and testing. The book is intended to be a stand-alone text, rather than a supplement to Horowitz's original text.

The book is divided into 26 chapters with each chapter covering the material required to complete a hands-on lab described at the end of the chapter. The end-of-chapter labs correspond to the weekly labs that students would complete in the university course. Of course, to complete the lab exercises, one must have access to the required circuit components and standard test equipment (oscilloscope, function generator, power supplies, breadboard, etc.).

There is very little math in Learning the AoE. Instead, Hayes attempts to develop the reader's practical skills and intuitive understanding of electronics. I teach a second-year electronics course and one of the things I like most about the course is that it introduces students to new mathematical techniques (solving differential equations and complex algebra, for example). Learning the AoE takes a completely different approach and makes no apologies!

The lab projects that are described at the end of each chapter are truly impressive. Some of my favourites include the AM radio, a working op-amp built from transistors, using infrared light to wirelessly transmit an audio signal (the audio signal is encoded onto the infrared light using frequency modulation), and digital-to-analog converters designed using resistor ladders. I also found the qualitative discussions of the Nyquist sampling theorem and aliasing particularly illuminating.

As a final remark, I think it would require a major investment of time for someone with no prior electronics experience to really benefit from studying Learning the AoE. For example, Part VI of the book covers microcontrollers, a topic with which I have no prior experience. I was not doing the lab exercises and, as a result, I found that I did not really gain much knowledge and/or insight from reading this part of the book. To get the most value from this text, one would have to do the suggested lab exercises. In a university setting, students typically always have an expert (lab instructor or TA) on hand to help them get through difficult laboratory tasks in a timely manner. You may not have that luxury if you're using this book as a self-study guide!

Jake Bobowski
University of British Columbia Okanagan

Problem Book in Relativity and Gravitation, by A.P. Lightman, W.H. Press, R.H. Price, and S.A. Teukolsky, Princeton University Press, 2003, pp. 599, ISBN 978-0-691-17778-6, price 150.00.

Learning special and general relativity is harder for students than it seems. Textbooks can often be confusing and lead the reader to paradoxes even if one thinks that one has a good grasp of the concepts. A way to obtain a deep understanding of relativity is through many exercises. PROBLEM BOOK IN RELATIVITY AND GRAVITATION is the best resource for that purpose. It is aimed at advanced undergraduate students and graduate students who would like to go through a variety of exercises.

Learners still need an ordinal textbook on relativity as this book has neither general explanations of concepts of relativity, nor definitions of mathematical terminologies such as manifolds or tensors, except for small notes at the beginning of each section. Because of this, I recommend this book for students who have already studied relativity once, and those who would like to test their knowledge and see how deeply they have understood the subject. Of course, the book is also accessible to students who are currently studying relativity as a complemment to their own textbooks. No book is perfect and I must admit that most of the problems are addressed for students in physics, hence, this book is not for students in mathematics who intend to seek physics as an application of Riemannian geometry.

A remarkable aspect of the book is that good solutions for all exercises are provided. These solutions are given in detail, and yet delivered in a mathematically simple manner. Some solutions become relatively long in order to avoid using too many mathematical theorems that are not familiar to physicists, but most of them are compact and they introduce some tricks to reduce the length of derivations. Readers already familiar with the notation, and who have a good grasp of the concepts of relativity should be able to follow the solutions without any trouble.

The first five sections deal only with special relativity. Readers study relativistic physics in flat spacetimes, which includes Lorentz transformation, particle decays and applications to elec- tromagnetism. Thus, these sections are useful for students in particle physics and other fields to learn relativistic physics. After many problems in flat spacetimes, readers are introduced to geometrical exercises of curved spacetimes in section 6 to 12. Even though there is no mathematical explanation of what curved spacetimes are, readers can gradually come to understand concepts of curved spacetimes and differences with flat spacetimes.

For students in gravitational physics, sections 1 to 12 are warm-ups. They should have developed a good foundation of Riemannian manifolds as well as computational techniques in curved spacetimes after going through these sections. Finally, exercises in the physics of curved spacetimes such as black holes and cosmologies are given in section 13 and after.

PROBLEM BOOK IN RELATIVITY AND GRAVITATION provides a variety of interesting exercises, and I believe it would help readers achieve a clear understanding of relativity. It is a fairly old book covering only classical exercises, which should be complemented with recent developments in gravitational physics. I nonetheless highly recommend this book for students who would like to pursue gravitational physics.

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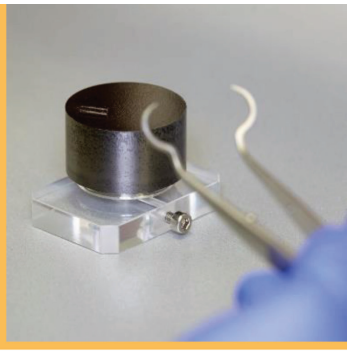
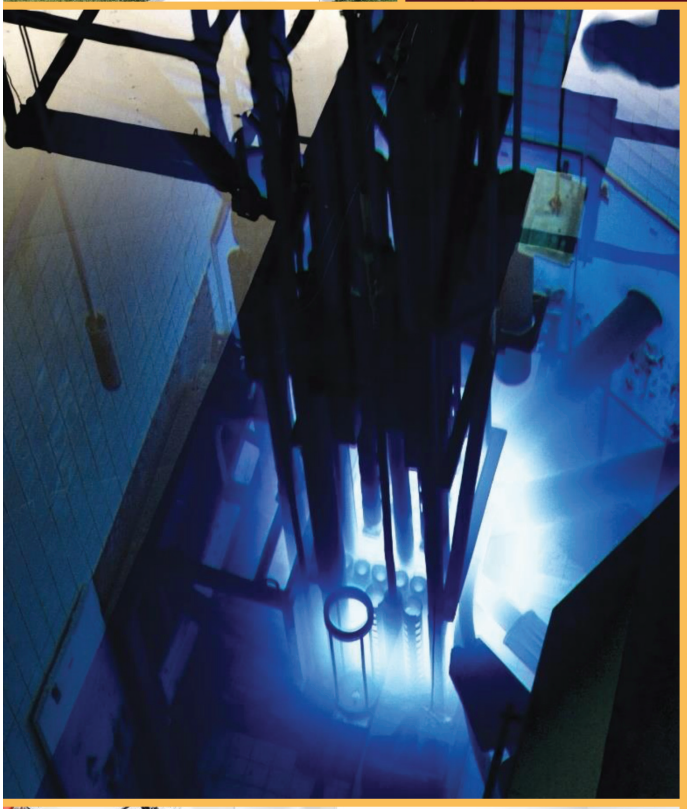

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