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BrightnESS²

Bringing Together a Neutron Ecosystem for Sustainable Science with ESS

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Grant Agreement Number: 823867

Deliverable Report

D2.4: Report on user needs in South Africa

(Neutron sciences in South Africa: Current landscape and future direction)

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1. Project Deliverable Information Sheet

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3. List of Abbreviations and Acronyms

ACNS	Australian Centre for Neutron Scattering
AfCA	African Crystallographic Association
AFRA	African Regional Cooperative Agreement
AFRIMETS	Intra-Africa Metrology System
ANSDAC	African Neutron and Synchrotron Data Analysis Competency
ANSTO	Australian Nuclear Science and Technology Organisation
BIUST	Botswana International University of Science & Technology
BrightnESS²	Bringing Together a Neutron Ecosystem for Sustainable Science with ESS
CARR	China Advanced Research Reactor
CARST	Centre for Applied Radiation Science and Technology
CATSA	Catalysis Society of South Africa
CIPM MRA	International Committee for Weights and Measures Mutual Recognition Arrangement
CPUT	Cape Peninsula University of Technology
CSIR	Council for Scientific and Industrial Research
CSNS	China Spallation Neutron Source
DESY	Deutsches Elektronen-Synchrotron
DMRE	Department of Mineral Resources and Energy
DSI	Department of Science and Innovation
EC	European Commission
ECM-21	European Crystallographic Association
ECS-5	5th European Crystallographic School
ENSA	European Neutron Scattering Association
ESRF	European Synchrotron Radiation Facility
ESS	European Spallation Source ERIC
EURADOS	European Radiation Dosimetry Group
HEI	Higher Education Institution
Hercules	Higher European Research Course for Users of Large Experimental Systems
HPRU	HIV Pathogenesis Research Unit
HZB	Helmholtz-Zentrum Berlin für Materialien und Energie
IAEA	International Atomic Energy Agency
ILL	Institut Laue-Langevin (France)
IRSN	Institut de Radioprotection et de Sûreté Nucléaire (France)
iThemba LABS	iThemba Laboratories for Accelerator Based Sciences
IUCr	International Union of Crystallography
JINR	Joint Institute of Nuclear Research (Russia)
J-PARC	Japan Proton Accelerator Research Complex
KIC	Knowledge Interchange & Collaboration
LANL	Los Alamos National Laboratory
MLZ	Heinz Maier-Leibnitz Zentrum (Germany)
MPR	Multi-Purpose Reactor
NBLC	Neutron beam line centre
NIST	National Institute of Standards and Industrial Technology (USA)
NMU	Nelson Mandela University
NPL	National Physical Laboratory (UK)
NRF	National Research Foundation
NWU	North-West University
OPAL	Open Pool Australian Lightwater

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ORNL	Oak Ridge National Laboratory (USA)
PIK	Petrova and Konopleva Reactor (Russia)
PSI	Paul Scherer Institute (Switzerland)
PTB	Physikalisch-Technische Bundesanstalt (Germany)
RDCs	Regional Designated Centres
RU	Rhodes University
SACI	South African Chemical Institute
SAFARI-1	South African Fundamental Atomic Research Installation
SAINTS	Southern Africa Institute for Nuclear Technology and Sciences
SAIP	South African Institute of Physics
SANEDI	South African National Energy Development Institute
SANS	Small Angle Neutron Scattering
SET	Science, engineering and technology
SNS	Spallation Neutron Source (USA)
SSC	Separated Sector Cyclotron
STEM	Science, technology, engineering, and mathematics
SU	Stellenbosch University
SWOT	Strength, Weaknesses, Opportunities and Threats
UCT	University of Cape Town
UFH	University of Fort Hare
UFS	University of the Free State
UJ	University of Johannesburg
UKZN	University of KwaZulu Natal
UNESCO	United Nations Educational, Scientific and Cultural Organization
UNIZULU	University of Zululand
UP	University of Pretoria
USA	United States of America
QMN	Quasi-monoenergetic neutron
WP2	BrightnESS² Work Package 2

4. List of Figures

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5. List of Tables

Table of Contents

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6. Executive Summary

Neutron scattering techniques are very versatile investigative tools of microstructural phenomena in materials, using high flux, low energy neutron beams in conjunction with specialised instruments located at large research centres. These techniques find application in diverse fields of scientific and engineering disciplines such as the study of the molecular structure inside materials which can be directly linked to the physical and chemical properties experienced in the everyday world. While it is applicable to most chemical elements it has a particular focus on light elements, especially hydrogen. Thus, it is highly complementary to synchrotron studies with X-rays that excel for the heavier elements. Neutron scattering provides observables that are readily calculable, thus modelling and neutron scattering are a natural partnership. There are a small number of centres for neutron scattering worldwide as the production of neutrons in sufficient quantities for useful science requires highly specialised facilities.

South Africa has participated actively within Work Package 2 (WP2) of the BrightnESS² project of the European Commission (EC), aimed at "Establishing a common roadmap and implementation strategy for future neutron capability". Within this activity, South African access to the European neutron science community and facilities is on offer to enable its researchers to become an integrated part of the community. Within the BrightnESS² consortium, the South African partners, Necsa SOC Ltd and NRF-iThemba LABS, facilitated the groundwork for this report, by engaging with the science community to determine the user needs in South Africa for neutron techniques (D2.4) on behalf of the Department of Science and Innovation (DSI) as coordinated by Dr Daniel Adams (Chief Director: Basic Sciences and Infrastructure). Activities encompassed two in-person workshops in South Africa, August 2019 (M8) and June 2020 (M18). Due to the severe impact of the COVID-19 pandemic from March 2020, the second workshop was replaced by ten mini-symposia conducted as on-line virtual events (M20 – M21). An overview of the schedules, scientific programs and participation with the two events are respectively given in Appendix 1 and Appendix 2. The latter were typically arranged as 2.5 hour virtual sessions that comprised talks by international and national experts, with involvement of inexperienced neutron users, concluded with consultative discussions. This format enabled much larger participation substantiated by extensive international expert inputs.

The overall objectives with these events were to consolidate the South African neutron community, attract new interest, to assess short and long term needs, as well as identify consensus from the community on modalities for international access, with special interest in the European neutron landscape and the European Spallation Source ERIC (ESS) being established in Lund, Sweden as the future premier neutron scattering facility. The outcome of the Workshops and relevant background information is contained in this document to advise the DSI towards their consideration on the level and extent of National support required, as well as international facility access, to facilitate and drive neutron science in South Africa as an imperative component and contributor to a knowledge-based economy in the short, medium and long terms.

The key outcomes of the Workshops are:

- South Africa has a small, but vibrant, multi-disciplinary neutron science community that performs high-level research utilising neutron techniques both at the National facilities, SAFARI-1 and iThemba LABS, as well as at leading international facilities.
  - Access is on peer review of submitted research proposals within open User Access programs. This mostly occurs on an ad hoc basis via personal contacts.
  - South Africa does not contribute financially to the beam time or facility infrastructure use at international facilities.
- Flagship international centres are extremely well resourced having on offer instruments that cover the full spectrum of neutron scattering applications, benefitting diverse disciplines that include physics, chemistry, mineralogy, biosciences, material sciences, agricultural sciences, medical sciences, palaeontology, heritage sciences, engineering, product manufacture and beneficiation, etc.
  - The beam time demand generally oversubscribes the instrument availability by more than 200%.
- The ESS, to be commissioned in 2023, will be a multi-disciplinary research facility focussed on an extensive suite of neutron scattering facilities utilising the world's most powerful neutron source. It will provide unique research opportunities within materials research, enabling scientific breakthroughs addressing some of the most important societal challenges in research related to materials, energy, health and the environment.
  - The research infrastructure is owned by 13 European nations, with international partnerships pursued. South Africa has been invited to join in an official capacity.
- Two world-class neutron diffraction instruments exist at the SAFARI-1 Research Reactor:
  - Respectively applied to the niche applications neutron powder diffraction and neutron strain scanning:
    - The diffraction instruments are equipped with in-situ sample environments that enable temperatures 1.5 K < T < 1800 K.
    - The neutron strain scanner capability is an active participant with Task 2.3A of the BrightnESS² project [[1]], with set aims the standardisation of measurement approaches and the establishment of a Neutron Quality Label for this technique.
  - Comprehensive studies are possible in the niches listed, which in addition can contribute preliminary results towards enhancing the scientific merit and likelihood of success of proposal that require specialised spectroscopic and scattering techniques at forefront international centres.
  - The modernisation of the neutron imaging facility is in process.
  - Capacitation and utilisation of these facilities should be substantially expanded as a priority to accommodate an enhanced local User Base and present first-line hands-on training in these exciting techniques in collaboration with the Higher Educational Institutions.

[1] R.S. Ramadhan, S. Cabeza, T. Pirling, S. Kabra, M. Hofmann, J. Rebelo Kornmeier, A.M. Venter, D. Marais, Quantitative analysis and benchmarking of positional accuracies of neutron strain scanners, Nuclear Instruments and Methods in Physics Research, A, 999 (2021) 165230. https://doi.org/10.1016/j.nima.2021.165230

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- Experienced South African neutron users have established collaborations with prominent practitioners and facility personnel (instrument scientists), in many cases from necessity to complement capabilities that do not exist in South Africa. These include magnetism, crystallography, engineering applications (residual stress and texture), energy storage and conversions systems (Li-ion batteries and hydrogen fuel cells), structural biology and lifesciences, palaeontology and heritage sciences. These collaborations should be maintained with continued financial mobility supported.
- Frequently used international facilities by South African researchers are: Australian Nuclear Science and Technology Organisation (ANSTO) Australia; Institut Laue Langevin (ILL) France; ISIS Neutron and Muon Source, UK; Joint Institute of Nuclear Research (JINR), Russian Federation; Paul Scherer Institute (PSI) Switzerland, National Institute of Standards and Industrial Technology (NIST) USA, Oak Ridge National Laboratory (ORNL) USA.
  - These are to access techniques and capabilities not existing locally, such as triple axis spectrometers, long wavelength (cold) neutrons with related techniques (such as small-angle neutron scattering, reflectometry), higher neutron fluxes (for better positional resolution) and special in-situ sample environments such as gas loading studies and in-operando studies requiring electrochemical cells and electrolysers, as well as deuteration laboratories for contrast variation studies.
- Many inexperienced neutron users have expressed interest in the benefits and value addition neutron techniques could add to their research. Similarly with the international situation, there is a general lack of familiarity (sensitivity) to what the techniques can offer, as it is seen to be the province of purely fundamental research, largely for condensed matter physics. The workshops have clearly dispelled these perceptions revealing a wealth of information that can be provided to most scientific and engineering disciplines within both academic and industrial focused research.
  - Specialities that can be vastly incorporated in South Africa include topics related to catalysis, geosciences, organic and inorganic chemistry, nanosciences, structural biology and lifesciences. These mostly require in-elastic diffraction techniques and scattering applications, frequently in conjunction with isotope substitution (deuteration) and labelling.
- The initiative to have the SAFARI-1 research reactor replaced by 2030 with a modern high flux Multi-Purpose Reactor (MPR) is very well received. It is essential that the MPR provides thermal and cold neutron beams to an extensive suite of neutron beam line instruments, equipped with a broad spectrum of in-situ sample environments, underpinned by multi-skilled and experienced personnel.
- Appropriate levels of funding will be required from the DSI to invest in the development of local facilities, as well as enable inherent growth in the South African neutron science community, both in size and stature, to the social and scientific benefit of South Africa, as well as all of Africa and the world community.
  - It is important that mechanisms be created to ensure long term sustainability and career prospects to accommodate students trained in neutron beam line techniques to the benefit of the MPR and its facilities.
- For the existing mobility programs on offer by the National Research Foundation, the South African neutron science community reiterated the essential need for continued government financial support to be implemented in a more-timely manner to fund travel, accommodation and

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subsistence for anyone in the community who is awarded beam time at a neutron research facility through peer reviewed proposals.

- With the ESS becoming the future flagship neutron science facility, future access would become an essential component of South Africa's neutron science program. The ESS has invited South Africa to become a Scientific Member with the membership level and cost to be determined. Similarly to all international centres, access will be governed by stringent procedures, preferentially based on a formalised financial contribution. The level of membership and financial contribution should be negotiated based on future anticipated usage.

7. Background

7.1. Neutron history and science

The significant interest and utilisation of neutrons in scientific research dates back to their discovery in 1932 [[2]][[3]]. The inherent value that their particle and wave duality contributes to scientific research was quickly identified and applied to measurements of neutron cross-sections in the 1940s, followed by innovative utilisation by crystallographers and condensed-matter physicists in the 1950s. The development of "cold" neutron sources in the 1970s, facilitated delivery of high flux long-wavelength neutrons, which attracted chemists and later biologists to neutron scattering. During the last decade, engineers, materials and earth scientists, palaeontologists, etc. entered the fray by exploiting the value addition neutron scattering and absorption studies contributed in their respective fields.

Neutrons interact with matter through all four forces, the strong, weak, electromagnetic and gravitational interactions, but it is the interaction via the strong force which makes neutrons a unique and ideal probe in condensed matter, having significant advantages over other forms of radiation in the study of microscopic structure and dynamics. The following main advantages have resulted in neutrons becoming increasingly important for research by virtue of their unique properties:

- *The wavelengths of thermal neutrons are similar to atomic spacings*. This property is directly exploited to provide structural information over nine orders in length scale (10^{-5} to 10^{4} Å), i.e. measurements are possible over length scales ranging from that of the wave function of the hydrogen atom to those of macromolecules.
- *Neutrons interact primary with the atomic nuclei, whereas X-rays interact with the diffuse electron cloud*. This has major advantages, such as enhanced sensitivity to detecting light atoms (such as hydrogen) in the presence of heavier ones, and to distinguish neighbouring elements. In addition, since the scattering cross-section of an atom generally varies between isotopes of the same element, exploitation of isotopic substitution methods to yield information on structural and dynamics is possible in great detail. This facilitates the use of contrast variation, which enables contrasting out parts of a complex system, for example the nucleic acid or the protein component of a virus.

[2] F. Mezei, History of neutrons and neutron scattering. In: F. Bassani, G.L. Liedl, P. Wyder (Eds). Encyclopedia of condensed matter physics. Amsterdam: Elsevier (2005) 76-83. ISBN:0-12-227610-8

[3] T.E. Mason, Pulsed Neutron Scattering for the 21st Century. Physics Today (2006) 59(5), 44–49. https://doi.org/10.1063/1.2216961

- *The energies of thermal neutrons are similar to the energies of atomic motions.* Neutrons can be delivered over a wide range of energy scales, from neV associated with polymer reputation (thermal motion), through to molecular vibrations and lattice modes, to eV transitions within the electronic structures of materials.
- *Neutrons possess a magnetic moment*. The neutron's magnetic moment is ideally suited to the study of the microscopic magnetic structures and magnetic fluctuations that underpins magnetic phenomena in materials.
- *Neutrons only perturb the experimental system weakly*. This greatly facilitates interpretation and often means that neutron scattering provides the most reliable scientific results in areas as diverse as the structure of water or the strain mismatch in superalloys used in turbine blades.
- *Penetrating, non-destructive investigations*. Due to the very weak interaction of neutrons with matter, experiments are non-destructive, even for complex, delicate biological materials. This also permits examinations of the interior of materials making them a genuine microscopic bulk probe which allows the routine use of complex environments such as furnaces, cryostats, and pressure cells, and enables the study of bulk processes under realistic conditions.

Today neutron scattering techniques are extensively used to provide fundamental microscopic information on the structure and dynamics of materials in the pursuit of our understanding of interactions in condensed matter. Applications are in fields as diverse as materials science, chemistry, biology, the earth sciences and physics. It has made outstanding contributions to detailed understanding of technically important materials such as plastics, proteins, polymers, fibres, liquid crystals, ceramics, hard magnets and superconductors, as well as understanding fundamental phenomena associated with phase transitions, quantum fluids and spontaneous ordering. The benefits and contributions of neutron scattering techniques were formally recognised with the awarding of the 1994 Nobel Prize for Physics to Bertram Brockhouse (Canada) and Clifford Shull (USA) for their pioneering efforts in the 1950s [[1]].

7.2. Neutron Production

Neutrons are abundant throughout nature. Along with protons and electrons, they form the basic building blocks of the material world. Neutrons are tightly bound together with protons in the nucleus at the centre of an atom. The most common methods of creating free neutron beams for materials research are by means of nuclear fission of uranium fuel in a reactor, or through spallation, where a high-power accelerator fires a particle beam into a metal target to release neutrons. These two processes are shown in Figure 1.

Figure 2 shows the advancement in thermal neutron flux levels attained with neutron sources over the last 9 decades. Initially free neutrons were produced with particle-driven accelerators, followed by fission neutrons from nuclear reactors in the 1940s to the present. Nuclear reactors dominate the neutron production arena due to their high neutron brightness. The neutrons from such steady-state sources are produced continuously with high energies (MeV). These neutrons become useful in neutron scattering applications when thermalized to meV energies with a broad band of highly selectable wavelengths. The energy distribution of the neutrons can be shifted to higher energies

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(shorter wavelengths) by allowing them to come into thermal equilibrium with a “hot source” (self-heating graphite block at 2400 K), or to lower energies with a “cold source” (such as liquid deuterium at 25 K). The resulting Maxwell distributions of energies have the characteristic temperatures of the moderators.

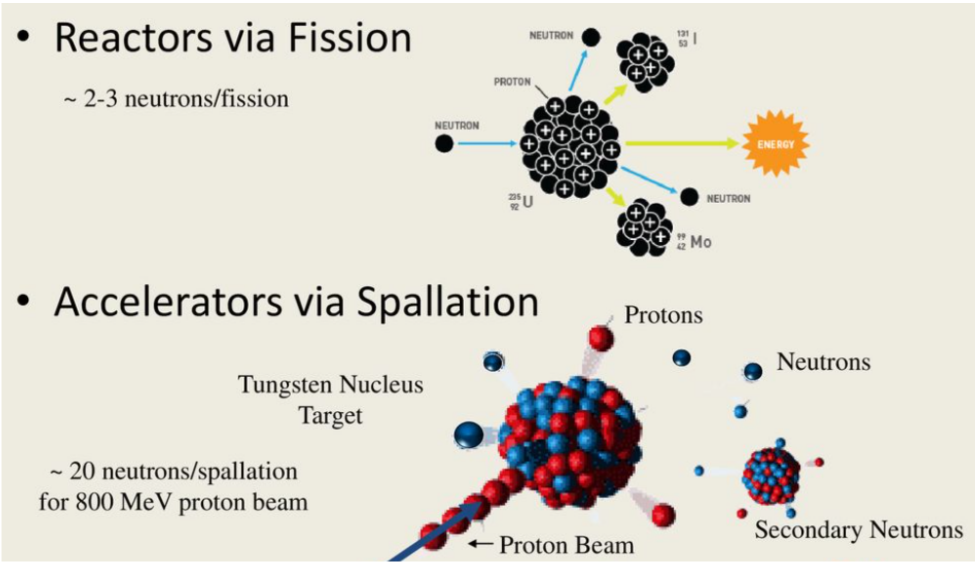

Figure 1: Depiction of the two dominant methods of producing free neutrons for use in neutron scattering applications, i.e. fission and spallation.

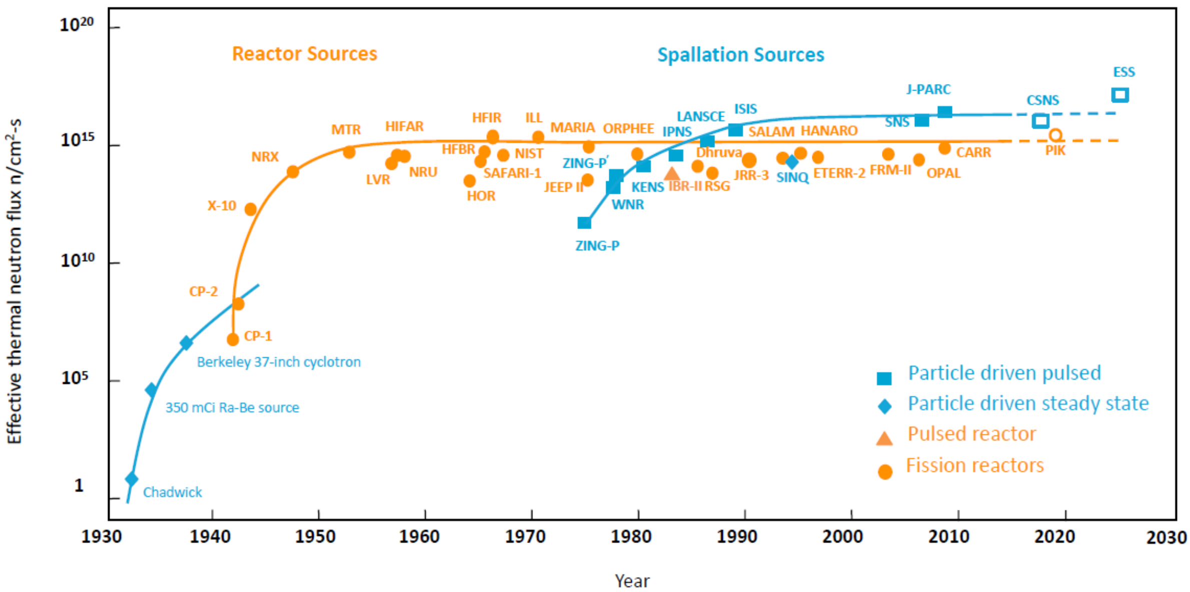

Figure 2: The evolution of thermal neutron source fluxes since the discovery of the neutron in 1932 [3].

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Since the 1980's, accelerator-based pulsed sources resurged as an alternative option pushing the envelope even further with the highest neutron fluxes attainable today. In this method, neutrons are released by bombarding a heavy-metal target with high-energy particles from a high-power accelerator – a process known as spallation. The low heat dissipation in this process allows pulsed sources to deliver higher neutron brightness with significantly less heat generation in the target as compared the most advanced steady-state sources.

Spallation facilities produce powerful bursts of fast neutrons that after moderation into slow and cold neutron sources, enable studies of a very broad range of applications in pure and applied neutron science. Such facilities are large scale infrastructures typically constructed and operated by large international consortia with substantial research budgets supporting extensive international user communities such as is available in the USA, Europe and the Far East.

The time-averaged flux (neutrons per second per unit area) of even the most powerful pulsed source is low in comparison with reactor sources. However, judicious use of time-of-flight techniques that exploit the high brightness in the pulse compensate for this. Although steady-state and spallation neutron sources each render unique capabilities and advantages with respect to neutron scattering applications, the two different modes of producing free neutron beams offers highly complementary probes of matter.

7.3. Neutron applications

Neutrons play a prominent and in many ways a definitive role towards our understanding of the material world by revealing where atoms are, and what they do. Neutron scattering enables study of the structure and dynamics of atoms and molecules over an enormous range of distances and times: from micrometres to one-hundred-thousandth of a micrometre, and from milliseconds to ten-million-millionths of a millisecond (see figure). While other techniques can provide information either within the same spatial range or the same temporal range as neutrons, neutron scattering provides a unique combination of structural and dynamic information **Error! Reference source not found.**.

Techniques based on their scattering from the microstructures of matter enable determination of the positions and motions of atoms and magnetic phenomena. By employing the wavelength range, and magnetic and nuclear moments, in conjunction with their weak interaction with matter, various application techniques, summarized in Figure 3, may be employed to study time and length scale (structure and motion) phenomena.

[4] https://europeanspallationsource.se/science-using-neutrons

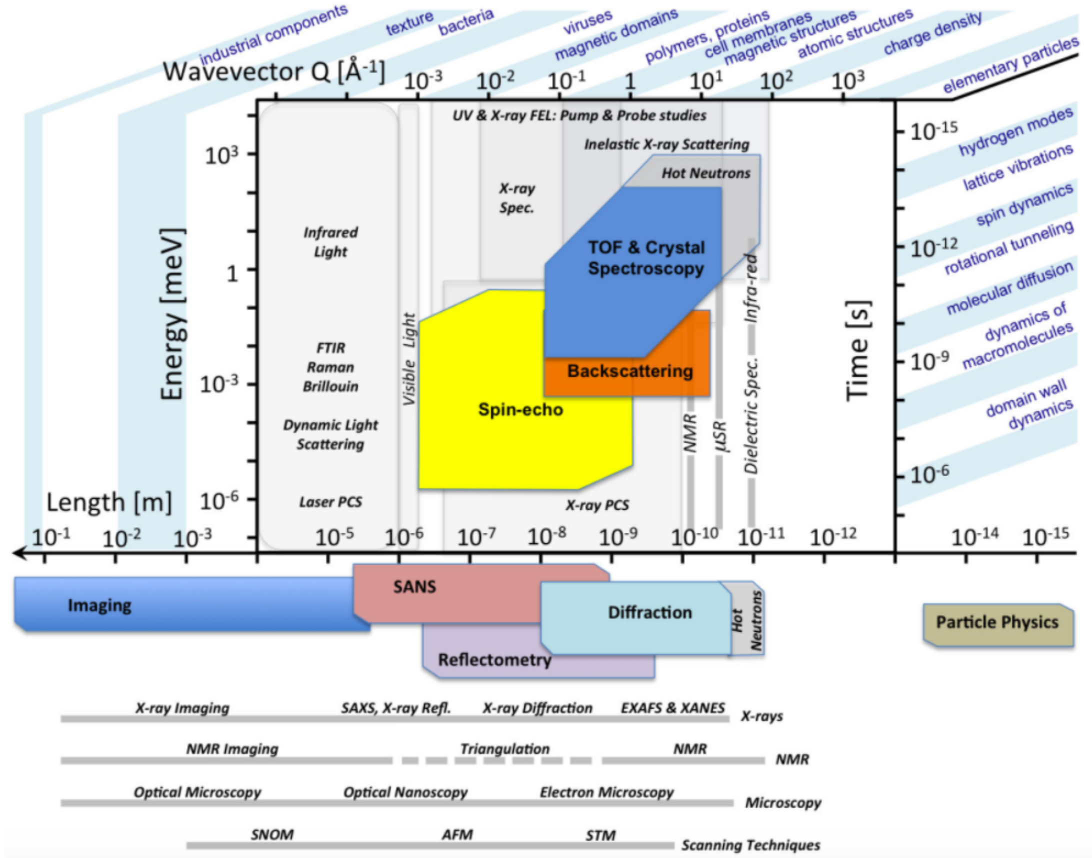

Figure 3: Probing structure and motion [4].

Major technological advances and challenges such as the dramatic revolutions in transport and manufacturing, the growth of computing and the internet and the steady increase in average life span, have their origin in understanding and exploiting the physics and chemistry of materials. The goal of modern materials science is to understand the properties of matter on the atomic scale, and to use this knowledge to optimise the properties or develop new materials. Neutron scattering techniques contribute vital information to these quests and successes ranging from studies of geological samples, understanding of human evolution from the study of prehistoric artefacts, to the development of new materials for energy production and storage, as well as processes that improve the performance of manufactured components have been achieved. By combining neutron scattering techniques with in-situ controlled sample environments, dynamics of chemical reactions at interfaces for chemical and biochemical engineering, food sciences, drug synthesis and molecular biology can be studied, in many cases non-invasively and non-destructively. Specifically the superior penetrating capabilities of neutrons facilitates probing deep into solid objects such as turbine blades, gas pipelines and welds to give a unique microscopic insight into the strains and stresses that affect the operational lifetimes of these crucial engineering components. Studies of nano-particles, low-dimensional systems and magnetism provide information that will impact the next generation computer and IT technology, data storage, sensors and superconducting materials. Neutrons furthermore enable studies of chemicals which affect the environment, polymers and plastics, materials for health – from new materials for hip implants to gels that can help babies with cleft palates. Neutron scattering techniques thus find vast application in many science, engineering and technology (SET) sectors as depicted in Figure 4.

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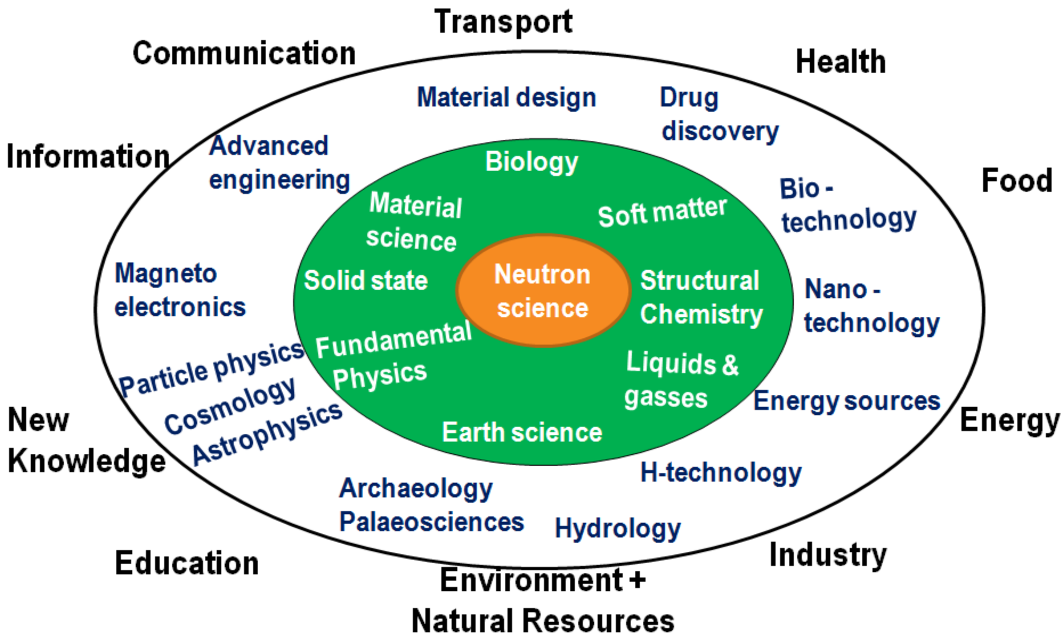

Figure 4: Applications of neutron sciences in SET sectors.

7.4. Landscape of neutron scattering facilities

Notwithstanding neutron scattering having been pioneered in North America, Europe is home to the world's most intense reactor at the Institut Laue-Langevin (ILL), France, and one of the world's most intense pulsed sources, the ISIS Facility at the Rutherford Appleton Laboratory in the UK. This will be substantially expanded with the next generation source, the European Spallation Source ERIC (ESS) which will have the highest neutron brilliance yet achieved. The ILL was commissioned in 1972 and has since maintained the distinction as the most powerful reactor source through substantial periodic upgrades and modernisation. Recent research reactor additions on the neutron landscape have been FRM II at the MLZ Germany, OPAL at ANSTO in Australia, CARR in China and PIK in Russia. A number of facilities are currently under construction with the RA-10 facility in Argentina being in an advanced stage. A number of spallation sources have recently been upgraded or commissioned, such as ISIS in UK (2nd target station), J-PARC in Japan, the SNS in the USA and CSNS in China.

Europe contains most of the research reactors, followed by Asia, with a growing interest from Africa (i.e. Tanzania, Ethiopia, Uganda and Zambia) to expand their nuclear science and technology programmes, including establishing new research reactors to complement the exist facilities that present thermal power ranging from 0.1 kW to 22 MW. There are 11 new neutron sources under construction and 14 planned world-wide [5].

[5] International Atomic Energy Agency, "Research Reactor Data Base". http://nucleus.iaea.org/RRDB/RR/ReactorSearch.aspx?filter=0

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Figures 5, 6 and 7 provide broad overviews of facilities where neutron beam instruments are in operation at both research reactor- and accelerator-based neutron sources [6].

Figure 5: Facilities using accelerator-based neutron sources. Total facilities encompass 146 located in 31 countries. These comprise 31 compact accelerator-based neutron sources, 84 generators and 11 spallation sources [6].

Figure 6: Facilities equipped with neutron scattering instruments. Total instruments encompass 362 located in 23 countries. These comprise 128 diffractometers, 104 spectrometers and 130 other instruments such as small angle scattering, neutron reflectometery, etc. [6].

Figure 7: Facilities equipped with neutron imaging instruments. Total facilities encompass 54 in 37 countries. These are located at 4 spallation sources, 2 non-spallation accelerator-based sources, 1 at a pulsed research reactor and 47 at research reactors [6].

7.4.1. Neutron scattering instrument suite at the European Spallation Source ERIC

The ESS is currently under construction in Lund, Sweden. When complete, it will provide a suite of 22 world-leading instruments for use by the neutron user community, shown in Figure 8, arranged around a spallation neutron target and moderator assembly, fed by a 5 MW proton accelerator. The facility, including all the instruments, is designed to offer world-leading performance, with new and unique instrumental capabilities not currently available at existing facilities providing the means to maximise scientific output and achieve breakthroughs across a broad spectrum of physical and biological sciences. By reducing the length of time required to conduct experiments, the ESS will facilitate the use of neutron scattering for example in time-dependent (i.e. "real-time") and kinetic studies, to analyse smaller samples and subsequently weaker signals, to a higher resolution in space and time, and to studies under more extreme conditions. The ESS is thus expected to expand the functionality of neutron-based experiments in strategic fields such as life sciences, engineering, nanoscience, geology and materials science. All instruments were designed to make optimal use of inherent strengths due to the unique design of the ESS neutron source namely a long-pulse, high flux, flexible resolution and large bandwidth. This results in an order-of-magnitude gain in performance averaged over the 15 instruments, compared to the best-in-class instruments currently operating. The instruments are chosen to maximise the breadth and depth of the envisaged scientific impact.

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In particular the high source brightness can be used in a number of transformative areas:

- Measuring very small amounts of sample, or to probe volumes/ areas of larger, non-uniform samples.
- Very fast measurements, giving access to kinetics on the tens of ms time scale
- Performing parametric studies, covering large volumes of parameter space such as temperature, flow conditions, magnetic field, pressure, etc.
- Studying weak effects, i.e. small cross-section events requiring high counting statistics.
- Polarised-neutron studies, allowing the separation of coherent, incoherent and magnetic scattering, again at the expense of beam intensity.

Further details can be found in [[7]].

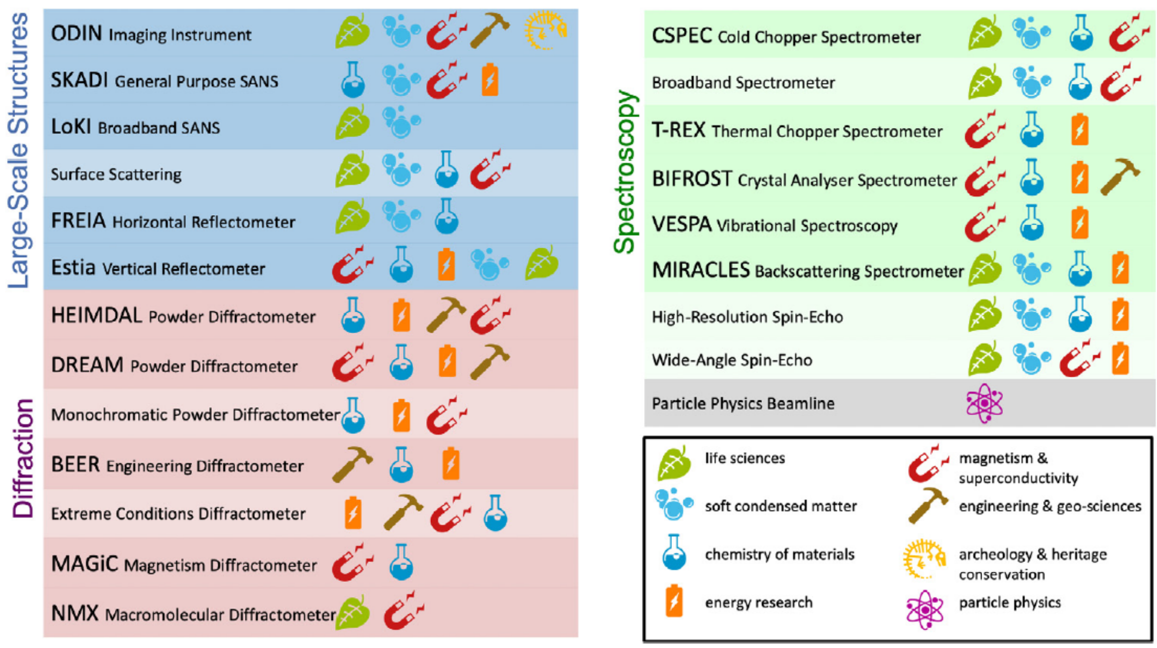

Figure 8: ESS instrument suite. Highlighted and named instruments (e.g. ODIN) are those which are currently in construction. The others are the remaining instruments from the Technical Design Report reference suite, which serve as placeholders for instruments 16–22. The main scientific communities addressed by the instruments are indicated with the symbols shown [[7]].

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[6] K.H. Andersen, D.N Argyriou, A.J. Jackson, J. Houston, P.F. Henry, P.P. Deen, R. Toft-Petersen, P. Beran, M. Strobl, T. Arnold, H. Wacklin-Knecht, N. Tsapatsaris, E. Oksanen, R. Woracek, W. Schweika, D. Mannix, A. Hiess, S. Kennedy, A. Schreyer, The instrument suite of the European Spallation Source, Nuclear Instruments and Methods in Physics Research, A 957 (2020) 163402. https://doi.org/10.1016/j.nima.2020.163402

7.4.2. Large-scale neutron research facilities in South Africa

7.4.2.1. Necsa

SAFARI-1 (South African Fundamental Atomic Research Installation) [[8]] is a tank-in-pool type research reactor with a licensed operating thermal power of 20 MW. This national asset is located at Pelindaba, 30 km west of Pretoria, South Africa, and owned and operated by Necsa SOC Ltd. The reactor project was initiated in 1960 and was commissioned in March 1965. SAFARI-1 has now been in routine operation for more than 56 years and is a major producer of medical and industrial isotopes for both domestic and international clients. It also provides neutron beam lines for scattering applications as a User Access Facility. To fulfil this role it operates more than 300 days per annum. It is a very well managed facility underpinned by rigorous maintenance management and an aging management plan that ensures safe and reliable operation. It is expected to be in operation until 2030.

Beam line facilities at SAFARI-1 are equipped for the applications of neutron powder diffraction (PITSI instrument [[9]]), as well as neutron strain scanning (MPISI instrument [[10]]), with a neutron radiography facility being upgraded (INDLOVU [[11]]).

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7 W.J. Strydom, A.M. Venter, C.B. Franklyn and F.C. de Beer, The Role of Safari-1 in Industry and Academia, Physica Scripta T97 (2002) 45. DOI:10.1238/Physica.Topical.097a00045

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The instrument characteristics of the diffraction instruments are summarised in **Error! Reference source not found.**.

Table 1: Characteristics of neutron diffraction instruments at SAFARI-1

Beam component	PITSI instrument	MPISI instrument
Monochromator Horizontal and vertical focused	Hor. and ver. focus adjustable at take-off angles (wavelengths): Take-off angle: 70° 90° Si(331) 1.43 Å 1.76 Å Si(551) 0.87 Å 1.07 Å	Hor. focus adjustable; Ver. focus fixed. Take-off angle 83.5° giving wavelengths: Si(331) 1.67 Å Si(333) 1.49 Å Si(011) 5.11 Å
Beam size	Slit: Hor: 1 – 20 mm Ver: 1 – 50 mm	Slit: Hor: 0.3 – 5 mm Ver: 0 – 20 mm
	Radial collimator to reduce background	Radial collimators: FWHM 1, 2, 5, 10 mm
Sample stage	Huber integrated XYZ with capacity 250 kg and 250 mm travel for each axis	Huber integrated XYZ with 250 kg and 250 mm travel for each axis; ¼ cradle with integrated phi
Sample setup	Theodolites + Neutron camera	Telecentric camera, laser levels, theodolites
Detector	Pseudo area detector: 15 x Reuter Stokes tubes giving active area 660 mm (hor) x 375 mm (ver)	Denex 300 x 300 mm2 area detector
	Two-theta range: 10° ≤ 2θ ≤ 120°	Two-theta range: 10° ≤ 2θ ≤ 110°
Resolution	Δd/d = 3 x 10-3	Δd/d = 3 x 10-3
Sample environments	Top-loader vacuum furnace: 400 K < T < 1800 K Bottom-loader cryostat: 4.5 K < T < 320 K Top-loader cryostat: 1.5 K ≤ T ≤ 800 K	
Data acquisition	All functionalities fully programmable SICS (SINQ Instrument Control System) Gumtree: drop down menus; Script files	
Data format	NeXus, HDF5 encoded	
Data processing	ScanManipulator	

7.4.2.2. **iThemba LABS**

iThemba Laboratories for Accelerator Based Sciences (iThemba LABS) is a national facility of the National Research Foundation in South Africa. Activities at the facility are based around a number of sub-atomic particle accelerators located at their Cape Town and Johannesburg campuses. The largest of these, a K-200 separated sector cyclotron (SSC), accelerates protons to energies of 200 MeV, and heavier particles to much higher energies. Smaller accelerators include two injector cyclotrons, one providing intense beams of light ions, and the other, beams of polarized light ions or heavy ions, and a 6 MV Van de Graaff electrostatic accelerator. Accelerators at the Johannesburg campus include a 6 MV tandem Van de Graaff electrostatic accelerator and two low energy electrostatic accelerators for ion implantation and other surface science studies.

iThemba LABS brings together scientists working in the physical, biological and material sciences. The facilities provide opportunities for modern research, advanced education and the production of unique radioisotopes [[12]]. The focus is on providing research with radiation for scientific purposes through the acceleration of charged particles using the SSC, the Van der Graaff Accelerator and other appropriate technologies.

At iThemba LABS, there is a purpose-built facility for the production and use of high-energy neutron fields. The SSC can generate secondary quasi-monoenergetic neutron beams (via (p,n) reaction) with peak energies ranging from 30 MeV to about 200 MeV through the acceleration of protons in the energy range of 25 MeV to 200 MeV. A beam pulse selector may be used to suppress a chosen fraction of proton bunches to enlarge the time interval between pulses, which allows time of flight measurements to be carried out. Typical currents for 100 MeV are about 5 mA in unselected mode and 500 nA at the repetition rate of 2.5 MHz. For 200 MeV, a current of 300 nA can be delivered at a frequency of 26 MHz. The spread in time of a proton bunch is about 1 ns. The 7Li (p, n) 7Be reaction is typically employed to produce neutrons, although natural beryllium and carbon targets have also been used from time to time. Neutron beams are formed by linear collimator apertures (5 cm x 5 cm) in the 2.6 m thick shielding wall that separates the neutron production area (Li target) from the experimental area. The shielding wall consists of a 2 m thick inner layer containing approximately equal proportions of iron and concrete and a 0.6 m thick outer (downstream) layer of borated wax or borated polyethylene. Neutron beams are typically produced at angles of 0^o and 16^o to the proton beam, although apertures at 4^o, 8^o and 12^o are also available. The energy spectra of the neutron beams generated by the p + Li reaction at neutron emission angles of 0^o and 16^o have two main components: the first is a high-energy (quasi-monoenergetic) peak of energy a few MeV less than that of the incident protons; the second is a low-energy continuum extending from the high-energy peak towards lower energies. The high-energy peak is prominent in the 0^o spectrum but decreases rapidly in intensity with increasing neutron emission angle. The spectrum and intensity of the low energy continuum is almost independent of angle for angles up to 16^o. Thus, subtracting a measured detector response produced in the 16^o beam (after appropriate normalization) from that measured at 0^o yields an effective measurement associated with a nearly monoenergetic neutron beam.

7.4.3. Future South African neutron research facilities

7.4.3.1. Multi-Purpose Reactor at Necsa

With the SAFARI-1 Research Reactor approaching the end of its useful operational lifetime, a project is being overseen by the Department of Mineral Resources and Energy (DMRE) in consultation with amongst others the Department of Science and Innovation (DSI) to replace it with a Multi-Purpose

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11 https://tlabs.ac.za/

Reactor (MPR). The major application areas envisaged are neutron scattering in material and biological research, isotope production and industrial applications. It will be a high flux facility equipped with a thermal as well as a cold neutron source to provide neutrons of required energies to beam line instruments respectively accommodated in the reactor beam hall, as well as into a neutron guide hall using low loss super-mirror neutron guides. The neutron beam line centre (NBLC) will be a large-scale facility available to users worldwide, equipped with state-of-the-art instrumentation to fully exploit the neutron beams produced for niche applications. It is envisaged that the NBLC, as a national laboratory, should remain the leading institution in neutron scattering science in the African continent and contribute to the international landscape.

The MPR will be equipped with a suite of beam line instruments such as neutron powder diffraction (respectively high-resolution and high intensity), engineering and material science, single crystal diffraction and neutron imaging. These are the most relevant neutron beam techniques for materials research, vibrational spectrometers for the study of lattice and magnetic dynamics, to the investigations of large scale phenomena in structural and biological systems using reflectometry and small-angle neutron scattering. By further exploiting the properties of neutrons, all the techniques can be combined with polarization analyses, as well as extensive sample environments for in-situ parametric studies under simulated operational and extreme conditions. As an example, the layout of such as modern facility is given in Figure 9 which shows a conceptual image of the Australian Centre for Neutron Scattering (ACNS) at ANSTO, Australia, with instruments in the reactor beam hall area, as well as in the neutron guide hall.

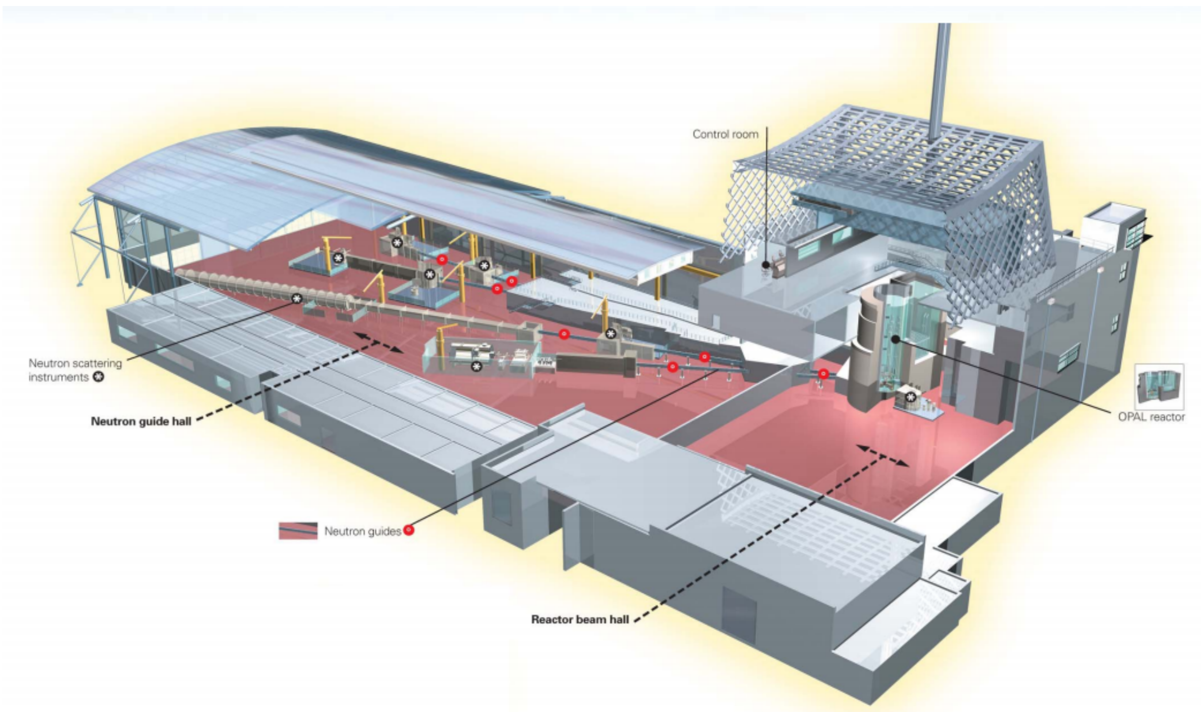

Figure 9: Conceptual view of the beam line instruments at the ACNS [13].

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12 https://www.ansto.gov.au/our-facilities/australian-centre-for-neutron-scattering

7.4.3.2. **iThemba LABS**

The neutron beam facility at iThemba LABS has been used for fundamental physics research [14], cross section measurements [15], radiation biology experiments [16] and detector development and calibrations [17], especially for dosimetry at flight altitudes and in space.

The facility was recently designated as the laboratory in South Africa for neutron metrology in the energy range 30 – 200 MeV by the National Metrology Institute of South Africa, in line with the CIPM MRA (International Committee for Weights and Measures Mutual Recognition Arrangement) and AFRIMETS requirements. There are ongoing developments in partnership with the University of Cape Town, PTB (Physikalisch-Technische Bundesanstalt in Germany), IRSN (Institut de Radioprotection et de Sûreté Nucléaire in France) and NPL (National Physical Laboratory in UK) to redesign the neutron beam vault, improve the beam quality and fluence characterisation methods for future experiments [18]. The planned upgrade of the iThemba LABS neutron vault facility that ensures traceability of the neutron fluence data in full compliance with metrology standards [19] to the neutron science community by 2023.

iThemba LABS actively participates in the European Radiation Dosimetry Group (EURADOS) Working Group (WG) 11, 'High Energy Reference Fields'. EURADOS coordinates research, development and harmonization in the area of radiation dosimetry. iThemba LABS has provided EURADOS WG 11 with a well-characterized quasi-monoenergetic neutron (QMN) source in the energy domain above 30 MeV [20].

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13 Domula et al., New Nuclear Structure and Decay Results in 76Ge-76As Systems, Nuclear Data Sheets 120 (2014) 44-47.

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14 Ndlovu et al., Measurements of Cross Sections for High Energy Neutron Induced Reactions on Co and Bi, EPJ Web of Conferences 239 (2020) 01025. https://doi.org/10.1051/epjconf/202023901025

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15 Nolte et al., Relative Biological Efficiency of 192 MeV Neutron Radiation for the Induction of Chromosome Aberrations in Human Lymphocytes of the Peripheral Blood, Proceedings of Science, FNDA (2006).

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16 Buffler et al., Irradiations at the High-Energy Neutron Facility at iThemba LABS, EURADOS Report 2016-2 (2016).

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17 Ndlovu et al., Upgrade of the fast neutron beam vault at iThemba LABS to a metrology facility, JACoW Publishing (2019). ISBN: 978-3-95450-205-9. https://doi.org/10.18429/JACoW-Cyclotrons2019-TUP012

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18 Mosconi et al., Characterisation of the High-energy neutron beam at iThemba LABS, Radiation Measurements 45 (2010) 1342 – 1345.

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[19] Trompier et al., A comparison of the response of PADC neutron dosemeters in high-energy neutron fields, Radiation Protection Dosimetry 161 (1-4) (2014) 78 – 81

8. South African stakeholder engagements

This project forms part of Work Package 2 of the BrightnESS² (Bringing Together a Neutron Ecosystem for Sustainable Science with ESS) project of the European Commission aimed at establishing a strategy to deliver neutrons for Europe and beyond. A specific activity under Task 2.2 is to afford South Africa the opportunity to determine "User Needs" from its neutron scattering community with suggested ways to accommodate their present and future needs. This determination was done in the form of two stakeholder consultation Workshops. Workshop 1 was organized in August 2019 at iThemba LABS Cape Town as a closed meeting with a targeted audience of approximately 40 experienced and occasional users of neutron techniques at laboratories such as ILL (France), PSI (Switzerland), MLZ (Germany), ISIS (UK), NIST (USA) and OPAL (Australia). Participants were mostly within the fields of materials science, magnetism and engineering. In addition, researchers that could potentially benefit from the use of neutron techniques were also invited. A report on this workshop is provided in Appendix 1 First South African BrightnESS2 Workshop

An outcome from this event was the identification of ten scientific Thrusts within which South African research could immediately benefit, namely:

- Biological and life sciences
- Catalyses
- Crystallography: Organic chemistry
- Crystallography: Inorganic chemistry
- Engineering applications
- Energy storage and conversion materials
- Geosciences
- Magnetism
- Nanomaterial
- Palaeontology and heritage sciences

For each of these Thrusts, prominent scientists and engineers were identified to coordinate the second Workshop aimed at a much larger participation. This was scheduled for June 2020, but had to be reconsidered due to the COVID-19 pandemic that curtailed travel and meetings. An alternative modality for this Workshop was the hosting as ten separate specialised virtual mini-symposia on the respective Thrusts with an example given in Figure 10. Participation was invited from existing contacts from the meeting conveners, Thrust Coordinator, as well as communications with Deans of Research at all universities. This modality further enabled participation by topical experts internationally. A report on this workshop is provided in Appendix 2. Second South African-BrightnESS2 Workshop

. Each symposium allowed a discussion session on ideas and expectations regarding the future role of neutron scattering and access/utilization of local and international facilities. These need to be seen in context to facilities existing in South Africa (Necsa's SAFARI-1 research reactor and iThemba LABS facilities) and internationally that includes the enormous potential that access to European facilities and the ESS as flagship facility can offer. To ensure adequate utilisation and access, there was a need to determine the extent South Africa should invest in ensuring access.

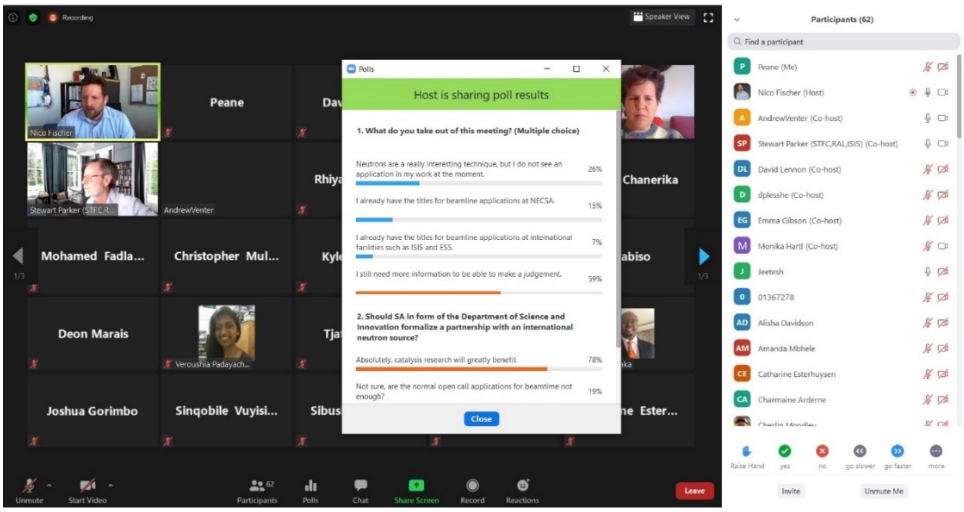

Figure 10: Screen shot of one of the online mini-symposia.

The aim of the workshops was to adequately inform participants on the value addition that neutron scattering techniques can offer in expanding existing research techniques towards furthering their research with the focus on determining:

- Compelling science questions and issues that can be addressed with neutron techniques;
- What are the niche scientific areas that these could contribute to;
- What is the format of access we require to South African facilities at Necsa and iThemba LABS, as well as abroad with the ESS;
- What capabilities do we need to develop as a country so that we can optimise the value addition that neutron techniques can offer?

8.1. **South African prominent investigators within neutron science community**

Notwithstanding a small community, a well-experienced and knowledgeable cohort of South African neutron users exists that use local as well as international facilities on a regular basis. Access to such facilities is possible through User Programs. Within this mechanism, user submitted proposals are adjudicated (peer reviewed) for scientific impact by the facility Advisory Committees. Successful proposals are granted use of specialised equipment and expert personnel support to ensure maximal success with the research aims. Typically, synchrotron facilities are accessed on the same way. As part of a formal agreement with the South African synchrotron users, travel and subsistence are supported financially by the KIC (Knowledge Interchange & Collaboration) program of the NRF [[21]].

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[21] https://www.nrf.ac.za/division/funding/knowledge-interchange-collaboration-kic

Table 2:Users of neutron facilities internationally based on personal initiatives, i.e. peer reviewed project proposal submissions

Researcher	Institution	Speciality	Facilities used
Prof André Strydom	UJ	Magnetism	ILL, ISIS, PSI,
Prof Alet Prinsloo	UJ	Magnetism	SAFARI-1, ANSTO
Prof Charles Sheppard	UJ	Magnetism	SAFARI-1, ANSTO
Prof Andrew Venter	Necsa	Magnetism; Engineering; Energy storage and conversion materials; Standardisation	SAFARI-1, ANSTO, FRM II, ISIS, PSI, Hanaro, HZB, LANL, JINR
Dr Esna du Plessis	SASOL	Crystallography	SAFARI-1, ILL
Prof Danie Hattingh	NMU	Engineering	ILL, ISIS
Prof Natasha Sacks	US	Engineering	SAFARI-1; ANSTO
Dr Mark Newby	Eskom	Engineering	ILL, ISIS, SAFARI-1
Dr Daniel Glaser	NLC	Engineering	SAFARI-1, ISIS
Dr Deon Marais	Necsa	Engineering	SAFARI-1, ISIS; JINR
Mr Robert Nshimirimana	Necsa	Engineering	ISIS, PSI, Hanaro, Maria
Prof Trevor Sewell	UCT	Biology	NIST
Dr Gavin Owen	Wits	Biology	ILL
Prof Maria Papathanasopoulos	Wits	Biology	ILL
Dr Frikkie de Beer	Necsa	Energy storage and conversion materials	NIST
Prof Andy Buffler	UCT	Fundamental and applied nuclear science	iThemba LABS, PTB, IRSN
Dr Tanya Hutton	UCT	Fundamental and applied nuclear science	iThemba LABS, PTB, IRSN
Dr Zina Ndabeni	UCT-iThemba LABS	Fundamental and applied nuclear science	iThemba LABS, JINR
Dr Peane Maleka	iThemba LABS	Fundamental and applied nuclear science	iThemba LABS, JINR

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Table 3: Users of South African neutron facilities in collaboration with instrument scientists. This is in addition to the previous table

Researcher	Institution	Speciality	Facilities used
Prof Ernst Ferg	NMU	Crystallography; Energy systems	SAFARI-1
Prof Dave Billing	Wits	Crystallography; Energy systems	SAFARI-1
Prof Joao Paulo Nobre	Wits	Engineering	SAFARI-1
Prof Pieter Pistorius	UP	Engineering; Phase transitions	SAFARI-1
Prof Roelf Mostert	UP	Engineering; Phase transitions	SAFARI-1
Prof Waldo Stumph	UP	Engineering; Phase transitions	SAFARI-1
Prof GT van Rooyen	UP	Engineering	SAFARI-1
Prof Thorsten Becker	US	Engineering	SAFARI-1
Prof Robert Knutzen	UCT	Engineering	SAFARI-1
Prof Claudia Polese	Wits	Engineering	SAFARI-1
Prof Kenneth Ozoemena	Wits	Energy systems and conversion materials	SAFARI-1
Dr. Mark Herbert	UWC	Fundamental and applied nuclear science	iThemba LABS
Dr. Charlot Vandevoorde	iThemba LABS	Radiation Biology	iThemba LABS

8.2. **SWOT analysis of South African neutron science**

Strengths

- Excellent beam line infrastructure exists at flagship facilities internationally.
- A firm base of experienced neutron science with established national and international networks exits in the South African research community.
- SAFARI-1 as a well-managed national asset that operates more than 300 days per year.
- Two world-class neutron diffraction instruments exist at SAFARI-1, equipped with in-situ temperature sample environments covering 1.5 K < T < 1800 K. These are optimised for the applications neutron powder diffraction and neutron strain scanning.
- iThemba LABS is one of the four facilities in the world that can provide quasi-monoenergetic neutron beams in the energy range 30 MeV to 200 MeV, with the other three in Japan [[22]]. With the ongoing upgrade to a metrology facility, this will be one of the prime neutron facilities in this energy domain.

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22 Pomp et al., High-energy quasi-monoenergetic neutron fields: existing facilities and future needs, Radiation Protection Dosimetry 161 (1-4) (2014) 62 – 66.

Weaknesses

- Limited funding. Travel funding by the NRF is not linked to the approval of beam time proposals;
- Not all neutron scattering techniques can be performed at the existing local facilities. No facilities existing at SAFARI-1 for inelastic scattering techniques, or sample preparation that entails deuteration.
- Very small staff complement exists at Necsa to support beam line research. This needs to be substantially expanded to achieve the aims envisaged with the MPR.

Opportunities

- Keen interest is expressed by inexperienced neutron users from the catalysis, nanosciences, chemical crystallography, as well as structural biology and lifesciences communities to expand their suite of research techniques with the incorporation of neutron techniques.
- Access to international facilities within their User Access Programs based on peer reviewed projects.
- Benefits of research and training opportunities inherent to an association agreement with the ESS;
- Increase the international reputation of South African STEM disciplines.
- Establish a South African regional Centre of Excellence in neutron sciences to the scientific benefit of sub-Saharan Africa.
- Exploitation of South African niche advantages, such as palaeontology and heritage studies (Paleoanthropological “Cradle of Humankind “UNESCO World Heritage site with its unique fossil repositories on pre-human life forms), local and tropical diseases, the rich local geological environment, the mineral and mining environment, manufacturing and beneficiation environment.
- Exploiting existing pockets of expertise in fields such as extreme temperatures, magnetism, energy systems and conversion materials, nanotechnology.
- Strengthening internationally competitive national facilities at iThemba LABS and Necsa (SAFARI-1) with respect to sample environments, as well as commissioning of modernized neutron radiography facility at SAFARI-1, etc.
- MPR project equipped with an extensive suite of neutron beam line techniques.
- Formal training opportunities in neutron sciences at tertiary institutions with incorporation of site visits and hand-on practical’s at the facilities of iThemba LABS and SAFARI-1.

Threats

- Remaining operational lifetime of SAFARI-1.
- MPR not maturing to fruition.
- Large portion of STEM community not aware of the benefits of neutron sciences and techniques towards advancing their research.

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8.3. Compelling science activities and niches that can be addressed with neutron techniques

The following research topics of interests have been identified from consultations with the Thrust Coordinators and their liaisons with existing and potential user communities:

Chemical crystallography:

This is a flourishing discipline in South Africa, with active research groups at the Cape Peninsula University of Technology (CPUT), Nelson Mandela University (NMU), Rhodes University (RU), Stellenbosch University (SU), University of Cape Town (UCT), University of Fort Hare (UFH), University of the Free State (UFS), University of Johannesburg (UJ), University of Kwa-Zulu Natal (UKZN), University of Pretoria (UP) and University of the Witwatersrand (Wits), as well as within the research division of SASOL. These research groups all produce high-quality publications in international peer-reviewed journals in the field. The following aspects are being studied within the South African context:

- Pharmaceutical applications:
  - Drug development (NMU, SU, UCT, UFH, UFS, UKZN, Wits);
  - Analysis of polymorphism, cocrystallisation and salt formation of active pharmaceutical ingredients with coformers that are "generally regarded as safe" in order to achieve better solubility and bioavailability (CPUT, RU, SU, UCT, Wits);
  - Investigation of drug-substrate interactions (UCT, UFS, Wits).
- Materials chemistry, with the following applications:
  - Development of new metal-organic and molecular frameworks for sorption, sequestration and sensing of a variety of guests, such as CO_2, water and organic solvents (NMU, SU, UCT);
  - Development of new magnetic materials (UP, SU);
  - Development of new compounds that are active in a wide range of catalytic reactions (SASOL, NMU, SU, UFS, UJ, Wits);
  - Development of new photoactive compounds (NMU, SU, UCT, Wits);
- Crystal engineering, to obtain a fundamental understanding of the role of intermolecular interactions in the formation of crystals (CPUT, SU, UCT, UKZN, Wits).

Catalysis:

In-elastic neutron vibrational spectroscopy has particular advantages over optical spectroscopy in the study of catalysis due to:

- Neutron penetrability;
- Sensitivity to hydrogen (deuterium);
- No energy deposition in samples;
- No selection rules;
- Simplicity of interaction (neutron – nucleus) enables quantitative calculations;
- More accurate determination of atomic positions and thermal parameters.

Typical studies encompass initial growth mechanisms of meso-structured silica-surfactant particles; Thermal conductivity in semiconducting materials such as clathrates (thermoelectric materials); Hydrogenation (heterogeneous catalyst) reactions; Water-spitting phot-catalysis; Diffusion of ionic

liquids in nano-pores in supercapacitors; Metal hydrides – green energy; Solid oxide fuel cells with tunable conductivity.
Applications generally utilise elastic (powder diffraction and total scattering) and neutron in-elastic techniques in collaboration with in-situ (real time) studies to determine mechanisms of catalytic reactions. In many cases it may be essential to perform deuterium substitution to improve the "hydrogen" visibility.

Energy storage and conversion systems:
Neutron techniques are well-suited to render unique structural insights in the study of battery materials, as well as energy conversions systems such as hydrogen fuel cells. This is possible due to: Finding light atoms (such as H, D, Li); Distinguishing similar elements (Ni, Mn, Co, V); Enables complex in-situ experimental setups (ex-situ, in-situ, in-operando – real time). Amongst others the following are typical research topics:

- Studies of oxygen vacancy concentrations and co-defects for doped oxide systems. looking at the influence of different dopants.
- Electrochemical delithiation;
- Phase ordering (occupancy);
- Electrochemical in-situ neutron experiments to study the potential dependent hydrogen absorption concentrations or difference between absorption and adsorption in an oxide system. The same for oxygen vacancy or co-defect concentration/stability.

Geosciences:
Neutron techniques can render information on the phase composition, crystallographic texture, magnetic phenomena, residual stress, inclusions, phase contents (visualisation) in borehole essaying samples, etc. of geological formations.

- Metamorphic rocks (high temperature – high pressure transformations, recrystallization) such as quartzites and marble (Calcite vs dolomite);
- Sedimentary phyllosilicates such as clays, shales, slates, mica, chlorite;
- Precipitates such as calcite changes in stalagmites and carbonate concretions;
- Residual stresses in marble (natural conditions, as well as in-situ compression loading combined with temperature);
- Sedimentology: Iron formation in chemical sedimentary rock (banded vs granular iron formation);
- Characterisation of base metal sulphide and platinum group mineralization in the Merensky Reef;
- Carbonados;
- Meteorites.

Lifesciences and structural biology:
Lifescience research faces many challenges in the study of biological processes that occur from the atomic and molecular size to the cellular scale. Neutrons are powerful probes for the study of biological samples as they are very sensitive to the presence of hydrogen. Using the unique properties of neutron-based scattering methods, researchers can study biological systems on a range of time and size scales, providing unique insight into a broad range of topics: from agriculture, medical devices, biofuels, to societal health challenges (e.g. cancer, diabetes, dementia, HIV). Neutron techniques

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enable atomic resolution macromolecular crystal structures, solution studies of biological complexes, structure and dynamics of biomembranes.

A desirable characteristic of neutrons for biology has to do with hydrogen, which us the most abundant element in biological systems. Photons and electrons interrelate with the atomic electric field with one electron hydrogen is at the limit of visibility to X-rays while neutrons can interact with nuclei, protons have a strong and negative scattering length. The isotope (deuterium) has a stringer scattering length which is positive. This different sensitivity of neutrons to hydrogen and deuterium allows for improved visibility of specific parts of complex biological systems through isotope substitution.
Isotopes of the same element to have different scattering lengths for neutrons therefore allowing the technique of isotope substitution to be used to yield structural details, in biological molecular structures the common isotopic substitution is $2H$ for $1H$. Neutron profit from the fact that the scattering length densities are not directly connected to electron densities. Neutron scattering provide the possibility of contrast variation with D_2O/H_2O mixtures this therefore allows to select specific components in the structure

The HIV Pathogenesis Research Unit (HPRU) at Wits University has focused on the development of an effective prophylactic HIV vaccine which utilizes a novel immunogen called Env-2dCD4_S60C that consists of a human two domain CD4 with an S60C mutation covalently bound to gp120 monomers or cleaved, soluble gp140-GCN4 trimers (Env). In several independent rabbit immunogenicity studies conducted in our laboratory, Env-2dCD4_S60C elicited potent broadly NAb against HIV-1 Tiers 1, 2, 3, HIV-2 and SIV pseudoviruses. This observation strongly indicates that Env-2dCD4_S60C complexes could provide similar effects in humans and should be considered as a viable candidate for an effective preventative and/or therapeutic vaccine against HIV-1. Prior to initiating further preclinical development of Env-2dCD4_S60C subunit vaccine immunogens in rhesus macaques, it would be critical to define and fine map the Env-2dCD4_S60C complex epitope structures which correlate to the potent viral neutralization. We will thus gain insights into the underlying mechanisms of the antiviral activity that will guide strategies for optimizing CD4-based immunogens that will likely provide protection from infection. Due to the difficulties experienced with higher resolution X-ray crystallography studies of Env and CD4, Small Angle Neutron Scattering (SANS) studies will assist with starting to biophysically characterise the gross structure and dynamics of the Env-2dCD4_S60C complex, as well as its individual constituent proteins, Env and CD4. Similar research projects have been performed collaboratively at the ILL (France) in conjunction with their deuterium facility.

<u>Magnetism:</u>
The study of magnetism in solids is traditionally one of the most intensively applied scientific areas that use neutrons as a microscopic probe. Magnetic properties of matter, magnetic excitations, short-range and long-range magnetic order as well as temporal magnetic correlations are very profitably surveyed using neutron scattering, -and in many instances with no parallel in any other method of investigation. Currently, examples of areas attracting much interest in magnetism communities are:

- Spin-orbit coupling in strongly correlated electron materials and the disentanglement of spin- and orbital degrees of freedom in local-magnetic moment spin systems.
- Unconventional quantum criticality and the accumulation of configurational entropy at very low temperature.

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- Ground states of magnetic and geometric frustrated spin systems, -among these the highly anticipated but enigmatic quantum spin liquid state.
- Low-lying magnetic ordering phenomena, the discovery of exotic magnetic quasiparticles, and new states of matter.
- Symmetry and topology in magnetism - including among other subjects the anomalous Hall effect, the spin Hall effect, and skyrmion lattices

Neutrons for engineers:
The essential question to answer; should the South African engineering user community focus on access to international facilities or should we rather strengthen the local capabilities and infrastructure. The importance of neutron scattering in a modern economy is way beyond being a useful research technique as there is enough tangible evidence of engineers using neutron scattering techniques in addressing global challenges facing society as well as the potential to assist with technological advancement that have immediate and long-term economic impact. It is essential that both local and existing international collaborations be maintained.

Engineering and more applied research are built on a foundation of fundamental investigations and techniques developed over the last 30 years, so it is crucial to continue such basic work to underpin the theories and technologies of tomorrow. Neutron experiments provide definitive data for the manufacturing industry, which has informed light weighing, lean design and process optimisation, resulting in reduced energy needs. Materials testing data have given aerospace companies confidence in new alloy compositions and manufacturing techniques.

Neutron facilities have unique requirements for advanced components and equipment, if you invest in the local facility, it could be used to challenge local suppliers to innovate and develop new technologies. Partnerships with large research centres can support small businesses by giving them the security and confidence to embrace new areas of activity. SA businesses have benefited from work done at neutron-scattering centres through technology development and knowledge transfer. Important to note that “Big Science” serves engineering, materials science, life science, information science, and the overarching aim of promoting innovation for economic growth. From publication available it is clear that neutron facilities support experimental work performed by engineers. Latest addition to the neutron landscape will be the European Spallation Source ERIC (ESS) in Sweden, most powerful neutron source in the world. The context of current SA challenges and opportunities are:

- Residual strain experiments applicable in both research and industrial applications.
- Studies of phase transformations in materials, using *in-situ* heating and cooling facilities.
- Societal benefits accruing from continued development of Safari1 and neutron facilities for engineers
- Economic benefits
- International standing and hence collaboration benefits
- Technological, industrial and research training benefits
- Benefits accruing from taking a holistic view of top rank SA imaging and materials characterisation facilities providing a national vision and runs experimental access to academia and industry.

Neutrons for palaeoanthropology and cultural heritage:

The scientifically rich repositories of fossils existing at many sites in South Africa and the greater continent, are indispensable in unravelling pre-historic lifeforms as well as human evolution. The contributions neutron techniques in conjunction with synchrotron techniques can offer in these quests have are well known and well documented in leading scientific journals.

8.4. Training in neutron sciences and applications

Notwithstanding no formal hands-on training programs existing that incorporate the SAFARI-1 facilities, at stages, honours level students do participate (on ad-hoc outreach initiatives) with some hands-on practical at the SAFARI-1 neutron diffraction facilities. Post-graduate students from many universities are though routinely supported on individual cases with their research investigations. The following training courses linked to Necsa and iThemba LABS are presented in South Africa:

- Necsa personnel present annual courses at honours and masters levels on neutron diffraction and imaging techniques to students of the CARST (Centre for Applied Radiation Science and Technology) centre of NWU.
- iThemba LABS personnel present training courses at postgraduate level to students at various universities around country via the SAINTS (Southern Africa Institute for Nuclear Technology and Sciences) initiative, and partner universities at other African countries (BIUST (Botswana); University of Dar Es Salaam (Tanzania), etc.).

A recent South African initiative has been the ANSDAC (African Neutron and Synchrotron Data Analysis Competency) Workshops run during 2018 and 2019 by UCT (Nico Fischer) within the SA-UK (ISIS Neutron and Muon Source; Diamond Light Source; University of Glasgow) initiative. This training is lecture based. An essential expansion of such programs, needs to include hands-on familiarisation of the facilities at SAFARI-1 and iThemba LABS.

Some annual training courses run in European countries:

- Hercules (Higher European Research Course for Users of Large Experimental Systems). This 11-month school, established in 1991, provides training for students, postdoctoral and senior scientists from European and non-European universities and laboratories, in the field of Neutrons and Synchrotron Radiation for condensed matter studies (Biology, Chemistry, Physics, Materials Science, Geosciences, Industrial applications). It includes lectures, practicals, tutorials, and visits of Large Facilities: ALBA in Barcelona, KIT in Karlsruhe, DESY and European XFEL in Hambourg, ELETTRA and FERMI in Trieste, ESRF and ILL in Grenoble, SOLEIL in Paris-Saclay, and PSI in Villigen [[23]].

- Oxford School on Neutron Scattering [[24]]. This two week course is intended for scientists and engineers who are new to the field of neutron scattering. Lectures and tutorials covering the theory and practice of neutron diffraction and spectroscopy are given by international experts. Students gain a comprehensive grounding in modern techniques and applications at both continuous and pulsed neutron sources and have the opportunity to hear about the latest research being carried

[23] https://nmi3.eu/about-nmi3/education/neutron-schools/hercules.html; hercules@hercules-school.eu

[24] https://www.oxfordneutronschool.org/

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out with the technique. The first week of the school introduces students to the core concepts of neutron scattering, neutron sources and instrumentation, neutron diffraction and spectroscopy. The second week splits tuition into three focused science areas, physics, chemistry and soft/bio, and provides lectures on neutron techniques and concepts which are most relevant to each area. Each lecture will be accompanied by a tutorial session. The students will also have the opportunity to visit the ISIS Pulsed Neutron and Muon Facility in Didcot, and to attend a number of evening lectures from prestigious names from the neutron community.

- Biannual Summer School on Neutron Detectors and Related Applications hosted by University of Trento, Italy. The aim of the school is to illustrate principles, methodologies and most recent applications of neutron detection technologies. In particular, the school tackle various arguments that span from neutron-matter interaction principles suitable to neutron detection, materials for neutron detectors, signal processing, Monte Carlo simulation codes to interdisciplinary applications of neutrons.

9. Discussion

9.1. Objectives

The main goal of the SA-BrightnESS² Workshops was to increase the knowledge, visibility and opportunities of neutrons to the South African academic and industrial communities, and also promote innovative multidisciplinary research that incorporate neutron techniques. The objectives, identified and set as outcomes of the mini-symposia are discussed.

Short-term objectives (0 – 3 years):

- Develop and expand the neutron science user community:
  - Engage with the government departments DSI and DMRE to establish dedicated endorsed neutron scattering programmes with universities. This will encapsulate the establishment of formal training course and research projects for students at a Hons, MSc and PhD levels, and establishment of nCap lecturer positions.
  - Link to existing initiatives such as ANSDAC (African Neutron and Synchrotron Data Analysis Competency) and SAINTS (Southern African Institute for Nuclear Technology & Sciences) to encourage hands-on training at Necsa and iThemba LABS facilities.
  - Continue involvements with the CARST (Centre for Applied Radiation, Science and Technology, NWU), and MANus/MatSci (UWC and UNIZULU) programs.
  - Arrange annual neutron scattering schools and conferences with involvement of invited international experts (form institutions such as ANSTO, ESS, Hanaro, ISIS, JINR, MLZ, NIST, etc.)
  - Placement of post-graduate students at leading international neutron centres, such as the ESS for direct skills and experience creation. It becomes essential that career prospects are established to entrench sustainability and knowledge hubs.
  - Establish a viable management structure for the neutron science community.

- Encourage and commit to neutron science studies nationally and internationally:
  - Engage with the DSI to contribute to the development and expansion of national equipment and infrastructure that are necessary to support complementary and preparatory work, to contribute to the formulation of successful proposals and the training of students.
  - Continue financial mobility support (NRF – KIC) and streamline the process to enable researchers' beamline access at international neutron science centres, to complement techniques not existing in South Africa.
  - Enter into a formal relationship with the ESS to ensure essential access of South African scientists to techniques and infrastructure not available in South Africa.
- Promote human capacity development:
  - Encourage and train larger numbers of students in fundamental as well as applied neutron sciences. Important aspects are sample preparation and data analysis software.
  - Encourage HEI's to include neutron science modules on beam line techniques at honours level curriculum.
  - Involve expertise from Necsa and iThemba LABS.
  - Include hands-on familiarisation at these facilities.
- Give support to the MPR project:
  - Solicit stakeholder inputs with respect to the optimal instrument suite required for the MPR.
  - Conduct a design study, including costs, for beam line instruments at the MPR. It may be important to involve other African countries and the International Atomic Energy Agency.
  - Preserve the existing relevant engineering technical expertise.

Mid-term objectives (3 – 5 years):

- The establishment of University Chair(s) in Neutron Scattering with associate funding for scholarships towards such projects (an NRF call for neutron science projects). Imperative to engagement with industry.
- As a DSI endorsed activity, coordinate with SACI (South African Chemical Institute), SAIP (South African_Institute of Physics)_and CATSA (Catalysis Society of South Africa), as well as Heads of Departments of Chemistry, Engineering, Geology, Lifesciences, Mineralogy, Physics, etc. to establish nGAP lecturer positions.
- Coordinate with DSI, NRF, specialist institutes (SACI, CATSA, SAIP), University Deans of Research and Heads of Departments towards establishment of joint chairs in neutron sciences with European universities (such as Technical University of Munich, University of Lund, Oxford University) that have direct links to neutron scattering institutes.
- Continue submitting proposals to the DSI/NRF for direct government investment in neutron science.
- Expand the neutron science community and its utilisation of neutron science techniques nationally and internationally, including the ESS.
- Continue growing the analytical infrastructure required for state-of-the-art neutron sciences.
- Engineering design of the beam line instruments at the MPR.

Long-term objectives (5 – 10 years):

- Continue expansion of the neutron science community and its utilisation of neutron science techniques nationally and internationally, including the ESS.
- Building and commission the beam line instruments at the MPR.
- Existence of a number of active academic chairs in South African University Departments where eligible students are trained in the use of neutron science techniques as the primary instrumentation for their research.
- Existence of international linkages with universities such as Technical University of Munich (Germany), University of Lund (Sweden), University of Oxford (United Kingdom), etc. that are closely associated with research reactor centres.
- Encourage the government to invest in expanding the staff complement at the national facilities to drive the growth of a topflight South African neutron science community.

9.2. Projected evolution of science portfolio

Originally developed for use in basic research in physics and in chemistry, neutron scattering has since found new uses within a wide range of fields, ranging from more traditional disciplines such as biology and geology, materials science, engineering science, and environmental science, to a number of emerging, high-growth research areas such as nanoscience, life sciences, polymer science, and soft condensed matter physics and biology.

It is generally recognized that neutrons have special properties that enable neutron scattering to provide unique information not attainable by use of other probing techniques such that neutron scattering should be seen as a necessary complement to other techniques.

Internationally competitive scientific research is being performed in South Africa in all of the identified Thrust areas. There is an opportunity to have these extensive expanded on with the incorporation / accessibility of neutron scattering techniques. With the involvement of post-graduate students, develop and vest expertise that can be utilised to build the research capabilities and communities at SAFARI-1 and MPR.

The establishment of a (South) African Neutron (Scattering) Association should be pursued, with membership of the European Neutron Scattering Association (ENSA) pursued as an initiating vehicle. A known chapter that has benefitted from such an association is the South African Crystallographic Society within the European Crystallographic Association. Amongst others the benefits have been the hosting of the ECM-21 (European Crystallographic Meeting) in South Africa in 2003, as well as expert inputs and participation with the recent ECS-5 (5th European Crystallographic School) at Stellenbosch University in 2018. Presently the establishment of the AfCA (African Crystallographic Association) is being pursued as a separate chapter from the IUCr (International Union of Crystallography) to be representative of the African continent.

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9.3. Benefits and financial implications for science & technology in South Africa

In support of the government's Vision 2030, this initiative provides an opportunity to support research for human resource development and the provision of core national neutron source facilities in order to create knowledge, thereby positioning local research and innovation to contribute to growth. Increased access to local facilities will boost training and development, thus opening up opportunities for competitive and beneficial science to be undertaken at large global research infrastructures like the ESS. The fundamental scientific knowledge acquired and the technology transfer through this participation will benefit society and play a key role in addressing many aspects of our challenges towards:

- National System of Innovation
- Knowledge-based economy
- High level of research / materials beneficiation / product development
- Employment of experts at MPR
- Industrial research that can have financial impact

Universities and research institutes are important driving forces underlying technological and industrial development. There is a fundamental relationship between research and higher education on the one hand and the international competitiveness of the economy on the other, although the essence of a knowledge-based economy is exploitation rather than simply adding to the knowledge base. Like all major research fields with a medium- and long-term application potential, neutron science contributes to innovation through interactive learning involving an innovation system or innovation clusters with many different players.

The content of this report highlights the potential benefits that can be derived from this field for stimulating a National Innovation system. It is well known that a functioning innovation system is an integral part of a country's strategic advancement/development. This report highlights the need in South Africa to competently build an innovative and technological business policy, taking a more long-term perspective, to create necessary conditions for the development of science and technology.

In addition, it is necessary to stimulate market mechanisms for independent financing of universities and research institutes, as well as to develop the practice of private initiatives and investment in the development of innovative activity.

The workshops highlighted the continuing studies on industrial components using neutron diffraction techniques, particularly in residual stress and materials characterisation. Previous neutron diffraction experiments on high integrity industrial components have resulted in very significant cost benefits to the South African power generation industry. An example of this is discussed.

Eskom's Research business unit partnered with Nelson Mandela University to develop the novel WeldCore® technique. A specially designed machine enables a coring tool to machine out a sample of 7mm diameter and approximately 25mm length from a thick walled component. The hole is repaired by the same machine using a Friction Hydro Pillar Processing weld. This process has been used to evaluate the rotor discs of eight high pressure turbine rotors which would otherwise have required

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immediate replacement at a cost of R100 million per unit. Validation of the technique involved detailed metallurgical assessment during weld process parameter development and through thickness residual strain analysis by neutron diffraction at the Institut Laue Langevin in France (experiment 1-01-58).

The NMU and Eskom research team won the 2011 National Science and Technology Forum Awards category for "Research leading to an innovation by a team" as well as the SA Premier Business awards 2014. This technique has been successfully implemented in three other outages on main steam pipe components, with savings of up to R50 million per group of components. The WeldCore® technique has been patented, and can be used on high integrity components across the power and petrochemical industry to reduce downtime, extend lifetime of equipment and reduce the risk of catastrophic failures.

10. Recommendations

South Africa has a small, but vibrant, multi-disciplinary neutron science community that performs high-level research utilising neutron techniques both at the National facilities, SAFARI-1 and iThemba LABS, as well as at leading international facilities. Experienced South African neutron users have established collaborations with prominent practitioners and facility personnel (instrument scientists). Many inexperienced neutron users have expressed interest in the benefits and value addition neutron techniques could add to their research. Similarly to the international situation, there is a general lack of acquaintance (sensitivity) with what the techniques can offer, as they have traditionally been seen as the province of purely fundamental research, largely for condensed matter physics.

Encourage and build an African collaborative agenda with countries that have research reactor installations through the programs of the International Atomic Energy Agency (IAEA) and specifically their AFRA (African Regional Cooperative Agreement) for Research, Development and Training Related to Nuclear Science and Technology program. Linkages already exist with Algeria and Morocco. iThemba LABS through AFRA has applied to host the Regional Designated Centres (RDCs) in Nuclear Instrumentation. Training at iThemba LABS is co-ordinated by the Southern African Institute for Nuclear Technology and Sciences (SAINTS) that accommodates post-graduate students (from Masters to Doctoral levels) registered with various universities across South Africa and partner universities in other African countries (Algeria, Botswana, Eswatini, Lesotho, Tanzania, Nigeria, Morocco, Cameroon, etc.) Other initiatives can be further explored by revisiting inter-governmental bi-lateral agreements.

Appropriate levels of funding will be required from the DSI to invest in the development of local facilities, as well as enable inherent growth in the South African neutron science community, both in size and stature, to the social and scientific benefit of South Africa, as well as all of Africa and the world community. It is important that mechanisms be created to ensure long term sustainability and career prospects to accommodate students trained in neutron beam line techniques to the benefit of the MPR and its facilities.

Flagship international centres are extremely well resourced having on offer instruments that cover the full spectrum of neutron scattering applications, benefitting diverse disciplines that include physics, chemistry, mineralogy, biosciences, material sciences, agricultural sciences, medical sciences,

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palaeontology, heritage sciences, engineering, product manufacture and beneficiation, etc., to the extent that beam line access is generally more than 200% oversubscribed.

Based on consultation with the South African research community with the Stakeholder Workshops the following is recommended:

- Training the next generation of neutron scientists should be a strategic necessity. Strongly motivate for the incorporation of neutron scattering techniques in university course work as part of education and training, as well as promoting the capabilities of the techniques to various science and engineering fields.
- Build on existing national capacity towards full exploitation of the capabilities and potential of the facilities at SAFARI-1 as a bridge to modern international flagship facilities. Invest in expanding the neutron beam laboratories as a national user facility. When fully exploited, it could accommodate a large percentage of the South African requirements, to enable easy access and run of the mill facilities.
- Government to provide a dedicated channel to facilitate financial assistance with the maintenance of unique and highly specialised equipment at the SAFARI-1 facilities.
- Government to financially support expansion of the experimental capabilities existing at the SAFARI-1 facilities, such as in-situ reaction studies.
- Replacement of SAFARI-1 with a well-equipped MPR needs to be seriously considered and pursued to ensure sustainability in neutron beam research to meet future user needs and grow the user base.
- Capitalization to expand the experimental capabilities such as in-situ reaction studies at SAFARI-1 that can be directly transferred to the MPR. An MPR replacement would be required in the future to meet user needs and grow the user base.
- Retain and strengthen NRF (KIC) financial support for continued access to high-brightness neutron sources internationally, such as ESS (future), ILL, ISIS, MLZ, NIST, PSI, etc. to complement and expand the techniques that do not exists in South Africa such as access to modern facilities equipped with in-elastic neutron capabilities, small-angle neutron scattering facilities and reflectometry.
- The South African government to explore the formation of an official partnership with the ESS to ensure that the South African training, research interests and capabilities (such as access to deuteration facilities) can be expanded and stimulated.

The main challenges are: (i) to implement a suite of state-of-the-art neutron scattering instruments at SAFARI-1; (ii) to build a solid neutron scattering user community; (iii) to train the human resources necessary for defining, implementing, operating and using the instruments. This poses a challenge to a laboratory aiming to become the leading institution in neutron science in Africa. A five-year outreach program needs to be implemented with the launching of the project, to target different audiences (national, regional, international and in-house scientists and technologists, decision makers, industry, general public) and through different channels (mailing lists, websites, brochures, topical meetings and workshops, presentations at national and international conferences, etc.).

11. Acknowledgments

The seminal role played by Dr Daniel Adams (DSI) to have South Africa included as an active participant within the BrighnESS2 project. Funding provided from the BrightnESS² project to facilitate the South African activities. All expert inputs received from ESS personnel under the leadership of Prof Dr Andreas Schreyer, as well as other international participants with the mini-symposia. iThemba LABS and Necsa personnel that did the ground work and facilitated the interactions. Authors of this document, i.e. Prof Andrew Venter and Mr Robert Nshimirimana from Necsa, and Dr Peane Maleka from iThemba LABS.

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13. Appendix 1 First South African BrightnESS2 Workshop

First South African Workshop on Capacity Building: Neutron Research in Collaboration with BrightnESS² partners

Date: 13 - 14 August 2019

Venue: NRF-iThemba LABS Auditorium, Cape Town, South Africa

Chairpersons: Dr. Peane Maleka (NRF-iThemba LABS) and Prof. Andrew Venter (Necsa)

Overview

The First South African Workshop on Capacity Building: Neutron Research was held at iThemba LABS, Cape Town on 13-14 August 2019. The workshop brought South African research scientists, engineers and technologists together with their counterparts from ESS. The meeting was hosted by the South African consortium (iThemba LABS and Necsa) led by the country's Department of Science and Innovation (DSI) and the National Research Foundation (NRF), included 14 participating universities, institutions and industrial partners.

The main focus for the workshop was an exchange of ideas on collaboration opportunities presented by the two national facilities, iThemba LABS and Necsa, in connection with the construction of ESS. Additionally, the workshop served to supplement the neutron-based research and innovations at iThemba LABS and Necsa, and explored the need for South Africans to consider an expansion in these fields. Given the focus areas at the South African facilities, there is always a need for the researchers to have access to global neutron sources that can provide complementary research opportunities.

The anticipated outcomes of the workshop were to:

- Familiarise potential new users to the existing research prospects that neutron sciences can offer;
- Compilation of a database of all relevant role players (researchers and institutions) within the area of neutron research in SA; the available expertise, current researchers that are actively involved, capabilities and infrastructure;
- Agree on the areas on neutron research of relevance to SA;
- Explore the need to enter into a partnership with ESS to enhance the neutron research capacities and capabilities in SA; and
- Agree on the high impact research areas that will form the basis for the collaboration with ESS;

The main outcome of this workshop, thematic areas on interests were identified for the South Africans, namely (Neutrons for Engineers; Crystallography: Organic Chemistry; Magnetism; Geosciences; Energy Storage & Conversion Materials; Palaeontology & Heritage Conservation; Catalysis/synthesis; Crystallography: Inorganic Chemistry; Nanomaterials; Life Sciences & Biology) and would be the main

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focus for follow-up workshop. The anticipated outcome of the second workshop was to finalise the document required to formulate the neutron research activities in South Africa, current status (Strength and Weaknesses) and future aspirations (Opportunities and Threats).

COVID-19 Pandemic regulations in early 2020 led to the cancellation of all in-person events across South Africa, a directive that is still in force currently. This prevented the 2nd South African Workshop planned for June 2020, from taking place. A meeting between all stakeholders (DSI, Necsa, iThemba LABS, and Thrust Coordinators) decided to replace the 2nd South Africa workshop with a series of virtual mini-symposia. An added advantage of hosting virtual mini-symposia was that experts from the ESS and other international facilities can be involved with the events.

Participants of the First South African Workshop at iThemba LABS, August 2019.

List of delegates participated during Workshop 1 at iThemba LABS

	Name	Affiliation
1	Albertus Smith	University of Johannesburg
2	Aletta Prinsloo	University of Johannesburg
3	Amogelang Bolokang	Council for Scientific and Industrial Research
4	Andre Strydom	University of Johannesburg
5	Andre Venter	Nelson Mandela University
6	Andreas Schreyer	European Spallation Source ERIC, Sweden
7	Andrew Jackson	European Spallation Source ERIC, Sweden
8	Andrew Venter	Necsa SOC Ltd
9	Andy Buffler	University of Cape Town
10	Bruce Mellado	University of the Witwatersrand and iThemba LABS

11	Catharine Esterhuysen	University of Stellenbosch
12	Charles Mokonoto	Department of Science and Innovation
13	Charles Sheppard	University of Johannesburg
14	Charlot Vandevoorde	iThemba LABS
15	Clifford Nxomani	NRF
16	Daniel Hattingh	Nelson Mandela University
17	Danny Adams	Department of Science and Innovation
18	Deshenthree Chetty	Mintek
19	Esna du Plessis	Sasol
20	Frikkie De Beer	Necsa SOC Ltd
21	Karen Cloete	NRF-iThemba LABS
22	Ken Andersen	European Spallation Source ERIC, Sweden
23	Kenneth Ozoemena	University of the Witwatersrand
24	Kudakwashe Jakata	University of the Witwatersrand
25	Lowry Conradie	NRF-iThemba LABS
26	Malik Maaza	NRF-iThemba LABS and UNESCO UNISA Africa Chair
27	Mlungisi Nkosi	NRF-iThemba LABS
28	Monika Hartl	European Spallation Source ERIC, Sweden
29	Nico Fischer	University of Cape Town
30	Nico Orce	University of the Western Cape
31	Ntombi Ditlopo	Department of Science and Innovation
32	Peane Maleka	NRF-iThemba LABS
33	Pieter Pistorius	University of Pretoria
34	Reinhard Botha	Nelson Mandela University
35	Robin Woracek	European Spallation Source ERIC, Sweden
36	Rudolph Nchodu	NRF-iThemba LABS
37	Sisa Pityana	CSIR-National Laser Centre
38	Suprakas Sinharay	Council for Scientific and Industrial Research
39	Tankiso Modise	Necsa SOC Ltd
40	Tanya Hutton	University of Cape Town
41	Thomas Leadbeater	University of Cape Town
42	Trevor Sewell	University of Cape Town
43	Willie du Preez	Central University of Technology, Free State
44	Zina Ndlovu	NRF-iThemba LABS
45	Zoë Fisher	European Spallation Source ERIC, Sweden

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brightness²

Workshop program, Day 1: 13 August 2019

First South African Workshop on Capacity Building: Neutron Research in Collaboration with BrightnESS² partners		
Date	Day 1: 13 August 2019	
Venue	NRF-iThemba LABS Auditorium	
Chairperson(s)	Dr. Peane Maleka (iThemba LABS) and Prof. Andrew Venter (Necsa)	
Time		
08h30 - 09h00	Arrival and Registration	All
09h00 - 09h10	Safety brief and Induction	NRF-iThemba LABS RSHEQ Department
09h10 - 09h30	Welcome Address	Dr. Nxomani (NRF-Deputy CEO)
09h30 - 10h30	Opening Address	Dr. Adams (DST Chief Director)
10h30 - 11h00	NRF-iThemba LABS overview	Dr. Nchodu (NRF-iThemba LABS Deputy Director)
11h00 - 11h30	Coffee/Tea break	All
11h30 - 12h00	ESS Introduction and Overview	Prof. Dr. Andreas Schreyer (ESS Director of Science)
12h00 - 12h30	ESS Instruments for slow, thermal and fast Neutrons: Current and future Opportunities	Ken Andersen
12h30 - 13h00	Life Science and Pharmaceutical Research	Zoë Fisher
13h00 - 13h30	Soft Matter Challenges	Andrew Jackson
13h30 - 14h30	Lunch break	All
14h30 - 15h00	Structural and Light Weight Materials	Robin Woracek
15h00 - 15h30	Chemistry, Catalysis and Energy	Monika Hartl
15h00 - 16h00	Time for general Q & A	ESS Delegation
16h00 - 16h20	Cofee/Tea break	All
16h20 - 16h35	NRF-iThemba LABS neutron beam facility	Zina Ndlovu
16h35 - 17h05	Radiation Biophysics at NRF-iThemba LABS	Charlot Vandevoorde
17h05 - 17h35	Neutron diffraction at SAFARI-1 complemented by X-ray diffraction	Andrew Venter
17h35 - 18h00	Neutron Radiography at Necsa	Frikkie De Beer
18h00 - 20h00	Social Event	All
20h00 - ??	**Departure to Hotel**	

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Workshop program, Day 2: 14 August 2019

First South African Workshop on Capacity Building: Neutron Research in Collaboration with BrightnESS² partners		
Date	Day 2: 14 August 2019	
Venue	NRF-iThemba LABS Auditorium	
Convenor	Department of Science and Technology	
Time		
09h00 - 09h30	Workshop briefing	DST delegate
09h30 - 11h00	Breakaway discussions: Slow/Thermal Neutrons	venue to confirmed
	Breakaway discussions: Fast Neutrons	venue to confirmed
11h00 - 11h30	Coffee/Tea break	All
11h30 - 12h30	Breakaway discusions and reporting	All
12h30 - 13h00	SA topical champions and Action Plans for Workshop 2	All
13h00 - 14h00	Lunch break	All
14h00 - 16h00	iThemba LABS Facility Tours	
14h00 - 16h00	Departure to Airport*	
16h30 - 17h00	Departure to Hotel*	

14. Appendix 2. Second South African-BrightnESS2 Workshop

Capacity Building: Neutron Research in Collaboration with BrightnESS² partners

Date: June 2020 -

Venue: Venue close to Necsa, Pelindaba, North West Province, South Africa

Chairpersons: Dr. Peane Maleka (NRF-iThemba LABS) and Prof. Andrew Venter (Necsa)

Overview

The purpose of this phase of the project was to involve the research community at large by having topical sessions run by Thrust Coordinators identified during Workshop 1. The meetings needed to give high-level overviews of the applications and hot research topics, supported by talks from experienced South African neutron users, as well as people that have research questions that could possibly answered by neutron techniques. The workshop had to be informative and interactive. It was envisaged to run the workshop during June 2020, to ensure maximal participation by academia.

Due to the COVID-19 pandemic, large gatherings were not possible. In consultation with the Thrust Coordinators the decision was made to have Workshop 2 replaced by individual mini-symposia run on a virtual basis over the period August 2020 to January 2021. This enabled much larger international participation to provide expert inputs. Using existing contacts internationally, and referrals from the ESS, it was possible to have at least one topical expert per mini-symposium. Details on the mini-symposia are indicated in Table A2.1, with Tables A2.2 to A2.11 giving specific details on each. Tables A2.12 to A2.21 summarise the participants with each event. Note that these have been completed as complete as possible, but due to the visual platform and open participation platform, not all participants could be identified from their login details. The envisaged outcome of each mini-symposium was to provide information towards:

SWOT analysis specifically related to our research interests and from this identify:

- What are the compelling science questions and issues that can be addressed with neutron techniques?
- How can we engage meaningfully in these questions?
- What are the niche scientific areas that these could contribute to?
- What is the format of access do we require for South African facilities at Necsa (SAFARI-1) and iThemba LABS, as well as abroad with the ESS (European Spallation Source ERIC)?
- What capacities do we need to develop as a country so that we can optimize the value adding that neutron techniques can offer?

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Table A2.1: Details on mini-symposia

Thrust Area	Coordinator(s)	Date and time
Neutrons for Engineers	Dr. Mark Newby (Eskom Holdings) Prof. Danie Hattingh (Nelson Mandela University)	05 August 2020; 14:00 - 16:00
Crystallography: Organic Chemistry	Prof. Catharine Esterhuysen (Stellenbosch University)	25 August 2020; 10:00 - 12:00
Magnetism	Prof. André Strydom (University of Johannesburg)	07 September 2020; 14:00 - 16:00
Geosciences	Prof. Albertus Smith (University of Johannesburg)	10 September 2020; 10:00 - 12:00
Energy Storage & Conversion Materials	Prof. Kenneth Ozoemena (University of the Witwatersrand)	15 September 2020; 14:00 - 16:00
Palaeontology & Heritage Conservation	Dr. Amélie Beaudet (University of Cambridge; University of the Witwatersrand)	18 September 2020; 14:00 - 16:00
Catalysis /synthesis	Prof. Nico Fischer (University of Cape Town)	22 September 2020; 13:00 - 15:00
Crystallography: Inorganic Chemistry	Prof. Dave Billing (University of the Witwatersrand)	23 September 2020; 11:00 - 13:00
Nanomaterials	Prof. Ray Suprakas (CSIR) and Prof. Malik Maaza (iThemba LABS)	28 September 2020; 14:00 - 16:00
Life Sciences and Biology	Prof. Maria Papathanasopoulos (University of the Witwatersrand)	19 January 2021; 10:00 - 13:00

Table A2.2: "Neutrons for Engineers" mini-symposium, 05 August 2020 via MS Teams platform, coordinated by Dr Mark Newby (Eskom Holdings) and Prof Danie Hattingh (Nelson Mandela University).

Time	Topic	Speaker
14:00 - 14:20	Review of previous neutron diffraction experiments with an industrial focus	Mark Newby (Eskom Holdings)
14:20 - 14:40	Evaluation of the Laser Shock Peening Process for Turbine Blade Application using Neutron Techniques	Daniel Glaser (National Laser Centre)
14:40 - 15:00	The use of neutron diffraction in physical metallurgy research in the Department of Materials Science and Metallurgical Engineering	Pieter Pistorius (University of Pretoria)
15:00 - 15:15	Overview of neutron diffraction facilities at SAFARI-1	Deon Marais (Necsa SOC Ltd)
15:15 - 15:40	Comparative assessment of industrially relevant techniques and ESS capabilities	Axel Steuwer (University of Malta)
15:40 - 16:00	Development of Position Paper: Open discussion	All speakers

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Table A2.3: "Neutrons for Chemistry" mini-symposium, 25 August 2020 via ZOOM platform, coordinated by Prof Catharine Esterhuysen (Stellenbosch University).

Time	Topic	Speaker
10:00 - 10:30	Neutron scattering in industry	Esna du Plessis (SASOL)
10:30 - 10:45	Chemistry and material science using neutrons	Monika Hartl (ESS)
10:45 - 10:55	Neutron powder diffraction facility at SAFARI-1	Andrew Venter (Necsa)
10:55 - 11:20	Perspectives on how access to neutron techniques at SAFARI-1, iThemba LABS and ESS could benefit research	Alice Brink (UFS) Susan Bourne (UCT) Delia Haynes (SU) Manuel Fernandes (Wits) Catharine Esterhuysen (SU)
11:20 - 12:00	Discussion and Feedback	All speakers

Table A2.4:"Neutrons for Magnetism" mini-symposium, 07 September 2020 via ZOOM platform, coordinated by Prof André Strydom (University of Johannesburg).

Time	Topic	Speaker
14:00 - 14:05	Welcome	André Strydom (UJ)
14:05 - 14:20	Neutron diffraction facility at SAFARI-1	Andrew Venter (Necsa SOC Ltd)
14:20 - 15:00	An update of the European Spallation Source ERIC and the cold time of flight spectrometer, CSPEC, as a future tool for the study of magnetic excitations	Pascale Deen (ESS)
15:00 - 15:20	Neutron scattering: an indispensable tool for studying magnetism in correlated electron systems	André Strydom (UJ)
15:20 - 15:40	Neutron diffraction studies in Cr based bulk alloys, thin films and nanoparticles (I)	Aletta Prinsloo (UJ)
15:40 - 16:00	Neutron diffraction studies in Cr based bulk alloys, thin films and nanoparticles (II)	Charles Sheppard (UJ)
16:00 - 16:30	Open discussion on way forward / Closing Comments	All speakers

Table A2.5:"Neutrons for Geosciences" mini-symposium, 10 September 2020 via ZOOM platform, coordinated by Prof Albertus Smith (University of Johannesburg).

Time	Topic	Speaker
10:00 - 10:05	Welcome	Bertus Smith (UJ)
10:05 - 10:50	Neutron diffraction for Geosciences: texture and stress analyses	Vladimir Luzin (ANSTO)
10:50 - 11:05	Facilities at Necsa in support of Geosciences	Andrew Venter (Necsa)
11:05 - 11:25	X-Ray CT and early Earth biological textures	Bertus Smith (UJ)
11:25 - 11:45	X-Ray CT and applications to minerals processing	Carene Mouton (UJ)
11:45 - 12:05	X-ray CT shows ellipsoidal inclusion-free halo around cubic phase in Brazilian carbonado: First strain analysis of pre-solar material?	Sharad Master (Wits)
12:05 - 12:30	Open discussion on way forward / Closing Comments	All speakers

Table A2.6:"Neutrons for Energy Storage & Conversion Materials" mini-symposium, 15 September 2020 via ZOOM platform, coordinated by Prof Kenneth Ozoemena (University of the Witwatersrand).

Time	Topic	Speaker
10:00 - 10:05	Welcome	Kenneth Ozoemena (Wits)
10:05 - 10:35	The unique structural insights and challenges of using neutron diffraction to study battery materials	William Brant (Uppsala University, Sweden)
10:35 - 11:05	Small angle neutron scattering as a tool to probe battery electrodes	Charl Jafta (ORNL, USA)
11:05 - 11:20	The application of neutron scattering for lithium-ion battery	Mesfin Kebede (CSIR, South Africa)
11:20 - 11:35	Sharing research experience with powder neutron diffraction analysis for energy storage materials	Aderemi Haruna (Wits, South Africa)
11:35 - 11:50	Large-scale research facilities for technological and economic development	Dean Barrett (Wits, South Africa)
11:50 - 12:05	Facilities at NECSA	Andrew Venter (NECSA)
12:05 - 12:30	Open discussion on way forward / Closing Comments	All speakers

Table A2.7: "Neutrons for Palaeontology & Heritage Conservation" mini-symposium, 18 September 2020 via ZOOM platform, coordinated by Dr Amélie Beaudet (University of Cambridge; University of the Witwatersrand).

Time	Topic	Speaker
14:00 - 14:05	Welcome	Amélie Beaudet (UC and Wits)
14:05 - 14:50	What neutron imaging can tell us about our distant ancestors	Burkhard Schillinger (MLZ, Germany)
14:50 - 15:10	Neutron tomography in Palaeontology	Amélie Beaudet (University of Cambridge and Wits)
15:10 - 15:30	The use of Neutron and X-ray imaging in Palaeontology and Heritage Conservation	Robert Nshimirimana (Necsa)
15:30 - 16:30	Questions and discussion on way forward / Closing Comments	All speakers

Table A2.8: "Neutrons for Catalysis" mini-symposium, 22 September 2020 via ZOOM platform, coordinated by A/Prof Nico Fischer (University of Cape Town).

Time	Topic	Speaker
13:00 - 13:10	Welcome and setting the scene	Nico Fischer (UCT, SA)
13:10 - 13:30	Examining the temporal behaviour of the hydrocarbonaceous overlayer on an iron-based Fischer Tropsch synthesis catalyst	David Lennon (Univ. of Glasgow, UK)
13:30 - 13:35	Q&A	
13:35 - 14:00	Neutron techniques in industrial catalysis development and research	Esna du Plessis (SASOL, SA)
14:00 - 14:05	Q&A	
14:05 - 14:20	Exploring catalytic reactions with neutron scattering	Monika Hartl (ESS, Sweden)

14:20 - 14:40	The ISIS Neutron and Muon Source	Steward Parker (ISIS, UK)
14:40 - 14:55	Neutron powder diffraction facility at SAFARI-1	Andrew Venter (Necsa, SA)
14:55 - 15:30	General discussion on the need and opportunities of the SA Catalysis community	All speakers

Table A2.9:"Neutrons for Chemistry: Crystallography: Inorganic Chemistry" mini-symposium, 23 September 2020 via ZOOM platform, coordinated by Prof Dave Billing (University of the Witwatersrand).

Time	Topic	Speaker
10:30 - 10:40	Welcome and Introduction	Dave Billing (Wits)
10:40 - 11:20	Scientific Capabilities of the DREAM Diffractometer at ESS	Mikhail Feygenson (ESS)
11:20 - 11:40	A neutron diffraction study of the heterogeneity problem of retained austenite in cast-iron grinding balls	Ernst Ferg (NMU)
11:40 - 12:00	Neutron powder diffraction facility at SAFARI-1	Andrew Venter (Necsa)
12:00 - 12:20	Correlation of ferroic orders in multiferroics materials for energy applications	Daniel Wamwangi (Wits)
12:20 - 12:40	Structure and thermoresponsive behaviour of porous and non-porous borophosphates	Wilson Mogodi (UCT)
12:40 - 13:00	Structure Property Correlation in SOFC/SOEC electrolytes	Dave Billing (Wits)
13:00 - 13:30	Questions and discussion on way forward / Closing Comments	All speakers

Table A2.10: "Neutrons for Nanomaterials" mini-symposium, 28 September 2020 via ZOOM platform, coordinated by Prof Suprakas Sinha Ray (CSIR) and Prof Malik Maaza (iThemba LABS and UNISA).

Time	Topic	Speaker
14:00 - 14:05	Welcome	Suprakas Sinha-Ray (CSIR) and Prof. Malik Maaza (iThemba LABS&UNISA)
14:05 - 14:30	Applications of Scattering in Polymer Nanocomposite Research: An overview	Jayita Sinha Roy (CSIR)
14:30 - 15:00	Investigating Nanomaterials with Neutrons - Current and Future Opportunities"	Andrew Jackson (ESS)
15:00 - 15:30	A journey in the world of Neutron Reflectivity	Alain Gibaud (University of Le Maine)
15:30 - 15:50	Surface & interface phenomena in nanostructures by neutron reflectometry	Malik Maaza (iThemba LABS & UNISA)
15:50 - 16:05	Neutron powder diffraction facility at SAFARI-1	Andrew Venter (Necsa)
16:05 - 16:30	Questions and discussion on way forward / Closing Comments	All speakers

Table A2.11:"Neutrons for Life Sciences and Biology" mini-symposium, 19 January 2021 via ZOOM platform, coordinated by Prof Maria Papathanasopoulos (University of the Witwatersrand).

Time	Topic	Speaker
10:00 - 10:10	Introduction: Background on SA-BrightnESS2 project Welcome	Andrew Venter (Necsa, SA) Maria Papathanasopoulos (WITS, SA)
10:10 - 10:25	General intro to neutrons & life sciences	Zoë Fisher (ESS, Sweden)
10:25 - 10:40	Examples of how X-ray and Neutron scattering can aide at updating markers for atherosclerosis development	Marité Cárdenas (Malmö University, Sweden)
10:40 - 10:55	SANS for structural and dynamical studies of biomacromolecular complexes in solution	Frank Gabel (Institut de Biologie Structurale, France)
10:55 - 11:10	The relative importance of different technologies for protein structure determination from the perspective of a South African Structural Biologist	Trevor Sewell (UCT, SA)
11:10 - 11:25	Hidden secrets of enzyme mechanism revealed by neutron crystallography: heme peroxidases	Peter Moody (University of Leicester, UK)
11:25 - 11:40	The use of small-angle neutron scattering (SANS) to understand dynamic changes in CD4 structure implicated in HIV-1 infection	Gavin Owens (WITS, SA)
11:40 - 11:55	Neutron Scattering in integrated structural biology; Closing remarks and summary	Trevor Forsyth (ILL, France)
11:55 - 12:05	·Substrate position and hydrolysis in the amidases ·Future prospects for Neutron Scattering in South Africa	Stanley Makumire (UCT, SA) Andrew Venter (Necsa, SA)
12:05 - 13:00	General discussion	All speakers

Table A2.12: Participants list with "Neutrons for Engineers" mini-symposium, 05 August 2020

No.	Name	Institute	Email
1	Peane Maleka	iThemba LABS	pmaleka@tlabs.ac.za
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Table A2.13:List of participants with "Neutrons for Crystallography, Organic Chemistry" mini-symposium, 25 August 2020.

No.	Name	Institute	email
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Table A2.14:List of participants with "Neutrons for Magnetism" mini-symposium, 07 September 2020.

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Table A2.15:List of participants with "Neutrons for Geosciences" mini-symposium, 10 September 2020.

No.	Name	Institute	email
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Table A2.21:List of participants with "Neutrons for Life Sciences and Biology" mini-symposium, 19 January 2021.

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