

CURRENT LANDSCAPE AND FUTURE DIRECTION FOR NEUTRON SCATTERING IN SOUTH AFRICA



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1. Introduction

Neutron scattering techniques are very versatile research probes applied to the instigation of microstructural phenomena in materials, using high flux, low energy neutron beams in conjunction with specialised instruments. They find application in diverse fields of the sciences, health, agriculture and engineering to assist in understanding the properties of matter on the atomic scale. Major technological advances and challenges have their origin in understanding and exploiting the physics and chemistry of materials such as the dramatic revolutions in transport and manufacturing, the growth of computing and the internet and the steady increase in life expectancy. Neutron scattering facilities are highly specialised and exist at research centres worldwide.

This publication is an output from South Africa's active participation within Work Package 2 (WP2) of the BrightnESS² (Bringing Together a Neutron Ecosystem for Sustainable Science with ESS) project [1,2] of the European Commission (EC), aimed at "Establishing a common roadmap and implementation strategy for future neutron capability". Benefits to the South African research community include establishing contacts with international counterparts, familiarisation of typical applications and access to the European neutron science community and facilities. Within the BrightnESS² consortium, the South African partners, Necsa SOC Ltd. and NRF-iThemba LABS, facilitated the engagement of the science community on behalf of the Department of Science and Innovation (Basic Sciences and Infrastructure), to promote neutron science in South Africa as an imperative component and contributor to a knowledge-based economy in the short, medium and long term. This was accomplished with workshop sessions held in South Africa during August 2019, followed by ten topical on-line mini-symposia held virtually from September 2020 to January 2021. The overall objectives with these events were to engage the South African neutron community, attract new interest, to assess short and long term needs, as well as identify modalities for international access, with special

interest in the European neutron landscape and the European Spallation Source ERIC (ESS) that is being established in Sweden as the future premier Neutron Scattering facility.

1.1 History and properties of neutrons

The significant interest and utilisation of neutrons in scientific research dates to their discovery in 1932 [3]. The inherent value that their particle and wave duality contributions 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 ($> 4 \text{ \AA}$) neutrons, which attracted chemists and later biologists to neutron scattering. During the last decade, engineers, materials and earth scientists, as well as palaeontologists, to name but a few, entered the fray by exploiting the value addition neutron scattering and attenuation studies contributed to research in their respective fields.

Neutrons interact with matter through all four forces, namely, the strong, weak, electromagnetic and gravitational. The interaction via the strong force makes neutrons a unique and ideal probe in condensed matter, with significant advantages over other forms of radiation in the study of microscopic structure and dynamics. The following main characteristics equip neutrons as increasingly important probes for research by virtue of their unique properties:

- » Subatomic particles. Neutrons are subatomic particles with similar mass as protons, but with neutral electrical charge.
- » 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 \AA), 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 primarily 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, the scattering cross-section of an atom generally varies between isotopes of the same element, enabling exploitation of isotopic substitution methods to yield information on structure and dynamics in great detail. This facilitates the use of contrast variation in complex systems, for example studying the nucleic acid or the protein component of a virus.
- » 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 reptation (thermal motion), through to molecular vibrations and lattice modes, to eV transitions within the electronic structures of materials.
- » Neutrons possess a magnetic moment. The magnetic moment is ideally suited to the study of microscopic magnetic structures and magnetic fluctuations that underpins magnetic phenomena in materials.
- » Neutrons perturb the experimental system weakly. This greatly facilitates interpretation and often neutron scattering provides the most reliable scientific results in areas as diverse as the structure of water or the strain mismatch in superalloys as found 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 rendering them a true microscopic bulk probe which allows the incorporation of complex sample environments such as furnaces, cryostats, and pressure cells that 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 understanding interactions in condensed matter which can be directly linked to the physical and chemical properties experienced in the everyday world. 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. Neutrons furthermore enable studies of chemicals which affect the environment, materials for health – from new materials for hip implants to gels that can help babies with cleft palates.

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 non-invasively and non-destructively.

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.

The benefits and contributions of neutron scattering techniques to science were formally recognised with the joint awards of the 1994 Nobel Prize for Physics to Bertram N. Brockhouse (Canada) and Clifford G. Shull (USA) “for pioneering contributions to the development of neutron scattering techniques for studies of condensed matter” in the 1950s [4]: Brockhouse “for the development of neutron spectroscopy”; Shull “for the development of the neutron diffraction technique”.

1.2 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 neutrons are released by bombarding a heavy-metal target with high-energy particles from a high-power accelerator. These two processes are shown in Figure 1.

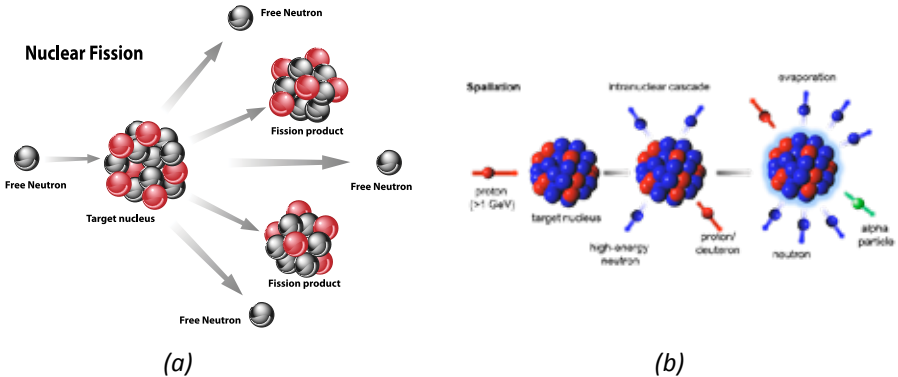


Figure 1: Two dominant methods of producing free neutrons for use in neutron scattering applications, i.e. (a) fission and (b) spallation (Source: <https://elena-neutron.iff.kfa-juelich.de/neutron-facilities/>).

Figure 2 shows the advancement in thermal neutron flux levels attained over the last 9 decades. 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) that become useful in neutron scattering applications when thermalized to meV energies. The thermalisation process results in neutrons with a broad band of highly selectable wavelengths of angstrom (\AA) dimensions, where the Maxwell distribution of energies are characterised by the temperatures of the moderators. The energy distribution of the neutrons can be shifted

to higher energies (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).

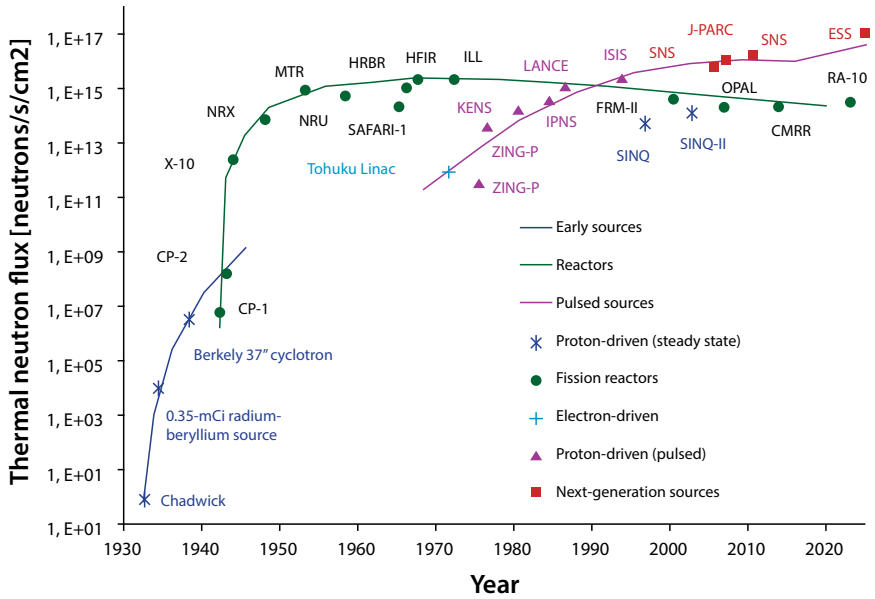


Figure 2: The evolution of thermal neutron source fluxes since the discovery of the neutron as adapted from [5].

Developments in accelerator-based pulsed (spallation) sources are pushing the envelope with modern facilities rendering the highest neutron brightness attainable today. Spallation facilities produce powerful bursts of fast neutrons that after moderation render slow and cold neutrons sources that enable studies of a very broad range of applications in pure and applied neutron science.

Notwithstanding the time-averaged flux (neutrons per second per unit area) of the most powerful pulsed source being low in comparison to reactor sources, these two modes of producing free neutron beams offers highly complementary probes of matter. Neutron facilities are large scale infrastructures that welcome international User utilisation and collaborations from diverse fields of interest.

1.3 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 the study of the structure (positions) and dynamics (motions) 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. While other techniques can provide information either within the same spatial range or the same temporal range, neutron scattering provides a unique combination of structural and dynamic information [6].

By employing the appropriate wavelength range, and magnetic and nuclear moments, in conjunction with their weak interaction with matter, various application techniques, summarized in Figure 3, are employed to study time and length scale (structure and motion) phenomena.

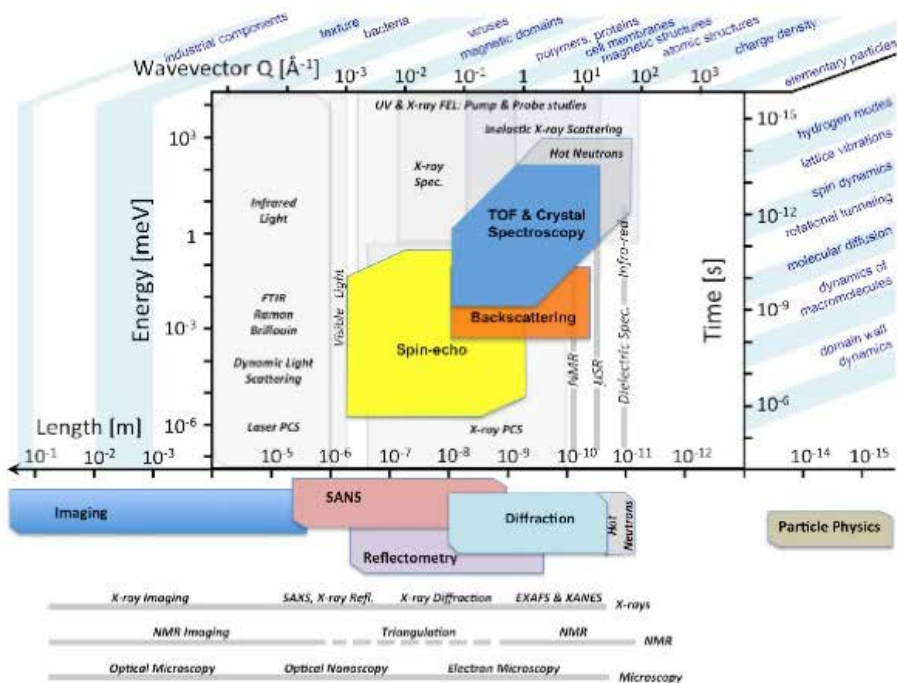


Figure 3: Applications of neutron scattering techniques to study structure and motion [6]. For comparison, the typical length scales probed by complementary techniques are shown at the bottom.

Neutron scattering techniques thus find vast application in many science, engineering and technology (SET) sectors as depicted in Figure 4.

1.4 Landscape of neutron scattering facilities

Most of the neutron sources exist in Europe followed by Asia, with a growing interest from Africa (i.e. Ethiopia, South Africa, Tanzania, Uganda and Zambia) to expand their nuclear science and technology programmes. There are 11 new neutron sources under construction and 14 planned world-wide. Figures 5 and 6 indicate the distribution of operational accelerator-based and research reactor neutron sources [7].

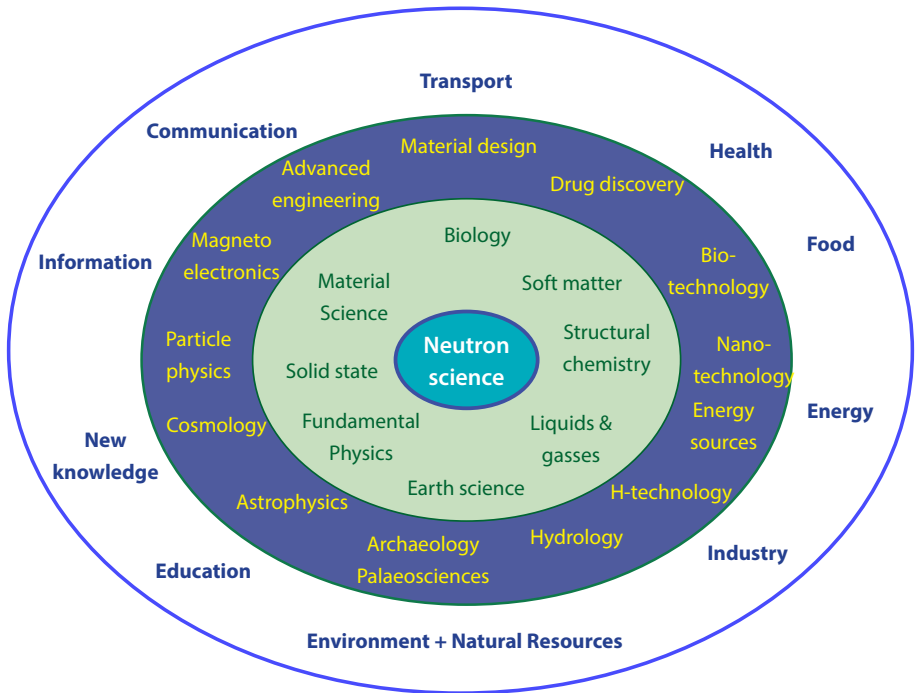


Figure 4: Applications of neutron sciences in SET sectors.

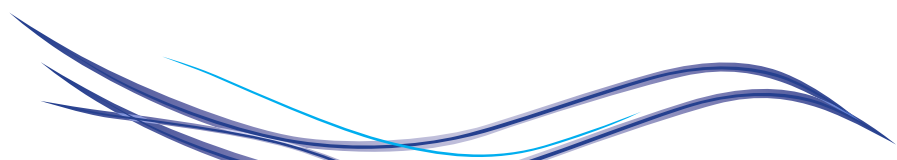
Recent research reactor additions have been FRM-II (at the MLZ Germany), OPAL (at ANSTO in Australia), CARR (in China) and PIK (in Russia). A number of facilities are currently under construction with the RA-10 facility in Argentina being in an advanced stage. A number of spallation sources have recently 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.



Figure 5: Facilities with 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 [7].



Figure 6: Facilities equipped with neutron scattering instruments. Total instruments encompass 362 located in 23 countries. These comprise 128 diffractometers, 104 spectrometers, 130 other instruments such as small angle scattering, neutron reflectometry, etc. There are 54 neutron imaging instruments (lower flux requirement) in 37 countries, 4 at spallation sources, 2 non-spallation accelerator-based sources, 1 at a pulsed research reactor and 47 at research reactors [7].















































































1.4.1 Neutron scattering instrument suite at the European Spallation Source ERIC

The ESS is currently under construction in Sweden as the most advanced spallation neutron source that employs a long-pulse, high flux, flexible resolution and large bandwidth. This results in an order-of-magnitude gain in performance of its instruments. The ESS will provide a suite of 22 world-leading instruments, shown in Figure 7. The facility, including all the instruments, is designed with due consideration of new and unique instrumental capabilities, to provide the means to maximise scientific output and achieve breakthroughs across a broad spectrum of physical and biological sciences. The superior brightness will facilitate the use of neutron scattering 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 study under more extreme conditions a number of transformative areas such as:

- » 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.
- » Parametric studies, covering large volumes of parameter space such as temperatures, flow conditions, magnetic fields, pressures, 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.

Further details can be found in [8].

Large-Scale Structures	ODIN Imaging Instrument					
	SKADI General Purpose SANS					
	LoKI Broadbands SANS					
	Surface Scattering					
	FREIA Horizontal Reflectometer					
	Estia Vertical Reflectometer					
Diffraction	HEIMDAL Powder Diffractometer					
	DREAM Powder Diffractometer					
	Monochromatic Powder Diffractometer					
	BEER Engineering Diffractometer					
	Extreme Conditions Diffractometer					
	MAGIC Magnetism Diffractometer					
	NMX Macromolecular Diffractometer					
Spectroscopy	CSPEC Cold Chopper Spectrometer					
	Broadband Spectrometer					
	T-REX Thermal Chopper Spectrometer					
	BIFROST Crystal Analyser Spectrometer					
	VESPA Vibrational Spectroscopy					
	MIRACLES Backscattering Spectrometer					
	High-Resolution Spin-Echo					
	Wide-Angle Spin-Echo					
	Particle Physics Beamline					

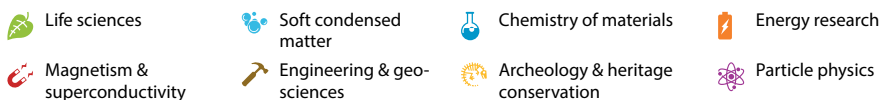


Figure 7: ESS instrument suite. Highlighted and named instruments (e.g. ODIN) are currently in construction. The others are the remaining instruments from the Technical Design Report reference suite, which serve as placeholders for instruments 16–22. The main scientific communities addressed by the instruments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

1.4.2 Large-scale neutron research facilities in South Africa

1.4.2.1 Necsca

SAFARI-1 (South African Fundamental Atomic Research Installation) [9] 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 Necsca SOC Ltd. The reactor project was initiated in 1960 and commissioned in March 1965. SAFARI-1 has now been in routine operation for more than 57 years and is a major producer of medical and industrial isotopes for both domestic and international clients. It also provides neutron beam lines 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 at least 2030.



Figure 8: *Paramic view of the 20 MW SAFARI-1 research reactor building.*

Beam line facilities at SAFARI-1 are equipped for the applications neutron powder diffraction (PITSI instrument [10]), as well as neutron strain scanning (MPISI instrument [11]), with a neutron radiography facility under modernisation (INDLOVU) [12].

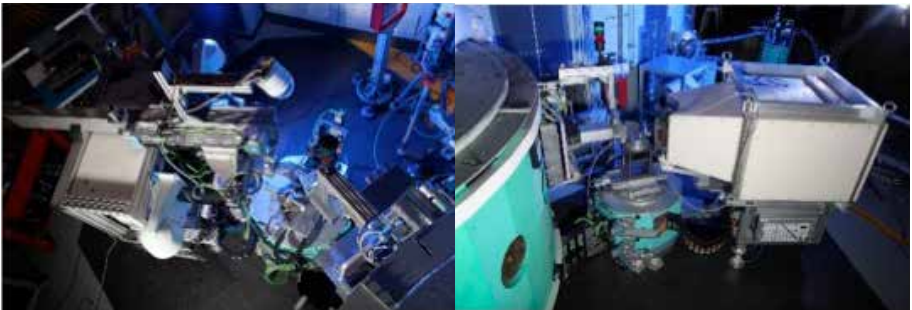
Table 1: Characteristics of neutron diffraction instruments at SAFARI-1

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

Beam component	PITSI instrument	MPISI instrument
Detector	Pseudo area detector: 15 x Reuter Stokes tubes giving active area 660 mm (hor) x 375 mm (ver)	Denex 300 x 300 mm ² area detector
	Two-theta range: $10^\circ \leq 2\theta \leq 120^\circ$	Two-theta range: $10^\circ \leq 2\theta \leq 110^\circ$
Resolution	$\Delta d/d = 3 \times 10^{-3}$	$\Delta d/d = 3 \times 10^{-3}$
Sample environments	Top-loader vacuum furnace: $400 \text{ K} < T < 1800 \text{ K}$ Bottom-loader cryostat: $4.5 \text{ K} < T < 320 \text{ K}$ Top-loader cryostat: $1.5 \text{ K} \leq T \leq 800 \text{ K}$	
Data acquisition	All functionalities fully programmable SICS (SINQ Instrument Control System) Gumtree: Graphical user interface & command line script files	
Data format	NeXus, HDF5 encoded	
Data processing	ScanManipulator	



Figure 9: Neutron diffraction facility at SAFARI-1.



(a)

(b)

Figure 10: Close up views of the neutron diffraction instruments (a) MPISI and (b) PITSI at SAFARI-1.

1.4.2.2 iThemba LABS

NRF-iThemba Laboratories for Accelerator Based Sciences (iThemba LABS) is a national facility of the National Research Foundation. Activities 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, respectively providing intense beams of light ions and beams of polarised light ions or heavy ions, as well as 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 surface science studies.



Figure 11: Separated Sector Cyclotron at the NRF-iThemba LABS Cape Town campus.

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 [13]. The focus is on providing research with radiation for scientific purposes through the acceleration of charged particles using the SSC, the Van der Graaff Accelerators and other appropriate technologies.

The SSC generates secondary quasi-monoenergetic neutron beams (via the (p,n) reaction) with peak energies ranging from 30 to about 200 MeV through the acceleration of protons in the energy range 25 to 200 MeV. A beam pulse selector suppresses a chosen fraction of proton bunches to enlarge the time interval between pulses, which allows time of flight measurements. The ${}^7\text{Li} (p, n) {}^7\text{Be}$ reaction is typically employed to produce neutrons, although natural beryllium and carbon targets have also been used from time to time. The energy spectra of the neutron beams generated by the $p + \text{Li}$ reaction at neutron emission angles of 0° up to 16° have two main components namely a high-energy (quasi-monoenergetic) peak of energy a few MeV less than that of the incident protons and a low-energy continuum extending from the high-energy peak towards lower energies. The spectrum and intensity of the low energy continuum is almost independent of angle for angles up to 16° . Thus, subtracting a measured detector response produced in the 16° beam (after appropriate normalization) from that measured at 0° yields an effective measurement associated with a nearly monoenergetic neutron beam.

1.4.3 Future South African neutron research facilities

1.4.3.1 Multi-Purpose Reactor at Necsa

With the SAFARI-1 Research Reactor approaching the end of its licenced lifetime, a project is 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 Reactor (MPR). This project was approved by Cabinet on 14 September 2021 [14].

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 thermal as well as cold neutron sources to provide neutrons with a variety of 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. The NBLC is envisaged to be the leading institution in neutron scattering science on the African continent and contribute to the international landscape.

It is envisaged that the MPR will be equipped with a suite of state-of-the-art beam line instruments comprising neutron powder diffraction (respectively high-resolution and high intensity), engineering and material science, single crystal diffraction, as well as neutron imaging. These are the most relevant neutron beam techniques for materials research. These will be complemented by 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 should be combined with polarization analyses, as well as extensive sample environments for in-situ parametric studies under simulated operational and extreme conditions. As examples of such modern facilities [15], [16] and [17] typically show the layout of beam lines instruments in the reactor beam hall as well as in the neutron guide hall areas of the installations.

1.4.3.2 Neutron beam facility at iThemba LABS

The neutron beam facility at iThemba LABS is used for fundamental physics research [18], cross section measurements [19], radiation biology experiments [20] and detector development and calibrations [21], especially for dosimetry at flight altitudes and in space.

The facility is designated as the South African neutron metrology laboratory in line with the International Committee for Weights and Measures Mutual Recognition Arrangement (CIPM MRA) 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 [22].

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 [23].

2. South African stakeholder engagements

This project formed part of Work Package 2 of the BrightnESS² project of the European Commission. A specific activity under Task 2.2 was to afford South Africa the opportunity to determine the “User Needs” of its neutron scattering community with suggested ways to accommodate their present and future needs. This determination has been done in the form of two stakeholder consultation Workshops. Workshop 1 was organized in August 2019 at iThemba LABS Cape Town 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. An overview of this workshop is provided in Appendix 1: First South African BrightnESS² Workshop. An outcome from this event has been the identification of ten scientific Thrusts within which the 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 researchers were identified to coordinate the second Workshop aimed at a much larger participation. This was scheduled for June 2020, but had to be reconfigured due to the COVID-19 pandemic that prohibited travel and meetings from March 2020. As an alternative approach, this Workshop was hosted as ten specialised virtual topical mini-symposia on the respective Thrusts. Participation was invited from existing contacts from the meeting conveners, Thrust Coordinators, as well as communications with Deans of Research at all prominent South African universities. This modality further enabled participation by topical experts internationally. An overview of this workshop is provided in Appendix 2: Second South African-BrightnESS² Workshop. The aim of the workshops was to inform participants on the value addition that neutron scattering techniques can offer in expanding their battery of existing research techniques with the focus on determining:

- » Compelling science questions that can be addressed with neutron techniques;
- » The niche scientific areas that these could contribute to;
- » The format of access required to South African facilities, as well as abroad including the ESS;
- » Capabilities that need to be developed as a country so that we can optimise the value addition that neutron techniques can offer.

2.1 South African prominent investigators within neutron science community

Notwithstanding being 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 achieved through their User Programs. Within this mechanism, user submitted proposals are adjudicated (peer reviewed) for scientific impact by the Advisory Committees of the relevant facilities. Successful proposals are granted use of specialised equipment and expert personnel support to ensure maximal success with the research aims. Travel and subsistence is regularly supported financially by the KIC (Knowledge Interchange & Collaboration) program of the NRF [24].

2.2 SWOT analysis of South African neutron science

Following the two Workshops, a thorough SWOT analysis was performed with the following outcomes.

Strengths:

- » A firm base of experienced neutron science with established national and international networks exists in the South African research community.
- » SAFARI-1 as a well-managed national asset is operated more than 300 days per year.
- » Two world-class neutron diffraction instruments exist at SAFARI-1, equipped with in-situ temperature sample environments covering $1.5 \text{ K} < T < 1800 \text{ K}$. These are optimised for the applications neutron powder diffraction and neutron strain scanning.

- » iThemba LABS is one of four facilities in the world that can provide quasi-monoenergetic neutron beams in the energy range 30 MeV to 200 MeV [23]. With the ongoing upgrade to a metrology facility, this will be one of the prime neutron facilities in this energy domain.

Weaknesses:

- » Notwithstanding the information era, large portion of the SET community are unaware of the applications and benefits of neutron sciences and techniques towards advancing their research.
- » Beam line facilities at SAFARI-1 are overall inadequately resourced:
 - A very small staff complement exists to establish research infrastructure and support beam line research.
 - Amongst others, no facilities exist for small angle scattering, inelastic scattering, reflectometry, or sample preparation/contrasting that require deuteration.
- » Inadequate funding support to Users. Bursaries to students utilising neutron scattering techniques in their research, and travel funding not linked to approved beam time awards.

Opportunities:

- » Strengthening internationally competitive national facilities at iThemba LABS and SAFARI-1 with respect to sample environments, as well as commissioning of modernised neutron radiography facility at SAFARI-1, etc.
- » Exploiting existing pockets of expertise in fields such as extreme temperatures, magnetism, energy systems and conversion materials, nanotechnology.

- » The growing neutron scattering community in South Africa, stimulated by the availability of advanced local research infrastructure, will fuel this growth and develop to a much greater extent than using instruments abroad.
- » Keen interest is expressed by non-experienced neutron users from the catalysis, nanosciences, chemical crystallography, as well as structural biology and life sciences communities to expand their suite of research techniques with the incorporation of neutron techniques.
- » Formal training opportunities to students and non-experts in neutron sciences with incorporation of site visits and hands-on practical work at the facilities of iThemba LABS and SAFARI-1. Sharing scientific expertise for experimental planning, execution, and analysis of data and results.
- » Complementing the advanced local research infrastructure through access to international facilities (within their User Access Programs based on peer reviewed projects) and formal agreements.
- » Benefits of research and training opportunities inherent to an association agreement with the ESS.
- » Establishment of 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.

- » MPR project equipped with an extensive suite of neutron beam line techniques.

Threats:

- » Remaining lifetime of SAFARI-1.
- » MPR not maturing to fruition.
- » Impact of loss of local research capability and experience on the ability of researchers to compete for beam time at major international facilities.
- » Notwithstanding excellent beam line infrastructure existing at flagship facilities internationally, successful beam time awards are very competitive with in many cases inadequate to meet research objectives.

2.3 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. 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 cofomers 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 CO₂, water and organic solvents (NMU, SU, UCT).
 - Development of new magnetic materials (UP, SU).
 - Development of new compounds that is 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:

Applications generally utilise elastic (powder diffraction and total scattering) and neutron in-elastic techniques in conjunction with in-situ (real time) studies to determine mechanisms of catalytic reactions. 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) that 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 photo-catalysis; Diffusion of ionic liquids in nano-pores in supercapacitors; Metal hydrides – green energy; Solid oxide fuel cells with tuneable conductivity.

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: Large interaction with 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 assaying samples, etc. of geological formations. Typical applications are as follows:

- » 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.

Life sciences and structural biology:

Life science 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 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 is the most abundant element in biological systems. Photons and electrons as probes of hydrogen are at the limit of visibility to X-rays, whilst neutrons are adversely affected by hydrogen that has a strong, but negative, scattering length. The isotope (deuterium) has a stronger

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.

Neutron scattering provide the possibility of contrast variation with D₂O/ H₂O mixtures which therefore allows the selection of specific components in the structure.

The following topics in life sciences are of interest within the South African context:

- » Development of an effective prophylactic HIV vaccine - HIV Pathogenesis Research Unit (HPRU) – University of the Witwatersrand.

A novel immunogen called Env-2dCD4_S60C (consists of a human two domain CD4 with an S60C mutation covalently bound to gp120 monomers or cleaved, soluble gp140-GCN4 trimers (Env)) is considered as a viable candidate for an effective preventative and/or therapeutic vaccine against HIV-1. High resolution X-ray crystallography studies were inconclusive. Small Angle Neutron Scattering (SANS) studies are assisting 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 in conjunction with their deuterium facility [25].

- » Development of enzyme mechanisms for drug target in tuberculosis - Department of Integrative Biomedical Sciences - University of Cape Town. Research is focussed on minimising disease progression by specifically targeting proteins using small molecules designed by rational processes using molecular and structural biology tools. Research focuses on the enzyme mechanisms of the nitrilase superfamily (amidases and nitrilases). These thiol enzymes play a range of roles in cellular processes involved in biosynthesis and post-

translational modification in plants, animals and fungi. While X-ray crystallographic studies and electron microscopy (experimental sciences used to determine the atomic and molecular structure of proteins) have yielded some excellent clues, a recent collaboration with the ESS (Deuteration and Macromolecular Crystallisation (DEMAX) platform) and ILL has been established towards determining the neutron structure of this amidase, in which the hydrogen atoms (neutron contrast enhanced through deuteration) that will form the basis of proposing a novel mechanism [26].

Magnetism:

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.
- » 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:

Engineering and 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. The importance of neutron scattering in a modern economy goes 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.

Neutron experiments provide definitive data for the manufacturing industry [27], which has informed light weighing, lean design and process optimisation [27], resulting in reduced energy needs. Materials testing data have given aerospace companies confidence in new alloy compositions and manufacturing techniques.

Partnerships with large research centres can support small businesses by giving them the security and confidence to embrace new areas of activity. In the context of current SA challenges, potential 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 SAFARI-1 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 allow experimental access to academia and industry.

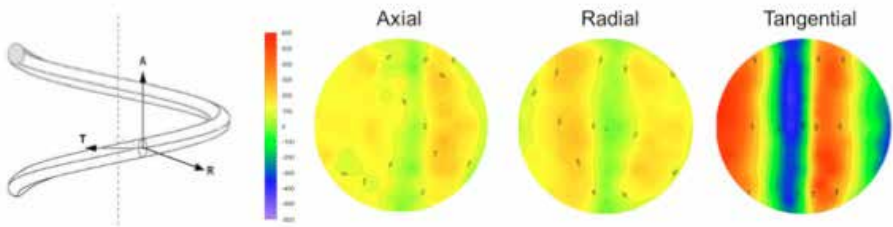


Figure 12: Residual stress field in a helical coil spring [28].

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 life forms as well as human evolution. The contributions neutron techniques in conjunction with synchrotron techniques can offer in these quests are well known and well documented in leading scientific journals.

2.4 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 work at the SAFARI-1 neutron diffraction facilities. Post-graduate students from many universities are routinely supported on individual projects with

their research investigations. The following training courses linked to Necsa and iThemba LABS are presented in South Africa:

- » Annual courses at honours and masters levels on neutron diffraction and imaging techniques - CARST (Centre for Applied Radiation Science and Technology) centre of NWU.
- » 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 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.

A number of annual training courses run in European countries:

- » Hercules (Higher European Research Course for Users of Large Experimental Systems). This 11-month school 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, and Industrial applications). It includes lectures, practical work, tutorials, and visits of Large Facilities such as ALBA in Barcelona, KIT in Karlsruhe, DESY and European XFEL in Hamburg, ELETTRA and FERMI in Trieste, ESRF and ILL in Grenoble, SOLEIL in Paris-Saclay, and PSI in Villigen [29].

- » Oxford School on Neutron Scattering [30]. This two week course is intended for scientists and engineers who are new to the field of neutron scattering. 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 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 is accompanied by a tutorial session. The students visit the ISIS Pulsed Neutron and Muon Facility in Didcot, and attend 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 school illustrates 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.

3. Key outcomes from African stakeholder engagements

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. The following provides a condensed list of the key outcomes from various African stakeholder engagements:

- » Facility access is based 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 presently 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 2027, 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 (membership level and cost to be determined). Access would become an essential component of South Africa's neutron science program.
 - 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.
- » 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 $1.5 \text{ K} < T < 1800 \text{ K}$.
 - 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.
- » 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 life sciences, 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 electrolyzers, 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 subsistence for anyone in the community who is awarded beam time at a neutron research facility through peer reviewed proposals.

4. Acknowledgments

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Local participants with the workshops and mini-symposia from:

Council for Geoscience

Council for Scientific and Industrial Research

Department of Innovation

Department of Minerals and Energy

Eskom Holdings

Impala Platinum, Rustenburg

iThemba LABS

Mintek

National Laser Centre

National Research Foundation

Necsa SOC Limited

Nelson Mandela University

North West University

Sasol Research and Technology

South African National Energy Development Institute

Stellenbosch University
University of Cape Town
University of Johannesburg
University of KwaZulu-Natal
University of Limpopo
University of Pretoria
University of South Africa
University of the Free State
University of the Witwatersrand

Internationals participants with the workshops and mini-symposia from the institutions:

Australian Centre for Neutron Scattering, ANSTO, Australia
European Spallation Source, Sweden
Heinz Maier-Leibnitz Zentrum (MLZ), Germany
Institut de Biologie Structurale, France
Institut Laue-Langevin, France
Malmö University, Sweden
Oak Ridge National Laboratories, USA
Science and Technology Facilities Council, ISIS Neutron and Muon Source
Rutherford Appleton Laboratory, UK
University of Glasgow, UK
University of Le Maine, France
University of Leicester, UK
University of Malta, Malta
Uppsala University, Sweden

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6. 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 workshop brought South African research scientists, engineers and technologists together with their counterparts from ESS. The meeting 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 was an exchange of ideas on collaboration opportunities presented by the two national facilities, iThemba LABS and Necsa, in connection with the construction of the 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; and Life Sciences & Biology. These “Thrusts” would be the main focus for the 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).

7. Appendix 2: Second South African BrightnESS² Workshop

Capacity Building: Neutron Research in Collaboration with BrightnESS² partners

Date: August 2020 - January 2021

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

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

The COVID-19 Pandemic regulations in early 2020 led to the cancellation of all in-person events across South Africa. 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 run on a virtual basis over the period August 2020 to January 2021. An added advantage of hosting virtual mini-symposia was that experts from the ESS and other international facilities could be involved with the events.

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.

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 can be provided via the facilitators. The envisaged outcome of each mini-symposium was to provide information towards a 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 Necsca (SAFARI-1) and iThemba LABS, as well as abroad with the ESS (European Spallation Source)?
- » 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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