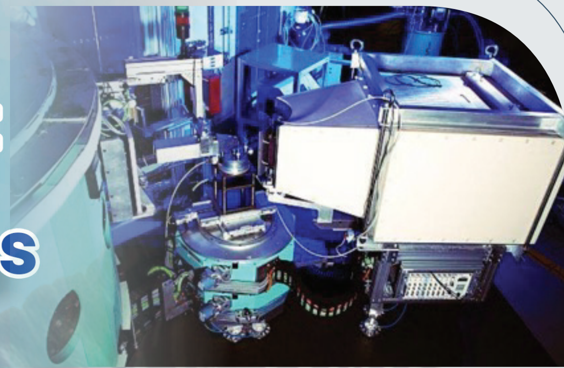
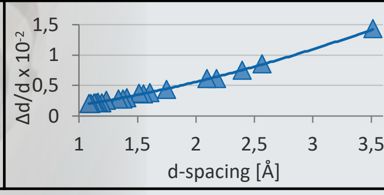
PITSI Facility

The Powder Instrument for Transition in Structure Investigations



Instrument parameters		
Si Monochromator	(331)	(551)
λ at $2\theta_M = 90°$	1.76 Å	1.07 Å
Beam size [mm]	Variable slits: Hor: 5 - 15 Ver: 5 - 48	
Temperature sample environments [K]	Vacuum furnace: $400 < T < 1800$ Bottom-loader cryostat: $4.5 < T < 320$ Top-loader cryofurnace: $1.5 \leq T \leq 800$	
Sample mounting	4-Position sample changer	
Detector	614 mm (hor.) × 375 mm (ver.) Oscillating radial collimator Range: $10° \leq 2\theta \leq 115°$	
Flux at sample position	~ 10^6 neutrons $cm^{-2}s^{-1}$	
Resolution		

The PITSI instrument enables medium-resolution neutron powder diffraction capability for the study of atomic and magnetic phenomena in solid and powdered polycrystalline materials. It is specifically equipped with a radial oscillating collimator that enables insertion of in-situ sample environments for low and high temperature studies.

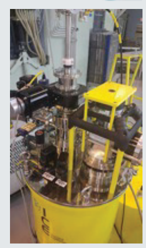
PITSI is located at the SAFARI-1 nuclear research reactor of the South African Nuclear Energy Corporation (Necsa) SOC Ltd. to complement and extend the capabilities of Necsa's X-ray diffraction instruments. Advantages include:

- Scattering off nuclei as opposed to the electron cloud.
- Interaction strength is atomic number independent, sensitive to light elements and can distinguish between neighboring elements in the transition metals, actinides and lanthanides series.
- Unlike X-rays, do not suffer form-factor fall off.
- Interaction between the magnetic moment of the neutrons with unpaired electrons in materials enables studies of magnetic phenomena.
- Superior penetrating capabilities enables non-destructive in-situ parametric studies, such as function of temperature, pressure, magnetic field, etc.
- Sensitivity to H and Li enables in-situ studies of chemical exchange in energy-storage systems such as hydrogen fuel cells, Li-ion batteries, as well as batteries in general.

4-positions sample changer

Vacuum furnace

Bottom-loader cryostat



Top-loader cryofurnace

Access to PITSI is through scientific merit within the open access User Program where results are published in the open literature. Commercial (proprietary) access is also available.

Contact useroffice@necsa.co.za to apply for beam time and general enquiries.

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South African Nuclear Energy Corporation SOC Limited

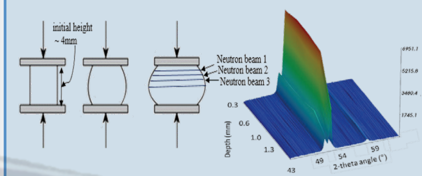
Application areas

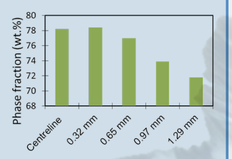
Neutron powder diffraction is a versatile technique that find application in fields such as material science, physics, chemistry, geosciences, energy, and cultural heritage. It allows researchers to study crystal and magnetic structures, analyse phase transitions, investigate intermolecular interactions, and analyse archaeological artefacts and cultural heritage materials.

Project examples

Depth-resolved measurements

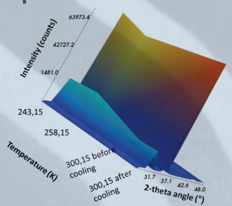
Depth-resolved chemical phase content in uni-axially loaded steel samples to determine the strain-induced martensite as function of depth (neutron beam designations in the sketch). The neutron gauge volume defined with a 0.3 mm vertical input slit.

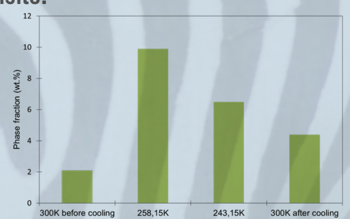




Phase transitions at low temperatures

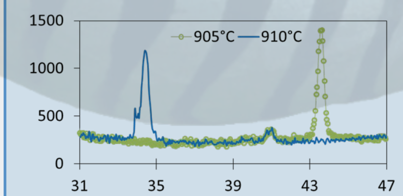
Low temperature phase composition studies of a welded steel containing both austenite and martensite to determine the temperature induced martensite.

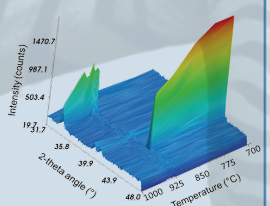




Phase transitions at high temperatures

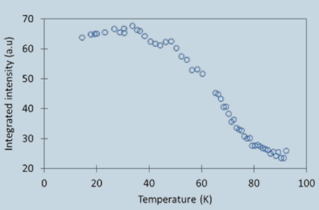
High temperature phase composition studies in pure iron (ferrite) to determine the phase transition from ferrite to austenite at temperatures above 900°C.

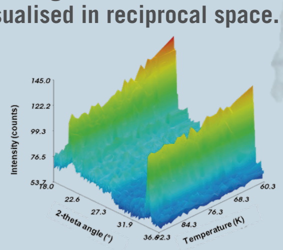




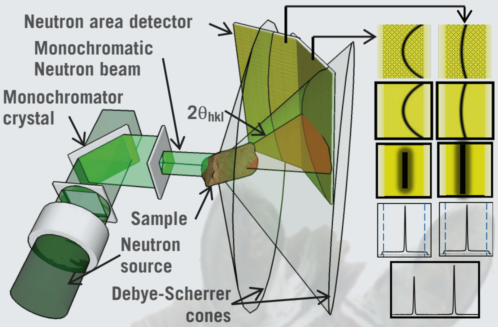
Magnetism

Low temperature study of the magnetic ordering in a nanoparticle chromite to determine the magnetic phases and transition temperatures. The advantage of neutrons is that the magnetic ordering is directly visualised in reciprocal space.





The neutron powder diffraction technique



A polychromatic beam of thermal neutrons delivered by SAFARI-1 is monochromated using either Si(3 3 1) or Si(5 5 1) reflections. The monochromatic beam is directed through a primary aperture to fully, or selectively, illuminate a polycrystalline sample positioned on the sample table. The diffracted beam passes through a radial oscillating collimator (ROC) to reduce scattered contents from sample environments such as cryostats and furnaces before impinging the neutron detector.

The wave characteristics of the neutron beam undergoes constructive interference with the atomic nuclei within the sample, that lead to distinct Debye-Scherrer cone distributions. These are detected by a 2D neutron detector to render their precise angles and intensities. The PITSI detector subtends 20°. To record a comprehensive diffraction extent, data are acquired in sequential detector frames. The resulting data is integrated to generate diffraction peaks.

Data analysis involves performing flat field and geometric corrections, followed by normalization and the removal of detector edge effects. Sequential datasets are stitched together to form a complete diffraction pattern.

Rietveld refinement is employed on the data to obtain detailed information about the crystal structure, including atomic positions, occupancies, thermal vibrations, and other structural parameters. This furthermore allows for chemical phase quantification in multi-phase samples.

Samples

Solids

Typical samples: Rods 5 mm in diameter by 50 mm in length.

Powders

Contained in vanadium tubes 5 mm in diameter by 50 mm in length.

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