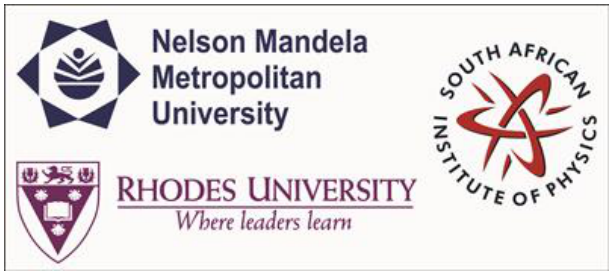

Contribution ID: **212** Type: **Oral Presentation**

Data processing at the Necsa neutron diffraction facility

Wednesday, 1 July 2015 15:20 (20 minutes)

Abstract content
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The South African Nuclear Energy Corporation SOC Ltd. (Necsa) recently completed major instrument upgrades to the Neutron Diffraction Facility (NDIFF) at the SAFARI-1 research reactor. With this, a method was needed to facilitate data processing of both the Powder Instrument for Transition in Structure Investigations (PITSI) and the Materials Probe for Internal Strain Investigations (MPISI) instrument.

As only minimal standardisation of neutron diffraction instruments and their data processing software exists, available packages were not directly compatible with the NDIFF instrument modalities. A number of diffraction data processing frameworks (such as Mantid and GumTree) are available, but these tend to be very expansive and have a steep learning curve, which needs to be overcome in order to add functionality. New purpose-built software named ScanManipulator was consequently created for NDIFF.

In order to produce a complete diffraction pattern from datasets at different detector angles as measured on PITSI, the data first undergoes a number of procedures, which was automated with the new software. This includes flat field and geometric correction, data cropping, normalisation, scaling and stitching. Treated data can be exported to a Fullprof compatible format enabling quantitative Rietfeld analysis.

ScanManipulator can be connected to the control system of MPISI thereby providing it with near real-time data originating from the 2D position sensitive neutron detector. The necessary corrections and normalisations are automatically applied as new detector data becomes available. Peak parameters resulting from automated peak fitting of the corrected data are evaluated against statistical criteria and used to adjust the measurement time within the control loop. The use of this protocol also leads to a reduced spread in standard deviation values of d-spacing between successive measurements.

ScanManipulator thus provides a platform to perform automated processing of diffraction data emanating from the NDIFF instruments.

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Session Classification: NPRP

Track Classification: Track B - Nuclear, Particle and Radiation Physics