

**Report:**  
**Constituting**  
**Instrument Advisory Team Meeting**  
**for *Kookaburra***

**26 September 2008**



*Kookaburra*  
(*Dacelo novaeguineae*)

**Duncan McGillivray**  
*Spokesman*

## INTRODUCTION

The Bragg Institute at ANSTO plans to install a very low-Q neutron scattering instrument (*Kookaburra*) at the OPAL research reactor. This instrument will extend the Q-range of the existing SANS instrument *Quokka* by two orders of magnitude.

The ANSTO workshop "Pushing Small-Angle Neutron Scattering at OPAL to Smaller Q" was held in November 2007, and was attended by 39 participants representing universities, Commonwealth institutes, overseas facilities and industry. At that workshop a scientific case for an ultra-small angle scattering instrument was developed, and two options for such an instrument were defined: a classical Crystal-USANS and the newer Spin-Echo SANS (SESANS) technique. At that workshop it was decided that the final choice between them would depend on both calculations of performance and the results from standard experiments performed at leading facilities overseas, in addition to a judgment about the relative importance and usage levels for weak and strong scattering samples.

## INSTRUMENT ADVISORY TEAM (IAT)

Following on from this workshop, a one-day constituting Instrument Advisory Team (IAT) meeting took place at ANSTO on 26 September 2008. The *Kookaburra* IAT was asked to:

- Represent the Australian ultra small-angle neutron scattering community
- Verify the scientific justification for a low-Q neutron scattering instrument
- Contribute intellectually to the instrument development
- Appoint a Spokesperson to
  - Advocate the instrument at meetings
  - Help prepare documents
  - Chair upcoming IAT meetings

As well as establishing the IAT, the meeting's goal was to get feedback from the Australian USANS community on the two proposed options for this instrument, and recommend which might best serve their research needs. The potential location for the instrument (on a cold-guide or thermal guide) was also discussed.

## IAT MEETING PARTICIPANTS (14)

|                       |                                                  |
|-----------------------|--------------------------------------------------|
| - Buckley, Craig      | Curtin University                                |
| - Garvey, Chris       | ANSTO/Environment                                |
| - Gilbert, Elliot     | ANSTO/Bragg                                      |
| - Hamilton, Bill      | ANSTO/Bragg                                      |
| - Hanley, Tracey      | ANSTO/Bragg                                      |
| - Heinemann, André    | ANSTO/Bragg                                      |
| - Hoffmann, Lee       | Flinders University                              |
| - Klose, Frank        | ANSTO/Bragg                                      |
| - Knott, Robert       | ANSTO/Bragg                                      |
| - Mata, Jitendra      | Australian National University                   |
| - McGillivray, Duncan | Auckland University ← <i>Appointed Spokesman</i> |
| - Rehm, Christine     | ANSTO/Bragg                                      |
| - Reynolds, Philip    | Australian National University                   |
| - Ruggles, Jeremy     | University of Queensland                         |

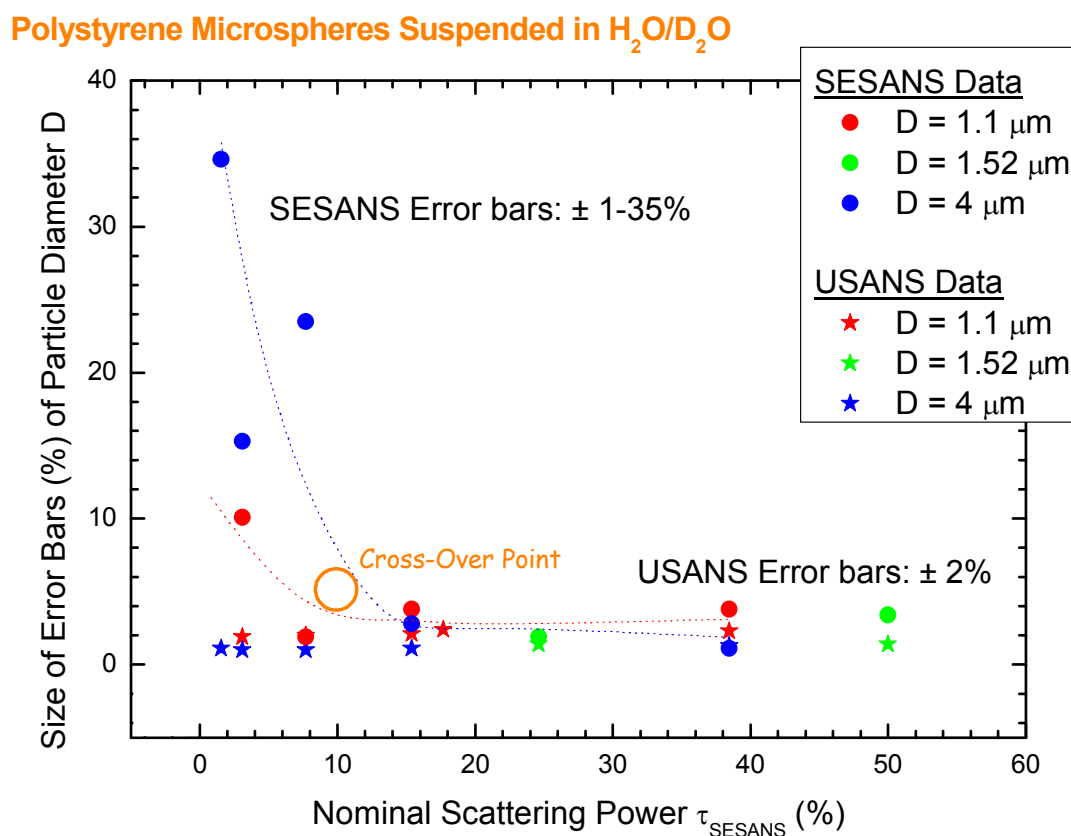
## INSTRUMENT SCIENTIST REPORTS

In the morning sessions, the Instrument Scientist Christine Rehm (CR) presented the IAT with the current status of the *Kookaburra* project including initial estimated instrument performances, as well as neutron scattering measurements performed on a set of standard samples using the BT-5 USANS instrument at NIST and the SESANS instrument at Delft Reactor Institute. The standard samples consisted of solutions of polystyrene microspheres of varying particle diameters and scattering powers.

CR's presentations can be downloaded by following the links below:

- [CR IAT Meeting Presentation Part I - Kookaburra Options](#)
- [CR IAT Meeting Presentation Part II - Round-Robin Experiments \(completed\)](#)
- [CR IAT Meeting Presentation Part III - Expected Performances](#)

Based on the experimental results presented in Part II CR concluded that Crystal-USANS and SESANS had similar performances for the standard samples measured except at low scattering, where SESANS performs significantly worse. The cross-over point below which SESANS is uncompetitive is judged to be approximately 10% in nominal scattering power. Note that this number is based on a direct comparison of the instruments at NIST and at Delft. Clearly, the cross-over point will shift towards a lower number if a future Crystal-USANS/SESANS instrument set up at OPAL is compared.



**Figure 1: Results of Crystal-USANS/SESANS round-robin tests on standard samples: determination of particle radius**

## USER PRESENTATIONS

A selection of users' science cases and instrument-of-choice considerations was presented to the IAT as follows (these presentations can be downloaded by following the links below):

- [\*Studies of Red Blood Cell Shape Changes and Lysis\*](#)  
Chris Garvey, ANSTO
- [\*USANS Studies on Packing of Hard Spheres and High Internal Phase Emulsions\*](#)  
Jitendra Mata, ANU
- [\*What I'd like to Measure at Lower Q - A Personal Perspective\*](#)  
Elliot Gilbert, ANSTO

## DISCUSSION & CONCLUSIONS

### 1) Crystal-USANS vs. SESANS

*Conclusion: A conventional Crystal-USANS instrument is preferred to a SESANS instrument.*

This recommendation is based on the following benefits of Crystal-USANS:

- Crystal-USANS is low technical risk compared to the highly complex SESANS method
- More experience at OPAL to realize a conventional Crystal-USANS, less dependence on overseas input/know-how
- Greater user familiarity with the technique, leading to a more rapid build-up of user base
- Larger range of analysis software/analytical models available
- Greater flexibility in sample environment, no concern about interfering with the magnetic fields of a SESANS
- SESANS much more sensitive to neighbouring instruments
- There are difficulties measuring magnetic or steel samples with SESANS
- Costs for both types of instruments are comparable, as are performances (except in weakly-scattering samples, where SESANS performs poorly)
- Construction times should be shorter for Crystal-USANS

The IAT recognized that as SESANS is a newer technique it may have greater potential for development, and the installation of such an instrument should be considered at a later stage.

As Crystal-USANS may be slower than SESANS, it was felt that including an operating option of a low-resolution bent crystal should be considered for kinetic measurements.

### 2) Location of instrument

Two possible locations for the Crystal-USANS instruments were discussed: either at the thermal guide TG3 or at the cold guide CG3. Considerations include:

- Space requirements: More available space on CG3, upstream from *Platypus*
- Performance requirements: There will be significant performance enhancements at either position compared to the Crystal-USANS at NIST BT-5. Direct comparisons for cold vs. thermal guide positions at OPAL needed to be calculated at the time, and are now attached below.
- Multiple scattering: Undesirable multiple scattering increases with  $\lambda^2$

- 4 Å neutrons (at the cold guide position) will cause multiple scattering in strongly scattering samples: an exchangeable  $\lambda \approx 4 \text{ \AA} / \lambda \approx 2 \text{ \AA}$  operation mode should be considered to accommodate weakly *and* strongly scattering samples

**TABLE 1: Performance characteristics for Crystal-USANS instruments**

|                                                                                                             | NIST BT-5<br>in Reactor Hall         | NIST BT-5<br>in Guide Hall              | TG-3 at OPAL                            | CG-3 at OPAL<br>$\lambda = 4.x \text{ \AA}$ | CG-3 at OPAL<br>$\lambda = 2.x \text{ \AA}$ |
|-------------------------------------------------------------------------------------------------------------|--------------------------------------|-----------------------------------------|-----------------------------------------|---------------------------------------------|---------------------------------------------|
| Reactor power                                                                                               | 20 MW                                | 20 MW                                   | 20 MW                                   | 20 MW                                       | 20 MW                                       |
| $\lambda$                                                                                                   | 2.38 Å                               | 4.43 Å                                  | 2.38 Å                                  | 4.43 Å                                      | 2.32 Å                                      |
| $d\phi_s/d\lambda d\Omega(\lambda)$<br>( $\text{cm}^{-2} \text{ \AA}^{-1} \text{ s}^{-1} \text{ sr}^{-1}$ ) | $9.4 \cdot 10^{11}$                  | $4.2 \cdot 10^{11}$                     | $2.5 \cdot 10^{12}$                     | $2.1 \cdot 10^{12}$                         | $1.9 \cdot 10^{12}$                         |
| $\Delta\lambda$                                                                                             | 0.1410 Å                             | 0.0816 Å<br>( $m_{\text{Hor}} = 1.2$ )  | 0.0744 Å<br>( $m_{\text{Hor}} = 3$ )    | 0.1699 Å<br>( $m_{\text{Hor}} = 2.5$ )      | 0.0463 Å<br>( $m_{\text{Hor}} = 2.5$ )      |
| $\Delta\lambda/\lambda$                                                                                     | <b>5.9%</b>                          | <b>1.8%</b>                             | <b>3.1%</b>                             | <b>3.8%</b>                                 | <b>2.0%</b>                                 |
| Crystal                                                                                                     | Si(220) 3x3                          | Si(111) 5x5                             | Si(220) 3x3                             | Si(111) 5x5                                 | Si(311) 5x5                                 |
| $\Delta\theta_D$<br>Darwin half width                                                                       | $3.72 \cdot 10^{-6}$ rad             | $9.07 \cdot 10^{-6}$ rad                | $3.72 \cdot 10^{-6}$ rad                | $9.07 \cdot 10^{-6}$ rad                    | $2.40 \cdot 10^{-6}$ rad                    |
| $q_{\text{min}}$                                                                                            | $2.0 \cdot 10^{-5} \text{ \AA}^{-1}$ | $2.6 \cdot 10^{-5} \text{ \AA}^{-1}$    | $2.0 \cdot 10^{-5} \text{ \AA}^{-1}$    | $2.6 \cdot 10^{-5} \text{ \AA}^{-1}$        | $1.3 \cdot 10^{-5} \text{ \AA}^{-1}$        |
| $\Delta\theta_{\text{Ver}}$                                                                                 | 0.0110 rad                           | 0.01533 rad<br>( $m_{\text{Ver}} = 2$ ) | 0.01234 rad<br>( $m_{\text{Ver}} = 3$ ) | 0.02299 rad<br>( $m_{\text{Ver}} = 3$ )     | 0.01200 rad<br>( $m_{\text{Ver}} = 3$ )     |
| $\Delta\Omega_{\text{Source}} = 4 \cdot \Delta\theta_D \cdot \Delta\theta_V$                                | $1.6 \cdot 10^{-7}$ sr               | $5.6 \cdot 10^{-7}$ sr                  | $1.8 \cdot 10^{-7}$ sr                  | $8.3 \cdot 10^{-7}$ sr                      | $1.2 \cdot 10^{-7}$ sr                      |
| $T_L$                                                                                                       | 0.31                                 | 0.50                                    | 0.49                                    | 0.66                                        | 0.66                                        |
| Gain from<br>vertical focus                                                                                 | 3.1                                  | 2.6                                     | 3.0                                     | 3.6                                         | 3.6                                         |
| $\phi_B$ ( $\text{cm}^{-2} \text{ s}^{-1}$ )                                                                | <b>20,800</b>                        | <b>25,000</b>                           | <b>51,000</b>                           | <b>700,000</b>                              | <b>25,000</b>                               |

From these calculations a very significant performance advantage exists for operation at the CG3 cold-guide at  $\lambda \approx 4 \text{ \AA}$ . Concerns about multiple scattering for strongly scattering samples can be addressed using a  $\lambda/2$  mode when necessary (although at much reduced sample flux – comparable to current BT5).

*Conclusion: A position at the cold-guide CG3 appears the most promising option.*

## OUTLOOK

The next IAT meeting is expected to be called in June 2009.