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Report:

2nd

Instrument Advisory Team Meeting for *Kookaburra*

7 September 2009

Kookaburra
(Dacelo novaeguineae)

Duncan McGillivray
Spokesman

INTRODUCTION

On 7 September 2009 the *Kookaburra* IAT members met to discuss the preliminary instrument layout and design as well as the expected performance of the *Kookaburra* USANS instrument.

IAT MEETING PARTICIPANTS (10)

- Dutta, Naba	University of South Australia
- Gilbert, Elliot	ANSTO
- Hanley, Tracey	ANSTO
- Holden, Peter	ANSTO
- Knott, Robert	ANSTO
- Mata, Jitendra	ANSTO
- McGillivray, Duncan	Auckland University, *Spokesman*
- Rehm, Christine	ANSTO
- Ruggles, Jeremy	University of Queensland
- Russell, Rob	ANSTO

INSTRUMENT SCIENTIST REPORTS

The Instrument Scientist Christine Rehm presented the IAT with the current status of the *Kookaburra* project. Fig. 1 shows the location of the *Kookaburra* instrument at the cold-neutron guide CG3 at the OPAL reactor upstream of the *Platypus* reflectometer. The instrument will be set up in a temperature-controlled hutch (roof not shown for clarity) with a footprint of about 6 m by 5 m. The main components of the instrument are the premonochromator, a monochromator stage, an analyser stage as well as a transmission detector and a main detector (detectors not shown in Fig. 1). The course of the neutron beam is indicated.

Fig. 2 shows details of the USANS instrument including the monochromator and analyser stage, a multi-position sample holder, transmission and main detector. The monochromator stage as well as the analyser stage comprises a base plate which holds two channel-cut perfect Si crystal monochromators, Si(111) and Si(311); and their motion control (tilt, rotation, translation).

It is planned to operate *Kookaburra* at two different wavelengths to accommodate both weak and strong scattering samples. This approach requires two sets of Si(111) (transporting λ = 4.4 Å to be used for weak scatterers) and Si(311) (transporting λ = 2.3 Å to be used for strong scatterers) channel-cut perfect crystal monochromator and channel-cut perfect analyser crystals. The base plate will be rotated by 180° to move either the channel-cut perfect Si(111) monochromator or the channel-cut perfect Si(311) monochromator into the neutron beam.

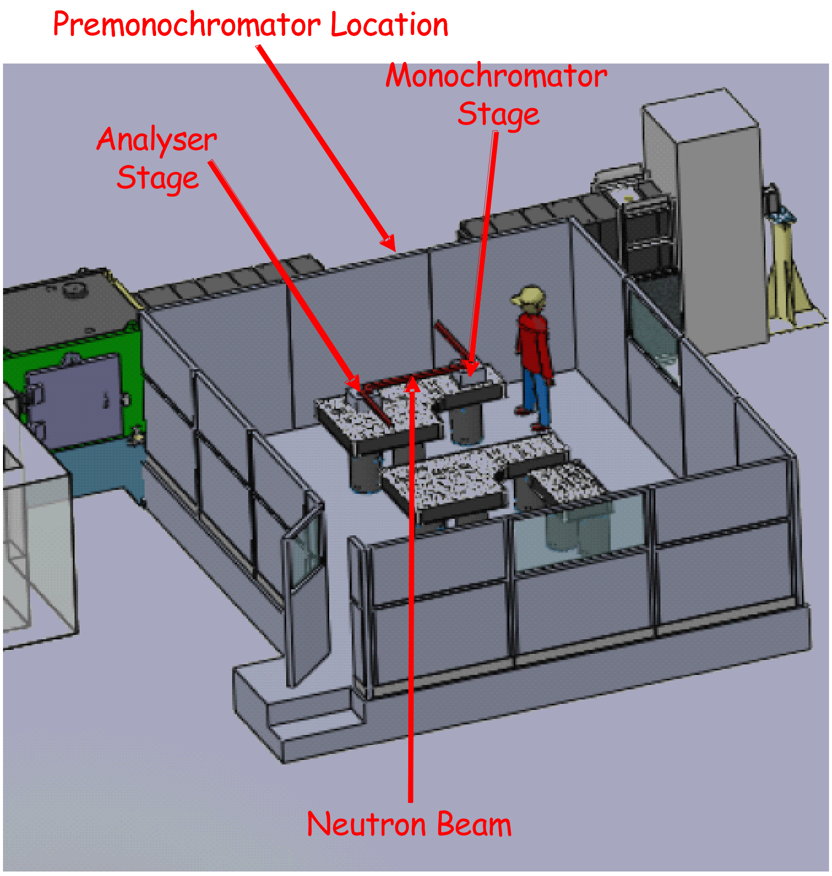

Figure 1: Location of *Kookaburra* USANS instrument at cold-neutron guide CG3

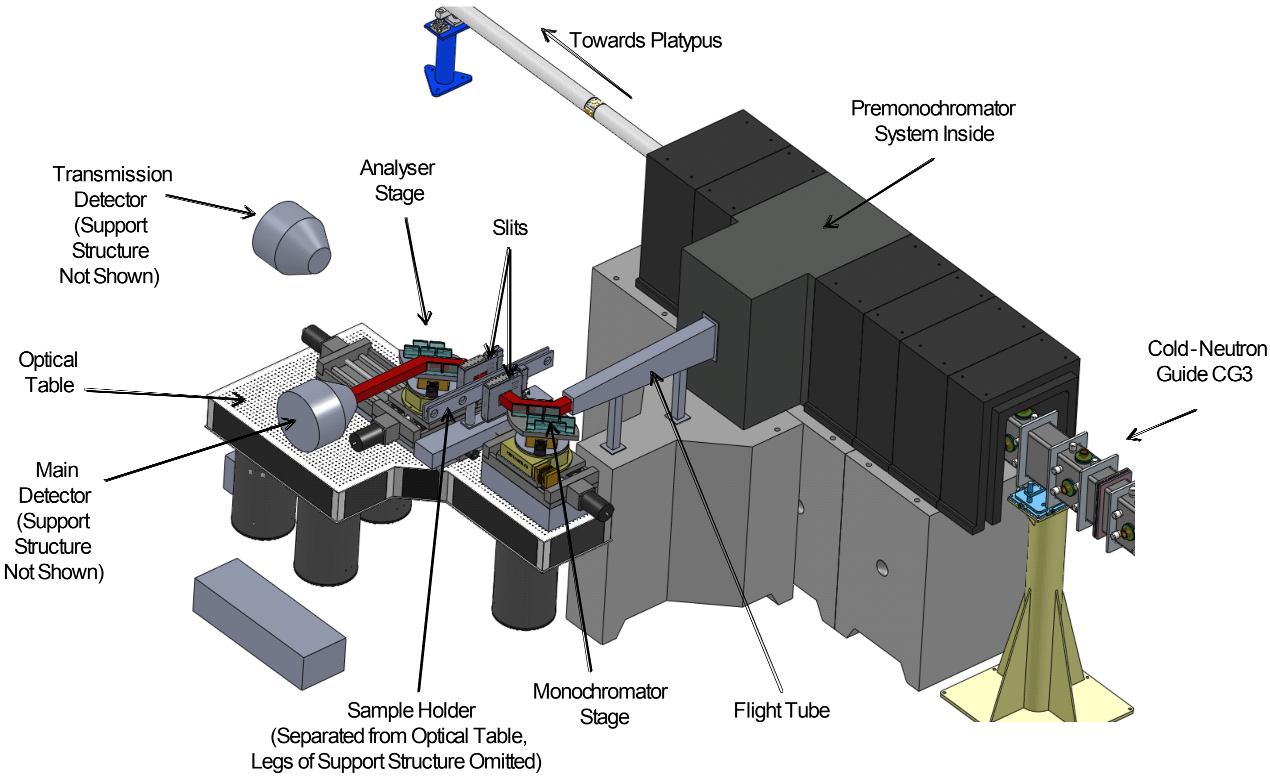

Figure 2: Details of the USANS instrument with monochromator and analyser stage mounted on an optical table

DISCUSSION

The following questions/suggestions were raised by IAT members, and comments are given in *blue*:

- Can we place the Si(111) premonochromator crystal in the upper half and the Si(311) premonochromator crystal in the lower half of the cold-neutron guide CG3?

  It seems to be non-practical to operate the ≈ 2 Å and the ≈ 4 Å neutron beams with vertical offset. Furthermore, Kookaburra seeks to optimise the beam intensities by vertically focusing the 18 cm tall beam [Si(111) and Si(311) will be focused separately].

- The IAT notes that for USAXS instruments at synchrotrons, the crystals are placed on separate optical tables. Given that this is likely to be a cheaper option, and also increases the space flexibility around the sample position for sample environment (the current model implies some form of supporting bench above the optical table for sample, limiting the possible environments), we recommend that this option be considered for feasibility.

  The current design suggests a custom-manufactured single optical table for the monochromator and analyser crystals.

- Estimate the overshooting of the neutron beam at the channel-cut crystals.

  This overshooting has been calculated in one dimension, and needs to be done in two dimensions.

- Consider using a neutron guide between premonochromator and monochromator.

  In the ideal case, the premonochromator is the same perfect crystal Si(111) or Si(311) as the downstream channel-cut perfect Si monochromators and analysers. Neutrons will only transmit premonochromator, USANS monochromator, and USANS analyser if a particular combination for wavelength and horizontal scattering angle is fulfilled. If for a given transmitting wavelength the horizontal angle is changed on the order of $5 \cdot 10^{-5}$ deg during the passage from one crystal to the preceding one, the neutron will not transmit the next crystal downstream.
  A vertically focusing neutron guide between the premonochromator and the first perfect crystal could theoretically be used to increase the beam intensity at the sample. However, even very good neutron guide surfaces have variations in the surface normal direction of ± 0.01°.
  Therefore, in practice, a vertically focusing guide surface will change the horizontal angle of the neutron upon reflection.
  In addition, all USANS experts (John Barker from NIST, Michael Agamalian from ORNL, and Dieter Bellmann formerly from GKSS) do not believe that a focusing guide is a viable option for maximising flux on sample. They, however, agree that a focusing premonochromator could be used for this purpose. Andreas Freund (formerly ILL and ESRF) will help devise the conceptual design and specifications for all crystals required for the USANS instrument.

- Consider placing the translation stage on top of the rotation stage to move the channel-cut crystal to the centre of rotation (rather than placing the rotation stage above the translation stage).

  In the current design the horizontal translation stage will be used to position the first facet of the perfect crystal monochromator into the optimal neutron beam position. This is done once and never changed afterwards. The perfect crystal monochromator does not need to be in the

rotation centre of the rotation stage because the maximum rotation angle during a USANS measurement is 0.1° which relative to the 55 mm beam size leads to only an insignificant change in the location of the crystal by $8.4 \cdot 10^{-5}$ mm.
The options for stacking the stages will be carefully analysed with the vendor of the motion stages.

- How stable are supporting structures made from Al when the ambient temperature varies?

  Small translational movements of 23.1 $\mu m \cdot m^{-1} \cdot K^{-1}$ due to thermal expansion effects are not an issue. USANS is only highly sensitive to changes of the horizontal scattering angle. An accuracy of 5×10^{-5} deg in angle should be stable during the measurement of the Darwin plateau which typically requires about 10 min. Thermal-expansion induced changes in angle occur when materials with different expansion coefficients are firmly connected. Our design tries to minimise this by always using only Al as the only material.

- Should we have a temperature-controlled hutch like at the Geesthacht USANS instrument?

  Yes, we definitely should have a temperature-controlled hutch similar to the ones used at Geesthacht and Juelich. I've talked with USANS instrument scientists from both facilities, and they strongly recommend such feature to protect the instrument against temperature gradients.

- Consider using a flexible Z spacer for small/medium sized sample environment.

  This will be considered.

- Will *Kookaburra* be able to use polarised neutrons?

  The use of polarised neutrons will be considered as there are efforts by other groups using e.g. magnetic prisms (E. Jericha et al., TU Wien) or ^{3}He polarisers and analysers. For the latter, we need to consult with Hal Lee to see if it would work when a 12 T magnet is used in the experiment. This issue will be discussed at the next IAT meeting.

- The premonochromator will focus on routine sample position, i.e. when large sample environment is used, the beam will not be focussed on the new sample position. Calculate how sensitive the focal point is.

  Monte Carlo simulations will be performed to evaluate beam focussing conditions.

- What will be the layout of the two premonochromators? Will the crystals be sandwiched like at the Geesthacht USANS instrument or will we have two separately operated premonochromators? - Will the bending of the premonochromators be flexible? - Consider using a multi-facet premonochromator.

  In December 2009 options for the premonochromator system will be discussed with the crystal expert Andreas Freund (formerly ILL, ESRF).

- Shielding calculations are required.

  As soon as the mechanical layout of the premonochromator system has been finalised, shielding calculations for the premonochromator system and for the complete USANS instrument will be performed. We need to know exactly which and how much material is in the beam before shielding calculations can commence.

- Are higher order wavelengths a problem because the scattering power is proportional to the wavelength squared?

  No. This is firstly due to the absence of second-order neutrons for the odd-index reflections of Si(111) and Si(311), and secondly due to the only very low intensities for third and higher order reflections.

- Consider using a shielding box for the channel-cut crystals with temperature control.

  The premonochromator and both USANS perfect crystals should be at the same temperature. According to calculations performed by John Barker from NIST, the temperature gradient between crystals need only be maintained to within 0.83°. However, each crystal will be surrounded by a Cd and Boron lined shielding box.

- Consider cooling the channel-cut crystals.

  *I have discussed this option with Jack Carpenter from IPNS, and he thinks that cooling the crystals to reduce (can't eliminate) thermal diffuse scattering is quite **impractical**.*

- Consider having a fixed distance between monochromator and analyser of about 100 cm.

  This option is currently being evaluated. Both John Barker from NIST and Dieter Bellmann (formerly Geesthacht Neutron Facility) agree that having a fixed spacing between monochromator and analyser crystals with the correct focus will result in a loss of intensity not bigger than about 20%. We will perform Monte Carlo calculations to make the choice quantitative (both in horizontal and vertical direction). - It is clear that having a fixed spacing will help save money and make a more robust instrument.

- Perform beam calculations: Divergences, angular acceptance, etc.

  Monte Carlo and analytical calculations for estimating the beam performance are currently underway.

- The options for the floor of the hutch are a 20 cm floor elevation, true floor with steps for people who need to get to the relatively high sample position or keep as flexible space, using a ramp. he proposed design suggests a false floor and steps or a ramp. The IAT believes that this will reduce the sample environment flexibility, and increase the footprint of the instrument enclosure, as well as making it more challenging to move heavy equipment into the sample area. Overseas experience with ramp access also suggests that this gives rise to complications. A flexible space, with stepping stones if required, is recommended as a preference.

  The USANS instrument needs a temperature-controlled enclosure in order to ensure that the lattice constants of the perfect crystals remain equal at all locations within the beam line. This ensures that all crystals are at the same temperature. Temperature gradients need to be below 0.8° according to a calculation by John Barker (NIST).
  The limited roof height will allow a small local crane or lifting device within the temperature-controlled enclosure. The capacity of this crane/lifting device will likely be restricted to approximately 200 kg. This kind of weight will not be a problem for a false floor and a ramp. Heavier equipment like high-field magnets will be craned into the instrument enclosure through a hatch in the roof. From a safety perspective, an uneven floor using stepping stones is not desirable.

- Should we have a temperature-controlled sample changer?

  Yes, such sample changer will be designed at a later stage.

- Reduce instrument background (flight tube, neutron beam), keep beam enclosed as much as possible.

  Background reduction will be one of the main design features for the USANS instrument.

- Consider the possibility of an independent second sample station: The IAT notes that there is consideration in the medium term of extending this instrument to include a second sample position, probably utilising a bent crystal analyser for kinetic measurements, and ideally capable of operating independently. It is important that the requirements of this extension be factored into the planning for the current instrument as much as possible, to avoid later necessity for modifications.

OUTLOOK

The next IAT meeting is expected to be called in February 2010.