**ISIS International Beamline Review: MAPS, MARI and TOSCA**
**17th – 18th September 2013**

## 1. Executive summary

The Panel was impressed with the breadth and depth of the science being delivered by the set of three instruments and their associated operational/managerial teams. There was clear evidence of high impact outputs in the areas of condensed matter physics, electron correlated systems, magnetism, molecular spectroscopy, solid state chemistry and catalytic science. However, it was noted that the productivity in terms of outputs for both MAPS and MARI could be improved; the number of publications for the period 2008-2013 for MAPS, MARI and TOSCA are respectively 30, 44 and 153.

The proposed business cases for MAPS and TOSCA were progressive and well justified, whereas the proposed actions for MARI over a roughly 5 year time horizon seemed a little speculative and, possibly, deviated some way from the instrument's core capability in inelastic scattering studies of polycrystalline solids.

The Panel recognized the landscape of a reduction in the number of neutron scattering facilities in Europe over the coming 5-10 years and confirms ISIS has a major role to play in delivering valuable neutron capacity for Europe for at least a 10-20 year time horizon. To this end, it must invest in valued assets within the TS-1 instrument suite. In order for ISIS to remain competitive in terms of high specification instrumentation in the area of inelastic neutron scattering, the Panel endorses the majority of the proposed up-grades on all three instruments. The details of these up-grades are outlined in the Proposals section.

The up-grades should be made as soon as possible. This initiative will refresh the instrument suite and ensure that ISIS maintains its active user community in the subject areas highlighted above. Furthermore, it is anticipated that, via a number of exemplar case studies, the resulting investment will additionally attract new users. Primarily, the work will feature fundamental studies led from academic research teams but a significant fraction of that work in areas such as functional materials (*e.g.* thermoelectrics and

magnetic materials) and heterogeneous catalysis will link with industrial interests that connect with a knowledge-led dynamic economy. In this way, these activities directly correlate expertise and training opportunities in the central domain of the EPSRC portfolio.

**Prioritization**

The guides for the three instruments take priority of funding. Within that scheme, both MAPS and TOSCA share the highest priority. The upgrade for MARI is imperative for its continued operation.

## 2. Background

ISIS management is putting into place a system of light periodic reviews for its instrument suite. The reviews carried out by panels of international experts will provide the Director of ISIS with an opinion on the current status of the instruments concerning excellence of science, technical performance and business case. Based on this evaluation the panels will comment on routes to be taken in order to strengthen the instruments' performance making them able to compete successfully on the international level for the decade to come.

The panel composed of David Lennon (Glasgow University; chair), Ken Andersen (ESS), Richard Catlow (UCL), Bella Lake (HZB), Hannu Mutka (ILL), Helmut Schober (ILL) and Tobias Unruh (University of Erlangen) was entrusted with the review of the instruments MARI, MAPS and TOSCA. The panel would like to thank ISIS management and all the staff involved for the sound preparation of the review. The written documentation the panel was provided with contained the relevant information in a structured and succinct way. However, a difference in the quality was perceivable. The panel recommends for future reviews the use of a common template that would ensure that the opinion of the panel is formed on the basis of comparable input. The panel equally appreciated the clear guidelines received from the ISIS management concerning the scope of the review exercise. The oral presentations were an ideal opportunity for the panel to start an in-depth discussion with the instrument teams. The panel was impressed by the enthusiasm that transpired from the presentations. The answers given to the various questions demonstrated that the teams had thought thoroughly about both the science that was to drive their instruments in the future as well as the technical upgrades needed to prepare for the concomitant challenges in terms of sensitivity and resolution. The visits of the instruments including target station two allowed the panel to further firm up their conclusions. Important details like the obsolescence of vital instrument components and the anticipated mitigation of the associated risks could be addressed.

The panel is aware that this review is the first of its kind and that the instruments that were included were chosen judiciously on grounds of high potential for upgrades. The

panel would have appreciated getting an overview of the entire activities in inelastic scattering situating the instruments under review in a broader context. A cover document would have been helpful. The internal expertise of the panel and the discussions with the instrument teams was fortunately sufficient to cover this matter.

The panel saw its task in giving a clear prioritization of investments for the presented instruments. However, the panel wants to point out that this prioritization has to be seen in the context of the full instrument suite. Being first or last out of the three instruments chosen for this review should not be interpreted as being first or last out of the full ISIS instrument suite.

# 3. MAPS

## 3.1 Background

Commissioned in 2000 MAPS was the first PSD chopper spectrometer. It was a pioneering instrument which set the direction for future spectrometers both at reactors and spallation sources, *e.g*. IN5 MERLIN SEQUOIA *etc*., and was game-changing in allowing excitations to be viewed with an order of magnitude more detail. It was designed for high energy epithermal neutrons, with emphasis on low dimensional magnets and cuprate superconductors as well as crystal field excitations. Its particular strengths are its large bandwidth of incident energies (few meV to eV), its fine resolution of ~2% of the incident flux, its exceptionally low background and its ability to access to low wavevector transfers with good resolution even at high energy transfers.

## 3.2 Sucesses

Over the years MAPS has been highly successful in mapping excitations in cuprate and iron-based superconductors and exploring quantum magnetism and model systems for precise testing of theories. Remarkably it has proved effective for measurements of catalysts providing a complementary role to TOSCA. This strength was completely unforeseen when MAPS was originally conceived and we offer our congratulations for the ability of the ISIS scientists to accommodate new directions. Although the number of MAPS publications is not high, we note however that they are exceptionally highly cited. In particular, the problem in quantum magnetism lies in finding an adequate theoretical model and the time-consuming data analysis of complex and highly pixelated datasets, making the time to publication quite long. We are also impressed by the strong national and international user base of MAPS.

## 3.3 Challenges

MAPS remains a very strong and highly competitive instrument, but with new instruments coming online often at higher power sources it is facing increasing competition. In particular these instruments are outperforming MAPS in the low energy range (20-50meV). For example MERLIN has more flux at low energies by a factor or 5-10 although with poorer wavevector- and energy-resolution. At the higher flux sources

like SNS and JPARC there are new competitors especially Sequoia at SNS which has a factor of 15-25 more flux at 20-50meV and a factor 2-3 at high energies. HRC at JPARC is also expected to out-perform MAPS. These instruments are new, and are being improved continuously in terms of flux and background; they may also be upgraded in the near future.

### 3.4 Proposed solutions

Three proposals are envisaged for MAPS which will improve the flux especially at low energies and the overall performance. The most important is the addition of a guide, which would give gains of ~x10 at low energies making it comparable to MERLIN while retaining its superior wavevector and energy-resolution. This upgrade is essential. A further gain in flux can be achieved by upgrading the moderator by removing the Gd-poisoning on the side facing MAPS. This, in addition to the upgrade of the guide, would make MAPS comparable to SEQUOIA in flux over the full energy range. Finally the addition of a broad band disk chopper would remove the problem of frame overlap which can make the high energy transfer region unusable especially at elevated temperatures. Such a disk chopper is routine now on other instruments, and this upgrade would also allow other types of Fermi chopper to be used adding flexibility in flux-resolution matching, *e.g*. a straight Gd chopper. An additional benefit is that the disk chopper would also allow rep rate multiplication to be performed on MAPS using the $\pi$-pulse. Finally, it should be mentioned that these upgrades do not compromise the initiatives proposed for other instruments and scientific fields.

### 3.5 Future profile

We believe that the business-case for MAPS is secure and that the current research areas of strongly correlated electron systems and catalysis will remain important in the foreseeable future. Nevertheless we urge the MAPS team to continuing being open to new research areas.

## 4. MARI

It is well recognized by the reviewers that MARI bridges the resolution gap between MERLIN and LET. It further closes the gap of the dynamic range between MAPS and LET. The instrument is regarded by the reviewers to be essential for applications ranging from excitations in magnetically ordered phases and frustrated magnetic systems to phonon density of states of functional materials and disordered materials like glasses. The proposed strong science case for MARI in soft matter research could, however, not be approved by the reviewers. Specifically, the references to (i) the dynamics of bio-active molecules in solution and (ii) the dynamics of bi-layers, micelles, vesicles and membranes were both poorly justified. Moreover, such an initiative represented a large jump from the instrument's established market of dynamics of functional materials; justification for the latter being readily evidenced by a significant number of high impact publications in that area from a diverse and respected user base.

The large array of non-position sensitive detectors provides powerful and efficient neutron detection which makes MARI preferentially suitable for powder samples. A substantial increase in flux would bring MARI in a position to boost the capacity for experiments on powders which is a strongly requested area in the user program. Another upcoming field is the relation between dynamics and function of the vast number of new functional nanomaterials. A corresponding MARI upgrade would be to allow MAPS and MERLIN to extend their focus on single crystalline samples.

With respect to the need of fast user access to experimental results it is recommended to set up a MARI-Express service to the community. This is particularly important for communities like materials scientists developing new preparation routes and substance classes rapidly.

It is regarded to be essential to offer and include theory and computing support like first principle methods calculations and simulation methods to the MARI user program. This should be provided to the users preferentially at the very beginning of the preparation of experiment proposals.

Accordingly the following recommendations are given:

- An essential flux increase is indispensable for MARI to become competitive with ISIS spectrometers and with respect to the international landscape of spectrometers. Thus the installation of an m=3 neutron guide is regarded to be crucial and highly recommended.
- The MARI instrument is regarded as an essential part of the ISIS instrument suite. Respecting the foreseeable reduction of neutron sources in Europe the MARI upgrade is regarded to be a sustainable investment for the future.
- The future scientific program focused on functional materials and excitations in magnetic systems is regarded to be sustainable and is strongly supported.
- The user program has to be supported by sufficient manpower at the instrument. At the same time a strong integration of theoretical and computational support is indispensable at MARI. Thus a second instrument scientist specialized to these issues needs to be integrated at MARI.

# 5. TOSCA

## 5.1 The Case

The document we received as well as the presentation and the tour at the instrument site gave us an impressive overview on the capacities of this instrument that has kept a leading role in the field of inverted geometry spectrometers dedicated to chemical spectroscopy. TOSCA is serving a wide range of users of broad range of origins; it is easily accessible to non-experts in neutron scattering. One can also appreciate the effort put into the development of sample cells and equipment for gas handling. The scientific output, both in terms of publications and also with respect to educational effort (20 theses since 2008) is outstanding, not to forget the impressive return of 0.8 papers/accepted experiment. This successful period is now entering in a new phase due to international competition. At SNS and ILL new projects have resulted or are going to produce competitive and/or complementary instruments and there's need for action to maintain the level of excellence. The staffing of the instrument is reported to be on convenient level and capabilities of data analysis are adequate for the present scientific areas, but some additional effort is called for in terms of disordered materials. It is expected to take care of this *via* scientific collaborations. Management need to ensure that future recruitment maintain the excellence of data analysis capabilities that have an integral part of the past success.

## 5.2 Suggested Improvement

The proposed action is to install a guide that will boost the capacity of the instrument by a good order of magnitude over a broad band of energies, further enhanced when considering the projected TS1 upgrade. This would alleviate the problems encountered when studying weakly scattering samples, many of which are industrially relevant systems. One can expect an interesting expansion to non-hydrogenous materials.

## 5.3 Recommendations

The panel agreed that the guide upgrade has to be taken up with the highest priority. Estimated cost is about £1M, The TS1 upgrade is an independent project but clearly of primary interest in what concerns TOSCA.

It was considered that the diffraction capacity is worth improvement along the lines proposed in the report, with an investment of £200k. The development of the on line RAMAN spectroscopy and the filter analysis are interesting options for technical development, but considered of lower priority by the panel.

The presentations, both TOSCA and MAPS, made a clear point on the synergy of using these two instruments for studying catalysis, and it is foreseen that the upgraded TOSCA instrument with the upgraded MAPS will immediately reinforce the capacity in this scientific field. Along with this synergy one can foresee that complementary use of IN1-Lagrange at the ILL can bring up interesting opportunities, as evidenced at the recent Dynamics of Molecules and Materials meeting in Glasgow (DMM-II).

## 6. Formal Proposals

The proposals listed below by instrument are strongly recommended by the Panel.

MAPS.

- The addition of a m=3 guide to increase incident neutron flux;
- The installation of a broad band pass disk chopper before the Fermi chopper to remove possibility of breakthrough of a $\pi$ pulse in the spectra.
- Redesign of the moderator to remove the Gd poisoning on the face that views the MAPS spectrometer. This will further increase available flux to the instrument.

MARI

- The provision of a m = 3 waveguide to enhance the flux available to the spectrometer.
- To concentrate on a work programme examining the dynamics of functional materials (e.g. phonons, collective excitations and soft modes in thermoelectric materials) of disordered and polycrystalline solids.
- To provide sufficient instrument scientist support to maintain and develop a comprehensive user programme.
- To provide computational support to exploit developments in computer simulations of polycrystalline and amorphous solids that could supplement the experimental measurements.

TOSCA

- The provision of a high m guide to enhance the flux available to the instrument.
- To improve the diffraction capability of the instrument. The possibility of being able to perform modest resolution diffraction studies on materials undergoing spectroscopic analysis is seen as a promising development that will lead to enhanced capability primarily in the area of materials science.

## 7. Highlights

- The proposed upgrades to MAPS are essential to allow it to continue leading the field of single-crystal excitations in strongly correlated electron systems. MAPS has pioneered the use of large arrays of PSDs for measuring excitations in single crystals. It now finds itself in a global landscape of about 10 similar instruments, mainly at higher-power sources than ISIS. The proposed MAPS upgrades will bring it up to the same level as the new world-leading instruments such as Sequoia at SNS.
- The current low flux on MARI makes an upgrade imperative for the continued operation of the instrument. This will allow MARI to focus on measuring excitations in functional materials, benefiting from its high flux in the 10-30meV region combined with its good high-angle detector coverage.
- The MARI upgrade will allow it to take over a significant part of the work on powders and disordered materials currently performed on MAPS, Merlin and LET, increasing the capacity of those instruments for delivering cutting-edge single-crystal work.
- The proposed TOSCA upgrade is needed for it to be competitive with the new and coming world-leading instruments such as Vision at SNS and Lagrange at ILL.
- TOSCA has opened up the area of neutron molecular spectroscopy, bringing in a large chemistry-based user community to neutrons. This is reflected by its very impressive publication record, averaging 0.8 papers per experiment.
- A future upgrade to TS1 would significantly increase the performance of all three instruments at a very small fraction of the investment cost of the instruments.
- To ensure an optimum return on investment, it is highly recommended to provide a sufficient level of manpower support per instrument.

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