Report of the 2011 KENS Science Advisory Committee

Summary

Over the last thirty years, KEK has developed and maintained an excellent reputation for the exceptional quality of their instrument and device development for neutron research. This tradition has certainly continued with their participation in the Materials and Life Sciences Facility (MLF) at J-PARC where they have produced an impressive suite of instruments and maintained their world-leading neutron device developments. These instruments have already produced excellent science and have exceptional potential for the future. In particular, the development of instruments tailored for application-driven research is to be commended.

These impressive accomplishments have been attained in spite of the fact that both the instrument development activities and the quantity of scientific output are severely constrained by existing staffing levels. This is a longstanding issue at KENS which has been highlighted by many previous advisory committees. KEK has responded to this issue by seeking short-term funding and expanding on its long and admirable history of successful partnerships for the development and operation of neutron instrumentation. For example, KEK secured funding from NEDO and ERATO for instrument development projects which encompass participants from industry, universities and government institutes. Clearly, KENS has been able to achieve a great deal in spite of severely constrained funding.

This resourcefulness is to be commended, but also carries significant risks. For example, approximately ⅔ of the budget for the neutron program at KEK is derived from short term sources, much of which is scheduled to end this financial year. Without a substantial increase in stable, sustained funding, it will be very difficult to support the staff necessary to maintain ongoing activities, including instrument operations at J-PARC. While in the past, KENS has responded by forming a variety of collaborations and partnerships to augment the inadequate staff, fully exploiting the world-class KEK instruments at J-PARC cannot be accomplished without a professional staff dedicated to producing user science. In this respect it is worth noting that the KEK instruments are substantially understaffed compared to SNS, ILL, or ISIS. Although it was difficult to ascertain the exact staffing levels, staffing on KEK instruments is certainly < ½ and probably < ⅓ of these facilities on a per instrument basis. Doubling the permanent staff for neutron instrument operations would begin to alleviate this disparity and would significantly enhance the scientific output of the KENS operated instruments.

This is not to diminish the importance of developing partnerships. KEK has been very successful in developing a variety of collaborations and partnerships to augment the in-house staff, and the committee strongly endorses continuing and expanding this approach. For example, KEK has extensively partnered with university teams to build and operate instruments and has created important international collaborations with other pulsed neutron facilities. This outstanding tradition must be maintained and should be expanded to include some of the national institutes in the Tsukuba area (*e.g.* NIMS), other university groups and additional international facilities. In the opinion of the committee, multi-university teams will be required to fully exploit the capabilities of the KEK instruments at the MLF even if funding can be secured to double the permanent KEK staff for instrument operations. In other words, KEK should

continue this admirable tradition of developing alliances that are successful in outstanding instrumentation leading to excellent science.

The most important single collaboration for the neutron program at KEK is with JAEA at the MLF in J-PARC. It is essential that this relationship be carefully managed so that users feel a common experience when performing an experiment at the MLF. Clearly both organizations recognize this and have taken steps to ensure this. For example, they have jointly developed a single proposal system. It is also important that the KEK instruments continue to take full advantage of any centralized services at the MLF, for example sample environment support, software development, *etc.* rather than trying to duplicate these essential services.

The management of the Institute of Material Structure Science (IMSS) presented a plan to develop "science centers" which span neutrons, x-rays, and muons. This is a fine concept, but it will require care to get it to work well. In particular, the "groups" within the centers will attempt to secure short-term funding for their science projects. This funding can then be used to bring post-docs and graduate students to IMSS. The committee fully endorses this approach to taking full advantage of the synergies between neutrons, x-rays and muons. In addition, IMSS management indicated a desire to develop "an instrument development team". For example, detectors are a common need within IMSS and something where being part of KEK at Tsukuba is a major advantage for the neutron program. The committee noted that KENS has a long and distinguished tradition in instrument and device development that must be maintained. We believe that this will require that this "team" identify mechanisms for training post-docs and students.

It is essential for any organization to actively set priorities as it is usually better to do a few things well. This is especially true when funding is severely constrained. However, the need to secure short-term funding means, that of necessity, the priorities at KENS have been largely set by the availability of *ad hoc* funding. In spite of this difficulty, the committee feels it is important that KENS articulate its priorities and vision more clearly. This requires considering both IMSS strengths and the external context. Then it is reasonably straightforward to decide which instruments and devices to develop. For example, priority areas for KENS could potentially include material structure, neutron physics, and magnetism.

During the period between the closing of the KENS neutron source and the start of operations at MLF, KENS operated an "inter-university program" to fund travel to overseas facilities. The committee found that this program was fully successful in providing university researchers access to pulsed neutron capabilities outside Japan in this period.

Finally the committee would like to express its sincere gratitude for the quality of the information during their review and for the hospitality we were shown. We eagerly anticipate the future technical and scientific achievements from the exceptionally dedicated KENS staff.

1. Management

The Institute of Materials Structure Science (IMSS) is one of the research organizations (Institute of Particle and Nuclear Studies; IMSS; Accelerator Laboratory; Applied Research Laboratory) within the KEK. The primary goal of the IMSS is to understand the structure of multifunctional materials by the complementary utilization of synchrotron, neutron, muon, and positron facilities and the efficient operation of inter-university programs. Instrumentation at the Photon Factory and the MLF are at the center of this strategy. In particular, the MLF is a world-leading facility which provides neutrons and muons for the scientific and engineering community through a variety of access mechanisms including peer reviewed proposals. In addition, the Photon Factory has been upgraded as a competitive 3rd generation synchrotron radiation source, while the KEK Energy Recovery Linac (ERL) will be the first ERL-based advanced light source. Due to this advanced infrastructure, the IMSS will be able to perform world-class research into materials structure using a variety of techniques. To take maximum advantage of this outstanding research infrastructure, the IMSS has been developing strategies and action plans.

1. Partnership between KEK (IMSS) and JAEA

The KEK (IMSS) needs to continue to manage its partnership with JAEA in operating instruments within the MLF at J-PARC, deciding which additional instrumentations should be developed and for promoting this facility to the scientific community so that it will lead to new science and advanced technologies in Japan and in the world.

2. Budget

Approximately 2/3 of the KENS budget now comes from temporary sources and much of this funding will expire in this financial year. This is a critical situation as KENS will be unable to sustain many of its current programs (which even now are severely underfunded) without additional resources. In order to take full advantage of the substantial investment at J-PARC, the IMSS must secure stable, continuous financial support that will allow robust operation of the instruments at the MLF. In particular, the IMSS needs financial resources to support: (1) the operation of the facilities including salaries, beamlines, utilities, *etc.*; (2) continuing instrument construction including detectors and so on; and (3) budget for R&D including hiring temporary staff such as graduate students and postdoctoral fellows. IMSS should prepare a well-considered budget plan that includes a long term strategy for KENS. This plan will articulate the needs and required funding which should include a mix of new, stable funding and short-term funding for instrument construction and scientific programs that will be necessary to achieve them. And with severe budget difficulties likely to arise from the expiration of short-term funding, it is essential that top KEK management be actively engaged in solving the current budget difficulties.

3. Manpower

The IMSS (KENS) has endeavored to provide adequate manpower, seeking funding from a wide-variety of sources. Unfortunately, the number of staff is still inadequate to operate the MLF instruments at a minimal level. It is critical that the IMSS (KENS) obtain more manpower. It seems that KEK might consider ways of redistributing staff among its organizations, giving more manpower to KENS. In addition, KENS should try to increase its promotion of inter-university programs and create more active relationships with universities, ultimately bringing more people into the KENS program. To achieve this, IMSS needs to secure additional funding (including short-term research funds on a relatively small scale). Inadequate staffing has long been an issue for KENS, but it has now become a critical threat to the long-term scientific success of KEK instruments at the MLF and to the world-renowned neutron instrument development activities at KENS. Thus it is essential that the top management of KEK provide special attention to this issue.

4. Research

It looks that the IMSS has excellent strategies for research into the structure of multifunctional materials based on their state-of-the-art neutron, muon, and synchrotron facilities. In particular, the KENS may further need to refine its strategy focusing on key science areas. This will entail developing a well-prepared budget and manpower plan and clear path to its realization. In addition, all scientific staff members should be encouraged to seek research funds, which can be used to employ graduate students and postdocs.

5. Roles and contributions to the science community in Asia and the world

The J-PARC and PF are the centers of advanced research infrastructure in Asia as well as in the world. The IMSS needs to work together with the countries in Asia and Oceania as well as elsewhere in the world to develop a network to promote advances in science. As part of this effort, KENS together with other institutions including Japan Atomic Energy Agency will host the first AONSA conference on neutron scattering (1^{st} AOCNS) at Tsukuba this autumn. KENS is to be commended for the work they have done in this area and are encouraged to expand these efforts.

II. Science

The scientific and technical achievements carried out so far in KENS have contributed significantly to the progress of condensed matter research and neutron physics worldwide. The scientific output is of high quality in the areas where KENS staff are active, particularly when the severely constrained resources are considered. However, the volume of scientific output is constrained by their heavy responsibilities to design, construct, and operate instruments at J-PARC. To maintain a science program together with the increased demands of operating the new instruments, the group must find a way to increase staff numbers. They are advised to aim for a minimum of 2 scientists per instrument, with instruments that have very high turnover of users potentially needing more.

Scientific output would also be significantly enhanced by a PhD program in collaboration with university user groups. The “science centers” within the IMSS could provide the necessary framework for accomplishing this goal, if adequate research funding can be secured.

1. Soft Matter Science

Neutrons are exquisitely suited to the study of soft condensed matter. At KENS, beamlines have been planned for the soft matter sciences. Some beamlines (in particular, the neutron reflectometer beamline) had been operational at KENS and were transferred to the MLF. In this case, there is a complete instrument tied to the strategy on the science and technology.

The first instrument for soft matter research at the MLF was the KEK reflectometer called SOFIA. At present, the progress of improving the beamline and conducting initial experiments has been going well. However, there is a serious lack of staff members dedicated to SOFIA. In addition, improved detectors are necessary for this instrument to reach its full potential.

The construction of a SANS instrument is a key part of the instrument development plan. Every effort should be made to bring this essential instrument into operation as soon as possible. This will require bringing additional manpower to the construction and operation. In addition, this instrument will benefit from the development of advanced high performance detectors.

The construction of a neutron spin echo instrument is also is in the beamline construction plan. The committee approves of the plan to defer development of a Mezei type instrument as the complexity of such an instrument makes the cost prohibitive. The committee believes that the development of the planned NRSE instrument should be accelerated, which will require bringing additional manpower to the construction and operation of this essential instrument.

Finally the committee notes that a comprehensive plan for soft matter research at the MLF is necessary and that it may reveal that additional instruments might be necessary to address the many opportunities for expanding soft matter science at the MLF.

2. Hard Matter Science

In this field, the traditional strengths of the group are in the magnetism of metals and insulators (now mostly focused on transition metal systems), strongly correlated electron materials, and cuprate superconductors. Their work in this area is internationally recognized. Inelastic neutron scattering with single crystal samples is the group's primary experimental technique. They have benefitted from collaboration with world-leading Japanese groups who have produced large, high quality, single crystals of these materials.

Under the Japan-UK collaboration, important work on the hole-doped cuprates $(La,Ba)_2CuO_4$, $YBa_2Cu_3O_{6+x}$, and related materials was carried out at ISIS, mostly using the MARI and MAPS spectrometers. These experiments provided key evidence for the universality of the nature of the spin waves (showing the characteristic "hourglass" excitation spectrum) in the high-Tc cuprates. The work was subsequently extended to the study of electron-doped systems such as $La(Pr,Ce)CuO_4$ when large single crystals became available. More recently, the group has also made important progress in our understanding of the new Fe-based superconductors, with, for example, a recent collaboration between KENS and TIT scientists in studying the excitations in LaFeAsO.

The group has studied diluted antiferromagnets as model systems for percolating networks. A distinctive type of magnetic excitations (fractons) is observed in these systems, and the results are used to test theories based on the so-called single length scaling postulate. Experiments using the high-resolution IRIS spectrometer at ISIS on Mg-doped $RbMnF_3$ provided the first quantitative evidence for the predicted dynamical properties of fractons.

The development of position sensitive detectors covering a wide angular range means that chopper spectrometers are the instrument of choice on pulsed neutron sources for studying excitations. The HRC spectrometer constructed at J-PARC by the KENS group complements the other chopper spectrometers at the MLF. Commissioning experiments had begun, prior to the March 11 disaster. Measurements on the model 1D antiferromagnet $CsVCl_3$ indicated that the performance of the spectrometer is as expected from the design calculations. It has the potential to become a world-leading instrument in the future when the facility is operating at the 1 MW level.

The proposed polarized neutron chopper spectrometer utilizing a cross-correlation method is a particularly challenging instrument proposed for J-PARC/MLF. This spectrometer promises to clarify novel and complex spin dynamics of condensed matter. However, to overcome the remaining technical issues, such as the development of a high-speed mechanical disk chopper and clarification of the optimal measurement conditions, collaboration with the CORELLI project at the SNS is highly recommended.

Diffraction studies of crystallographic and magnetic structures are also an area where the KENS group has made important contributions. The new Super-HRPD diffractometer, constructed by the group at J-PARC, is an outstanding instrument with world-leading high resolution. It will be particularly valuable, for example, in precision measurements of lattice distortions at phase transitions, hence illustrating the coupling of the lattice to orbital, charge, and spin densities. *Nature* papers have already been published as a result of work carried out on Super-HRPD, in collaboration with users in Japan and elsewhere. One example of this collaboration is the study of $SrRuO_3$ by Je-Geun Park *et al*. from Seoul National University which reveals changes of the different Ru-O bond lengths at the ferromagnetic transition. Collaboration with Park's group also produced an earlier *Nature* paper on the giant magneto-elastic coupling in multiferroic hexagonal manganites.

The group is therefore very well placed to exploit the new neutron spectrometers at J-PARC. Moreover, within the framework of the IMSS Condensed Matter Research Centre, they have the opportunity to collaborate with colleagues using complementary techniques employing x-rays and muons.

3. Diffraction & Energy Materials

A range of complementary powder diffractometers are in operation at J-PARC. As noted in the previous section, the super high resolution powder diffractometer Super-HRPD reaches with $\Delta d/d = 0.035\%$ the best resolution in the world and at the same time, provides high intensity. The concept of the new diffractometer SPICA looks very impressive and provides an excellent tool for time-resolved studies. Among the scientific achievements are phase transitions of functional materials like multiferroic or ferroelectric systems (e.g. lead free piezoceramics) or superconductors like $SrRuO_3$. The high intensity diffractometer allows data collection in the range of milliseconds coming close to acquisition times on synchrotron facilities. Specialized sample environment has been constructed for hydrogen storage materials.

A new complete data acquisition and refinement system, called Z-code, is under development. It combines Rietveld and pair distribution function techniques (PDF). Furthermore, texture analysis and absorption corrections are included. Two NEDO funded projects started successfully. Both include partners from industry, universities and other research centers. The loading system for hydrogen storage allows the study of charge and discharge of metal hydrides especially to determine the time needed to make hydrogen available. Furthermore exchange reactions between deuterides and hydrides may yield thermodynamic data. It is, however, not clear how the structural studies are linked to the development of fuel cells.

The other project of energy storage is related to Li-battery research. Neutron diffraction studies are extremely important to understand the migration of Li-ions during charge and discharge of the battery and to understand the formation of texture and voids in the electrode material. The structure of a new Li-compound with the best Li-mobility has been elucidated. Additional efforts are necessary to improve the sample environment for in-situ studies. The different parts of the battery were studied by the partners of the consortium. A strategy has so far not been demonstrated for the use of particular materials for cathode, anode or the electrolyte. The ultimate goal (in current density, durability *etc*.) is not yet well defined. Other special tools for *in-situ* studies of functional materials (*e.g.* field dependent studies in piezoceramics) are mandatory.

4. Neutron Physics

KEK is a natural home for studies of the neutron itself. Neutron physics currently conducted or planned at KENS include a neutron lifetime measurement and a search for the electric dipole moment (EDM). These are certainly of great importance in the fields of particle physics and astrophysics. In the former experiment, the precision of τ_n expected to be achieved in near future might not be in itself be world leading, but due to its unique method taking advantage of the neutron optics techniques developed at KENS, the experiment has the potential of solving the present puzzle of a significant discrepancy between the two most precise measurements. The plan of the EDM experiment involves a few novel techniques of manipulating and rebunching of ultra-cold neutrons, again capitalizing on their neutron-optics technology. The ingenuity of this group attracts a number of young physicists, and in fact several able postdoctoral researchers from particle and nuclear physics fields are actively working in this group. Although this type of study requires a considerable time to complete, step-by-step publications of results may be desirable in order to make progress more evident to people in other fields and to convince the neutron community of its significance more clearly.

By virtue of the augmented neutron intensities now and in near future at J-PARC, a number of experiments other than the above two are likely to become feasible soon at KENS, and therefore it may be the time to start considering a scheme of accepting experimental proposals from outside universities.

The neutron physics group is also continuing its involvement in the development of small-sized neutron sources. The presence of such a neutron source at universities would provide opportunities for students to do neutron physics studies. At least, an in-house neutron source at universities should enable neutrons to be included in their curriculum, so that neutrons become one of the standard techniques for young scientists.

III. Device Development

KENS has a long and distinguished history in the development of new instruments and devices. Many instruments at pulsed neutron sources worldwide can trace their provenance to developments at KENS. Thus it is essential to neutron science world-wide that this strength of KENS be preserved.

1. Detectors

The world-wide shortage of ^{3}He has made the procurement of future large area detectors for spectrometers such as the HRC to be prohibitively expensive. This is a significant issue at the MLF and it is crucial that new types of detectors for neutron scattering be developed and there is a search for new detector technologies. KEK is a natural home for a program to develop new detector technologies as this is an issue for synchrotrons as well.

KENS is working on this issue on two fronts. The first is to develop a 1D position sensitive neutron detector Multi-Pixel Photon Counter (MPPC) with Hamamatsu. These detectors, intended to be a suitable direct replacement of ^{3}He-PSD, are based on a ZnS scintillator. The position along the detector is determined with charge division and a resolution of 2.8 mm has already been demonstrated on a detector 32 cm long. This resolution is better than required for the vast majority of instruments for inelastic neutron scattering. The primary remaining challenge is to increase the efficiency which is only 29% of that of a ^{3}He gas detector. The degree of insensitivity to γ rays must also be quantitatively established.

The second focus area is on the development of 2D detectors with both high position resolution and capable of a high counting-rate. Such detectors would be of interest for neutron imaging, SANS, off-specular reflectrometry etc. Efforts in this area include GEM (gas electron multiplier) with Ohshita on BL21 at the MLF and B-doped micro channel plate.

2.Neutron Optics

KENS has developed many interesting optical devices for neutron research. For example, the magnetic lenses can provide polarized beams with exceptionally high polarizations. In addition, they may provide a new approach to creating SANS instruments with very good resolution. In fact, a test of this idea has already been carried out. But this is not the only focusing approach pioneered by KENS staff. They are also actively developing refractive lenses based on perfluoropolymer, Fresnel-shaped sheets which are pressure molded at high temperature. This promises to provide a less expensive and more flexible type of refractive lens than does MgF_2 which is typically employed for refractive neutron optics.

A novel electronic chopper is another interesting device which is being used on the neutron physics beam line NOP. This device consists of a flipper and a neutron polarizing mirror. It works on a polarized beam by electronically flipping the neutron spin so that it will pass through the mirror. When the flipper is switched off, the neutrons are reflected. Thus one can steer the beam electronically. This device is unmatched elsewhere in the world. The participation of students and post-docs in these activities will help ensure that the innovative spirit which is being exhibited by KENS staff will be maintained into the future, training a new generation in instrumentation issues.

3. ^{3}He Spin Filters

The importance of polarized neutron beams is continuing to increase. KENS has recognized this and has been actively pursuing the development of spin filters based on ^{3}He filled cells polarized by spin exchange optical pumping (SEOP). In fact measurements have already been performed at J-PARC and JRR-3M. We support these developments, but note that the ^{3}He polarizations achieved are still somewhat less than the world standard of 80%. We believe this gap can quickly be closed, and encourage KENS to actively consult and form collaborations with NIST and other leading facilities in the SEOP method.

APPENDIX A

COMMITTEE MEMBERSHIP

Dan A. Neumann (National Institute of Standards and Technology, USA)

Keith A. McEwen (University College London, UK)

Moonhor Ree (Pohang University of Science and Technology, Korea)

Hartmut Fuess (Universität Darmstadt, Germany)

Kazuyoshi Yamada (Tohoku University, Japan)

Koichiro Asahi (Tokyo Institute of Technology, Japan)

Jun Akimitsu (Aoyama Gakuin University, Japan)

Mitsuhiro Shibayama (The University of Tokyo, Japan)

APPENDIX B

AGENDA

June 20, 2011 (Mon.)

18:00- Welcome Dinner (German Restaurant ELBE @ Seibu Department Store 6F)

June 21, 2011 (Tue.)

9:00 Closed Session

Session-1 IMSS overview

10:00 Opening: Present Status of IMSS (O. Shimomura)

10:30 Overview of KENS (H. Seto)

11:30 Lunch

Session-2 Sciences in Elastic Scattering Instruments

13:00 Structure Analysis (T. Kamiyama)

13:30 Hydrogen Storage Materials (T. Otomo)

13:50 Soft Matter and Interfaces (N. L. Yamada)

14:10 break

Session-3 Sciences in Inelastic Scattering Instruments

14:30 Excitations in Solids (S. Itoh)

14:50 Slow Dynamics (H. Seto)

15:05 Polarization Analysis (K. Ohyama)

15:20 break

Session-4 Fundamental Physics and Devices

15:40 Fundamental Physics (H. M. Shimizu)

16:00 SANS & etc. (M. Furusaka)

16:10 Polarization Device R&D (T. Ino)

16:20 Counter R&D (S. Muto)

16:30 Group Photo

16:40 Closed Session

18:00 Reception (Lounge @ KEK Honkan Building)

June 22, 2011 (Wed.)

9:00 Closed Session

10:30 Summary

11:00 Adjourn

12:30 Lunch at Tokai (Japanese Restaurant Uoyasu)

13:30 J-PARC tour