

REVIEW  
OF  
THE NEUTRON SCIENCE LABORATORY KENS  
IN  
THE HIGH ENERGY ACCELERATOR RESEARCH  
ORGANIZATION, KEK

Summary and Recommendations  
of  
the KENS International Review Committee

February 2008

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*Glossary*

<Institutes>

KEK : High Energy Accelerator Research Organization

IMSS : Institute of Materials Structure Science

KENS : Neutron Science Laboratory, IMSS, KEK

JAEA : Japan Atomic Energy Agency

J-PARC : Japan Proton Accelerator Research Complex

IPNS : Intense Pulsed Neutron Source, Argonne National Laboratory, USA

LANSCE : Los Alamos Neutron Science Center, Los Alamos National Laboratory, USA

ILL : Institut Laue-Langevin, France

PSI : Paul Scherrer Institute, Switzerland

ICANS : International Collaboration on Advanced Neutron Sources

MEXT : Japanese Ministry of Education, Culture, Sports, Science and Technology

BATAN : National Nuclear Energy Agency of Indonesia

ITER : International Thermonuclear Experimental Reactor

ILC : International Linear Collider

PF : Photon Factory (a synchrotron radiation facility, IMSS, KEK)

SPring-8 : Third-generation synchrotron radiation facility (8 GeV), Hyogo

<Neutron Spectrometers at KENS, ISIS, LANSCE and JRR3>

LAM-40, LAM-80ET, LAM-D : Inverted geometry crystal analyzer spectrometers with different energy resolutions

SAN : Time-of-flight small angle neutron scattering spectrometer

ARISA : Advanced reflectometer for interface and surface analysis

SWAN : Small and wide angle neutron scattering spectrometer

WINK : Small/medium angle neutron diffractometer

INC : Inelastic neutron chopper spectrometer

HIT : High intensity total scattering spectrometer

VEGA : Versatile neutron powder diffractometer

SIRIUS : High resolution and high intensity powder diffractometer

HRP : High resolution powder diffractometer

FOX : Laue method single crystal diffractometer

EXCED : Extreme condition epithermal neutron diffractometer

CRISP : Neutron reflectometer with horizontal sample geometry

MARI : Chopper neutron spectrometer

MAPS : Chopper neutron spectrometer

PRISMA : Inverse geometry crystal analyser spectrometer and high resolution diffractometer

IRIS : High resolution quasi-elastic and inelastic neutron scattering spectrometer

OSIRIS : Long-wavelength diffractometer and backscattering pyrolytic graphite crystal analyser spectrometer

PHAROS : High-resolution chopper spectrometer

PONTA-NSE : Polarized neutron triple axis spectrometer

TOF : Neutron time-of-flight method

MEM : Maximum entropy method

## ***1. Executive Summary***

The Review of the KENS neutron scattering facility took place at a moment of change and was timely in being able to look back over the whole lifetime of the KENS source and to look forward to the full operation of the J-PARC third-generation spallation neutron source.

The Review was conducted in a positive atmosphere and the support of KENS and KEK staff is gratefully acknowledged. The Review team was composed of seven internationally recognised scientists covering a range of disciplines, four Japanese and three overseas scientists.

The committee was very positively impressed with the achievements of the KENS source over its twenty-plus-years lifetime and the dedicated efforts of the staff and management. This achievement has three major threads – the source itself, well-optimised – the novel instrumentation, in terms of its quality and diversity – and the remarkable scientific output of the facility.

What is outstanding is that these achievements have been realised with extremely limited resources when compared to global standards. Only the ingenuity of KENS leaders and staff, their dedication and commitment has allowed this to happen.

The success of KENS in terms of increasing the user community, creating strong networks around the world and, of course, the more tangible reality of having built and operated a pulsed spallation source which is respected both within Japan and around the world, has paved the way for Japan to embark upon the hugely ambitious J-PARC facility at Tokai.

The Review Committee has every reason to be optimistic about the future health of neutron scattering in Japan and congratulates heartily the whole team, past and present, of KENS in KEK. In particular, the Review Committee strongly recommends that the KENS group continues to keep and exercise the responsible for the very successful Inter-university programme in J-PARC, to form a new fruitful science network, to develop innovative techniques, to generate new science, and to maintain Japan's world-class scientific impact in this discipline.

## **2. Introduction of KENS Review**

The KENS Review of 2007, convened by the KEK Director General, took place on Wednesday and Thursday, 30 and 31 January, 2008, at KEK in the Seminar Hall of Building 4. The Committee members were C. J. Carlile, A. J. Hurd, H. Kamimura, Y. Matsushita, R. L. McGreevy, K. Suzuki, and H. Yoshizawa. After welcome and introductions by Professor O. Shimomura, Director of the KEK Institute of Materials Structure Science, and designation of Committee Co-Chairmans K. Suzuki and C. J. Carlile, and after reaching agreements as to procedures, an all-day programme of presentations and discussions followed. On Thursday the Committee met to discuss and formulate this report.

The charge of the Committee is first to evaluate the whole activities in the operation, performance, and scientific achievements of KENS since 1980. Secondly, the Committee was asked to review the status of the J-PARC (Japan Proton Accelerator Research Complex) project, which is a huge national project including the construction of a new MW-class pulsed spallation neutron source facility, JSNS (Japan Spallation Neutron Source). The third charge is to recommend how to keep and promote the activities of the KENS facility during the period of about three years between the shut-down of KENS and the start-up of JSNS. At the time of this meeting, sweeping changes are underway which affect KENS and its community of users.

KEK will complete building the new MW-class pulsed spallation neutron source facility JSNS at the end of 2007 collaborating with the Japan Atomic Energy Agency. Therefore, KEK proposed a scenario for the shutdown and decommissioning of KENS in 2005, as well as the move of scientific activities from KENS to JSNS. Reviewing the J-PARC activities and the scenario toward J-PARC is also charged to the Committee.

The first international Review Committee for evaluating the KENS activities was held in 1997. The committee concluded that there was a significant contribution by KENS to the progress of materials research and neutron physics in the world, but they recommended the increase in the number of KENS staff and the approval of the JHF (Japan Hadron Facility) project. This third Review Committee verifies the fulfillment of this recommendation.

Each reviewer presented to the co-chairmen his report of the subject charged to him. This booklet is a summary and recommendation of the Review Committee completed by collecting the reviewers' reports and arranging them under the responsibility of the co-chairmen. The result of the evaluation is reported to the Director General of KEK, Professor Atsuto Suzuki.

### **3. General Survey of KENS Activities**

#### **3.1 KENS Operations**

First conceived in 1978 and brought rapidly into operation on June 18<sup>th</sup> 1980, the KENS Facility has operated within various administrative frameworks but has in reality functioned as an inter-university research center within the High Energy Accelerator Research Organization (KEK) and its predecessors. Currently it sits within the Institute of Materials Structure Science IMSS together with muons and synchrotron radiation. KENS was the first pulsed spallation neutron source dedicated to neutron scattering applications, following prototype installations ZING-P and ZING-P' at Argonne. The rapid initial realization of the KENS source and its continuous record of source and instrumentation improvements, accompanied by a continuously increasing proton current, are significant achievements and result from the great competence and remarkably devoted commitment of all involved. In FY 2005 the strategic decision was taken to shut down completely the operations of the proton accelerator complex in order to concentrate both staff and financial resources to the then emerging new facility J-PARC at Tokai, of which KEK together with JAEA are partners. This decision had consequences, which required special initiatives to be directed towards the increased user base, which KENS had successfully nurtured.

By the time of its closure KENS operated with a 500-MeV proton beam at currents of up to 10  $\mu$ A at 20 Hz pulse repetition frequency. The target and moderator systems had been developed through a series of stages, many of which were highly innovative, to the final highly efficient Ta-clad W disk target, with optimized decouplers and poisoned moderators, with a Be-graphite reflector optimized for maximum neutron/cost ratio. These accomplishments, remarkable in many ways for a facility with limited resources, have proved to be decisive in placing KEK in the happy position of being capable, and credibly so, of co-operating in the design and realization of the world-class pulsed neutron source J-PARC just about to produce its first beam. This position results from the application of experience gained over the 26 years of operation together with the close and fruitful collaborations with many national and international neutron laboratories, such as those in the ICANS collaboration, notably ISIS, IPNS, and LANSCE, and relying heavily upon the pioneering electron linac sources at Tohoku and Hokkaido Universities.

A defining theme pursued from the very beginning of KENS up to the present is the tight coupling of the primary neutron source (the target) to the moderators, which has provided a ratio of slow neutron current to proton beam power which is at least double that of other similar installations. At the end of its operational life, KENS was receiving protons 2400 hours per year [100 days equivalent], operating with high reliability and a staff complement which was small by international standards. The companion muon research facility also received proton beam for 2400 hours each year. In parallel a ground-breaking medical research programme was pursued which investigated the feasibility of using protons for cancer therapy.

The KENS facility pursued continuous development resulting in a linear increase in beam intensity and improved delivery parameters that, viewed overall, are particularly impressive. This is a real achievement proving to be a springboard to the building of J-PARC. Reliability has been satisfyingly high, reflecting well on component quality and maintenance routines. It is clear that management decisions both with short-term operational goals and long-term strategic goals have proved to be very incisive, and have laid down the foundations which have allowed Japan to embark upon the ambitious J-PARC Facility.

The relatively low power of the source has had the benefit of allowing the KENS team to take

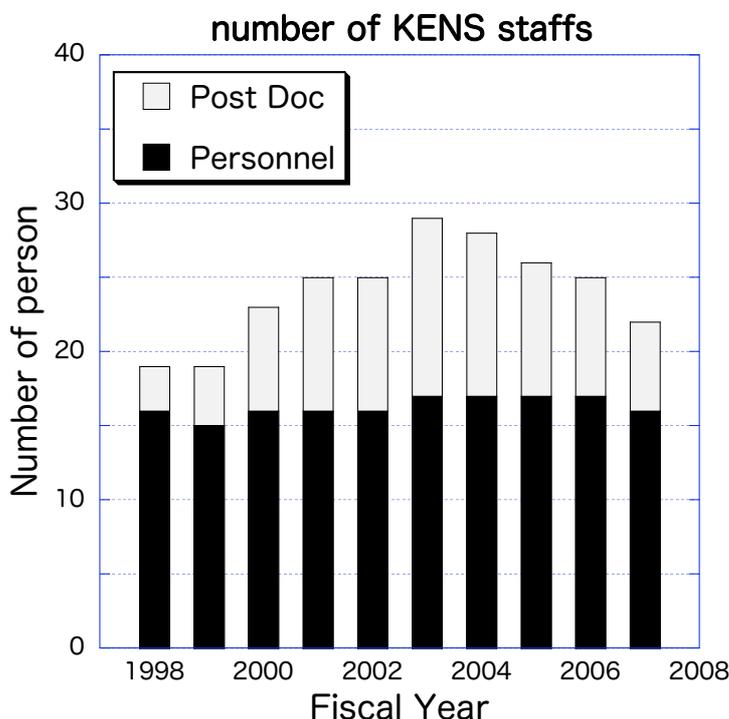
advantage of the opportunity to reduce dimensions wherever possible in order to benefit from “brightness and coupling”, as demonstrated by the tight coupling of the moderators to the source. This means that the path from the incident proton beam to the output of the moderated neutron beam has been kept to a minimum, and thus beam brightness losses have been kept to a minimum also. The ratio of thermalized neutrons-out, to high-energy protons-in was therefore much higher than has been achieved in higher power sources, meaning that good quality science could still be carried out. It is interesting to note that the ISIS second target station, although of a higher power than the KENS facility has also followed this approach. It was therefore essential that elements of this philosophy were retained in the design of the target and moderator assembly for J-PARC, despite the significantly higher power loads on the moderators.

The second experimental hall which had already been constructed in 1997 provided for the addition of six new instruments which had been prepared for almost immediate installation, including the transfer of instruments from the old experimental hall to the new one. Furthermore this allowed the opportunity to upgrade or to replace several instruments in the original hall. In the final years of operation, relevant to this section, what was impressive about the experimental halls at KENS to the new user or visitor was the very dense concentration of instruments and instrumentation in these halls and the evident air of activity. Pulsed-source instruments are very different in concept to those on reactor-based sources, and new initiatives have therefore had to be explored in order to capitalize upon the power of pulsed sources and the relative lack of development of the instrumentation. The situation today is very different from that in 1980 when pulsed source instrumentation was not perceived as being as effective as it is today, when it is accepted that the best pulsed source instruments can compete with or exceed the capabilities of the tried and tested equivalent reactor instruments. It is to the credit of KENS that it has contributed significantly to that change of view, and that was very evident in the instrument suite operational in the years from 2004 until the source was closed in 2005. There simply had not been the time available or the quantity of pulsed sources around the world to reach the levels of development which have been achieved at reactor sources.

Today the dearth of pulsed neutron experience is much less the case than in the early years of KENS. Ingenuity has had to be employed in order to catch up here. One saw much evidence for this process at KENS. The combination of instrument quantity and quality, as well as variety, impressed the observer. Small-angle scattering machines, high-resolution spectrometers, and diffractometers have helped to re-define the standards for instruments worldwide and have fed directly into the instrument suite at J-PARC, which will benefit from the KENS experience. We salute the management, the scientists, engineers and technicians of KENS for driving the continuing evolution of the instrument suite since 2004 despite knowing that one day, perhaps sooner than later, the operation of KENS would give way to that of J-PARC. It is clear that their motivation was governed by the goal of preparing the future. Equally well done, there has been a wide variety of groundbreaking, and ambitious, ancillary equipment which has been developed. One need look no further than the polarization filters which were developed despite the relative weakness of the source. Of course one of the possibilities at a source like KENS is the opportunity to pursue technical developments of this nature where they would be more difficult at the bigger sources. The final years were marked by a process of optimization and upgrade of already conceived ideas towards the new era to be heralded in by J-PARC.

### 3.2 Personnel

It is always striking to an outsider that all these achievements could have been carried through to fruition by a remarkably small and dedicated band of scientists and students. The activities of KENS have been supported by in-house staff, cooperating researchers from universities, local industry, and the “company people”. Since 1988, the total number of KENS in-house staff has been almost constant (14 to 17) including professors, associate professors, research associates, and technicians. Many efforts to increase the staff as well as the budget (external and internal) have been made. The number of post-doc fellows and research assistants (part-time) had increased up to 12 in FY2003, mainly by using the external budget. The total number of cooperative researchers (including B1-group researchers and students) reached 80 in FY2003. It is noted that the activities of KENS are actually supported by about 110 researchers.



This was clearly an effective approach for KENS, but we must raise the question as to whether this culture is the correct one for a source as powerful as J-PARC, where the user community will necessarily be much larger and the scientific disciplines welcomed to the facility will be increasingly wide. The transition from the professional neutron user and instrument builder, to the concept of neutrons as but one probe, albeit powerful, in the armoury of the materials researcher, will in our view require a rethink of this operational philosophy. Put into

the international context, a world-class neutron source operating 23 instruments for a user community of thousands would require a staff of around 7 per instrument, meaning a staff complement of around 160 people [*this excludes accelerator operations, this is simply neutron instruments*], including staff for sample environment laboratories, electronics, detectors, and instrument component development. Although KENS can call upon up to 30 such staff, trained and developed during the final years of operations, they must play the role of increasing the human resource capability in line with the building and coming-on-line of the instruments at J-PARC; we must emphasize this point very strongly. Of course such staff will require a correspondingly adequate operational and development budget.

### 3.3 Budget

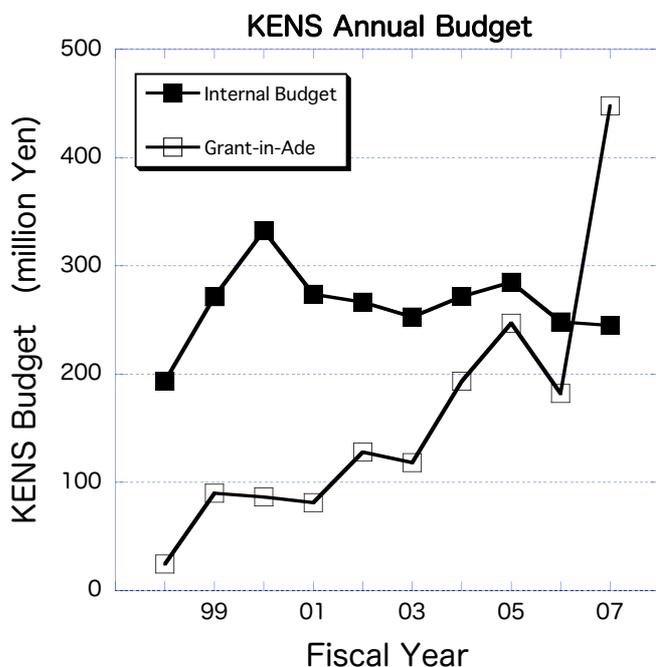
The budgets for upgrading the neutron source and constructing new spectrometers were approved in 1987, 1990 and 1995. However, running costs for operating the neutron source and instruments and for

performing experiments has shown essentially no fluctuation around 330 million Japanese Yen since starting the operation of KENS. This means that the average maintenance cost for each spectrometer currently has decreased to less than half of that in the beginning of KENS operation, because the number of spectrometers available for users is more than twice than at the present moment.

KENS staff have continuously received the Grant-in-Aid for Scientific Research from Monbusho since 1990. In particular, the travelling fund for Japanese scientists to visit ISIS under the Japan-UK agreement has been raised by KENS until 1996. KENS has also accepted payment from industry continuously since 1988, when industrial researchers use the KENS facility.

The special budget for upgrading the neutron source was approved in 2000. However, the annual budget for operating KENS, maintaining the neutron source, and improving the new spectrometers, around 250 million yen, has shown essentially no change.

Since 1997, KENS staff have received many continuously-increasing Grants-in-Aid for Scientific Research, while the original budget of KENS is almost constant. During the period of JFY1998-2003, KENS received funding from the Japan-UK contract. Furthermore, in the period of JFY2004-2008,



KENS staff will receive Grants-in-Aid for proceeding with KENS International Collaborative Research (including the Japan-UK collaboration) as well as for developing new neutron science fields for the J-PARC project.

As a benchmark it should be remarked that the budget of the Science and Projects Divisions of the ILL in order to run the totality of the neutron user programme on about 30 instruments was around 30M€, including staff costs. We would find it difficult to accept that the J-PARC neutron activities could be supported with a budget which is significantly lower.

### 3.4 Inter-University Research Programme

KENS users do not simply use the KENS facility, but are organized to join cooperative research groups (B1-group), which are responsible for the project science with their own instrument, design, operation, maintenance and improvement of instruments together with the in-house staff. In exchange for this obligation, a half of total machine time is preferentially allocated to these groups in addition to the money for supporting the research to be carried out using the spectrometer. According to the different function and degree of collaborations, the groups are classified into four categories. The leader of the group is very often an outside user. The groups and spectrometers in KENS correspond to each other.

Since the number of neutron beam holes and the funds for spectrometer construction are limited,

severe competition is unavoidable among the groups. Such a mechanism for the collaboration and competition in KENS, which has worked quite successfully, is a unique feature in the Japanese neutron community.

Each B1-group also has a strong obligation to act as a local contact for “pure” outside users. In return for such an obligation, KENS gives each B1-group about 50% of the total experimental time as well as financial support for research. Many research achievements in KENS have been produced by the B1-groups.

The Inter-University Research Programme accepts proposals from academic researchers. Each proposal is received, refereed by three referees, and reviewed by the Neutron Science Committee (PAC). Since 2002, the programme has accepted proposals twice a year. This has been working well. The increase of proposals in 2003 is due to doubling the yearly proposal opportunities.

There are three characteristic trends in the recent Inter-University Research Programme. One is oversubscription, which results in an increase in the number of rejected proposals. The second trend is a concentration on some specific scientific subject, mainly materials science. Third, in order to help advance these subjects, new instruments, SIRIUS, SWAN, ARISA, PORE, and EXCED, have been installed and some of the other instruments, SWAN, VEGA, INC, LAM-D, LAM-40, INC, and RAC, have been upgraded.

In 2002 KENS had about 700 registered users, the sum of all members in proposals. Almost all users of KENS come from outside the facility as visiting scientists and research students from universities and institutes in Japan. Although users from overseas are still relatively small in numbers, eight overseas proposals were received in FY2003.

### **3.5 Educational Activities**

KEK takes part in the Graduate University for Advanced Studies (Sokendai) under MEXT. Sokendai is a university for doctoral studies. Some KENS staff are members of Sokendai, and in addition to their KENS duties they also give lectures as at ordinary universities. Seven students have been supervised by KENS staff members during 1997 to 2003, and five of them obtained a PhD. In addition to their Sokendai affiliation, KENS staff members are frequently invited to be lecturers at external universities. It is also noted that KENS staff members are often asked to give introductory lectures for the general public, that is, other than researchers or university students. In recent years, people in industry are gradually becoming interested in using neutrons, and KENS staff are asked to give talks for them. KENS is an appropriate place to host training schools, and financial support for these and all such purposes is highly recommended.

### **3.6 International Collaboration**

In the Japan-UK collaboration in neutron scattering research, KENS has had the major responsibility for the exchange of scientists and engineering of instruments, particularly for the construction of the MARI spectrometer at ISIS. KENS scientists have played a key role in developing advanced techniques for measuring excitations in single crystals at pulsed sources. The development of such techniques at ISIS is an essential step towards the realization of next generation pulsed neutron sources world-wide.

KENS is a founder member of ICANS which has done so much to stimulate the development of

spallation sources world-wide. KENS served as the host of ICANS meeting in 1980 and 1990, and significantly contributed to every meeting of ICANS since 1980. As a part of ICANS collaboration, there have been more than twenty scientists exchanged in long-term stays between the KENS and foreign pulsed neutron facilities.

International collaborations are vitally important for continuing the scientific activity of neutron communities. The present close relationship with ISIS should be maintained and developed further. At the same time the future possibility of collaborations with Grenoble and Asian countries should be kept in mind, so that KENS becomes really international. Regular scientific meetings should be held in KENS to publicise its activities to broader international communities.

The second period of the UK-Japan Collaboration Programme on Neutron Scattering began in 1997, with an innovative chopper spectrometer MAPS constructed at ISIS. About 20 scientific proposals and 110 experimental days from Japanese universities and institutes have been approved each year.

The KENS-LANSCE and KENS-IPNS collaborations were also established in 1998 and 2000, respectively, under the umbrella of a high-level memorandum of understanding between KEK and the US Department of Energy. Both collaborations have been built on staff exchanges, and in the case of LANSCE they are intended to continue. (IPNS closed in January 2008.) Among the areas of collaboration, spallation physics and neutron reflectometry have been most active. In the transition to J-PARC and with the advent of new instrumentation at LANSCE starting in 2010, additional interactions should be pursued. Further, KENS has collaborated with Asian countries. The KENS-BATAN (Indonesia) Collaboration was established in 2003. Also in 2003, KENS promoted the Neutron Science Collaboration between Japan and Korea, and workshops have already been held in both countries. Collaboration with Taiwan for new spectrometers in J-PARC is now in the planning stage.

The KENS-ISIS link has been particularly fruitful, resulting in powerful inelastic spectrometers being built at ISIS and the technology transferred back to KENS instruments. These instruments rapidly became flagships in the world of neutron scattering. This technology will doubtless benefit the new instruments being built at J-PARC, thanks to the far-sightedness of KENS leaders. One tangible inheritance of these collaborations is the twice-yearly UK-Japan meetings, which operate on the scientific as well as the technological level.

For three decades now there has been a valuable and co-operative collaboration with international efforts in the technology of pulsed neutron sources. This is exemplified by the setting up of ICANS in the early 70s in which KEK scientists were leading figures. Profs. Ishikawa and Watanabe from the university and the KENS side, respectively, played key enabling roles. This collaboration has proved to be extremely effective, and it is to the credit of all concerned that world-wide efforts have been co-ordinated in this way. KENS personnel are to be congratulated for their initiative and openness here.

As a result, many scientific collaborations have been developed which have used the best qualities of the Japanese team and the overseas teams, for example, by one side providing high-quality samples and the other side, characterizing methods. As J-PARC becomes operational, there will be a concentration on getting the experimental programme on the road, but these collaborations will still retain a mutual benefit and without doubt must be nurtured.

#### **4. Neutron Source**

##### **(1980-1997)**

KENS is the first pulsed spallation source constructed for the purpose of being a full-blown research facility. KENS has operated successfully from its beginnings and has done much to prove the effectiveness of the concept, both worldwide and in the scientific community of Japan. A distinguishing feature of KENS is its high efficiency in converting protons to slow neutron beams, exploiting a very tightly coupled target-moderator geometry which sets a standard not met elsewhere and demonstrates a goal to which other designs must aspire. The use of only two moderators enhances this efficiency, notwithstanding the fact that the moderators serve a large number of beams and instruments. KENS also set new standards in neutron facilities development by the early use of a solid methane moderator and guide tubes.

Starting from 1 to 2  $\mu\text{A}$  proton current, KENS has steadily improved in performance and has reached 5  $\mu\text{A}$  over the course of the years. This, together with continuous improvements on the existing instruments and the addition of new innovative ones, allowed KENS to become an important user-oriented facility, attracting scientists not only from all over Japan but also from around the world. While the beam time allocated to KENS has remained roughly unchanged over the years, the number of research proposals accepted and completed successfully has grown almost linearly throughout the whole period and has reached an impressive number of 150 in recent years. This has become possible not only by adding new instruments to the existing suite, but also by upgrading earlier ones or replacing them with more efficient ones.

The continuing close collaboration with the Hokkaido University group and KENS is a great benefit to KENS and to the larger world effort in target-moderator-reflector assembly (TMRA) systems development. Collaborations set up within the framework of ICANS and with ISIS and PSI were similarly very helpful in accomplishing a highly efficient facility in the future project (the N-Arena of the JHF).

All these development and activities served exceedingly well to position the KENS group to arrive at highly-refined, efficient designs for the N-Arena of the Japan Hadron Facility. Furthermore, the collaboration formed with the KUR group on target thermal, hydraulic and mechanical engineering provided an excellent mechanism for the development in the future project too.

##### **(1997-2004)**

In 2000, KENS was renewed by replacing the whole TMRA with a new tantalum-clad tungsten target, which was fabricated by the HIP method. A gadolinium poison, giving a sharper pulse, was installed in the ambient moderator. The new target increased source intensity by about 20% compared to the former tantalum target. The cold neutron intensity of the former TMRA, which had decreased about 70% from its initial state, was recovered. The neutron performance was measured at several spectrometers. The cold neutron intensity is fully recovered and the epithermal neutron flux was increased as the neutronic design calculations had indicated. The scattered-neutron profile shows low background and becomes more symmetrical by the shortened tail. At the total scattering spectrometer, the radical distribution function shows better resolution in position. As a whole, it can be said that KENS in its latest configuration had a good capacity to investigate materials.

**(2004-2007)**

KENS investigated the ways to develop materials that have strong resistance against impact shock and irradiation for spallation targets and aerospace. Pitting phenomena in mercury targets was also investigated. In the next stage, material development and characterization will be promoted. As for material development, cladding or film coating on iron is needed by using a more improved method, such as laser pinning, as well as an optimized condition, even for the conventional method. Presently, CrN film formation with the molten salt method is being performed at Kyoto University. The characterization of materials and the material behaviour under impact conditions and radiation is very important to certify new materials and improve them.

## 5. Scientific Research Achievements

### 5.1 Soft- and Bio-Materials

(1980-1997)

The importance of neutron scattering for studying soft materials has arisen first from the labelling possibilities offered by the large difference in the coherent scattering length between hydrogen and deuterium, and secondly from the available  $Q$ -range, which allows exploration of distance scales from a few repeat molecular units up to the dimensions of whole molecules. A great advantage in the usage of pulsed neutron facility for the study of soft materials is to allow simultaneous measurements in a wide range of both momentum and energy space at the same sample conditions, because several phenomena observed in soft materials are resulted in complex conformational and morphological changes at different circumstances. These powerful neutron scattering techniques have been successfully applied in the studies of several polymer systems at the KENS facility.

A typical example is the investigation of structure and mechanism of physical gels using atactic polystyrene as a sample. When the crosslinking of polymers is of a physical nature, thermoreversible gels are formed. On cooling the polymer solution, a sol to gel transition is observed. The neutron scattering experiments of atactic polystyrene solution in carbon dioxide revealed that two mechanisms of physical gelation existed in different molecular conformations of polymer segments. Another scientific highlight done at KEK is the study of glass transition dynamics and relaxation processes of polymers. Using a quasielastic neutron scattering technique, the dynamics of amorphous polybutadiene was investigated as a function of temperature. A very fast motion of picosecond order was found at the so-called Vogel-Fulcher temperature  $T_0$ , suggesting that the fast process is a precursor of the glass transition. This fast process was assigned to a damped vibrational motion in the C-C torsional potential well. In addition to the fast process, a slow motion of 0.1 nanosecond order was observed above the glass transition temperature  $T_g$ . This slow process was assigned to an elementary process of conformational transition in a polymer chain, leading to structural relaxation above  $T_g$ . These experiments have been performed in the close collaboration among many scientists from several universities under the inter-university programme of KENS.

Currently inorganic ceramics and often transient materials between inorganic and organic state have been prepared from organic polymers specially designed as a precursor material. The KENS neutron instruments LAM-40, SAN and WINK have worked efficiently to find that a very high mechanical strength of Si-C-O(Ti) fibres (a kind of semi-soft material) is not simply related to an anisotropic fibre structure induced by the organic-to-inorganic conversion, but essentially originated from the formation of critically sized  $\beta$ -SiC crystalline nanoclusters embedded in Si-C-O amorphous matrix. Such as new category processing, which lies across conversion disciplines of organic and inorganic materials, might be a merging and promising area for pulsed neutron scattering characterization of dynamics and medium-range structure at the KENS facility.

Neutron scattering is also one of the useful tools to investigate the structures and dynamics of biomaterials. However, the neutron intensity of the present facility at KENS seems to be too low to elucidate biological phenomena in detail, although a few preliminary experiments related with biomaterials have been carried out. This would be realized in the near future by the use of the high neutron flux of J-PARC.

**(1997-2004)**

High-quality research in the fields of polymers and bio-materials has resulted from the use of the neutron reflectometer (ARISA), the small-angle neutron scattering (SANS) spectrometers (SWAN and WINK), and the inelastic neutron spectrometer (LAM-40). ARISA has been installed quite recently (2000) and opened for public users since 2002. Nevertheless, the reflectometer has already been producing quite good output and will certainly make further important contributions to surface science and technology. From SWAN and WINK came important contributions to examination of the static structures of polymers and bio-materials. We should note an outstanding research output obtained on keratin protein: results clearly proved that these spectrometers could help elucidate hierarchical structures extending over a wide length scale (from  $\sim 0.1$  nm to  $\sim 100$  nm). Exploration of such hierarchical structures and their cooperative dynamics will have an important impact on life science. LAM-40 has produced excellent research results on the dynamical aspects of glass-forming polymers. In conclusion, the high-level research activities attained so far in this field should be further extended to various research topics by attracting a greater number of external users.

**(2004-2007)**

Excellent research outputs in the fields of soft materials have continually resulted from the use of the small-angle neutron scattering spectrometers (SWAN and WINK), the neutron reflectometer (ARISA), and the inelastic neutron spectrometer (LAM-40). The activities have been maintained even after KENS shut down by the strong supports from two programmes, i.e., “UK-Japan collaboration programme on neutron scattering” and “Inter-University Research Programme on Pulsed Neutron Scattering at Overseas Facilities”. The reflectometer, ARISA, has been producing good outputs with the aid of CRISP at ISIS, for example the difference in diffusion behaviour between ring polymer molecules and linear counterparts has been clarified very clearly, and will certainly make further important contributions to surface and interface science and technology. Very useful and applicable contributions have been produced from SWAN and WINK by examining the static structures of polymers and bio-materials. One typical example we should note is the observation of abnormal protein aggregation. LAM-40, with assistance of MARI at ISIS, has proved the local dynamical structure of a glass-forming polymer in thin films. These results have been shown that these spectrometers are indispensable in investigating hierarchical structures of soft materials covering mesoscopic length scales. In conclusion, the high-level research activities attained so far in this field should be further extended to various research topics by attracting a greater number of external users.

## **5.2 Dynamics in Spin Systems**

The dynamics of magnetic materials produces the important information about the spin structures of these materials over a wide range of momentum  $Q$  and energy  $E$ . Thus the pulsed neutron with a wide wavelength band is suitable for exploring such dynamics. In this context the dynamics of magnetic materials has been one of the strongest research areas in KENS since the first user’s research programme started on June of 1980. These dynamical studies were performed by using the spectrometers at KENS, by the Japan-UK collaboration programme on neutron scattering and by the international collaborations of the Inter-University Research Program on pulsed-neutron scattering at overseas facilities. The KENS group has accomplished marvelous scientific achievements on various subjects in “Dynamics in Spin

Systems” over 26 years since 1980, in particular in the following areas: (1) Fractal structures of percolating magnetism realized in diluted antiferromagnets, (2) Magnetism in CoO with unquenched orbital angular momentum, and (3) Dynamical properties of high- $T_c$  superconductors. Highlights of their scientific achievements will be summarized in the following three subsections which cover the periods from 1980 to 1997, 1997 to 2004, and after 2004.

#### (1980-1997)

In this first period, KENS groups carried out a notable study in the forefront areas at that time, such as high temperature superconductivity and low-dimensional magnetism. Among these frontier areas, we will mention KENS notable activity on (i) the fractal structure of percolating magnetism realized in dilute antiferromagnets and (ii) spin dynamics in antiferromagnets.

##### i) Fractal structure in diluted antiferromagnets

Fractals are characterized by self-similarity and are described by the fractal dimension ( $D_f$ ). If an object reduced by a certain ratio becomes identical to a part of the original object, the object is a fractal and has self-similarity. It is recognized that a percolating network forms a fractal and a dilute antiferromagnet is the simplest ideal percolating network. When magnetic atoms in a parent antiferromagnet are randomly replaced by nonmagnetic atoms, the Néel temperature ( $T_N$ ) decreases as the magnetic concentration ( $c$ ) decreases, and  $T_N$  becomes zero at the percolation threshold ( $c_p$ ). In a percolating antiferromagnet (diluted antiferromagnet with  $c = c_p$ ), infinite spin clusters with fractal geometry are present. Since there existed a single-crystal sample and magnetic properties can be observed at the antiferromagnetic superlattice point separately from lattice properties, the coherent magnetic excitations (fractons) can be selectively investigated in percolating antiferromagnets. The high  $Q$ -resolution experiments can confirm unambiguously the scaling nature of the systems of percolating antiferromagnets. At the same time the nature of anomalous spin diffusion in percolating magnets can be clarified by the experiments carried out at very low energy transfer. KENS groups succeeded in the structural study of percolated magnetic systems  $\text{Rb}_2\text{Co}_c\text{Mg}_{1-c}\text{F}_4$  with various magnetic concentrations  $c$ , and they showed that the  $\text{Rb}_2\text{Co}_c\text{Mg}_{1-c}\text{F}_4$  system was clearly characterized by a fractal system with the fractal dimension of  $D_f = 1.89$ .

It should be noted that the fractal nature was directly observed by the line profile of the scattered neutron spectrum  $S(Q)$ . We highly appreciate the success of the first observation of “fractons” by the KENS group. Consequently this success of the observation of fractons has led to remarkable developments in the research of more complex percolating antiferromagnetic systems in later periods. About this development we will mention more.

##### ii) Spin dynamics in antiferromagnetism

The study of spin dynamics in antiferromagnetism was carried out by the KENS-UK collaboration which started during this first period. In this collaboration KENS groups clarified spin-dynamics of antiferromagnetism in high  $T_c$  oxides of parent  $\text{La}_2\text{CuO}_4$  and its Sr compounds using a unique spectrometer MARI, which could scan a wide range of  $Q$  and  $E$ . They also found the qualitative difference of the width of the spin wave in the limit of low temperature between  $S=3/2$  ( $\text{CsVCl}_3$ ) and  $S=2$  ( $\text{CsCrCl}_3$ ) spin systems. The remarkable activity of Japanese scientists in this collaboration can be seen

from the ease with which they obtained beam time on inelastic scattering spectrometers such as MARI and HET at ISIS in Rutherford Appleton Laboratory, because time on these machines was awarded purely on the basis of peer review of scientific proposals.

**(1997-2004)**

In this second period, KENS groups performed research on (i) 1 D antiferromagnets utilizing INC, MARI, and PRISMA spectrometers, (ii) high- $T_c$  superconductors by MAPS, (iii) magnetic quasicrystals by LAM-40, and (iv) percolating systems by IRIS, LAM-80ET, PRISMA, OSIRIS, and PONTA-NSE. Here, MARI, PRISMA, MAPS, and IRIS are the spectrometers installed at ISIS at the Rutherford Appleton Laboratory.

i) One-dimensional (1D) antiferromagnets

The dispersion relation for magnetic excitations at low temperatures and the  $T$ -dependence of the inverse correlation length in the spin systems of  $\text{CsNiCl}_3$  ( $S=1$ ),  $\text{CsVCl}_3$  ( $S=3/2$ ) and  $\text{CsCrCl}_3$  ( $S=2$ ) were measured by the inelastic neutron scattering experiments, and KENS groups confirmed the validity of the spin-dependent quantum renormalization scheme from the good agreement between experiment and theoretical prediction. The systematic studies of the spin-dependent quantum effects in 1D antiferromagnets are very impressive, and thus we appreciate their achievements as a very high level.

ii) High- $T_c$  superconductors

Among the high- $T_c$  (HTSC) cuprates, both  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  (LSCO) and  $\text{YBa}_2\text{Cu}_3\text{O}_{6+\delta}$  (YBCO) are the only HTSC systems in which the static and dynamical incommensurate properties in certain carrier concentrations have been reported. The time-of-flight technique with a pulsed neutron source is particularly well-suited for such wide- $Q$  and high-energy transfer measurements. The spin-correlations of the optimally doped superconductor  $\text{YBa}_2\text{Cu}_3\text{O}_{6.9}$  ( $T_c = 92.5\text{K}$ ) were extensively measured for wide energy- and wavelength- ranges on the MAPS spectrometer. The conclusions that incommensurability and intensity cannot be described by the stripe model is quite important and has opened a way for further discussion regarding the mechanism of high  $T_c$  superconductivity.

iii) Magnetic quasicrystals

Quasicrystals have distinct spatial symmetry characterized by highly ordered but non-periodic (quasiperiodic) atomic structure, which differs from both periodic and random structures. In order to understand the dynamics of quasi-periodically arranged spins, Zn-Mg-RE (RE: rare-earth) icosahedral quasicrystals were studied by inelastic scattering experiments using LAM-40. KENS groups showed the existence of the localized collective spin dynamics in the icosahedral Zn-Mg-Tb quasicrystal. This piece of work contributes to the understanding of the dynamical aspects of quasicrystals and should be highly appreciated.

iv) Percolating systems

The magnetic properties of a percolating network were investigated by using single crystals of the two-dimensional Ising system  $\text{Rb}_2\text{Co}_c\text{Mg}_{1-c}\text{F}_3$  and of the two- and three-dimensional Heisenberg systems  $\text{Rb}_2\text{Mn}_c\text{Mg}_{1-c}\text{F}_4$  and  $\text{RbMn}_c\text{Mg}_{1-c}\text{F}_3$ . It is impressive that with measurements of the critical scattering on

IRIS and LAM-80ET, KENS groups clearly correlated the percolation regime to the fractal structure in the square lattice. Although detailed studies have been continued in the next period, this work is unique and pioneering. We appreciate this work highly as one of highlights in KENS's scientific achievements in the area of pulsed neutron studies for spin dynamics.

**(2004-2007)**

In the meeting of the KENS review committee held on January 30-31, 2008, we have heard research activities after 2004. As regards the dynamics in spin systems, the following three research achievements were reported as scientific activities after 2004: (i) Fractons in percolating antiferromagnets; (ii) Magnetism in a  $d$ -electron system with unquenched orbital angular momentum; and (iii) Dynamical properties in high- $T_c$  superconductors.

i) Fractons in percolating antiferromagnets

An inelastic neutron scattering experiment on the percolation Heisenberg antiferromagnet,  $\text{RbMn}_c\text{Mg}_{1-c}\text{F}_3$ , with  $c = 0.4$  was performed at 1.5 K, well below  $T_N = 19.5$  K, using the IRIS spectrometer at ISIS. The magnetic concentration in this system ( $c = 0.4$ ) is close to the percolation threshold  $c_p = 0.312$ , and the crossover wave vector is estimated to be  $Q_c = 0.029 \text{ \AA}^{-1}$ , where behaviour nature can be observed at  $Q > Q_c$ . The dispersion relation of the observed magnetic fractons was well fitted to  $E(Q) \sim Q^z$  with  $z = 2.5 \pm 0.1$ . The value of  $z$  was in good agreement with the fractal dimension  $D_f = 2.48$  for this system. It has been postulated that fractons are characterized by a single length scale and the dynamical structure factor can be scaled as  $S(Q, \omega) = Q^{-y} F[Q \omega^{-1}]$  with an energy-dependent length scale  $\omega^{-1}$ . In the present experiment, the functional form of  $S(Q, \omega)$  was completely determined. This is the first experimental determination for the predicted dynamical properties of fractons. We appreciate highly this result as one of the highlights in the scientific achievements in the area of dynamics in spin systems.

ii) Magnetism in a  $d$ -electron system with unquenched orbital angular momentum

A magnetic moment is generated not only by a spin angular momentum  $S$ , but also by an orbital angular momentum  $L$ . KENS groups have tried to find an effect of unquenched  $L$  by the inelastic neutron experiments. For this purpose they chose CoO (NaCl-type crystal structure,  $T_N = 289$  K) as an object of study, because the orbital angular momentum  $L$  of a  $\text{Co}^{2+}$  ion is not quenched in CoO. In this case the appearance of two or more magnetic modes is expected as the contribution from unquenched  $L$ , although only one spin wave branch normally exists when one up moment is included in a magnetic unit cell with the case of quenched  $L$ . KENS groups have performed inelastic neutron scattering experiments on CoO for the high-energy-transfer region by using chopper spectrometers INC at KENS and PHAROS at LANSCE while for the low-energy region a triple-axis spectrometer installed at a steady-state neutron source was used. Indeed they observed two or more magnetic modes. In experiments using a single-crystal sample, dispersion relations of the two magnetic excitation modes below 70 meV are determined along the symmetric directions in the crystal. Moreover, magnetic excitations around 120 meV were also observed. The energy spectra on a powder sample suggest the existence of higher order magnetic excitations spreading up to around 200 meV. The magnetic modes were analyzed in connection with the exchange interaction through  $S$  with the freedom of an unquenched  $L$  of a  $\text{Co}^{2+}$  ion. It was found that the

magnitudes of the spin-orbit interaction and of the exchange interaction obtained from the analyses were comparable, indicating that these interactions had to be simultaneously considered without an approximation of the total angular momentum,  $J = S + L$ . The lowest two dispersion curves observed in experiments are interpreted as mixing and splitting between dispersive excitations of  $S_z$  ( $S$ -mode) and individual excitations of  $L_z$  ( $L$ -mode). We recognize that this result is a remarkable scientific achievement.

### iii) Dynamical properties in high- $T_c$ superconductors

KENS researchers consider that the coexistence of antiferromagnetic fluctuations and superconductivity may be important in the mechanism of high- $T_c$  superconductivity. From this standpoint they performed neutron scattering experiments using the MAPS chopper spectrometer at ISIS. All experimental results for the hole-doped systems of monolayer  $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$  and bilayer  $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$  showed similar "hourglass-like" spin excitations. In these spin excitation spectra four incommensurate peaks are observed in a constant energy plot at low energy and those disperse inwards toward an antiferromagnetic zone centre as the energy increases. At a characteristic energy which corresponds to  $\sim 50$  meV, a single peak is found at the antiferromagnetic zone centre. At higher energies, the excitations disperse outwards and form a square-shaped continuum. These results indicate that such hourglass-like dispersive excitations might be common to high- $T_c$  cuprates. In fact, after this discovery it was confirmed that the hourglass-like spin excitations are commonly observed in many systems with different rate of hole doping.

As regards the electron-doped systems, researchers in the KENS group have succeeded in growing large single crystals of electron-doped  $\text{Pr}_{1-x}\text{LaCe}_x\text{CuO}_4$  and in observing magnetic signals up to  $\sim 180$  meV on MAPS. At all of the measured values of  $x$ , a single peak centered at the  $(\pi, \pi)$  reciprocal position is confirmed. The spin excitation spectrum differs from conventional spin-wave excitation, although the present  $\text{Pr}_{0.89}\text{LaCe}_{0.11}\text{CuO}_4$  has a phase boundary located between the antiferromagnetic ordered and superconducting phases, but is similar to that of metallic antiferromagnets. They have also performed experiments on an over-doped  $\text{Pr}_{0.83}\text{LaCe}_{0.17}\text{CuO}_4$  on MAPS, and have found that the high-energy magnetic excitations at more than 100 meV observed in underdoped  $\text{Pr}_{0.89}\text{LaCe}_{0.11}\text{CuO}_4$  disappear in the over-doped system. These experimental results give important information in understanding the mechanism of the electron-doped high- $T_c$  superconductivity.

There is increasing evidence as for a strong electron-phonon interaction in high- $T_c$  superconductors. Recent systematic X-ray scattering measurements of  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  (LSCO) have revealed an enhancement of anomalous softening in the Cu-O bond-stretching phonon mode in the entire superconducting phase, suggesting a possible contribution of lattice vibration (phonon) to the superconductivity. Researchers in the KENS group have recently performed an experiment to investigate the spin-phonon coupling in the high- $T_c$  cuprates through the impurity effect on the phonons. For this experiment they have used the Fe-doped  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  system with the hole concentration of 0.12. By substituting a small amount of Fe for Cu, the SDW order is enhanced and CDW order is induced. They have prepared single crystals with total mass of 80 g and experiments were performed on PHAROS at LANSCE. Experimental result shows the inelastic neutron-scattering intensity around  $Q = (3, 0, l)$  at 13 K. The clear phonon branch from the in-plane Cu-O bond stretching mode can be seen in the energy range between  $\sim 70$  meV and 85 meV. They have found that the bond-stretching phonon with the anomalous peak-broadening is modified by Fe-doping, suggesting the interplay between the phonon and the stripe

formation of spin and charge.

In the spin systems the spin fluctuations play an important role in determining the magnetic properties and dynamical behaviours of magnetic materials. Thus the neutron scattering experiments play unique roles of extracting the information of atomic and spin structures in magnetic materials,  $S(Q, E)$  and  $\chi(Q, E)$ , respectively, in a wide range of momentum  $Q$  and energy  $E$ . The scientific research activities on the subject of “Dynamics in Spin Systems” by the KENS group over 26 years since 1980 have significantly contributed to the progress of the following subjects: (1) Fractal structures of percolating magnetism realized in diluted antiferromagnets, (2) Magnetic quasicrystals, (3) Magnetism in CoO with unquenched orbital angular momentum, and (4) Dynamical properties of high- $T_c$  superconductors.

As regards the fractal structures in dilute antiferromagnets, the KENS group succeeded in the complete determination of the dynamical structure factor of magnetic fractons in 2D and 3D percolating magnets for the first time. It is impressive that with measurements of the critical scattering on IRIS and LAM-80ET, the KENS group could correlate the percolation regime to the fractal structure. It is one of remarkable scientific achievements by the KENS group to have clarified the fractal structure for diluted antiferromagnets.

The success of the first observation of the remarkable effect due to the unquenched orbital angular momentum in the magnetic excitations of CoO is also highly appreciated as a notable achievement by KENS group. Finally we should mention that, by observing the hourglass-like spin excitations in hole doped LBCO and YBCO, KENS group and collaborating researchers have found that hourglass-like dispersive spin excitations may be common to hole-doped high- $T_c$  cuprates. We believe that this outstanding result will play an important role in determining the mechanism of high- $T_c$  superconductivity.

Although detailed studies should be continued, the work mentioned above are all unique and should be considered as remarkable scientific achievements in the area of pulsed neutron studies of spin dynamics.

### **5.3 Liquid and Amorphous**

**(1980–1997)**

Liquid and amorphous solids form a large part of the structured studies carried out in KENS since the start of its operation. Separation of centre-centre correlation and orientational correlation of molecules existing in the liquid state is a noteworthy success due to the use of short wavelength neutrons provided efficiently by the KENS neutron source.

The high  $Q$  measurement by HIT using the short wavelength neutrons gives the highly resolved short-range structure in the radial distribution function. This point has been fully applied to assign the atom-atom correlations in various kinds of multi-component glasses to find the role of chemical bonds in the topologically disordered materials. The high  $Q$  measurements also contribute to the classification of the short- and medium-range order such as atomic distance and the coordination number in metallic glasses. For example, the existence of the trigonal prismatic packing of six Ni atoms in Ni-B amorphous alloys was found.

Inelastic neutron scattering measurements using the LAM-40 clearly represent the identification of the so-called Boson peak (excess spectral weight in medium energy range around a few meV) in a  $\text{Pd}_{79}\text{Ge}_{21}$  amorphous alloy as due to the hinge-like motion between trigonal prismatic units.

Dynamical pair correlation functions of SiO<sub>2</sub> and GeSe<sub>2</sub> glasses were observed by using MARI. This method shed new light on the dynamic structure about the Si-O-Si bond angle and dihedral angle between SiO<sub>4</sub> tetrahedra in SiO<sub>2</sub> glass which is very difficult to obtain by other methods.

**(1997—2004)**

Studying the nano-scaled structure of liquids and amorphous solids is one of the ongoing activities of the KENS and ISIS facilities. Between 1997 and 2004, the main subject in this field shifted from metallic system to a non-metallic one, including aqueous solutions and hydrogenous materials. Based on experimental results obtained by using the spectrometers HIT, SWAN, LAM-40, LAM-D, LAM-80ET, INC in KENS, and MARI in ISIS, the excellent work completed so far has been published in 85 original papers.

These excellent activities are summarized:

- Static structure of energy materials; Observation of hydrogen atoms in hydrogen absorbing materials,
- In-situ measurement of molecular glass by using a novel cryostat,
- Mesoscale structure of aqueous solution,
- Collective motions in glasses,
- Dynamic structure of methane hydrate for a future neutron moderator,
- Hydrogen dynamics on the surface of nano porous silicon, and
- Structure of two-dimensional solids.

Two highlights are among the subjects previously mentioned: the study on the mesoscopic phase separation in a 1-propanol aqueous solution, which is well characterized by a mass-fractal model, and the detailed dynamical structure of the Boson peak in SiO<sub>2</sub> glass, in which the buckling motion of a six-fold ring is first observed.

The nano-scaled structure of liquids and amorphous solids is expected to be a major field for the coming J-PARC. Significant step-up of instrumentation and the supporting system for this field is needed to keep the activity going in J-PARC.

**(2004—2007)**

Multiple combinations of different probes and methods such as between neutron and X-ray, experiment and visualization by computers, small-angle scattering and total scattering, static and dynamic structure measurements and so on have been widely used in the study of liquid and amorphous solids during the period of 2004 to 2007. Especially, visualization of complicated random structure by large scale reverse Monte Carlo calculation provides a comprehensive approach to understand the characteristic behavior of liquid and amorphous solids.

Examples of the excellent works are shown:

- Visualized analysis of small angle neutron scattering intensity of alcohol-water mixtures

An anomalous behaviour in molar volume evolution of 1-propanol aqueous solution was found to originate from a characteristic change of the fractal dimension in the meso-scale solution structure observed by means of small and wide-angle neutron scattering. The meso-scale solution structure is well interpreted in terms of a double water-shell model visually shown by large-scale reverse Monte Carlo simulation.

#### -Structural origin of thermal stability of Cu-Zr-Al metallic glasses

Addition of a third element Al to Cu-Zr binary metallic glasses lowers its glass transition temperature due to stabilization of the super-cooled liquid state. Voronoi polyhedra-analysis based on neutron and X-ray diffraction data and reverse Monte Carlo simulation concludes that the fraction of icosahedral-type structure units increases by addition of Al. However, a low energy excitation observed around a few meV corresponding to Boson peak decreases by the addition of Al. The conventional relation confirmed between free volume and stability of liquid structure might be carefully examined from the nano-scale point of view by pulsed neutron scattering.

#### -Cation-cation correlation in molten CuI

CuI is well known to exhibit a very high Cu-ion conduction in the high temperature solid state, compared with CuCl and CuBr. However, in its molten state, Cu-Cu pair correlation is much stronger in CuI than in CuCl and CuBr where Cu-ions are uniformly distributed due to the repulsive force between Cu-ions. In fact, a first sharp diffraction peak due to Cu-Cu pair correlation appears at  $Q=0.86 \text{ \AA}^{-1}$  and Cu-Cu pair distance is completely overlapped with Cu-I pair distance in molten CuI. This suggests possible formation of covalent bond between Cu atoms. The relaxation time for Cu atom movement obtained from quasi-elastic neutron scattering peak width at  $Q=0.86 \text{ \AA}^{-1}$  gives a much longer value 1.6 ps than that expected from simple self-diffusion. How the dynamic behaviour and the local structure of Cu atoms are related to the diffusivity of Cu atoms is an interesting problem to be solved by using J-PARC facilities.

### 5.4 Crystallography

The important activity by the KENS powder diffraction group was the construction of a series of state-of-the-art level diffractometers which includes two famous diffractometers, Vega (versatile powder diffractometer) and Sirius (high resolution powder diffractometer). The group has also invested enormous efforts to develop TOF-engineering diffraction as well as high-pressure techniques for J-PARC. Some of the scientific achievements cover the determination of the structure of the high- $T_c$  cuprate superconductor, hydrogen-storage materials, and recent novel materials such as energy storage materials, oxygen sensors, ferroelectric memory materials, multiferroic materials. The special focus on the crystallography has been placed on the exploration of the relationship between the function and its relation to the crystallographic structure. Highlights will be summarized in three subsections which covers the period 1980 to 1997, 1997 to 2004, and after 2004.

#### (1980-1997)

The most remarkable achievement in the structural studies at KENS in this early period was the world's earliest determination of the high- $T_c$  superconducting material in 1987. As soon as the crystalline  $\text{YBa}_2\text{Cu}_3\text{O}_7$  was reported to undergo a transition to the superconducting state at 90 K, almost all of the solid state researchers began to address the problem. Among such world-wide movements, the scientists at KENS pioneered the determination of the detailed crystal structure of this substance using the HRP spectrometer. It is worthwhile mentioning that the achievement was brought in by an *ad hoc* 3 days extension of the operation of the proton accelerator at KEK. This pioneering work has been followed by a large amount of structural data of various classes of high- $T_c$  superconducting materials, which has

contributed to a broad understanding of novel mechanism of superconductivity.

**(1997 - 2004)**

In this period, a number of experiments have been performed on the single-crystal diffractometer (FOX), Epithermal diffractometer (EXCED) and on two powder diffractometers, versatile powder diffractometer (VEGA), and newly constructed high-resolution instrument (SIRIUS). Scientific efforts were concentrated on elucidating the relationship between material functions for practical applications and the structure of the materials themselves.

i) Single-crystal diffraction (FOX and EXCED)

Two-step ordering in an *fcc* crystal was first observed on the Pt-rich Pt-Mn alloy. With rising temperature, successive transformations, from the ABC<sub>6</sub>-type to Cu<sub>3</sub>Au-type transformation and then to a disordered *fcc* structure, were established. In addition, a variety of experiments have been carried out on the FOX spectrometer, for example, “SDW formation in the ordered Pt-12.5% at.% Mn alloy”, “Two-dimensional magnetic superstructure in a ternary alloy TbRu<sub>2</sub>Ge<sub>2</sub>”, “Multi-step metamagnetic phase transition under external magnetic field in TbRu<sub>2</sub>Si<sub>2</sub>”, and “Characteristic diffuse scattering in eta-Sn”. The excellent diffraction experiments on natural abundant Gd compounds were achieved with an epithermal neutron diffractometer, EXCED. One of the highlights is the confirmation of a peak at (1/2 1/4 1/4) from GdB<sub>6</sub>. It had been believed that this peak must disappear in Gd compounds because of the lack of orbital moment of gadolinium atom. This result completely renewed the concept of magnetic interaction of this class of compounds.

ii) Powder diffraction studies (VEGA and SIRIUS)

It should be emphasized that continuous efforts have been made to improve these two powder instruments, and their performance is literally at a state-of-the-art level. From work with these spectrometers, 99 publications were published from 1997 to 2004. Work conducted on these two instruments is categorized as “Structural studies on new materials and science”. Two of the important topics covered are “Ferroelectric random access memory materials” and “Origin of structural transition in the first pyrochlore superconductor Cd<sub>2</sub>Re<sub>2</sub>O<sub>7</sub> and its orbital ordering”. Development of the analysis method is crucial to powder diffraction studies. Along this direction, the development of the TOF/MEM method and its beautiful application to the study of a Li-ion conductor is one of the highlights in the powder diffraction studies conducted at KENS. An in-situ measurement of hydrogen alloys under hydrogen pressure offers another typical example of the strong instrumental support to new experimental techniques at KENS. Within a study of the solid oxide fuel cell, the structural evaluation of a new electrode material, the lithium manganese spinel, contributed to the improvement of battery performance, which would eventually contribute to open a new energy life.

**(2004-2007)**

i) Hydrogen storage materials

For future fuel cell cars, development of safe and large capacity hydrogen storage is crucial. Some of the key issues for the developments are how much hydrogen can be stored in the light of the weight

and/or volume of the alloys, how much of them can be reversibly utilized, working condition (temperature and pressure to absorb and release), lifetime, etc.

The hydrogen storage capacity of *bcc* solid-solution alloys, Ti-Cr-V, Ti-Mn-V and Ti-Cr-Mo, reaches about 2 H/M at room temperature. To clarify the so-called “dead storage” issue, the crystal structures of metal hydrides,  $(\text{Ti}_{0.45}\text{Cr}_{0.55-x}\text{Mo}_x)\text{-D}$  ( $x = 0.05, 0.10, 0.20, 0.30$ ), at various deuterium contents have been investigated by *in situ* neutron powder diffraction at various temperature. These works identified that in the dead storage state hydrogen atoms are trapped at a site with more Ti and less Cr. The crystallographic knowledge obtained in this work will be useful to develop less residual hydrogen materials by controlling local structure of hydrogen-storage alloys.

ii) Proton Conductivity in  $\text{K}_3\text{H}(\text{SeO}_4)_2$  - This work was performed with a combination of Neutron Diffraction and Inelastic Scattering

Fuel cells need a proton-conducting electrolyte membrane to conduct protons. The polymer fuel cell uses polymer electrolyte membranes. Among candidates of proton conductors,  $\text{M}_3\text{X}(\text{YO}_4)_2$  (M: K, Rb, Cs or  $\text{NH}_4$ ; X: H or D; Y: S or Se), the detailed crystal structure of  $\text{K}_3\text{H}(\text{SeO}_4)_2$  was studied in two distinct phases, the proton-conducting phase (phase I) and non-conducting phase (phase II) using the Vega diffractometer. Quasi-elastic neutron scattering (QENS) measurements were performed on the LAM80-ET spectrometer.

The crystal structures and scattering-amplitude-density distribution maps were obtained by a combination of the Rietveld method and maximum entropy method (MEM). It was found that the amount of the proton in the hydrogen bond region varies from 87% for the phase II to 21% for the phase I. From both the proton densities in the space of the inter- $\text{SeO}_4$  layers obtained by structural analyses and the diffusion constant obtained by QENS spectra analyses, the electric conductivity was calculated by the Nernst-Einstein relation, and the results were in well accord with those obtained from macroscopic electric conductivity measurements. The agreement suggests the inter- $\text{SeO}_4$  layer protons are conducting protons in these proton-conducting electrolyte membranes.

## **6. Neutron Instruments and Devices**

### **(1980-1997)**

KENS now has a suite of instruments that is able to cover a broad range of energy and momentum transfer, with suitable resolution. Several diffractometers (HIT, HRP and SAN) provide information on the static structure of materials over a range of length scales from sub-angstrom to fractions of a micron, and a suite of spectrometers (LAM-40, LAM-80, LAM-D, CAT, MAX and RAT) allow atomic and magnetic dynamics to be studied over a wide range of time scales.

Several of the neutron scattering instruments at KENS are based on innovative designs whose value can be judged by the fact that they have been imitated at other neutron sources. Examples include MAX (which is the forerunner of PRISMA at ISIS) and CAT and RAT (the forerunners of TFXA and EVS at ISIS). In other cases, clever instrument design has enabled scientists at KENS to make measurements in some fields of science that are fully competitive with those made at the world's best facilities. A case in point is the LAM-80ET instrument which, for measurements of  $Q$ -independent scattering, provides both similar resolution and similar count rates to IRIS spectrometer at ISIS, which has about 60 times greater proton beam power.

In the area of powder diffraction, one of the world experts in this field, Dr. J. Jorgensen of Argonne National Laboratory, has informed us that the KENS instrumentation is now more advanced than any in the world. A special symposium will be organized at this year's International Conference of Neutron Scattering to examine first results from SIRIUS and to plan an international strategy for advancing the state of the art even further. That new diffractometer sets a new standard for large solid angle detectors and their implementation through data acquisition and calibration.

WINK and SWAN are unique instruments designed in KENS and they simultaneously provide very wide  $Q$ -scan range of  $10^{-2}$  to  $10^2$  nm<sup>-1</sup>. Such a wide  $Q$ -scan will be surely a key strategy for exploring the overall structure of complicated amorphous systems between organic and inorganic materials.

Until recently, the KENS facility has suffered somewhat from the restrictions of space in the experimental area. While this has been largely overcome by clever arrangements of instruments in the crowded room, the new cold neutron hall completed in 1996 will enhance the effectiveness of the facility and its service to the scientific community.

Japanese scientists at KENS have recognized the importance of advanced neutron technology and novel sample environments, and have systematically moved forward in these areas. For example, the PEN instrument was one of the first (if not THE first) in the world to perform generalized polarization analysis by carefully controlling the magnetic fields around the sample. In another area, scientists in Europe and the USA are now beginning to emulate their Japanese colleagues by constructing high-field magnets, but it will be several more years before there is any serious competition to the 30 Tesla magnet that is available at KENS for the studies of the structure of magnetic materials.

Scientists associated with KENS have also advanced the state of the art in the area of neutron detection, by developing a linear position sensitive detector package with compact, integrated amplifiers having excellent positional resolution. This same technology, applied to increase the large- $Q$  range in the small angle diffractometer SWAN, exemplifies KENS's leadership in the push to larger numbers of data pixels in advanced time-of-flight instrumentation. On-going research on helium scintillation detectors is aimed at producing detectors that can handle 100 times the counting rate of present-day detectors and that

will therefore be well-suited for development at more intense neutron sources, such as that envisaged for future construction at the N-Arena in the JHF project.

The Review Committee recognizes the importance of the chopper spectrometer developments pursued jointly between KENS and ISIS. MARI and the forthcoming MAPS spectrometer not only provide access for the Japanese scientific community to state-of-the art spectrometers, but also represent important experience on which to build new instruments for the N-Arena.

Similarly, KENS scientists have had important input on the evolution of the reflectometer SPEAR at LANSCE. With the commissioning of HRF at J-PARC and a planned upgrade to SPEAR, this collaboration promises further benefits to both parties and the international scientific community.

An important feature of the instrument construction activity at KENS has been the way in which students and professors from Japanese universities have been involved. Not only has this contributed strongly to the education of students, but it has proved to be a very efficient way to construct many instruments without unduly augmenting the in-house staff. This method of involving the national community in the construction of instrumentation has not been widely used in the rest of the world, but is now being attempted in different guises at centres in other countries, partly because of the success that it has had at KENS. Observers from foreign centres conclude that there is much in this model that can profitably be applied in instrumentation programs at new facilities developing outside Japan, not only in the provision of instruments but also in governance of their utilization through the external instrumentation groups.

Opening his presentation to the Review Committee, Dr. M. Arai noted that “Our unique instrumentation has made KENS competitive with other more intense sources”. The Review Committee fully concurs with this view and congratulates the scientists who have been involved with instrument construction at KENS on their innovation and efficiency in building a suite of instrumentation which is truly world class.

#### **(1997-2004)**

A new high-resolution powder diffractometer, SIRIUS, was completed in 1998, a new reflectometer, ARISA, was constructed under the collaboration of KENS and a Japanese polymer group in 2000, and an eV-diffractometer, EXCED, was constructed in 2000. Further, the detector system of the single-crystal diffractometer FOX was improved in 1997. The high-intensity powder diffractometer VEGA and small-to-medium angle scattering spectrometer SWAN were improved using a Grant-in-Aid in 2002. The chopper spectrometer INC was improved with the PSD in 2003.

KEK and JAERI will construct 10 day-one instruments by the completion of the first phase of J-PARC in 2007. Among the 10 instruments, KEK is responsible for building four epoch-making instruments aiming at the observation of extremely high resolution in space and energy range:

i) High-performance neutron reflectometer with horizontal sample geometry

This instrument has an inclined beam line to make study of free liquid surfaces as well as liquid/liquid surfaces possible with the world's highest incident neutron intensity up to  $0.5\text{\AA}^{-1}$  in  $Q_z$ .

ii) Super-High-Resolution Powder Diffractometer

This is the world's highest resolution powder diffractometer for study of the structure of hybrid nano-scale novel materials. The resolution (0.03%) is comparable to the highest resolution of SR powder diffractometers. The combination of these high-quality data from SR-XRD and JSNS will definitely open

a new scientific window on materials structure study.

iii) High-Intensity Total Scattering Diffractometer

This is a high-intensity total scattering instrument to study liquid and disordered materials such as glass and amorphous solids in very high spatial resolution and at very high intensity, clarifying the structural hierarchy in materials for creating functions.

iv) High-Resolution Chopper Spectrometer

This is a high-resolution inelastic scattering instrument to study dynamics related to function and properties of a wide range of materials including a highly correlated electron system, magnetism, superconductor, amorphous materials, liquids, etc. The spectrometer covers very wide energy and spatial ranges.

v) R&D of neutron devices

Neutron scattering instrumentation requires continuous development. This depends greatly upon what can be termed “peripheral” devices, which in fact are intrinsic to the performance of any given instrument. An impressive program of such developments has taken place at KENS, within a relatively restricted set of resources. The vast majority of these developments will directly benefit the instrument suite at J-PARC.

Examples which can be quoted include the following:

- The building of  $t_0$  choppers – fruit of the collaboration with Mechanical Engineering Center at KEK and very necessary for J-PARC. This work is well along and a prototype is in operation. Collaborations with ISIS, IPNS, and SNS facilitated the work of all parties.

- The program of neutron detector development, particularly high count-rate position-sensitive detectors which will be essential for J-PARC. For neutron detectors, specific attention is going to micro strip gas counters (MSGC), which have the prospect for sub-millimeter resolution and high data rates. Tests show interesting results. These efforts connect to the gathering world collaboration on neutron detector development.

- Neutron helium-3 spin filters, where an impressive storage time has been achieved. A prototypical system, based on Rb spin exchange, is under test. Pumping and  $^3\text{He}$ -polarization lifetime questions are objects of study. The prototype system already gives results comparable with those in other laboratories, with whom the developers maintain communications.

- Particularly worthy of mention is the development of pulsed magnetic fields up to 32 Tesla (in collaboration with Tohoku University), which represents the highest available fields in the world for neutron scattering measurements. This will be especially valuable on J-PARC, where intensities in a single pulse will be particularly high and able to match the performance of this magnet.

- KENS played host to the International Neutron Optics conference in January 2004. Developments of neutron optical devices, a helium-free high-power refrigerator, and a device for polarizing protons in scattering samples are underway.

There are many developments both in Japan and worldwide in these areas, which complement the programs at KENS. The panel observes that many of these activities will benefit from close collaborations with other centers. It may even be possible to pool resources in order to achieve the optimum use of resources.

**(2004-2007)**

KENS are currently taking responsibility for nine of the potential 23 instruments at J-SNS. The

status of these is summarised in the table below.

<b>Instrument</b>	<b>Planning Status</b>	<b>Funding status</b>
Super high resolution powder diffraction (S-HRPD)	Operational May 2008	Funded
Total scattering diffractometer (V-HIT)	Operational March 2009	Funded
Fundamental Physics (NOP)	Operational March 2009	Funded
Horizontal sample reflectometer (HRF)	Pending	Funding agreed but not yet available
High resolution chopper spectrometer (HRC)	Pending	Funding agreed but not yet available
Micro focus SANS	Concept	Funding not yet available
High intensity Chopper Spectrometer	Concept	Funding not yet available
Diffraction under extreme conditions	Concept	Funding not yet available
Spin-echo spectrometer	Concept	Funding not yet available

The progress being made in the experimental hall at J-SNS is easily visible and there is every reason to believe that the construction/operation schedule for the first three of these will be met. Funding for the next two instruments has temporarily been diverted into the accelerator part of the project in order to maintain its schedule, but it is hoped that this will be changed during the next financial year. Further instruments are in the initial planning/concept stage and cannot realistically be expected to be in operation within the next few years even if funding becomes available.

SHRPD is planned to improve on the resolution of the equivalent instrument at ISIS, which has held the world leading position for nearly 20 years. It is not absolutely clear that significantly greater resolution will actually be needed for most experiments, but resolution can always be traded for count rate by grouping detectors, giving an exceptionally powerful instrument. Given the expected speed of SHRPD there will need to be substantial investment in automation such as cryogenic sample changers if it is to be effectively exploited.

VHIT forms a complement to SHRPD at the low resolution, total scattering end, with the high intensity powder diffractometer funded by Ibaraki prefecture in the middle. It is clearly planned to make significant use of structural modelling, for example reverse Monte Carlo, in analysis of data from this instrument. In order to be able to fully exploit such methods for the benefit of users KENS would be recommended to form a development partnership with some interested university(ies). Given the world leading high quality data that is now routinely being produced at Spring-8, there is a great opportunity to exploit the X-ray-neutron synergy by operating a coordinated research programme.

The construction of the beamline for neutron optics and fundamental physics is in progress at the J-PARC BL05 under the support of the Ministry of Education, Science, Sports and Culture, Grant-in-Aid for Creative Scientific Research. The beamline contains three beam branches, which provides high quality beams for the precision measurement of neutron decay parameters, neutron interferometry using multilayer interferometer accessing wide wavelength region and precise measurement of neutron scattering cross section for searching unknown medium range forces.

KENS is taking responsibility for optics and software development stretching across all of J-SNS instruments. The software development covers both data acquisition and basic data analysis, for which a common framework is being developed. Guidelines are then produced for interfacing more advanced (instrument/science specific) analysis, which tends to be the responsibility of individual instruments/scientists. The general software approach is very much in line with similar developments at e.g. SNS and ISIS. The same member of staff will be responsible for both VHIT and software development. This is not tenable even in the short term.

The optics and component development work is impressive in both its achievements and levels of innovation and imagination. Some of the works is 'blue skies' in that it is not directly intended for any instrument currently under construction or planned in the near future, but even if some of the specific ideas do not work out the general investment will undoubtedly be of long term benefit.

Refractive optics in the form of both prisms and Fresnel lenses, fabricated from novel polymeric materials, are being tested, though these are probably not yet close to real practical applications. The high  $m$ - and curved focussing super mirrors are much closer to applications. It is not absolutely clear whether the suggested design of multiple stacked micro-focus SANS instruments using these mirrors is entirely practical for user operation, but the concept is innovative and certainly the considerable shortening of the instrument that can be achieved will be a major benefit. There should also be important potential uses in for example the planned single crystal instruments or the residual stress instrument.

There is some work on polarisation devices such as  $^3\text{He}$  filters, but it is not clear if any thought has yet been given to the practical (and funding) implications of operating a  $^3\text{He}$  service on instruments. This should certainly be considered before too much effort and resources are spent on development.

Electronics development for long  $^3\text{He}$  position sensitive detectors, which are becoming a common feature of pulsed source spectrometers around the world, is addressing the common difficulty of achieving both the required resolution and count rate. A novel 'global/local' approach has been taken to the electrode layout on microstrip detectors to maintain the resolution but significantly reduce the electronics cost.

## **7. Future Scenarios**

The discovery of novel materials and innovative developments of devices has stimulated new sciences, led to new technologies and have given a huge impact on all of our lives. It should be the “food chain” of science and technology. There are so many examples of recent novel materials. Those are liquid crystals, advanced batteries, structural ceramics, dielectrics, ferro-electric, nano-crystals, catalysis, reaction interface, high temperature superconductor, hard materials and magnetic resistance materials. Additionally, in the 21st century the human genome project has been completed, and human beings have gotten the blueprint of their own life. However, this does not mean that we fully understand life even in its simplest forms, but indicates we have gotten the map of how to reveal the mystery of the life. One of the most important fields today is structural genomics. It makes the functions and dynamics of proteins clear, and also gives many effects on our actual lives. It should bring new cures for disease.

KENS is now constructing 1 MW pulsed spallation neutron source under the collaboration of JAEA, J-SNS. The peak flux is 100 times higher than that of the ILL, which is the most intensive reactor neutron source in the world. It can provide very unique and very innovative research-a circumstance offering the opening of new science fields. In such rapid growth of science and the technology, KENS is creating new world-leading projects (under KENS' initiative) which will play essential roles in the basic sciences. Those are (1) Reactive interface, (2) Protonics, (3) Basic quantum mechanisms, (4) Universality in complex nature and, (5) Fundamental neutron physics.

The main purpose of the “Reactive interface” is to measure the structure and dynamics at the bio-membrane interface, the electrical double layer as well as material transfer around electrode and formation process of phase-separated interface under an external applied field, and finally to understand mechanisms of signal transduction through the bio-membrane, mechanisms of electrochemical reaction around the electrode, and mechanisms of interface formation for composite materials, respectively. The purpose of “Protonics” is to resolve the structure and dynamics (including the transfer) of protons which are the key of understanding for the human activities and mechanism of biological kinetics as well as for the function of the novel materials such as performances of fuel battery. In the “Basic quantum mechanisms” project, the brand new elementary excitation of electronic orbitals that could possibly be an origin of giant magneto resistance GMR (the discovery of GMR has been awarded to Nobel Prize) as well as the detailed interaction between the electron-spin-phonon, that could derive useful quantum effects in the novel materials, will be researched. A purpose of “Univesality in complex nature” is to discover the universal structure and dynamics such as fractals, fractons and anomalous diffusion commonly observed in nature, materials and the life. The purpose of “Fundamental neutron physics” is to explore new physics beyond the standard model combining the achievements of neutron optics starting from the precision measurement of neutron decay parameters, improvement of the sensitivity of neutron interferometry and anomalous angular dependence of neutron scattering cross sections for seeking unknown medium-range forces.

Generally, by using the time-of-flight method, the pulsed neutron technique can give several benefits like a high energy-resolution, a high  $Q$ -resolution, a wide accessible range in the energy-momentum space and low background situations. Taking into account these benefits, characteristic instruments are realized. For example, the high-resolution instruments with reasonable intensity in a wide energy range will be realized, the energy resolution of which should be higher than that of light scattering measurements. Instruments with extremely large area detectors will be realized with a low background. It allows one to

observe widely distributed weak scattering from a quantum fluctuating system and short range correlations. Brillouin scattering will be realized using very small-angle detectors and a well collimated incident neutron beam. Measurements on small samples become possible by using focusing devices such as reflective and magnetic devices. Very short experiments will be possible which would allow studies on kinetics of both physical changes and chemical reactions and a much better exploitation of extreme environments.

KENS has developed several innovative instruments in the KENS facility, and staff understand well the advances of the pulsed neutron source. Based on this deep knowledge base, KENS plans 9 instruments in J-PARC, and at the beginning stage of J-PARC is constructing 5 instruments: a super high resolution powder diffractometer, total scattering diffractometer, horizontal refractometer, high resolution chopper spectrometer, and fundamental physics instrument. The performances of those instruments are among the highest in the world, and the challenge has been indispensable for promoting the KENS' staff initiative. In order to realize those innovative instruments, innovative devices are needed. KENS will collaborate with the Institute of Particle and Nuclear Studies (IPNS) which has sufficient experience for developing high speed electronic system and detectors, and will together establish a "world-leading center for the detector and devices" for continuous development on the KEK-Tsukuba campus.

KENS had developed about 13 powerful project teams called as the B1-group which involved about 100 researchers in the KENS facility (1980-2005). At the time of the KENS shutdown in JFY 2005, a new program "KENS-O" was established to transition activities to J-PARC. KENS again formed 5 project teams. The "KENS-O" program was very limited to the period of 2006-2008. KENS should safely transfer the original KENS activities into J-PARC, which will operate in 2008, through the KENS-O program.

Taking into account this time table and the framework of the inter-university program, KENS urgently formed five project teams to construct their own instruments in J-PARC and to promote the KENS initiatives of (1) Reactive interface, (2) Protonics, (3) Basic mechanism of quantum effect, (4) Universality in complex nature and, (5) Fundamental neutron physics, respectively. Those project teams are open for any researcher (including overseas researchers) who have good suggestion, good proposals, good skills and good expertise for topic. The project teams mainly work in the Tokai-campus, and promote their own projects. Here, the collaboration between the pulsed and the reactor neutron researchers is realized. Furthermore, owing to the powerful data-network system between Tokai-Tsukuba, the collaborative work between Synchrotron radiation (Tsukuba campus), Muon (Tokai campus) and Neutron (Tokai campus) team is strongly facilitated.

KENS originally belongs to the Institute of Materials Structure Science (IMSS) as a science division, and further doubles as members in the J-PARC center which is responsible for safety operating, maintaining, and developing the J-PARC facility. This sometimes leads the KENS teams into difficult situations. In order to discuss activities in the J-PARC neutron facility and to avoid difficulties, a sub-committee has been established within the J-PARC steering committee. The members of the sub-committee are Director of IMSS, Director of J-PARC center and Director of JAEA-side. KENS expects that this organization will work well.

KEK is responsible for inter-university program and promoting world-leading science in the fields of particle physics, nuclear physics, material science and life science with the accelerator complex. Although,

in principle, KEK should provide all of the required instruments for this promotion, it is difficult owing to short budget. Therefore, KENS plans to form a new University-union (or network), in which the KENS-initiative itself, the planning of future instrument-construction and the contribution by the university are discussed. The KENS-initiative is expected to grow as world-leading projects under this strong support from the University-union. KENS can contribute to educating young students (including students in Asia-Oceania) and to bringing in world-leading scientists for talks and collaborations. KENS will thus provide a great contribution to the University.

The KENS has capabilities for promoting world-leading projects, developing innovative techniques, educating young students and creating new science fields. KENS is always open. Following this KENS culture, KENS continuously establishes fruitful collaboration with world-leading laboratories and acts as a center of excellence.

## **8. Conclusions and Recommendations**

In 1997, the first KENS Review Committee was held for evaluating the scientific and technical achievements accomplished during the 17 years since KENS operation began in 1980, and concluded that the KENS facility was remarkably successful in promoting materials science and neutron physics research by means of a pulsed spallation neutron source and functioned at the world's highest standard. The second Review Committee pointed to the significant role of KENS to neutron science, its inter-university activities and the success of bringing the J-PARC project towards fruition, in 2004. KENS is now constructing a 1 MW pulsed spallation neutron source in collaboration with JAEA. J-PARC will provide really unique and innovative research opportunities and will give huge possibilities for opening up new science fields. In a phase of such rapid growth in scientific applications and their underlying technology, KENS is creating new world-leading projects (the KENS-initiative), which will play an essential role in basic sciences. These are (1) Reactive interfaces, (2) Protonics, (3) Basic quantum mechanisms, (4) Universality in complex nature, and (5) Fundamental neutron physics. Based upon their mature experience and knowledge acquired, KENS plans a total of 9 instruments at J-PARC. Already in the first phase of J-PARC, 5 instruments will be constructed. The performance of these instruments promises to rival the best in the world and they are indispensable for promoting the KENS-initiative.

The Committee extensively studied the achievements and activities carried out by KENS staff and users for 26 years of KENS operations via their oral presentations, written documents, and visitation of the facility site. The conclusions and recommendations of the Committee are as follows:

1. 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 facilities and the research are of the highest quality in particular when considered with the resources available. Staff productivity has continuously maintained a remarkably high level. Achievements accumulated in KENS are certainly helpful in realising the J-PARC project and cannot be substituted with any other ones. KENS has important capabilities in promoting world-leading projects, developing innovative techniques, educating young students and creating new science fields. KENS is always open for collaborative ventures, to their credit.
2. KENS continuously establishes fruitful collaborations with world-leading laboratories such as ISIS, IPNS and LANSCE, and acts as a centre of excellence both in Japan and on the world scene. These collaborations are certain to expand to Asian partners in Indonesia, Korea, China and Taiwan in the future, given the capacity of J-PARC. The Committee well recognizes that the J-PARC project must be a flagship in the world societies of neutron scattering and recommends that KEK promotes more valuable co-operative collaboration particularly in the development of pulsed neutron technology.
3. KENS had developed 13 powerful project teams, referred to as the B1-groups, which have involved about 100 researchers in the KENS facility (1980-2005). When KENS shut down in JFY 2005, a new program "KENS-O" was established. KENS formed 5 project teams again. The "KENS-O" programme is rather limited in a period of 2006-2008. These group systems have functioned quite efficiently so far as a

unique mechanism for the promotion of scientific activity, education, maintenance and development of instruments at KENS. KENS should safely transfer the group systems into J-PARC, which will operate in 2008.

4. KENS is responsible for building five day-one instruments: Horizontal Reflectometer (HRF), Powder Diffractometer (S-HRPD), Total Scattering Diffractometer (V-HIT), Chopper Spectrometer (HRC) and Fundamental Physics Instrument (NOP). KENS also plans to construct four other innovative instruments, such as SANS, High Intensity Spectrometer, Diffractometer under extreme condition and Spin-echo Instrument in the later phases of J-PARC. The Committee expects that these nine spectrometers installed at J-PARC will open challenging opportunities to the frontier of materials and life sciences as well as fundamental physics.

The Committee was rather surprised to find that the budget for the instrumentation has not been approved at the time of meeting in KEK. Therefore, the Committee strongly recommends that the five day-one instruments must be ready to be operated as soon as the J-PARC neutron facility started. In addition, the Committee expects that substantial arrangements for preparing the budget for 1) upgrading the above five day-one instruments, and 2) the construction of the other four instruments in the next phase.

5. KEK is responsible for the Inter-university programme and in promoting world-leading science therefrom. Therefore, KENS should form a new science network (University-union), and establish urgently project teams under this framework. The project teams are strongly expected to promote new science under the KENS-initiative that will grow into world-leading projects. The project teams should always remain open for any researchers (including overseas researchers) who have good suggestions, good proposals, good skills, and good expertise.

6. J-PARC will create possibilities for synergetic research with pulsed and reactor neutron beams, synchrotron radiation and muons. Also, KEK is located in Tsukuba city, where more than 80 government and private research organizations exist. The Committee therefore suggests that under this splendid situation for the total research on materials structures and dynamics that KENS should take the initiative to promote mutual collaboration in the field of materials structure research in Tsukuba and beyond.

7. Despite their excellent activities, the low number of in-house researchers is a serious concern. The Committee agrees with the proposal of KENS that the number of in-house staff must be increased by more than 30 in order to assure the future activities of KENS, especially with regard to the J-PARC project. A comparison with the resources available to the instruments on SNS would inform the decision-making process.

8. Finally, the Committee asks the Japanese government and KEK not to delay the construction of J-PARC behind its present time schedule. This is a very crucial point to be compatible with the collaboration and competition among ISIS, SNS, and J-PARC spallation sources and other leading neutron facilities world-wide.

The Review Committee congratulates the KENS team and wishes them well for the future!

## ***Appendix***

### **Conclusions and Recommendations (1997)**

The KENS facility has performed a remarkably successful function as the first pulsed spallation neutron source dedicated for condensed matter sciences and neutron physics since the beginning of operation in 1980. Pioneering works for the design and construction of neutron sources and instruments still continue at KENS. Much high quality research of a high international standard has been given from KENS to the scientific communities of physics, chemistry and biology in the world.

However, the situation has been significantly changed from when KENS started seventeen years ago. The user community of pulsed neutron scattering in Japan has been enlarged, in not only universities but also in industries, to approximately ten times compared with the start-up of KENS.

Outside of Japan, large-scale spallation pulsed neutron sources were installed at the IPNS in Argonne National Laboratory and the ISIS in Rutherford Appleton Laboratory after KENS. Furthermore, Europe and USA are actively planning new megawatt-class spallation neutron sources.

On the basis of the historical situation mentioned above, the KENS Review Committee has surveyed extensively the scientific and technical activities of the current KENS facility by hearing the presentation and/or by reading the written reports submitted from KENS. The KENS Review Committee concludes the evaluation and presents the recommendations as follows:

- The scientific and technical achievements carried out in KENS have contributed significantly to progress of materials research and neutron physics in the world. These researches are of very high quality in the world-wide standard. The productivity of the achievement has been maintained at a significantly high level despite of the shortage of neutron beam time in-house man-power at KENS.
- There is the difficult problem of the reduction of numbers of young scientists on the KENS staff. The numbers of KENS staff is far too small to support the rapidly increasing number of university users. The Review Committee strongly suggests that the number of the KENS in house-staff has to be increased at least to the twice of the present number for both the researchers and technicians over the next few years.
- The inter-university users program has been efficiently organized. The machine group system has functioned quite efficiently so far, as a unique mechanism for the maintenance and development of new instruments in KENS. However, it must be carefully considered that his mechanism will be still promising in the future of KENS. The personnel exchange between universities and KENS is extremely effective.
- The Neutron-Arena in the Japan Hadron Facility is a most necessary and timely project for developing the neutron scattering activity indispensable to materials science and technology in Japan.
- The Review Committee strongly recommends that the N-Arena in JHF project must become a key

strategy for Japanese scientists to continue the scientific contribution through pulsed neutron scattering to the peaceful progress of the world. In particular, KENS must be a Centre-of-Excellence for neutron scattering science in the Asian-Pacific region.

### **Conclusions and Recommendations (2004)**

In 1997, the first Review Committee was held for evaluating the scientific and technical achievements accomplished during the 17 years since the KENS operation began in 1980, and concluding that the KENS facility was remarkably successful in promoting materials science and neutron physics research by means of a pulsed spallation neutron source and functioned at the world's highest standard.

Since 1997 the KENS has much changed. A new tantalum-clad tungsten target was installed to provide a 20% increase of source intensity in 2000, and several instruments were newly constructed or improved. The most striking impact to the KENS is the year 2000 commencement of construction of a MW-class pulsed spallation neutron source, JSNS, based on the 3-GeV proton accelerator of the J-PARC project. Therefore, the second Review Committee was called up in June 2004 to survey the status of the KENS facility between 1998 and 2004. The charge given the Committee by the Director General of KEK, Professor Yoji Totsuka, is to evaluate the scientific and technical activities in KENS, to review the JSNS program in the J-PARC project, and to recommend a way to maintain its activities during the period between shut-down of PS and start-up of J-PARC.

The Committee extensively studied the achievements and activities carried out by KENS staff and users by hearing their presentations, reading the written documents, and visiting the facility site. The conclusions and recommendations of the Committee are as follows:

1. The scientific and technical achievements carried out so far in the KENS have significantly contributed to the progress of condensed matter research and neutron physics in the world. This research is of the highest quality according to the world-wide standard. The productivity continuously maintains a high level. Achievements accumulated in KENS are certainly helpful to realize the J-PARC project and cannot be replaced with any other ones.

2. KEK and JAERI will construct 10 day-one instruments by the completion of the first phase of J-PARC in 2007. Among 10 instruments, KEK is responsible for building four epoch-making instruments aiming at the observation of extremely high resolution in space and energy range:

- High-performance neutron reflectometer with horizontal sample geometry,
- Super-High-Resolution Powder Diffractometer,
- High-Intensity Total Scattering Diffractometer, and
- High-Resolution Chopper Spectrometer.

The Committee expects that these spectrometers installed at JSNS could open challenging doors to the frontier of materials structure such as mg-order small specimens, liquid/liquid interface, nano-scale hybrid material and electron-correlated materials under extreme environmental conditions.

3. It must be emphasized that KENS staff has been playing an indispensable role in the research and development of peripheral devices such as target, moderator, T<sub>0</sub>-chopper, polarization filters, detectors, data acquisition system, and so on, which are necessary to the JSNS program. In particular, the instruments to be installed at the JSNS cannot be built without the long-accumulated experience of the KENS staff.

4. The Committee was very surprised to find that the budget for the instrumentation has not been approved so far in KEK. Therefore, the Committee strongly recommends that the four day-one instruments for which KENS is responsible be constructed with monies raised during the shut-down term of the facilities related to the KENS. In addition, the Committee expects that substantial arrangements for preparing the budget for the construction of the remaining six instruments in the second phase begins earlier than previously planned.

5. KENS staff and users are facing the serious problem of how to keep and develop their activities after the shut-down of the KENS facility in 2005 until the start of the operation of JSNS in 2007. Therefore, the Committee suggests a special arrangement with the neutron partners, ISIS, IPNS, JRR3-M, and ILL, to support scientific activities of KENS staff and users during the period of no pulsed neutron source in Japan. This is an effective way to insure the manpower of young persons necessary when starting the operation of JSNS in 2007.

6. Despite their excellent activities, the low number of in-house researchers is serious. The Committee agrees with the proposal of KENS that the number of in-house staff must be increased by more than 30. Meeting the following needs is important to assure the future activities of KENS, especially with regard to the J-PARC project:

- (1) Drastic increase in the number of in-house researchers,
- (2) System of employing “senior post-docs”, which allows some excellent post-docs to stay more than two years but less than five years in total, and
- (3) An increased number of Ph.D. students who are associated with such national facilities as KENS. KENS staff should attract more young Ph.D. students to neutron scattering research by way of inter-university programs

7. KENS has intensively expanded the international collaboration outside Japan with pulsed neutron partners ISIS, IPNS, and LANSCE. These collaborations are certain to continue and expand to Asian partners in Indonesia, Korea, and Taiwan. The Committee well recognizes that the J-PARC project must be a flagship in the world societies of neutron scattering and recommends that KEK promote more valuable co-operative collaboration particularly in the development of pulsed neutron technology.

8. KEK has a splendid situation for the total research of materials structure, because the three different kinds of radiation source, neutron, light, and muon, are operated within direct-contact distance. KEK is located in Tsukuba city, where more than 80 government and private research organizations exist. Therefore the Committee suggests that KEK should take the initiative to organize a forum for promoting

mutual collaboration in the field of materials structure research.

9. Finally, the Committee asks the Japanese government and KEK not to delay the construction of J-PARC behind its present time schedule. This is a very crucial point to be compatible with the collaboration and competition among ISIS, SNS, and JSNS.