

World Premier International Research Center Initiative (WPI)

FY2011 WPI Project Progress Report (Post-Interim Evaluation)

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Common instructions:

* Unless otherwise specified, prepare this report from the timeline of 31 March 2012.

* So as to base this fiscal year's follow-up review on the document "Post-interim evaluation revised center project," please prepare this report from the perspective of the revised project.

* Use yen (¥) when writing monetary amounts in the report. If an exchange rate is used to calculate the yen amount, give the rate.

Summary of State of WPI Center Project Progress (write within the space of this page)

In FY2011, AIMR established a research environment to promote mathematics – materials science collaboration by expanding the Mathematics Unit, setting the three target projects, and establishing new types of researcher positions for the collaboration. These attempts were performed as part of the introduction of a new system towards progress from FY2012, and led to the following achievements.

"Conducting research of the highest world level"

The level of research at AIMR in the materials field has always been the highest in the world. In FY2011, AIMR's full-time PIs and their co-workers published 209 papers, with many appearing in high-impact journals such as *Nature*, *Science*, *Nature Materials*, and so on. They gave 117 invited presentations at international meetings, playing active roles in the global arena. External research funds increased in FY2011 (about 2.8 billion yen), indicating the world's high evaluation of AIMR's science level.

"Advancing fusion of various research fields"

Important results were produced by interdisciplinary fusion research. Based on these results, three target projects were established with the aim of seeking further achievements. Mathematics will play the role of a catalyst for the fusion of disciplines and this will give birth to a new paradigm for materials science methodologies. New researcher positions for such fusion have also been created.

"Globalization of the Institution"

Joint workshops at satellite institutions were held at the University of Cambridge in June 2011, and at the University of California, Santa Barbara, in January 2012. Global collaborations have been strengthened. The 5th Annual Workshop gathered 246 participants from 10 countries in February 2012, and the GI³ (Global Intellectual Incubation and Integration) Laboratory Program promoted personal exchanges between AIMR and partner institutions. AIMR helped non-Japanese researchers apply for external research funds, submitting successful applications to KAKENHI and CREST (Core Research for Evolutional Science and Technology), in order to create an environment attracting foreign researchers.

"Implementing organizational reforms"

A new evaluation system based on an international peer review was established to replace PIs and promote young researchers to such positions as Independent Investigators (IIs). The Research Support Center was established to provide researchers with a world-class research environment in which they can quickly begin experiments and theoretical calculations just after arrival. These new systems will attract great brains from around the world.

- Please concisely describe the progress being made by the WPI center project from the viewpoints described below.
- In addressing the below-listed 1-6 criteria, please place emphasis on the following:
 - (1) Whether research is being carried out at a top world-level (including whether research advances are being made by fusing fields).
 - (2) Whether a proactive effort continues to be made to establish itself as a “truly” world premier international research center.
 - (3) Whether a steadfast effort is being made to secure the center’s future development over the mid- to long term.
- Please prepare this report within 10-20 pages (excluding the attached forms).

1. Conducting research of the highest world level

The level of research at AIMR in the materials field has always been the highest in the world (the percentage of top1% papers produced is 2.6%). In FY2011 AIMR full-time PIs and their co-workers published 209 papers, with many appearing in high-impact journals such as *Nature*, *Science*, *Nature Materials*, *Nature Nanotechnology*, *Nature Physics*, *Nature Communications*, *Physical Review Letters (PRL)*, *Journal of the American Chemical Society (JACS)*, and *Advanced Materials*. They gave 117 invited presentations at international meetings in FY2011, with many being plenary lectures and keynote presentations.

In addition, researchers have received domestic and international scientific awards, including Fellow of the American Ceramic Society (Y. Ikuhara PI) and the Presidential Early Career Award for Scientists and Engineers Award (A. Khademhosseini Junior PI). External research funds increased over the fiscal year (about 2.8 billion yen), indicating the world’s high evaluation of AIMR’s science level. These facts are strong evidence of the high scientific level of AIMR.

The outcomes of research at AIMR vary widely from basic studies to applications (Figure 1). We have categorized the achieved research goals of FY2011 from the micro to macro level: **(1) observe and understand atoms and molecules**, **(2) control atoms and molecules**, **(3) create new materials**, and **(4) create new devices and systems**. These categories are based on a viewpoint of the hierarchy of structures and functions of materials, and correspond to our research strategy. Some example research results are listed below.

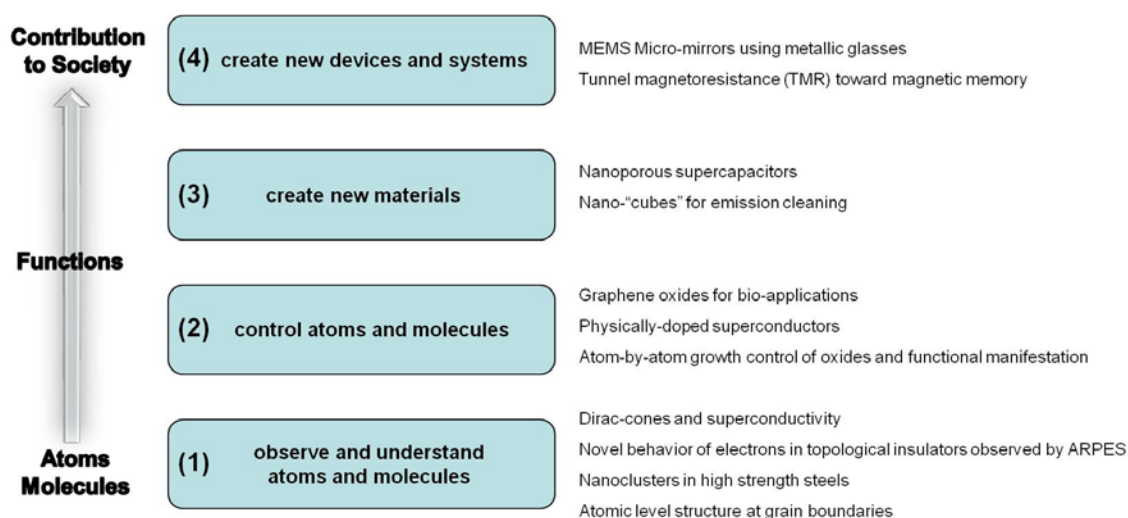


Figure 1 Outcomes obtained at AIMR in FY2011, listed from basic research (bottom) to applications (top).

(1) observe and understand atoms and molecules

Atomic level structure at grain boundaries

Structural defects play a crucial role in determining the physical and electronic properties of materials; especially, grain boundaries essentially influence the properties of polycrystalline materials. The self-trapped grain boundary defect is an important defect and should be investigated in terms of the distribution and role. However, it has been difficult to study due to the very low concentration of such defects. The researchers from AIMR developed a new methodology to elucidate such defects using an artificial ‘bicrystal’ consisting of two crystals cut along different crystallographic directions. The researchers analyzed the sample with a combination of electron energy loss spectroscopy, transmission electron microscopy measurements, and first-principles calculations using density functional theory. They discovered that titanium and calcium impurities segregate into grain boundaries. This atomic-scale information on point defects provides insight into structure-property interplay at the quantum level.

Z. Wang, M. Saito, K.P. McKenna, L. Gu, S. Tsukimoto, A.L. Shluger and Y. Ikuhara, Atom-resolved imaging of ordered defect superstructures at individual grain boundaries. *Nature* **479**, 380-383 (2011).

Nanoclusters in high strength steels

Using the latest microscopy technology, Cs-corrected scanning transmission electron microscopy (STEM) with a resolution of about 0.1 nanometers, atomic structures of oxide nanoclusters less than 4 nanometers in size were found in oxide-dispersion-strengthened (ODS) steels. Although an imaging of the cluster has not yet been achieved owing to the effect of the magnetic steel matrix so far, the atomic structure of the nanoclusters has clearly been identified by minimizing the magnetic effect through the preparation of ultrathin samples about 5 nanometers thick. The surprising result is that the nanoclusters have very defective rock salt crystal (NaCl-type) structures, yet are incredibly stable at high temperatures. This is the key to solving the mystery of why ODS shows outstanding resistance to radiation damage and high temperatures.

A. Hirata, T. Fujita, Y.R. Wen, J.H. Schneibel, C.T. Liu and M.W. Chen, Atomic structure of nanoclusters in oxide-dispersion-strengthened steels. *Nature Materials* **10**, 922-926 (2011).

Novel behavior of electrons in topological insulators observed by ARPES

Because of their use of electron spin, topological insulators are among the most promising materials for next generation electronics such as low energy computers. One of the most characteristic features of topological insulators is that electrons at the surface behave as particles having no mass (Dirac fermions). However, in this study, AIMR researchers discovered that electrons have mass in some topological insulators, a discovery that may possibly lead to a new type of spin electronics. They used an angle-resolved photoemission spectrometer (ARPES) with the world-best resolution, which they developed themselves. They measured the topological insulator, thallium–bismuth–selenium, and compared it with samples where selenium was partially replaced by sulfur. Increasing the sulfur content toward the thallium–bismuth–sulfur composition (not a topological insulator), “X”-shaped energy dispersion gradually fell and a gap opened up, indicated that the electrons were no longer massless. This discovery suggests new possibilities for applications of topological insulators in information storage.

T. Sato, K. Segawa, K. Kosaka, S. Souma, K. Nakayama, K. Eto, T. Minami, Y. Ando and T. Takahashi, Unexpected mass acquisition of Dirac fermions at the quantum phase transition of a topological insulator. *Nature Physics* **7**, 840-844 (2011).

Dirac-cones and superconductivity

Iron (Fe)-bearing superconductors, known as pnictides, were discovered by Japanese researchers from 2006 to 2008 and attracted much interest as a new type of high temperature superconductor with a special mechanism. At AIMR, a Dirac cone electronic structure has been discovered in this new superconductors (P. Richard, T. Takahashi et

al., *Physical Review Letters* **104**, 137001 (2010)) and investigations have continuously been performed. In 2011, the AIMR team studied the pnictide $\text{Ba}(\text{FeAs})_2$ and found that its linear magnetoresistance effect, one of the characteristics of a pnictide, is caused by a combination of two Dirac cones, one for electrons and also one for their opposite number, holes. This is an important finding for the exploration of new superconductors with higher critical temperature.

K.K. Huynh, Y. Tanabe and K. Tanigaki, Both electron and hole Dirac cone states in $\text{Ba}(\text{FeAs})_2$ confirmed by magnetoresistance. *Physical Review Letters* **106**, 217004 (2011).

(2) control atoms and molecules

Atom-by-atom growth control of oxides and functional manifestations

When two materials interface there is a high potential of producing new characteristics, for example, the electric conductivity of the interface of the two insulators lanthanum aluminate and strontium titanate. However, atom scale observation has not been achieved in such interface systems. In this study, the AIMR research group developed a high-resolution scanning tunneling microscopy combined with a pulsed laser deposition system and investigated the homo-epitaxial atom-by-atom growth process of a perovskite material, strontium titanate. They found that the specific surface can be prepared in a wide range of oxygen partial pressures in a reproducible manner. These investigations lead to the preparation of new heterostructures, or high quality thin films with exotic multifunctionality.

K. Iwaya, R. Shimizu, T. Hashizume and T. Hitosugi, Systematic analyses of vibration noise of a vibration isolation system for high-resolution scanning tunneling microscopes. *Review of Scientific Instruments* **82**, 083702 (2011).

R. Shimizu, K. Iwaya, T. Ohsawa, S. Shiraki, T. Hasegawa, T. Hashizume and T. Hitosugi, Atomic-scale visualization of initial growth of homoepitaxial SrTiO_3 thin film on atomically ordered substrate. *ACS Nano* **5**, 7967-7971 (2011).

Physically-doped superconductors

AIMR in collaboration with researchers from the University of Tokyo have succeeded in producing a superconducting state by artificially introducing large amounts of electrical charges into known materials, such as potassium tantalum oxide (KTaO_3). They created an electric double layer transistor structure using ionic liquid. By bringing the ionic liquid into contact with the surface of an electrical circuit containing the material, an electric double layer is formed at the material–liquid interface. By applying an electrical voltage to the gate electrode, large amount of carriers are doped into the material due to the large electric field in the electric double layer, compared to general field effect transistors (FETs). Since this method does not face the same limitations as chemical doping, this approach has great potential to discover superconductor systems that have not shown superconductivity by chemical doping.

K. Ueno, S. Nakamura, H. Shimotani, H.T. Yuan, N. Kimura, T. Nojima, H. Aoki, Y. Iwasa and M. Kawasaki, Discovery of superconductivity in KTaO_3 by electrostatic carrier doping. *Nature Nanotechnology* **6**, 408–412 (2011).

Graphene oxides for bio-applications

Graphene and its derivatives, such as graphene oxide, have attracted much attention due to their extraordinarily high mobility and wide range of applications. Research into these materials for biological and biomedical applications is also progressing. The interaction between graphene and biological materials such as proteins and cells is the most important factor for bio-applications, and varying reduction change is the most direct way to control this factor. In this study, researchers from AIMR demonstrated a way to optimize cell performance by controlling the reduction state of graphene oxide. Through the thermal reduction method, they controlled the reduction state and

found the optimum conditions for the adsorption of proteins, cell adhesion, cell proliferation and cell differentiation. Moderately reduced graphene oxide showed the highest performance in all cases. This result is fundamentally important for the future bio-applications of graphene materials.

X. Shi, H. Chang, S. Chen, C. Lai, A. Khademhosseini and H. Wu, Regulating cellular behavior on few-layer reduced graphene oxide films with well controlled reduction states. *Advanced Functional Materials* **22**, 751-759 (2012).

(3) create new materials

Nano-“cubes” for emission cleaning

Out of the array of rare earths and precious metals that fill automobile catalytic converters, a compound known as cerium oxide (CeO_2) play a special role in balancing oxygen. Higher efficiencies are expected if we can make nanocrystals. In AIMR, a new synthetic process to produce CeO_2 “nanocubes” that displays almost triple the oxygen storage capacity of typical CeO_2 crystals has been developed. Supercritical hydrothermal synthesis was used to produce these unique box-shaped crystals. The most important point of this technique is to cap the crystal surface by using organic molecules under supercritical hydrothermal conditions in which organic and inorganic materials can be combined. This technique will reduce the amount of precious metals used for catalytic emission cleaning.

J. Zhang, H. Kumagai, K. Yamamura, S. Ohara, S. Takami, A. Morikawa, H. Shinjoh, K. Kaneko, T. Adschiri and A. Suda, Extra-low-temperature oxygen storage capacity of CeO_2 nanocrystals with cubic facets. *Nano Letters* **11**, 361–364 (2011).

Nanoporous supercapacitors

As a technique for energy storage in future society, the importance of double-layer supercapacitors will increase. A team at AIMR has been working on building supercapacitors using transition metal compounds such as manganese dioxide (MnO_2), which can store charges at metal sites through an electron transfer process called ‘pseudocapacitance.’ The problem is that MnO_2 has low conductivity, and this limits charging and discharging speeds. The researchers solved this problem by making a supercapacitor constructed using an MnO_2 -plated gold film. First, they selectively etched a silver–gold alloy into a thin gold sheet permeated with numerous nanopores. They then grew MnO_2 nanocrystals directly into the pore channels using a gas-phase reaction. The supercapacitor device displayed excellent charge storage capacity with an energy density up to 20 times higher than that of other MnO_2 electrodes.

X. Lang, A. Hirata, T. Fujita and M.W. Chen, Nanoporous metal/oxide hybrid electrodes for electrochemical supercapacitors. *Nature Nanotechnology* **6**, 232-236 (2011).

(4) create new devices and systems

Tunnel magnetoresistance (TMR) toward magnetic memory

The demand for data storage system, low power, high speed and large storage density, is rapidly increasing. This demand could be satisfied by non-volatile magnetic memory (MRAM). New tunnel magnetoresistance (TMR) materials with both large magnetic anisotropy and low magnetic friction are required to realize high performance MRAM. Using a newly-developed system with an ultrashort laser pulse, a team at AIMR has discovered that an alloy of manganese and gallium is not only a strong magnet but also has switchable magnetization with low loss, a key requirement for fast, low-power non-volatile magnetic memory. This discovery offers unique promise for future magnetic random-access memory devices.

S. Mizukami, F. Wu, A. Sakuma, J. Walowski, D. Watanabe, T. Kubota, X. Zhang, H. Naganuma, M. Oogane, Y. Ando and T. Miyazaki, Long-lived ultrafast spin precession in manganese alloys films with a large perpendicular magnetic anisotropy. *Physical Review Letters* **106**, 117201 (2011).

Another example of an outcome corresponding to this category is described in the next section on “Advancing fusion

of various research fields” – **micro-mirrors using micro electro mechanical systems (MEMS) technology and bulk metallic glass as a material.**

Aside from the above, many high-level results were obtained in FY2011, for example, the surface properties of a polymer film were mapped using atomic force microscopy, the modulation of magnetism with inorganic-organic hybrid structures was achieved, super hybrid materials were created by supercritical hydrothermal synthesis, functionalized fullerenes was produced for lower-cost organic solar cells, and electrochemically-based biosensors were created.

Through the combination of innovative ideas and the state-of-the-art facilities and equipment of AIMR, such as spin- and angle-resolved photoemission spectrometer (spin-ARPES) with the world-best resolution and leading-edge microscopes having atomic resolution, a number of new phenomena have been discovered in the field of materials science. Some discoveries seem to have similar structures or properties and there is the possibility that common principles lie behind various materials. Based on these facts, it became clear that new viewpoints of mathematics are necessary for us to identify common principles. As described in the next section, interdisciplinary fusion research from a mathematical viewpoint will play an important role in creating new materials science. Along this line, we will further investigate the mechanism of functional manifestations from the atom scale to the macroscopic scale and develop a basis for creating new functional materials.

2. Advancing fusion of various research fields

Since FY2009 AIMR has provided the “Fusion Research Proposal Program” to help researchers promote interdisciplinary fusion research. In FY2011, 10 research subjects from 17 proposals were accepted and seed money has been provided. Researchers who were provided the fusion research money in FY2010 were offered an opportunity to make a poster presentation of results from their projects at Tea Time in FY2011 so that the results could be shared with other researchers and inspire more new ideas for fusion research.

In FY2011, the bigger challenge started. In March 2011, AIMR established the Mathematics Unit to accelerate fusion and create a new kind of materials science in AIMR. The Unit joined the existing four research groups for Bulk Metallic Glasses (BMG), Materials Physics, Soft Materials, and Device/System. The researchers of AIMR have frequently organized seminars in order to discuss current topics in materials science, physics, chemistry and the devices area, in order to improve mutual understanding between scientists and initiate fusion research activities. The reward of these efforts has been gradually emerging results. The progress of interdisciplinary research in AIMR is described below with examples of such results.

Common structure

(Fusion between BMG and Soft Materials)

One important example of the emerging results was obtained through the fusion research of the BMG Group and the Soft Materials (Polymer) Group. It is becoming clear that in BMG, shear transformation zones (STZs) of several nanometers which generate during plastic deformation have great effects on mechanical characteristics. The latest research by the BMG Group has revealed the existence of cluster structures of several angstroms in BMG (*Nature Materials* **10**, 28-33, 2011). Based on the existence of a short-range order and the lack of a long-range order, it is assumed that BMG contains structural fluctuations and many defective regions, leading to heterogeneity of a similar scale to STZs. The Polymer Laboratory of AIMR has succeeded in mapping the energy dissipation derived from the viscosity in micro-areas using AFM (*Macromolecules* **43**, 9049-9055, 2010) and this

method was applied to investigate heterogeneity in BMG. The analysis revealed that the nonuniform structure of the viscosity measured in BMG had a distinctive scale of 2.5 nm, which matched that of STZs. Therefore, the inhomogeneous distribution of viscosity and STZs are deeply related, which suggests that they dominate the macroscopic characteristics of metallic glasses.

One interesting point is that the measurement and analysis methods developed for polymers could be applied without modification to BMG. This suggests the existence of common principles between BMG and polymers. More specifically, there is a possibility that what is called a "cooperatively rearranging region (CRR)" in polymers is essentially the same as or very similar to a STZ of BMG, despite the different names. There are great expectations that a solution in mathematical framework to this issue will lead to the discovery of common principles and new physical facts that bridge different material systems.

[Ref.] Y.H. Liu, D. Wang, K. Nakajima, W. Zhang, A. Hirata, T. Nishi, A. Inoue and M.W. Chen, Characterization of nanoscale mechanical heterogeneity in a metallic glass by dynamic force microscopy. *Physical Review Letters* **106**, 125504 (2011).

Green catalysts

(Fusion between Soft Materials and BMG)

We learned from fusion research that exchanging a concept between disciplines can produce a new concept for materials. AIMR introduced the concept of "catalyst" (Soft Materials group) into the Bulk Metallic Glasses (BMG) group. Catalysis is an essential concept to control chemical reactions. Palladium is a well-known catalyst for organic synthesis, but unfortunately, palladium catalysts are toxic, expensive and difficult to separate completely from a final product. The synthetic chemist group of AIMR started to collaborate on palladium catalysts with the BMG group, and together they succeeded in developing a solid palladium-based "metallic glass" that can repeatedly catalyze carbon coupling reactions with negligible leaching of the catalyst into the solvent. By using palladium–nickel–phosphorus metallic glass and an electrochemical fabrication techniques, it became possible to create nanoporous palladium having a uniform distribution of pores of about 30 nanometers in diameter. Nanoporous structure provided not only a large specific surface area effective for reactions but also some special effects. Although nanoporous solids have simple relations with nano particles such as being "inside" or "outside," researchers found further difference between them. The coupling proceeded extremely efficiently even after reusing the nanoporous catalyst four times and the amount of palladium lost into solution during the reaction was less than 0.0005% of the precious metal in each cycle. The results of this fusion research give us hope for more innovation with geometric insight, such as the development of a robust "green" catalyst. The exchange of concepts between disciplines is very important to produce new concepts for materials.

[Ref.] S. Tanaka, T. Kaneko, N. Asao, Y. Yamamoto, M.W. Chen, W. Zhang and A. Inoue, A nanostructured skeleton catalyst: Suzuki-coupling with a reusable and sustainable nanoporous metallic glass Pd-catalyst. *Chemical Communications* **47**, 5985–5987 (2011).

Putting the spotlight on existing materials

(Fusion between Device/System and BMG)

Silicon is traditionally the material of choice in micromechanical innovations. The brittleness of silicon, however, limits the possible range of its applications. The fusion research team for micro electro mechanical systems (MEMS) and bulk metallic glasses of AIMR used metallic glasses as a tougher alternative to silicon in the development of enhanced micro-mirrors. Metallic glasses can bear heavier loads without starting to deform, and are thus ideal for micromechanical devices in which small components are repeatedly subjected to strong forces. They constructed a mirror structure by placing a round plate between two torsion bars that formed the axis for the mirror's movements. When in resonance with an oscillating external magnetic field, the mirrors followed the field and rotated more than

300 times per second without undergoing any damage. Tilt angles of over 70 degrees were demonstrated in this dynamic mode, and in larger static magnetic fields, the mirrors reached up to 270 degrees. Such unique use was never found in metallic glasses prior to the fusion research in AIMR. The need for MEMS devices has put a spotlight on a mechanical property that has not attracted attention so much thus far.

[Ref.] J.-W. Lee, Y.-C. Lin, N. Kaushik, P. Sharma, A. Makino, A. Inoue, M. Esashi and T. Gessner, Micromirror with large-tilting angle using Fe-based metallic glass. *Optics Letters* **36**, 3464-3466 (2011).

New idea in spintronics

(Fusion among many factors; physics, chemistry, microscopy, and device technology; mathematics in the future)

Integrating ideas and techniques among materials scientists specializing in semiconductors, device physicists skilled in electric double layer transistors, chemists operating liquid electrolytes, and physicists specializing in microscopy have led to a new possibility for the utilization of “spin.” The ability to switch the magnetic properties or electron ‘spin’ of a semiconductor in a similar way to charge in conventional devices opens up new possibilities for fast, low-power data storage and “spintronics” applications. The magnetic semiconductor materials needed for such applications at room temperature, however, have proved elusive as most magnets are either metals or insulators. AIMR has developed a magnetic semiconductor system with controllable ferromagnetism at room temperature. They used titanium dioxide containing a small amount of the magnetic element cobalt as a material and injected high concentration of charge by using a liquid electrolyte. The development of a magnetic semiconductor providing switchable magnetic properties at room temperature offers intriguing possibilities for high-performance devices.

[Ref.] Y. Yamada, K. Ueno, T. Fukumura, H.T. Yuan, H. Shimotani, Y. Iwasa, L. Gu, S. Tsukimoto, Y. Ikuhara and M. Kawasaki, Electrically induced ferromagnetism at room temperature in cobalt-doped titanium dioxide. *Science* **332**, 1065-1067 (2011).

These outcomes would have never been obtained if researchers from various fields had not been gathered at AIMR. It is expected that these results will lead to the creation of Green Materials which contribute to “energy harvesting,” “energy saving” and “environmental clean-up,” and contribute to green society as shown in Figure 2.

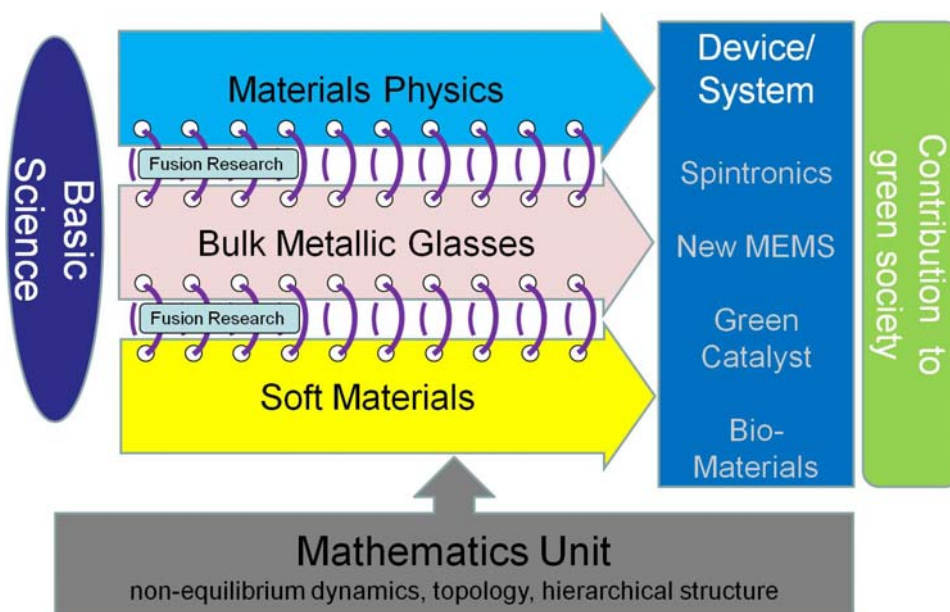


Figure 2 Schematic diagram showing the fusion of various research fields at AIMR.

Through the fusion research, we open the new paradigm of materials science through fusion of different disciplines. They include studies of

- a) structures and properties of the non-equilibrium materials, such as metallic glasses and polymers, as well as their formation mechanism and stability. Novel useful functions are expected to emerge based on a common principle inherent to non-equilibrium states
- b) functions originating from the “spin” of electrons, and functions related to the “topology of energy bands.” The relationship between “topology” and the activity of nanoporous metal catalysts has been also suggested as something to study. The exploration of novel materials and their multi-functions utilizing robust properties of topological features, which need a help from mathematics, is a key challenges.
- c) the hierarchical structures from atoms and molecules to macroscopic bulk materials, through short-range ordering (nano-clusters), long-range ordering (nano-crystals), crystals and poly-crystals levels. Importance of a bridge between scales and functional manifestation which derives from multi-scales has been understood. Interface is one of the keys.

We recognized that these items are significant viewpoints in the next-generation materials science and we set them as our target projects to be focused. By probing the three fields carefully and deeply, with the help of advanced mathematics, we will elucidate the mechanisms and common principles. The following three are our target projects and target materials and devices derived from the above categorization.

Three target materials

1) Non-equilibrium Materials based on Mathematical Dynamical Systems

This project targets, for example, metallic glasses, polymer glasses, block copolymers, bio-inspired materials, and super-hybrid multifunctional devices for green society.

2) Topological Functional Materials

This project targets, for example, spintronics materials, superconductors, and MEMS devices for energy-saving, along with nanoporous metal catalysts and new materials for photo-voltaic solar energy conversion and thermoelectric conversion for energy-harvesting.

3) Multi-Scale Hierarchical Materials based on Discrete Geometric Analysis

This project targets the identification of mid-range and long-range order in the atomic / molecular / cluster / domain arrangement and functional manifestation by creating the hierarchical structures. Interfacial processes from the atom/molecule level to macroscopic properties are also targets of this project aiming to understand the mechanism of functional manifestations. For example, grain boundaries for the improvement of electric conduction in devices, solid-liquid interface control for the improvement of friction problems for energy-saving, nanoporous supercapacitors for energy storage, and bio-inspired materials.

The organization for the mathematics – materials science collaboration has been strengthened in order to accomplish these target projects. Two professors (Motoko Kotani, the Deputy Center Director in FY2011, and Yasumasa Nishiura, the Leader of Mathematics Unit from February 2012) were appointed as to PIs of Mathematics Unit. Project Leaders and Project sub-Leaders were appointed in each project. They have organized study groups for each target project. Furthermore, in FY2011, six interface researchers have been assigned from 68 applicants via international recruitment (They will join AIMR in May, June and July in FY2012) – they are theoretical researchers, who will not belong to a specific PI. They will work together with some experimental laboratories, inspiring new experimental

targets, contributing discussions on experimental results and suggesting novel approach of materials control, based on their mathematical and theoretical expertise as shown in Figure 3. AIMR will assign a mentor as their supervisor.

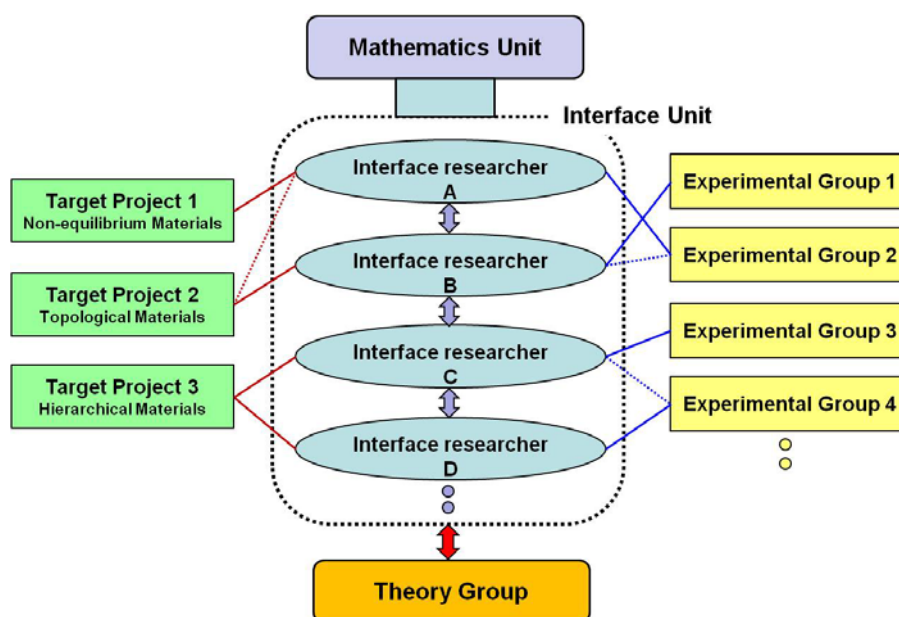


Figure 3 The research organization structure surrounding interface researchers.

3. Globalization of the institution

Describe what's been accomplished or recognized in the efforts to raise the center's international recognition as a genuine top world-level research institute, along with innovative efforts proactively being taken in accordance with the development stage of the center, including the following points, for example:

- Efforts being developed based on the analysis of number and state of world-leading, frontline researchers; number and state of visiting researchers; exchanges with overseas entities
- Proactive efforts to raise the level of the center's international recognition
- Efforts to make the center into one that attracts excellent young researchers from around the world (such as efforts fostering young researchers and contributing to advancing their career paths)

The International Relations Unit was established in the Administrative Division and started to further promote the globalization of AIMR. The unit supports foreign researchers not only in their research activities at AIMR but also with the daily life of their families. As of March 31, 2012, AIMR has 32 principal investigators (PIs) and 44% of them (14 PIs) are foreign researchers. More than 50% of all researchers are foreigners. In order to position AIMR into the flow of global brain circulation, public advertisements for the positions of associate professor, assistant professor and postdoctoral researcher were carried out for international recruitment and AIMR was able to employ talented researchers from around the world. As a concrete plan to enhance international partnership and collaborations, AIMR promoted the GI³ (Global Intellectual Incubation and Integration) Laboratory Program and sent and accepted young researchers via foreign PIs and 15 partner institutions. After the GI³ Laboratory Program was institutionalized in FY2009, the number of researchers exchanged between AIMR and overseas partner institutions increased, though it decreased in FY2011 because of the earthquake (15, 18 and 9 researchers in FY2009, 2010, and 2011, respectively). In order to create an environment which can attract foreign researchers, AIMR helped non-Japanese researchers to apply for external research funds, submitting successful applications to KAKENHI and CREST. The winning of a CREST grant by an AIMR foreign researcher (M.W. Chen PI) was a big achievement in FY2011.

In cooperation with three overseas satellites, which are the core of our comprehensive global collaborations, joint workshops were held at the University of Cambridge in June 2011, and at the University of California, Santa Barbara in January 2012, and consequently the name recognition of AIMR was raised. We are preparing to establish joint laboratories at satellite institutions. Global collaboration between AIMR and overseas satellites and partner institutions produced 21 papers in FY2011.

Our 5th Annual Workshop was held in February, 2012 and 246 participants from 10 countries attended it. Since the first workshop held in February 2008, the number of foreign PIs, adjunct professors and adjunct associate professors have increased and the number of participants is increasing year by year as well. In particular, mathematicians joined the workshop this time, allowing us to confirm our mission of seeing mathematics – materials science collaboration through deep discussion. AIMR researchers also attended many international meetings. They gave 117 invited presentations at international meetings in FY2011, with many being plenary lectures and keynote presentations. AIMR researchers introduce WPI and AIMR briefly at the beginning of every presentation to gain publicity.

In order to publicize AIMR further, advertisements for AIMR were printed in *Science* (Vol.333, 2 September 2011) and *Nature Asia-Pacific* (PUBLISHING INDEX 2011), and furthermore, targeting researchers, advertisements for *AIMResearch* was printed in *Nature* (Vol.481, 19 January 2012). Banner advertisements on the websites of those scientific magazines and in their e-mails were also carried out.

The Main Building of AIMR was completed in July 2011, and the “Combination Room” and “Multi-purpose Hall” were constructed in the building for active exchanges and discussion between researchers. Tea Time held on every Friday at such exchange spaces provides further opportunities to make and increase collaboration. These occasions also encourage exchanges between foreign researchers and Japanese researchers. Fusion research is also enhanced in such an atmosphere.

The research environment for researchers from abroad, including short-stay visiting researchers, will be improved by completing the “Research Support Center” which will include the “Common Equipment Unit” and “Computation-Aid Unit,” in FY2012. Through the support of this center, researchers will be able to start their research quickly after their arrival at AIMR.

4. Implementing organizational reforms

* If innovated system reforms generated by the center have had a ripple effect on other departments of the host institutions or on other research institutions, clearly describe in what ways.

In order for AIMR to further advance over the next five years, we focus on system reform in particular, centering on the appointment of researchers and reform of research organization toward mathematics – materials science collaboration.

1) AIMR has created new systems for human resources development. We have established a system for evaluation and promotion through international peer reviews. The research outcomes of the researchers over the past four years and the compatibility of their research with the AIMR’s new strategy were evaluated based on the judgment of an international referee and an interview by AIMR’s Executive Committee. Some PIs were replaced and two IIs were promoted as a result. AIMR has created an environment in which our six young researchers, three Junior PIs and three IIs can pioneer new research areas independently.

We also established a new type of research position, interface researchers. These researchers do not belong to any single laboratory, but form the “Interface Unit” as a whole. Six theoretical researchers have been appointed to the Interface Unit through international recruitment followed by an evaluation of all PIs. They will work together with

partner experimental laboratories to build a bridge between mathematicians and materials scientists. They will promote interdisciplinary fusion under the supervision of a mentor. Moreover, they will construct the basis of the new kind of materials science that we are aiming for in which we can predict new physical properties and functions based on mathematics and theories.

2) In FY2011, AIMR started preparations for and then management of the Research Support Center. The center consists of four parts: a Common Equipment Unit, a Computation-Aid Unit, a Mathematical Collaboration Unit, and a Researcher Support Office. This center will support not only domestic AIMR members but also short-stay visiting researchers including foreign PIs and researchers. Through strong support on the part of this center, even short-stay researchers will be able to promptly start their research in AIMR. This system will enhance exchanges of researchers and contribute to the facilitation of AIMR as the central hub of global brain circulation in the field. Furthermore, in cooperation with our In-house Council consisting of the heads of four departments and institutes at Tohoku University, we have established a research support system using an in-house network. This system makes it possible for us to utilize experimental equipment and computational resources.

3) System reforms at AIMR that have influenced Tohoku University

- i) The new salary system at AIMR gave rise to the creation of the "Distinguished Professor System" at the host institution, Tohoku University. Since the "Distinguished Professor System" has been recognized to be effective at strengthening research, the system has been updated for a second term and become a regular system in Tohoku University.
- ii) The various rules stipulated by AIMR were used as reference for administrative processing when new organizations at Tohoku University such as the "Tohoku Medical Megabank Organization" and "International Research Institute of Disaster Science" were established.
- iii) Manuals have been created for safety in environments where researchers with different backgrounds and cultures gather.

5. Efforts to secure the center's future development over the mid- to long term

* Please address the following items, which are essential to mid- to long-term center development:

- Future Prospects with regard to the research plan, research organization and PI composition; prospects for the fostering and securing of next-generation researchers
- Prospects for securing resources such as permanent positions and revenues; plan and/or implementation for defining the center's role and/or positioning the center within the host institution's institutional structure
- Measures to sustain the center as a world premier international research center after program funding ends (including measures of support by the host institution)

(1) Research plan, Organization, Human resources

In FY2011, AIMR advertised the clear strategy of promoting mathematics – materials science collaboration in order to create new materials science and contribute to society through the creation of new functional materials. Our mid-term goal is to provide a basis for common understanding among the existing four research groups via a mathematical viewpoint, and our long-term goal is to create revolutionary *Green Materials* by contributing to the advancement of the concepts of "energy harvesting," "energy saving" and "environmental clean-up." In terms of AIMR's long-term perspective, we seek to ensure a stable energy supply for future generations and provide a basis for environmental conservation through the use of new materials that can cause an evolutionarily change in our society and show the world what the future should be like.

In order to promote our new approach we have started the following activities.

- i) AIMR has set the three target projects described above and strengthened the organization for mathematics – materials science collaboration. Project Leaders and Project sub-Leaders were appointed for each project. Six interface researchers will join AIMR and take up the role of acting as bridges between materials researchers and mathematicians in early FY2012. A mentor will be positioned as their supervisor. Through the whole process for target projects, we will assure direct interaction between mathematicians / theorists and interface researchers / experimentalists so that each stakeholder can mutually benefit from research.
- ii) For human resource development, AIMR has created new systems (as described in 4-1). As a result, some PIs were replaced in order to enhance our new research direction, and three Junior PIs and three IIs were given an independent environment in which to pioneer research areas. Six young theoretical researchers have been appointed as interface researchers in order to develop new insights by bridging materials scientists and mathematicians (Figure 3). A Research Support Center (Common Equipment Unit, Computation-Aid Unit, Mathematics Collaboration Unit, and Researcher Support Office, details are in 4-2)) has been started, and it is expected to aid with smooth transitions to life at AIMR. A new framework to foster young researchers, through for example, training on presentations at the Researcher Support Office (in Research Support Center), has been discussed, and this will be organized in FY2012.

(2) Planning and enforcement: the number of researchers, research funds, position within Tohoku University, etc.

The promotion of AIMR and the construction of organizations within it are clearly positioned in the most important items in the Mid-Term Objectives and Plans of our host institution, Tohoku University. The University's new president has stated his organizational policy for Tohoku University as becoming a world leader through "Progress toward becoming a World-class University" and "Leading the Tohoku restoration." In order for Tohoku University, as a research institute, to progress toward becoming world-class, there is a need to promote materials science, which is the strongest research area of the university, and especially AIMR. AIMR is recognized to be the core existence for the promotion of world-leading research and formation of an international environment at Tohoku University. AIMR was established as an organization of Tohoku University from the beginning. As described in the initial application, AIMR will maintain its present scale and continue as a world top level research center for innovative materials science even after the end of the WPI program.

(3) How AIMR will continue to be "world top level research center" after completing the WPI program.

After completing this program, achievements made by the center will serve as a base for the development of the Tohoku University Advanced Institute for Materials Research, which will play a leading role in the promotion and internationalization of advanced research.

In Tohoku University, materials researchers are working in various departments and research centers. We have proposed to the president of Tohoku University the construction of an advanced institute for materials research where all materials research will be integrated with AIMR placed as a core. We believe that the establishment of such a center will be necessary for Tohoku University to become a true world leader in materials research.

Towards the realization of this, in FY2012, Tohoku University will establish a Task Force for the establishment of the integrated advanced institute for materials research in Tohoku University. Discussion will be made on the issues among the related departments and a concrete plan for the organization (the number of researchers and their position in the university, etc.). Moreover, the task force will discuss how to introduce and implement the new systems grown

in AIMR over the past five years into the whole university in order to promote system reform and further internationalization.

6. Others

* In addition to the above 1-5 evaluation items, only if there is anything else that deserves mention regarding the center project's progress, please note it.

In July 2011, the main building of AIMR was completed and an environment in which everything is “under one roof” was achieved. This has given the institute a sense of unity greater than ever before and built up strong ties among AIMR members.

The international guest house at Tohoku University – plans for which were based on the requests of AIMR to the University – is now under construction next to the AIMR main building and will be completed in FY2012.

In order to increase chances for personal communication among researchers including foreign PIs, “Tea Time Talk” and mini concerts during Friday Tea Time have been started. Once a month, AIMR members present their specialties, playing instruments, singing, dancing, etc., and such performances have had the effect of creating a good atmosphere at the center. We are planning to extend such events to the families of AIMR members.

7. Center's response to interim evaluation

Transcribe each item from the “Actions Required and Recommendations” section and note how the center has responded to them. However, if you have already provided this information, please indicate where in the report.

1) It is essential for Tohoku University to be sufficiently committed to supporting the new strategy and director.

[Action]

On April 1, 2012, a new directorial structure commenced at the host institution under the leadership of the University President, Susumu Satomi. In March 2012, the new Center Director (Motoko Kotani) and Administrative Director of AIMR met with the University President and confirmed that AIMR would remain at the core of efforts to strengthen research at Tohoku University, that support for AIMR would be prioritized, and that the independence of Center operations would be maintained. Visions were also exchanged on the integrated advanced institute for materials research, which is the University plans to establish after completion of the WPI program. Additionally, a standing task team led by the Executive Vice President in charge of Research will be established to assist the Center Director.

The In-house Council, comprising the heads of departments and research institutes that are deeply related to the Center, will be used to further enhance cooperation with related departments in Tohoku University.

2) AIMR's identity along with its new strategy in materials science should be clearly stated.

[Action]

Since its establishment, AIMR has continuously pursued the creation of new materials science and revolutionary functional materials by gathering researchers from various fields. The main goal is to promote the common understanding of materials based on a knowledge of different size scales from atoms to materials and different

materials such as metals, ceramics, polymers and biomaterials. There is no change in this concept. However, based on the results of discussion and collaborative research carried out during the first five years, we have further crystallized our mission: to discover common elements and universal principles among various materials and create a new kind of materials science which can predict new functions. To accomplish this mission, we have injected mathematical viewpoints into materials science and accelerated fusion research toward our goal. We have established the three target projects of: (1) Non-equilibrium Materials based on Mathematical Dynamical Systems, (2) Topological Functional Materials, and (3) Multi-Scale Hierarchical Materials based on Discrete Geometric Analysis.

In AIMR, material scientists and mathematicians join hands in explaining new phenomena measured by AIMR's top class equipment and elucidate the mechanism lying behind the structure-function relationship. The challenge of elucidating the mechanism of function manifestations and linking it to the creation of new materials is unprecedented in the world. Materials scientists from diverse backgrounds and mathematicians are gathered in a single place at AIMR and challenged to do ambitious investigations to create new materials with revolutionary functions that can contribute to society—that is the identity of AIMR.

3) Firm supporting systems should be provided to the director from material scientists and mathematicians as well as from the host institution.

[Action]

The Center Director frequently exchanges views with the four material group leaders so that AIMR can develop soundly as a center for materials science. Our International Advisory Board consisting of highly reputed personalities including Nobel Prize laureates also gives advice to the Center Director from a global perspective. Moreover, the Center Director's office is placed on the first floor, and an open-door policy will be implemented so that the Center Director will be able to answer the needs of researchers as best as possible, and so that the Center Director can work to carry out necessary system reform and construct a research support system. In February 2012, Professor Yasumasa Nishiura (Research Director of the Mathematics Program of CREST funded by the Japan Science and Technology Agency (JST)), an internationally respected authority on applied mathematics who has spearheaded cooperation between mathematics and the various scientific fields in Japan, joined AIMR as a PI and the leader of the Mathematics Unit. The Unit has commenced activities in a dynamic manner. Partnerships with the Applied Mathematics Forum (AMF), Tohoku University and other mathematical societies in Japan and abroad will be exploited in order to promptly distribute news of mathematics-materials science outcomes at AIMR to the world and to secure the superiority of AIMR.

As described above, the President of Tohoku University has confirmed his strong support for AIMR. As for the Administrative Division of AIMR, the Deputy Administrative Director in charge of research (Doctor of Science) and the Deputy Administrative Director in charge of management were created under the Administrative Director in an effort to strengthen the Division. Moreover, from April 2012, the Administrative Director, who is an experienced and distinguished materials science theorist, has been appointed to provide complete support in order to realize the concepts promoted by the Center Director from a scientific perspective.

4) The performance of the center's science and management will need to be watched carefully over the next two years.

[Action]

AIMR's ultimate objective in science is to discover new principles via collaborative research between materials science and mathematics and to create materials science which can predict new functional manifestations of materials based on discovered principles and then develop those materials. Towards the achievement of this objective, we will

clarify a concrete approach for materials science that incorporates mathematics over the next two years. We have established three target projects based on the PIs' proposals and a mathematical viewpoint and these three projects have been started under the direction of Project Leaders (materials scientists) and sub-Leaders (young materials scientists and mathematicians). These projects will be implemented based on AIMR's mission of creating new materials. In particular, with respect to materials with a high potential to be realized, we have organized study groups, and will concentrate AIMR's research toward these materials to ensure progress, making use of a clearly-defined research management system in the first two years.

The relationship between materials scientists and mathematicians exists on a diverse range of levels. The first stage of our cooperation is daily consultations regarding the operation of mathematics and the introduction of cutting-edge mathematics. The final stage is the development of mathematical models and discovery of new principles. Our objective for the ensuing two years is for experimentalists, theorists, and mathematicians to stimulate each other and experience the fact that such cross-interaction does engender novel ideas. This will allow researchers to understand the true significance of the new strategy. After several different groundbreaking research projects take form, we will provide a policy for the development of new functional materials. In this way, a mathematics atmosphere will permeate AIMR and allow us to explain the mechanisms of functions and discover new principles, as outlined in our mission. By achieving this we will create new materials science which can predict new functions of materials over the ensuing five years and establish a research institute that leads materials science in the world.

8. Center's response to the site-visit report used in the interim evaluation

Transcribe each item from the "7. Actions Required and Recommendations" section and note how the center has responded to them. However, if you have already provided this information, please indicate where in the report.

1. With no doubt, each PIs' activity is at a world-class level. However, it is difficult to judge if the WPI as a whole is presently at a world-class one or not. The overall impression of AIMR is not as high compared with that based on achievements of each individual PI. The main reason seems to be due to the fact that the mission as a whole is not fully confirmed by the members. All the members need to discuss and assess their achievements in terms of the common definition of "materials science" for this center.

[Action]

From March 2011, a monthly PI Meeting (started from December 2010) and Staff Meetings which all researchers above assistant professor level attend have been held regularly. All staff members have made continuous efforts to communicate with each other. In FY2011, the year before the start of the next five years of WPI, we discussed the identity of AIMR deeply and established the three target projects, based on 17 proposals from the PIs. We set the Leaders and sub-Leaders for each project and organized study groups which discussed each subject thoroughly. Each theme is expected to progress faster because of this. Besides the PI Meeting, monthly PI Lunch Meetings have been started and this also stimulates the PIs toward deeper communication and collaboration. Through the active discussion in FY2011, the atmosphere of AIMR has changed incredibly. All AIMR members are ready to accomplish our goal of creating a new type of materials science and establishing AIMR as a firm hub of global brain circulation. The improvement of the research environment through the establishment of the Research Support Center will also accelerate the evolution at AIMR.

2. AIMR is in a period of transition both in leadership and in its technical programs. The fusion efforts have not yet been very productive. Additional time should be granted to AIMR to allow the changes that are in

place to have a chance to mature.

3. After 4 years since its establishment, AIMR now seems to make every effort to establish as a WPI center, sharing the mission of WPI project with all members and carrying out a high level of materials science research. We sincerely hope that AIMR creates a new materials science by collaboration with mathematicians in the next five years.

[Action to items no. 2 and 3]

Mathematics – materials science collaboration and the creation of a new type of materials science through such collaboration is not easy. However, the challenge is ambitious and attractive, and there already exists an atmosphere in AIMR to face it squarely. As described above, AIMR undertook concentrated discussion and reforms in FY2011, creating a completely new atmosphere that is unlike that of any other institute in the world. We are ready to produce real fusion, learning from the struggle of the past five years.

The relationship between materials scientists and mathematicians exists on a diverse range of levels as described in 7-4. Step-by-step progress is important to accomplish our goal. First we will form an environment in which experimentalists, theorists, and mathematicians can understand each other, in order to make the mathematical way of thinking familiar for experimentalists and help mathematicians understand the rich world of materials. Next, through mutual discussion and the exchange of novel ideas, researchers with different expertise will inspire each other to perform unprecedented collaborative works. Since we are already seeing some buds of collaborative work, we will work to grow these and give them form over our next stage. Based on such step-by-step efforts, we will develop a basis for innovative mathematics – materials science collaboration and make a breakthrough that can produce new values for materials science in society.

4. It may collapse anytime if firm and versatile supporting systems are not well provided to the new director. So, this looks somewhat risky. To make it successful, all the PIs need to agree with this scheme sincerely and are committed to support strongly the director. The director in turn should have to learn the global tide and the history of “materials science,” since each discipline has its own definition of “materials science.”

[Action]

As already noted (see Section 7), AIMR has already started heading in a new direction as a single body. This is the first attempt to do this in the world. All the members of AIMR are enthusiastic about taking up global leadership. The Center Director is willing to make every effort to overcome the difficulties and make AIMR a unique research center that can bring about a paradigm shift in materials science. The director support system, that is, the advice from the International Advisory Board, discussions with group leaders (the Executive Committee of AIMR), and the collecting of opinions from AIMR members of various backgrounds through opportunities such as PI meeting and Staff Meetings, is working effectively.