

## Vision of the Director

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### 1. Scope

The history of the development of materials is that of progress of mankind itself. Whenever mankind has discovered new materials, such as stone implements, earthenware, ironware, metals, ceramics, or polymeric materials, our society has changed drastically, and along with changes in our society, new values have been created. It is not an overstatement that the ultimate goal of materials science is realization of the dreams of mankind.

The Advanced Institute for Materials Research (AIMR) was established in 2007, aiming to contribute to society through the creation of new and innovative materials by gathering researchers from all over the world in the fields of materials science, physics, chemistry, and engineering – fields in which Tohoku University holds a leading position in the world in its research. Since its foundation, while AIMR has consistently pursued top-level research in individual research areas, it has also put much effort to create new materials science by interdisciplinary research. Through those activities, we have identified the objectives of the AIMR as follows:

- (1) To elucidate fundamental principles lying behind functional manifestation common to different kinds of materials.
- (2) To build a basis for “predicting” new functions and new materials based on the newly-established principles.
- (3) To create Green Materials to contribute to "Energy Harvesting", "Energy Saving" and "Environmental Clean-up".

Now we have introduced a mathematical viewpoint to deepen common understanding of materials and accelerate our research activities towards the goal, which is our new characteristic. We shall establish a seamless and comprehensive materials research base where top level researchers with various backgrounds are gathered, and inspired each other daily. We believe this is the way to introduce new values for the next generation through development of materials science.

## **2. Management**

In order to achieve the above goals, we manage the operation of the institute as follows:

### **1) Research Environment and the Support System for Researchers**

As a center established under the WPI Program, it is essential to attract and gather top-level researchers from all over the world, and provide for them an ideal research environment. Researchers at AIMR should be able to concentrate on their studies like distinguished professors in the U.S. by being provided world top-level research facilities and equipment. For researchers from overseas, we also provide housing, assistance for the daily life of their family members, and information on Japanese culture and Japanese language learning.

Human resource development for the next generation is an important mission of the WPI research center, thus we provide sufficient support in their research environment for Junior PIs, independent investigators (young excellent researchers who can carry out their research activities on their own independently), associate professors, lecturers, assistant professors, and post-doctoral young researchers, so that they build their careers at AIMR, grow to be research leaders in the next generation in the flow of a global brain-circulation.

In addition, we need to streamline research activities within the organization, and establish a system for researchers, including newly employed researchers, to start and carry out their research without delay by making the Research Support Center with (1) Common Equipment Unit, (2) Computation-Aid Unit (3) Mathematics Collaboration Unit, (4) Researcher Support Office.

### **2) Internationalization**

Internationalization is the most important agenda for the WPI research center. In order to construct a “visible center,” AIMR will establish satellites and partner institutions in the world, and promote fusion and joint research on a worldwide scale. Out of 15 partner institutions in total, the following three institutions – the University of Cambridge; the University of California, Santa Barbara; and the Institute of Chemistry, Chinese Academy of Sciences – are designated as satellite institutions to carry out active research exchange by establishing a joint laboratory. The University of Cambridge has the Department of Materials Science and Metallurgy and that of

Chemistry, both famous for their strong basic study and the Isaac Newton Institute for Mathematical Science, a national and international visitor research institute, which is a globally well-known institute where Dr. Andrew Wiles proved the Fermat conjecture. The University of California, Santa Barbara, is famous for nanotechnology and conductive polymer material, and there is a strong tie between materials science and mathematics because the University is promoting the application of the fruits of their research for practical use. AIMR conducts allied research focused on soft materials and leverage its applied research with the Institute of Chemistry, the Chinese Academy of Sciences. The satellite function with these pioneering institutions is one of motives which make excellent researchers attracted to AIMR.

As a specific measures to promote global research alliances further, WPI operates its own exchange program called the GI<sup>3</sup> (Global Intellectual Incubation and Integration) Laboratory Program (which was institutionalized in 2009). As a result, while AIMR accepts excellent researchers and students who are active at the forefront of research, AIMR also actively sends researchers and students overseas to promote forcefully global fusion and tie-up research, and aims to establish a base of brain circulation in materials science.

### 3) Organization

In order to promote system reform, which cannot be accomplished by traditional old universities, the Center Director makes top-down decisions with my clear visions. In order to support the Center Director, the Center regularly holds the Executive Committee, consisting of the Director, the Administrative Director and group leaders, and the In-house Council, consisting of heads of related departments and research institutes, and the International Advisory Board gives advice to the Director from a global perspective.

AIMR consists of not only researchers but also Administrative Division officers. They aim to create a world top-level research center on their own initiative and to promote “visible administration.” In line with the vision of the Center Director, the Administrative Director, who is also a materials scientist, the Deputy Administrative Director in charge of research and the Deputy Administrative Director in charge of management will make an effort for the realization of an ideal research environment. Following the principle of WPI Program, the official language at AIMR is English. For

further smooth operation, the International Relations Unit has been established. The Administrative Division shall reform the host institution by taking pioneering measures which are free from conventional practices.

### **3. New approach: Materials science with the participation of Mathematics**

AIMR has focused its efforts on creating new materials science using innovative atomic and molecular control methods through “fusion research” and other interdisciplinary approaches, resulting in some outstanding results. Through successful research outcomes achieved by each research group, we have recognized the importance of focusing on functions of a wide range of materials. Innovative functional materials that give a future vision to human society can be created only by recognizing the process from atoms and molecules through to materials, devices and systems as a complex layered system and by elucidating the mechanism of the manifestation of functions in layers and between layers with a function as an indicator. During the course of these studies, we have recognized the importance of accelerating fusion and interdisciplinary research more actively and effectively.

In order to accelerate fusion research across those different disciplines in a more substantial way and to achieve a new scientific and technological breakthrough, AIMR has realized the necessity of the power of mathematics, which has a long tradition of providing a common language to all the fields of science and technology. Moreover, mathematics simplifies complicated and diverse phenomena and abstracts principles from them. Based on these principles, it may be possible to predict and create new functional materials. After intensive discussions, all the PIs and researchers of AIMR have now recognized the importance of the injection of mathematics at AIMR. We are convinced that mathematics will play a role of a catalyst to stimulate fusion research more extensively, thus creating a new materials science. This concept is in line with the initial concept of AIMR, which is the establishment of a new materials science through fusion research.

### **4. Concrete research plans**

In order to promote our new approach, AIMR has set target projects. The concept of setting target projects was generated as the fruit of our efforts to concretize math-materials science collaborations through the Joint Seminars and Math-Mate

Seminars that have been held since March 2011.

Each project will be carried out by an interdisciplinary team. This year, seventeen proposals were submitted by materials scientists, and after elaborating on them from the point of view of injecting mathematics, they were categorized into the following three projects based on intensified discussions at several PI meetings.

### **1) Non-equilibrium Materials based on Mathematical Dynamical Systems**

One of the major challenges in materials science is to synthesize multifunctional materials, in which multi-functions emerge based on non-equilibrium states, hybrid structures consisting of different types of materials, or the inhomogeneity of systems. Based on Mathematical Dynamical System, we focus on understanding mechanisms of dynamical structural formulation in non-equilibrium systems. This enables us to accurately control non-equilibrium and inhomogeneous materials and to achieve prescribed multi-functions under a given environment.

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**

Topology is a mathematical concept for describing a shape up to continuous deformation. It is also a tool to abstract essential properties from a complex shape and to make it into a simpler shape. One challenge in materials science using “topology” is to synthesize functional materials that are robust under environmental change but achieve highly sensitive properties at the same time.

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**

Innovative functional materials can be created only by recognizing the

complex multi-scale hierarchical structure in materials systems from the atom/molecule scale to the macroscopic scale of materials and devices. Therefore, the understanding and the use of the multi-scale hierarchy are the fundamental research processes of AIMR. At AIMR, precise structure analysis and control at each level of hierarchy from the atom/molecule scale will be carried out using top-level equipment and new technology.

In addition to experimental technology, AIMR will apply a mathematical method, namely Discrete Geometric Analysis to this hierarchical problem. Discrete Geometric Analysis can make a bridge between scales and take account of detailed geometric data. By employing these advanced tools, we are attempting to produce functional multi-scale hierarchical materials.

This project targets the identification of mid-range and long-range order in the atomic arrangement of bulk metallic glasses and interfacial processes from the atom/molecule level to macroscopic properties, such as grain boundaries for the improvement of electric conduction in devices and solid-liquid interface control for the improvement of friction problems for energy-saving.

Through the whole process of the target projects, direct interaction between mathematicians / theorists / experimentalists is assured so that each stakeholder can mutually benefit from the research.

These are very ambitious projects, and we have to take an arduous way to accomplish them. However, we would have never encountered this great opportunity without AIMR, thus in order to make the best of the opportunity, we dare to challenge these projects.

The relationship between materials scientists and mathematics exists on a diverse range of levels. The first stage of our cooperation is the daily consultation regarding the operation of mathematics and the introduction to cutting-edge mathematics. The final stage is to develop mathematical models and discover new principles. The world top-level cutting-edge instruments in AIMR can produce new data and discover new phenomena that nobody has found, and this will inspire the mathematicians / theorists to make new mathematical models. Having opportunities to deepen and develop mathematics makes a great impact on mathematicians and theorists in the world.

## **5. Contribution of mathematics to materials science and global trends:**

There is a world trend of science and technology cooperating with mathematics. As described above, in AIMR the contribution of mathematics to materials sciences has been started. This is the first attempt in the world to promote math-materials science collaboration at an institutional level. Consequently, our approach is just ahead of its time. We will lead global trends by initiating direct interaction between mathematics and materials science.