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Synthesiology

English edition

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MESSAGES FROM THE EDITORIAL BOARD

There has been a wide gap between science and society. The last three hundred years of the history of modern science indicates to us that many research results disappeared or took a long time to become useful to society. Due to the difficulties of bridging this gap, it has been recently called the valley of death or the nightmare stage (Note 1). Rather than passively waiting, therefore, researchers and engineers who understand the potential of the research should be active.

To bridge the gap, technology integration (i.e. *Type 2 Basic Research* – Note 2) of scientific findings for utilizing them in society, in addition to analytical research, has been one of the wheels of progress (i.e. *Full Research* – Note 3). Traditional journals, have been collecting much analytical type knowledge that is factual knowledge and establishing many scientific disciplines (i.e. *Type 1 Basic Research* – Note 4). Technology integration research activities, on the other hand, have been kept as personal know-how. They have not been formalized as universal knowledge of what ought to be done.

As there must be common theories, principles, and practices in the methodologies of technology integration, we regard it as basic research. This is the reason why we have decided to publish "*Synthesiology*", a new academic journal. *Synthesiology* is a coined word combining "synthesis" and "ology". Synthesis which has its origin in Greek means integration. Ology is a suffix attached to scientific disciplines.

Each paper in this journal will present scenarios selected for their societal value, identify elemental knowledge and/or technologies to be integrated, and describe the procedures and processes to achieve this goal. Through the publishing of papers in this journal, researchers and engineers can enhance the transformation of scientific outputs into the societal prosperity and make technical contributions to sustainable development. Efforts such as this will serve to increase the significance of research activities to society.

We look forward to your active contributions of papers on technology integration to the journal.

Addendum to Synthesiology-English edition,

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Synthesiology Editorial Board

Note 1 : The period was named "nightmare stage" by Hiroyuki Yoshikawa, President of AIST, and historical scientist Joseph Hatvany. The "valley of death" was by Vernon Ehlers in 1998 when he was Vice Chairman of US Congress, Science and Technology Committee. Lewis Branscomb, Professor emeritus of Harvard University, called this gap as "Darwinian sea" where natural selection takes place.

Note 2 : *Type 2 Basic Research*
This is a research type where various known and new knowledge is combined and integrated in order to achieve the specific goal that has social value. It also includes research activities that develop common theories or principles in technology integration.

Note 3 : *Full Research*
This is a research type where the theme is placed within the scenario toward the future society, and where framework is developed in which researchers from wide range of research fields can participate in studying actual issues. This research is done continuously and concurrently from *Type 1 Basic Research* (Note 4) to *Product Realization Research* (Note 5), centered by *Type 2 Basic Research* (Note 2).

Note 4 : *Type 1 Basic Research*
This is an analytical research type where unknown phenomena are analyzed, by observation, experimentation, and theoretical calculation, to establish universal principles and theories.

Note 5 : *Product Realization Research*
This is a research where the results and knowledge from *Type 1 Basic Research* and *Type 2 Basic Research* are applied to embody use of a new technology in the society.

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Contents

Development of novel chemical reagents for reliable genetic analyses

— Process from an original idea to marketing of a chemical product used for life science —

Yasuo Komatsu * and Naoshi Kojima

[Translation from *Synthesiology*, Vol.3, No.3, p.223-230 (2010)]

High performance genetic analysis is an integration of various inter-correlated technologies. Of all the technologies, chemical reagents are indispensible for modifying DNA or RNA, yet the total performance of genetic analysis is sometimes limited by the insufficient capability of reagents. We have developed novel chemical reagents to increase accuracy and sensitivity in genetic analysis. We describe the development process from obtaining the original idea to marketing of the products and discuss important factors in the process.

Keywords **:** Gene, genetic analysis, DNA, RNA, immobilization, detection, labeling, amino group

1 Goal of the research

Genes are the common language in all organisms and viruses, and decoding them to understand their functions is necessary to learn their essence. The technologies for decoding and analyzing genes were built on the accumulation of past researches. For example, the genetic decoding of an individual has recently reached a level where it can be completed within one hour[1], and it is also possible to analyze the massive and complex inter-genetic networks as well as the gene-protein networks[2]. With the development of such highly advanced genetic analysis technology, the genetic information are utilized in wide-ranging aspects of our social lives including medicine, foods, and security, as well as basic research. In the future, this technology is expected to advance even further with the progress in the engineering fields as well as the bioscience fields. At the same time, genetic information is expected to become more closely linked to our lives, and is likely to have greater influence on our society. Therefore, both high precision and high performance are required in the genetic analysis technology. However, it is not necessarily true that all elemental technologies integrated in genetic analyses have advanced to the same level as the evolving analysis systems with higher functions. Therefore, we focused on the performance of the chemical reagents, which are essential for the genetic analyses, and conducted research to improve the overall precision of the genetic analysis by enhancing the function of the reagents.

2 Scenario to realize the goal

Most of the genetic analysis methods are organized as a system where several current technologies are integrated around an innovative core technology. Here, parts of the existing elemental technologies are often used commonly in different genetic analysis technologies. The relationship is shown schematically in Fig. 1. For example, the "synthetic DNA" that binds to the target gene and the "labeling reagent" used for highly sensitive gene detection are representative elemental technologies used commonly in many genetic analyses.

Many researches are conducted to develop some novel core technology with much funds. However, some new problems might occur in the conventional technologies when they are linked up to the core technology, resulting in the decrease of precision of the whole system. Thinking that improvement and modification of the performance of a technology with high commonality may set off a ripple effect throughout several genetic analysis systems, we turned our attention to the technologies in overlapping fields and reviewed the issues. As a result, we focused on the aforementioned technologies of "synthetic DNA" and "labeling reagent", and challenged improvement in the precision of the overall genetic analyses.

3 Synthetic DNA linker and labeling reagent

From the 1990s to present, advanced genetic analysis devices such as the DNA chip (microarray) and next-generation high-speed sequencers have been developed, and these technologies continue to advance as we speak. In most of these analysis systems, the probe DNA (oligonucleotide) that binds sequence-selectively to the target gene is immobilized onto a solid surface of flat plates or microbeads. The immobilization is achieved by the covalent bond between the special chemically modified linker incorporated into the DNA and the reactive groups of the substrate surface (Fig. 2a). The linkers

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are also used to conjugate with fluorophores or drugs to the DNA (Fig. 2b). Under such circumstances, we determined that the "linkers" played an extremely important role among the "synthetic DNAs". Similarly, we thought that the reactivity of the reagents to "label" genes recovered from samples not only would affect the sensitivity in detecting minute amounts of genes (Fig. 2c), but also may lead to the development of nucleic acid drugs. Therefore, we focused on the issues in conventional linkers and labeling reagents, and aimed to develop a new type of reagent with higher performance. After describing the development and the product realization of the linker used for probe modification, we shall present the development of the labeling reagent.

4 Development and results

4.1 Development of the amino linker

4.1.1 Goal of the development

The DNA used as a probe is synthesized sequentially by coupling the four monomer building blocks - adenine, guanine, cytosine, and thymine, according to sequence information. At the same time, the linker needed for the immobilization of the DNA to solid surface is incorporated to the termini of synthesized DNAs by using the specific "linker reagent" at the final step of the synthesis. Although there are several types of linkers possessing the different functional groups, the amino linker with primary amino group is used most frequently for the chemical modification of DNA because of the chemical stability and the easy handling.

DNAs modified with the amino group (amino-modified DNA) are generally conducted by specialized DNA synthesis companies. In one process of this synthesis, defective DNAs failing in the linker incorporation must be separated from

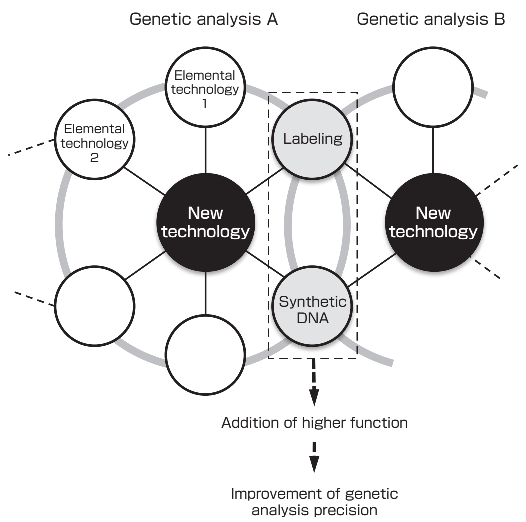

Fig. 1 Technological configuration of the genetic analysis system
The conventional technologies such as synthetic DNA (RNA) and labeling are used commonly in several genetic analysis systems, and also are related to pharmaceuticals.

Table 1 Advantages and disadvantages of amino linkers

	Conventional	First-generation	Second-generation
Advantages	• Stability • Cost • Performance	• Reactivity (> Conventional) • Purification (≧ Conventional)	• Reactivity (> Conventional) • Purification (≧ Conventional)
Disadvantages	• Purification • Reactivity	• Stability • Cost • Performance	• Cost • Performance

amino-modified ones. However, since the presence of an amino group presents only a slight chemical difference, it is difficult to conduct this separation in a short time period. On the other hand, due to the recent demand for comprehensive genetic analysis of whole genomes, it has become necessary to prepare several hundreds to several thousands of amino-modified DNAs in parallel. However, we imagined that the DNA synthesis companies were facing trouble in their synthesis and purification processes due to the use of the conventional linker. Also recently, there is an increased potential for oligonucleotide drugs such as aptamers and siRNA. In order to increase their functions *in vivo*, various functional compounds must be conjugated with oligonucleotides through the linker with high yields, and we thought there would be a high demand for increasing the reactivity of the amino group as well as simplifying the purification process (Fig. 2B, Table 1).

Therefore, we decided to develop a new amino linker that enabled both the high-purity high-throughput purification of amino-modified DNA (or RNA) as well as the high chemical modification efficiency, so it could be utilized in the recent comprehensive genetic analysis and the nucleic acid drugs.

4.1.2 Development of the first-generation amino linker

The conventional amino linker has a simple structure where a primary amino group is linked to the terminal of the straight carbon chain. We first developed a series of amino linkers which consist of a single aromatic molecule (Fig. 3, first-generation amino linker). We expected that the reaction efficiency would be enhanced by hydrophobic interaction between the aromatic residue and the target molecule. Also, we expected that the separation using the reverse-phase column chromatography would become easy because of the increased hydrophobic property of the amino-modified DNA molecule.

Several types of amino linker reagents with different distances between the aromatic and amino groups were synthesized (Fig. 3; L1, L2), and the chemical properties of the amino-modified DNA were examined. The first-generation amino linkers dramatically improved both efficiencies in the coupling to the primary amine and the purification compared to the conventional linker (Table 1)[3], and we applied for the patent jointly with a collaborating company for the first-generation amino linker in 2004.

4.1.3 Research for practical application

We planned the product realization of "high-performance DNA chip" with our joint research companies, by selecting the "ssN-linker" that showed the highest performance among the first-generation types as the terminal modification. The basic data concerning ssN-modified DNA was already completed at AIST, but in order to realize actual use by the bioscience users, it was necessary to clear three major issues: 1) synthesis of the linker reagent, 2) synthesis and purification of the amino-modified DNA, 3) fabrication of the DNA chip using amino-modified DNA and its performance evaluation (Fig. 4a). However, the joint research partner engaging in 3) could not conduct business in chemical synthesis of 1) and 2), and we became painfully aware of the difficulty of realizing a chemical reagent product for use in the biosciences field. Therefore, we set out to explain the function and advantage of the new linker to the chemical companies so that they would undertake the synthesis business of this linker. A certain custom chemical company showed interest in the ssN-linker, and we provided both the linker reagent and the DNA synthesis technologies to this company (Fig. 4b, c). While the technology transfer of mass synthesis of the reagent alone (1) was done easily, time was needed for the technology transfer of synthesis and purification of multiple DNA probes (2). This was because our protocol established in the AIST lab level did not directly fit with that used in the company operating synthesis and purification of several hundreds and thousands of DNAs with automatic machines. That is to say, the protocol had to be adjusted for automation. On the other hand, along with the synthesis work (1 and 2), we also worked on the fabrication of the DNA chip in which ssN-modified probes were immobilized onto the slide glass, and evaluated its function (Fig. 4b, c). Although the work of evaluating the functions of the linkers both upstream (1 and 2) and downstream (3) was extremely hard, for the actual use of the linker by the bioscience users, we believed it was necessary to establish the route and to indicate our product's superiority to the conventional technology. Therefore, we collaborated with the companies for this work. As a result, we demonstrated that our linker showed higher performance than the conventional reagents in all evaluations, and licensed the manufacture and sales of the ssN-linker modified DNAs to the DNA synthesis company, as well as the sales of DNA chip to the bioscience company.

4.1.4 Discovery of issues and interruption of product realization

For the commercialization of chemical reagents, the stability of the reagent itself and the DNA modified with the reagent are important check items. Since such stability test is generally time-consuming, it was started at AIST at nearly the same time as the technological transfer to the private sector. As a result, while the ssN-linker was stable in the form of a reagent, a slight amount of ssN-modified DNAs were decomposed to lack original property under severe heated alkaline conditions[4]. Since it was stable under ordinary conditions, it was not a major issue in practice. However, the usage and storage greatly depend on users, and we could not negate the possibility that this may develop into a critical problem after it was marketed as a product. Therefore, we decided to halt the licensing of the ssN-linker. We explained the situation to the people involved in both projects of DNA chip fabrication and DNA synthesis, and asked them to temporarily interrupt the projects. The instability of the ssN-linker was an unforeseen result. How much AIST should be involved in product realization including stability testing is a difficult issue. However, we must reflect on the point that we might have rushed the application (downstream) research involving the private companies immediately after discovering the new material, the ssN-linker.

4.1.5 Development of the second-generation amino linker

The interruption of the project was a major setback, and we also experienced a sense of defeat. However, we were

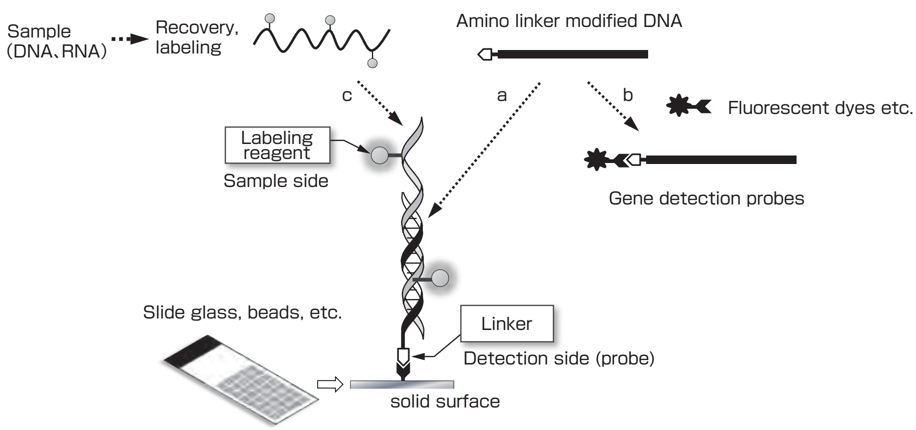

Fig. 2 Amino-modified DNA and labeling of nucleic acids
Amino-modified DNA is used for immobilization to the solid surface (a) or bonding with chemical substance (b).
The sample DNA (RNA) with the complementary sequence is labeled with the labeling reagent (c).

investigating the high reactivity of the ssN-linker along with the work of product realization and the basic research turned out to be fruitful. Soon, we found that the structure of the linker alters the chemical property of the neighboring primary amine increasing the reaction efficiency with the target molecule[4]. Since this structure was a new discovery not included in the patent for the first-generation product, we applied for a new patent, and this new structure was called the "second-generation amino-linker". Although several compounds belong to the second-generation type due to the common structure, we selected the highly stable "ssH-linker" as the next linker after various investigations (Fig. 3). Unlike the ssN-linker, the ssH-linker does not contain the hydrophobic group in the molecule, but it is possible to very quickly remove the hydrophobic group that protected the amino group under moderate conditions. This chemical property of the ssH-linker enabled the high-throughput purification easily by reverse-phase chromatography, and it was also confirmed that the conjugation efficiency of this linker with the target molecule was superior to the conventional amino-linkers (Table 1, Fig. 5). Moreover, the ssH-linker was chemically more stable than the ssN-linker, and had the advantage of the synthesis cost being almost the same as the conventional reagent (Table1).

Due to such superiority, we re-proposed the ssH-linker to the DNA synthesis company and the DNA chip manufacturing company, and requested the restart of the interrupted projects. Since it became possible to keep the unit price significantly low for the ssH-linker, the chemical synthesis company accepted it smoothly, while time was needed for getting approval from the DNA chip company that had been collecting data for the DNA chip using the ssN-linker. Later, the technological superiority of the ssH-linker was acknowledged by the two companies. We concluded a licensing agreement for the domestic DNA synthesis using the ssH-linker in 2006 with the DNA synthesis company. Also, in 2007 and 2008, the DNA chips using the ssH-modified probes were commercially produced.

The ssH-linker has higher reactivity to active esters compared to conventional amino-linkers, and its modified DNAs and RNAs show high-purity by high-throughput purification. In addition, the low cost of the reagent promoted the use of the linker in the DNA synthesis companies, and it is now on market worldwide by overseas chemical companies. The license of the lower priced ssH-linker meant the reduction of royalties for us, but we decided to license it so that as many companies and research institutes use our product as possible.

4.1.6 Development after licensing

The conventional amino linker has been used throughout the world for a long time, and it has been already built into the current genetic analysis systems. Therefore, it was not easy to replace the conventional linker by the new type having a different structure. This meant that after the license, we faced the difficulty of "selling a product or getting people to buy it." To steadily increase the use of our linker, we continued application researches to propose new usages other than genetic analysis, as well as scientific demonstrations through publication of papers. As a result, we were able to propose an alternative usage of this reagent in the oligonucleotide therapeutic field[5], and the demand for linkers is recently

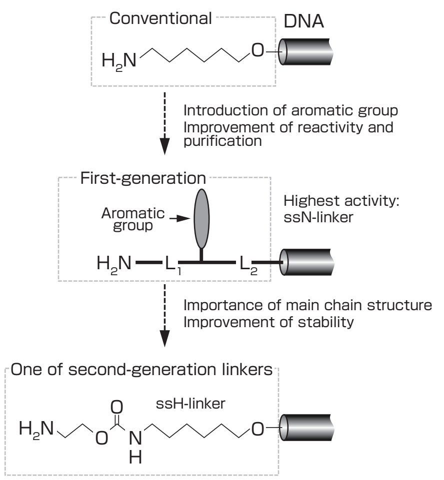

Fig. 3 Structures of the amino linkers bonded to the DNA and the flow of development

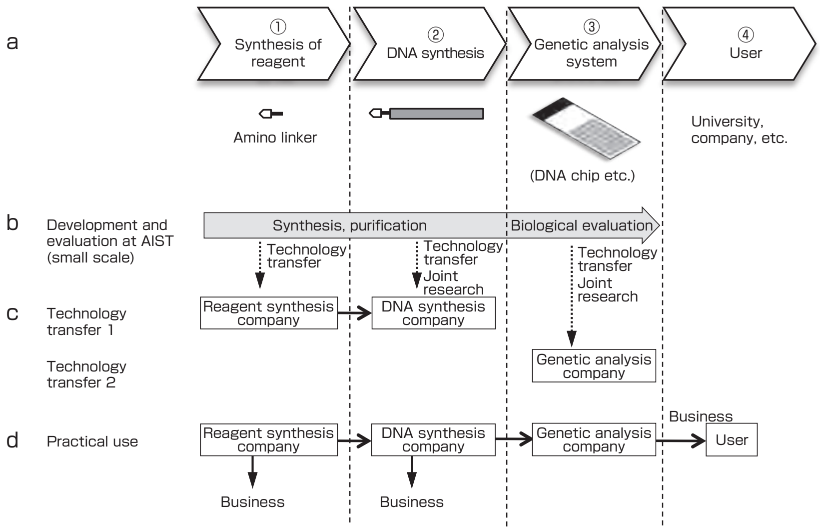

Fig. 4 Process from the linker reagent to the utilization of analysis system
Basic development and the construction and evaluation of the model system were conducted at AIST, and the efficacy of the performance was confirmed (b). Later, the technology was transferred to the private sector (c), evaluation of biological experiments were done at the genetic analysis company (c), and the route for utilizing the amino-linker reagent in bioresearch was established. Businesses are conducted for the reagent and products treated with the reagent.

rising in the new field. We feel it is important to continue R&D to seek new advantages to develop the technologies in the niche field, instead of simply ending with the licensing of the product.

4.2 Labeling reagent

In the development of the first-generation amino linker, we found that the amino group close to the aromatic residue reacts efficiently with the target molecules. To extend this principle to other issues, we planned the development of a reagent that labels nucleic acids isolated samples. Since the amino-linker is a reagent related to probe modification, we aimed to construct the complementary relationship by developing a superior labeling reagent.

To efficiently label DNA or RNA recovered from living samples, the binding efficiency of the reagents with nucleic acids is one of the important factors. While enzymes are useful for labeling of nucleic acids[6], the efficiency frequently depends on the target sequences. We thought that a labeling reagent could be a universally useful tool just like the amino linker, because it reacts with the "aldehyde groups" generated naturally or artificially in both DNA and RNA. Since there were already several marketed reagents labeling aldehydes, the developed product must have higher performance than the existing products. To obtain high reactivity to nucleic acid, we synthesized a reagent with linked aromatic group in proximity to the aminooxy group, which is known to react with the aldehyde group, using the know-how we obtained in developing the amino linker (the aromatic residue improves affinity to the nucleic acid) (Fig. 6). Since the incorporation of the hydrophobic group made the reagent poorly insoluble, we synthesized another compound which had a guanidino group of a positive charge. We expected the reagent molecule would not only increase the affinity to the negatively charged nucleic acid but also become water soluble. As a result of the reaction, the new labeling reagent with both the aromatic and the guanidino groups showed much higher reactivity to the aldehyde group in nucleic acid as compared with the commercially available reagent, and could sensitively detect aldehyde groups produced in the genomic DNA[7]. The reactivity can decrease the amounts of genes required for the analysis, and achieve highly sensitive gene detection. In addition, the synergetic effect of the aromatic and guanidino groups provided important findings for the creation of other functional molecules binding with nucleic acids. The patent was filed in 2007 for this product, and papers were presented at the academic societies in 2009. As a result, we received requests for samples from several research institutes, and its activity is under evaluation at this moment. We hope to have this labeling reagent used widely in society in the future.

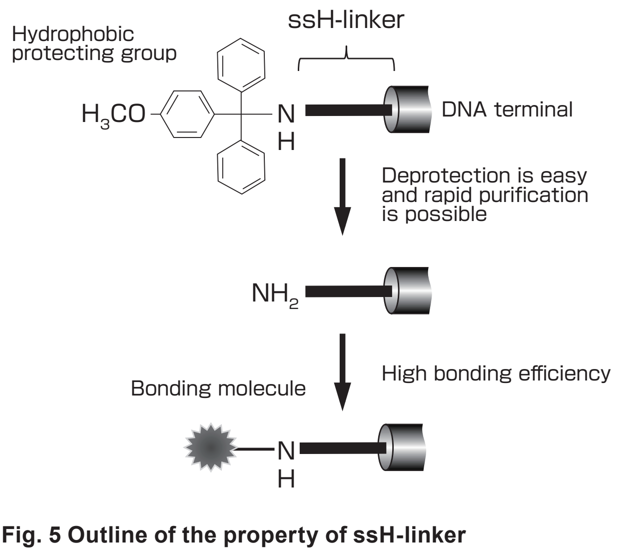

Fig. 5 Outline of the property of ssH-linker
The deprotection speed of the hydrophobic protecting group and reaction to the amino group increased.

5 Discussion

Since the "progress of the research" and "patents" were major points in our R&D, we shall discuss them in detail.

5.1 Progress of the research

The research was started in the latter half of 2003, and the reagent went on worldwide sale by 2007. There were several factors for this realization. As described above, the realization of a chemical reagent used in biological analyses must not only cover wide-ranging research fields from organic chemistry to biosciences, but solve several issues including stability and cost. To achieve valuable effects within the limited budget and human resources, we thought that a development of some universal technology was necessary. Therefore, we selected the research of the amino-linker that was used "commonly" in several analyses. While this was a

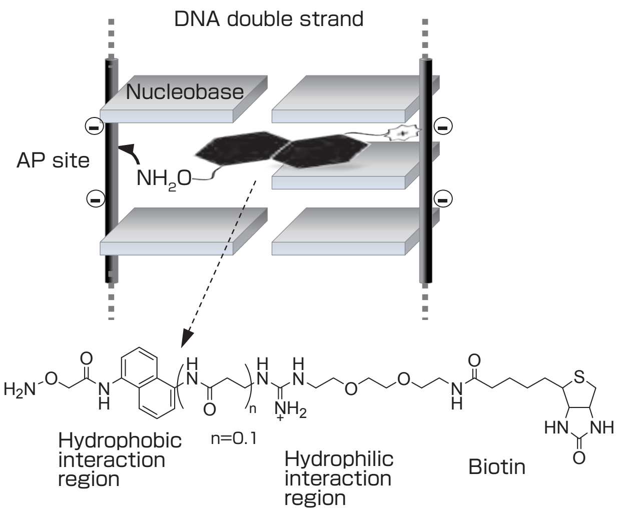

Fig. 6 Schematic diagram of the reaction with labeling reagent
The + and – indicate the positively charged guanidino group and the negatively charged phosphodiester group, respectively. The AP site is a structure of damaged DNA lacking the nucleobase, and possesses the aldehyde group.

"non-trendy topic" that had been considered to have nothing to be developed, we could perform the original researches (Factor 1). To quickly conduct the wide-ranging research, we held intense discussions with our collaborators. Such collaborations inside and outside of AIST were extremely important (Factor 2). In the improvement of the existing technology, particularly, the "speed" of the development seemed to be very important, and we carried out the research with practical use in mind from the development stage. While this may not be the best way, we believe it is very important to develop our technology speedily in life sciences which progress at an extremely fast pace (Factor 3). As the progress of our research was accelerated day by day, frictions were generated with the research environment systems. Therefore, there should be an environment that would minimize deceleration. Also, the development of the second-generation linker was important for the product realization, but this could not be accomplished without the continuous basic research on the chemical property of the first-generation linker. We realized that it was essential to pursue the basic research in practical realization (Factor 4). While four factors described above were derived as a result of the research, perhaps it was most important that we engaged in research with passion for contributing to society by producing valuable products, and joint research with private companies always reminded us that we were linked to society.

After licensing one product, we started the second research on the basis of our findings obtained from the first research (Fig. 7). However, to further broaden the potential of the licensed product, it was still necessary to continue working on the first research. Our tactics allowed quick extension of the first findings to wide-ranging fields, but two projects (the newly started research and the application of the licensed technology) had to be handled by two full-time employees, and this was extremely severe in terms of budget and physical capacity. Licensing is not the goal and researches are carried on. We should construct a research environment where researchers can carry out both basic and application researches smoothly.

5.2 On patent

For the developed reagent to be used in society, a patent is necessary in reality. In engaging in joint research with a private company, we placed extreme importance on patent from the beginning. Therefore, we were extremely careful about conducting preliminary patent survey for our project. As a result, novelty was recognized in Japan and overseas for the amino linker, the patent was accepted extremely quickly, and this led to the licensing. The patent for the labeling reagent will soon undergo patent examination, and we have received report that the developed reagent is novel.

On the other hand, much cost is required for a patent. We filed several related patents other than the main patent, but we withdrew the applications without moving on to examination requests or overseas applications for the patents that we thought would not be licensed, and narrowed down the items on our own. While patents cannot be obtained without budget, large amount of budget does not necessarily guarantee a product or a patent. Although the R&D and the handling of the patent reflect the organizational policy, we believe that if the practical use of technology is the goal, it is important to establish an environment that allows filing for

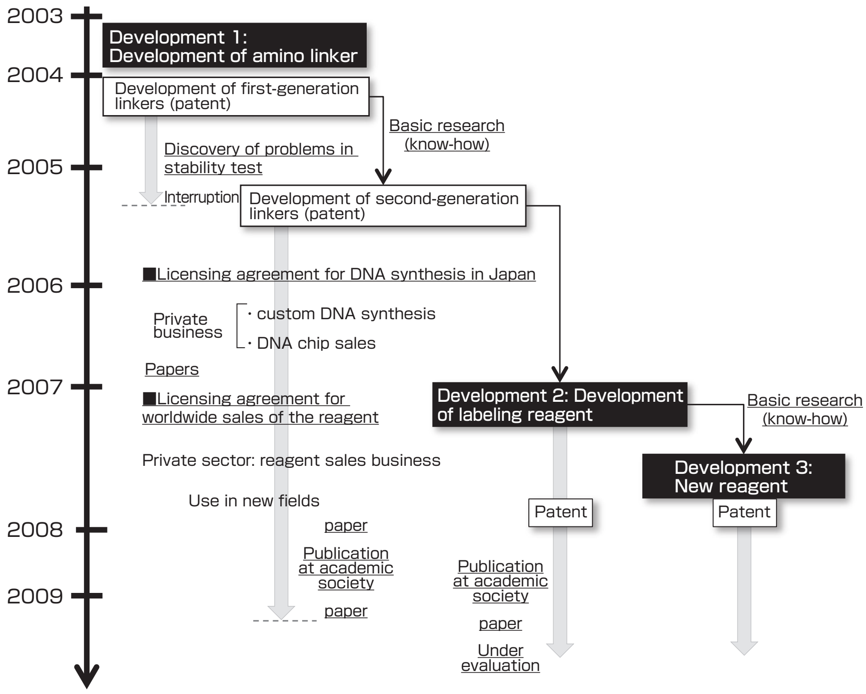

Fig. 7 Development of the R&D

good patents and supports such endeavors.

6 Issues for the future

In the development of the two types of reagents, the initial goal was achieved by conducting research to improve the performance of the existing reagents. However, we also realized that the existing technologies were deeply integrated into many systems, and time is needed for replacing them. Therefore, for the next development, we wanted to attempt an approach of proposing a totally new idea without concern for the immediate demand, and we recently developed a reagent that has unique properties (Fig. 7; Development 3). Although the details of this reagent are unpublished, we have filed for its patent. This third reagent has properties unseen before, but does not necessarily fulfill the users' specific demand. Therefore, unlike the earlier reagent developments, we have no image of the final product at this moment. For this third reagent, we must create the demand on our own, or present this technology to the world through papers and hope others will come up with ideas for its use.

Although there are numerous discussions on potential and demand (or "seeds and needs"), we have no idea which approach is the best from our experience in development. However, since unforeseen events do occur, there is the danger that if the researchers concentrate too much on potential and demand, they may become stalled and be unable to accomplish much. Both potential and demand are necessary to realize a product, and it is necessary to maintain the balance of the two in the process of research and revise them if necessary. We also believe that rather than setting licensing of the product as the goal, a venture spirit is needed for the true realization of a product.

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References

[1] J. Shendure and J. Hanlee: Next-generation DNA sequencing, *Nat. Biotechnol.*, 26, 1135-1145 (2008).
[2] H. Sara, O. Kallioniemi and M. Nees: A decade of cancer gene profiling: from molecular portraits to molecular function, *Methods Mol. Biol.*, 576, 61-87 (2010).
[3] N. Kojima, M. Sugino, A. Mikami, K. Nonaka, Y. Fujinawa, I. Muto, K. Matsubara, E. Ohtsuka and Y. Komatsu: Enhanced reactivity of amino-modified oligonucleotides by insertion of aromatic residue, *Bioorg. Med. Chem. Lett.*, 16, 5118-5121 (2006).
[4] Y. Komatsu, N. Kojima, M. Sugino, A. Mikami, K. Nonaka, Y. Fujinawa, T. Sugimoto, K. Sato, K. Matsubara and E. Ohtsuka: Novel amino linkers enabling efficient labeling and convenient purification of amino-modified oligonucleotides, *Bioorg. Med. Chem.*, 16, 941-949 (2008).
[5] N. Kojima, T. Takebayashi, A. Mikami, E. Ohtsuka and Y. Komatsu: Efficient synthesis of oligonucleotide conjugates on solid-support using an (aminoethoxycarbonyl) aminohexyl group for 5'-terminal modification, *Bioorg. Med. Chem. Lett.*, 19, 2144-2147 (2009).
[6] K. Cole, V. Truong, D. Barone and G. McGall: Direct labeling of RNA with multiple biotins allows sensitive expression profiling of acute leukemia class predictor genes. *Nucleic Acids Res.*, 32, e86 (2004).
[7] N. Kojima, T. Takebayashi, A. Mikami, E. Ohtsuka and Y. Komatsu: Construction of highly reactive probes for abasic site detection by introduction of an aromatic and a guanidine residue into an aminooxy group, *J. Am. Chem. Soc.*, 131, 13208-13209 (2009).

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Discussions with Reviewers

1 "2 Scenario to realize the goal"

Comment (Yoshifumi Jigami, Research Center for Medical Glycoscience, AIST)

In this section, the explanation of Fig. 1 is difficult to understand. It may be better if you specifically explain each "elemental technology" of the genetic analysis system and their mutual relationship, as well as the relationship with "labeling" and "DNA synthesis". Also, "conventional technology", "first-generation type (ssN-linker)" and "second-generation type (ssH-linker)" of Fig. 3 should be compared in a table that shows their properties, advantages and disadvantages. You should explain what has brought you to your "scenario to contribute to the improvement of precision of the overall genetic analysis" and explain why you "selected to fulfill the demand in the niche field" in that process. This will enable the readers to understand the authors' thinking processes.

Answer (Yasuo Komatsu)

I rewrote the text to clarify the explanation of the figure and the scenario. Also, I created a simple table that summarizes the advantages and the disadvantages of the amino linkers.

2 "*3.1.4 Discovery of the problem*"

Comment (Yoshifumi Jigami)

This is an important section that explains the motivation for the development of the second-generation amino linker and I think you should give a more detailed explanation. Particularly, there should be a more elaborate explanation of your decision and the situation why the discovered problem halted the licensing of the ssN-linker and interrupted the project.

Also, I think the significance in terms of synthesiology will be clear if you add your thinking and social situation behind "the decision to allow the developed product to be used by Japanese and overseas companies despite the decrease in royalties".

Answer (Yasuo Komatsu)

At the same time that ssN-linker showed high reactivity, it was also chemically unstable. The transformation of ssN-linker is confirmed only under limited conditions. However, the situation under which the users store the amino-modified DNA may vary greatly, and we could not eliminate the possibility that the linker may transform during storage and its function may decrease. This means that if such a compound with potential danger is released to the public sector, the company must carry the risk. Therefore, although the project was far in its course, we made a decision to develop a better linker. The background of making such a decision immediately before licensing was mainly from a thought that claims from users could be extremely troublesome to deal with, as well as a vague feeling that there was a possibility of some major problem in the future.

We considered licensing not only in Japan but overseas from the beginning of the R&D. We made this decision because having the developed technology used throughout the world will expand the possibility for evolution of this technology. For royalties, rather than AIST profiting, we thought it was more important that businesses would be conducted in the private sector as shown in Fig. 4.

3 "*3.2 Labeling reagent*"

Comment (Yoshifumi Jigami)

I think it would be more useful to the readers if you compare the property of the newly developed reagent with that of the conventional reagent and comment on how much and what kind of social impact will arise from future developments based on this new agent.

Answer (Yasuo Komatsu)

The high reactivity of the developed labeling reagent to the nucleic acid will lead to the reduction in the amount of reagent needed for the detection of minute amount of samples (reduction of background value). The characteristic in the structure of the reagent also provided an important finding in the creation of the nucleic acid recognition molecule other than the labels. I rewrote the text to emphasize these important points.

4 "*4.1 Development of the research*"

Comment (Hisao Ichijo, Tsukuba Center, Inc.)

I think it will be easier to understand and the readers will be able to see the choice of the research elements conducted in the R&D process, if you explain the process by which you arrived at the new labeling reagent.

Answer (Yasuo Komatsu)

If there was no development of the second-generation reagent, there would have been no realization, and this was a major point. As you indicated, I added the importance of this development in the discussion section.

Comment (Yoshifumi Jigami)

You state, "the fact that we selected a 'non-trendy development' turned out to be important (Factor 1)". If that is true, you should explain why this is important. You should also describe a specific situation how "the collaboration inside and outside the institute to conduct wide-ranging research for product realization (Factor 2)" has been carried out.

For the Development 3 of Fig. 7, please present a discussion on how the seeds-oriented research is different from the earlier needs-oriented research and what are your assumptions on how the difference of research methods affect the research results and what kind of ripple effect (social impact) there may be in "5 Future issues". Also, it seems you are returning to a seeds-oriented research from the earlier needs-oriented research, but as a researcher, why do you need such a return? I would like to hear the "thoughts" and "future dreams" of the authors based on this experience.

Answer (Yasuo Komatsu)

Pursuing a trendy topic means that the research may be an attempt to catch up to someone else, and may end up without ever catching up if we are lacking human resource power. On the other hand, technology that was once thought to be firmly established may develop problems due to new demands arising from changes over time. Therefore, we reviewed the technology that was considered firmly established, dug up its problems, and that led to good results for this particular case. I rewrote the part that explains the other factors that led to the success. I also added some text in Fig. 6.

For demand and potential, or "needs and seeds", we engaged in "needs-oriented" research in the first two R&D. However, as written in the text, if we are caught up by "needs" only, we must compete with (that is, replace) the similar, existing technologies. It may be difficult to replace the already entrenched technology even if the new technology is superior, and this requires time. We wanted to try the route of providing a technology with absolutely no similar product, and then move toward its product realization. Therefore, we began the development of the third reagent. However, such approach may land in a place where the demands are different. Therefore, I don't know what the best approach is, but both elements are required in practical use, and I personally think that a balance has to be struck and modifications made in the process of the research.

Development of laser-assisted inkjet printing technology

— Wiring technology to achieve high throughput and fine patterning simultaneously —

Akito ENDO* and Jun AKEDO

[Translation from *Synthesiology*, Vol.4, No.1, p.1-10 (2011)]

A new technology that can be easily adapted to various circuit designs and production in small lots has been requested in electronic device manufacturing where low cost device fabrication on large area is required. We have developed a laser-assisted inkjet printing technology which can achieve high throughput and fine patterning simultaneously. To realize fine patterning with low resistivity, ejected ink-droplets have been dried by laser irradiation to suppress expansion on a substrate, a problem often observed in a conventional inkjet process. Drawing of fine wiring with aspect ratio of 1 or above with line width of 10 μm or less has been achieved using this new approach. In this paper, the achievements of laser assisted inkjet printing technology is shown based on the needs that triggered this research and the solutions used to overcome the problems met during the R&D process.

Keywords : Ink-jet printing, throughput, fine pattern, wiring technology, low cost

1 Background

As the industrial structure becomes globalized, the electronic technology has become one of the major fields that support the Japanese economy and industry. Several new electronic devices are developed and produced with the advancement of technology. With this background, the price competition is becoming even fiercer, as there are differences in the values for quality and performance in Japan and abroad. Technological innovations are needed to ensure the competitiveness of the Japanese makers in the years to come I nthe world market.

As seen in the built-to-order (BTO) (system where the products are manufactured after receiving the order from the customer), customizations and differentiation of the electronic devices are done according to demand, and various tailor-made electronic devices and products are manufactured to meet the demands of the users throughout the world. As a result, an innovative manufacturing technology that enables high-diversity low-volume or high-diversity variable-volume production as well as shortened product cycle is becoming important. At the sites of development and production, efforts are spent on the diversification of functions, downsizing, further cost reduction, and high throughput by integrating the electronic devices with various functions. At the same time, small-lot production and short delivery time are achieved by the horizontal division of labor of the manufacturing process[1].

On the other hand, from the perspective of sustainability of industry, there is a high demand for technologies that are using minimum resources, minimum energy consumption and low environmental impact for the "manufacturing process" in the 21st century. The National Institute of Advanced Industrial Science and Technology (AIST) propose the concept of "minimal manufacturing", which is a concept for a production process that simultaneously solves the three elements that often contradict each other: "energy and resource saving", "high performance/new function", and "high productivity, low cost". By achieving minimal manufacturing, AIST aims to contribute to the sustainable development of Japanese manufacturing through environmental harmony and international competition.

The situation is no different in the field of electronics mounting. In the wiring technology that is the core of electronics product manufacturing, there is rising demand for high diversity and customization of the mounting of electronic circuitry and parts. Since photolithography technology used in silicon micromachining is a relatively high cost process, it is difficult to achieve high diversity using this technology. In the wiring for displays with large surface areas such as the flat panel display (FPD), achieving larger surface area is difficult because there are issues in the alignment of mask due to the fine-sizing, increased surface area, and multiple layering of the mask. Moreover, the photolithography process is a multistep process that involves among other steps the formation of the conducting metal film ,deposition and removal of the photoresist material, removal of the excess conducting metal, and washing. Large volume of waste liquid containing precious metals and harmful substances is produced, and energy and resource savings in these processes are necessary[1].

The inkjet printing technology that we are developing can form the desired conductive film only on the areas needed avoiding in this way the production of waste. With its on-demand and energy saving characteristics, it is a technology at the core of "minimum manufacturing" proposed by

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AIST. Since the waste liquid produced in the manufacturing process makes a heavy load on the environment, there are high expectations for the wire mounting process through the inkjet printing technology to achieve reduction of fabrication costs and reduce the production of waste[2][3].

But, before implementing the inkjet printing technology to wiring, there are problems that had to be solved, such as the high resistance of the conductor in the ink and the decreased throughput as the wiring became finer. In this paper, we report our research and progress toward the realization of a practical inkjet wiring under the minimal manufacturing concept.

2 Situation of the manufacturing technology for high-diversity production and the selection of technology to be developed

2.1 Integration of the IC chip in multiple function devices and the flow of technological development

To achieve downsizing, high function and low power consumption of the IC chip, the "system on a chip (SoC)"concept where various functions are integrated on a single chip was actively developed.

In the SoC, to integrate the functions on a single chip, the new process technology "system in package (SiP)" is used to realize the multiple functions. Here, the IC chips are inserted in a single package, or the module is created by combining the developed IC chips with the package. Currently, further downsizing and multiple functions are attained for the electronic products, and 3D integration is done by IC stacking where the IC chips are stacked inside the IC package to reduce the mounting surface area (Fig. 1). The 3D mounting technology for connecting the stacked IC chips is the key technology.

Until now, electric connection by flip chip mounting was done for the 3D mounting of the IC chips. Specifically, the solder ball and soldered pad are set on the input-output terminal of the IC chip, and the solder is melted by heating in a furnace to connect the electrode terminal (ball grid array). Another way to connect the electric terminals is by heating and supercharging the space between the IC chips.

However, as the IC chips are stacked, the bump became smaller and several problems became apparent, such as the difficulty of checking the connection fault, increased cost of bump installation, difficult installation of the fine Si through-via needed for interlayer connection, and the need for ultra-thin processing of Si substrate to keep the IC stack thin.

On the other hand, there are methods where the electric connection between the IC chip and the interposer or lead frame is done by wire bonding, (or) where the input-output terminal is brought to the surface by creating a step on the IC chip. However, there are several issues in wiring that are very difficult to solve. One such example is that is difficult to realize a densifications in the wire connection lines to the IC chip so that there is a limit in high-speed transmission due to increased inductance in the wires[4].

The developments of the 3D mounting technology that allows electric connection over the steps between the chips and the wires on the lateral side of the stacked IC chips are immediate concerns.

2.2 Characteristics of process technologies and the technological issues of the inkjet printing

With the recent integration, the design rule inside the IC chip was reduced from about 100 μm to submicron level, and the fine-sizing of wiring in the 3D mounting technology has become important. At the same time, high performance, energy and resource savings, increased production efficiency, and decreased cost are in demand for the wiring technology.

Figure 2 is a comparison of the wiring technologies that are put to practice or are expected to be put to practice, including the photolithography process technologies, micro contact printing (μCP) nano-imprinting, and screen printing, and the mask-less technologies, such as microchip integrated processing technology (MIPTEC) and inkjet printing.

In the photolithography process, the photosensitive organic substance is exposed in patterns to create a resist film, and the metal film formed on the substrate is etched to fabricate the desired pattern. The fine patterning depends on the diffraction limit of the mask that depends on the wavelength of light used for exposure, and this must be considered to

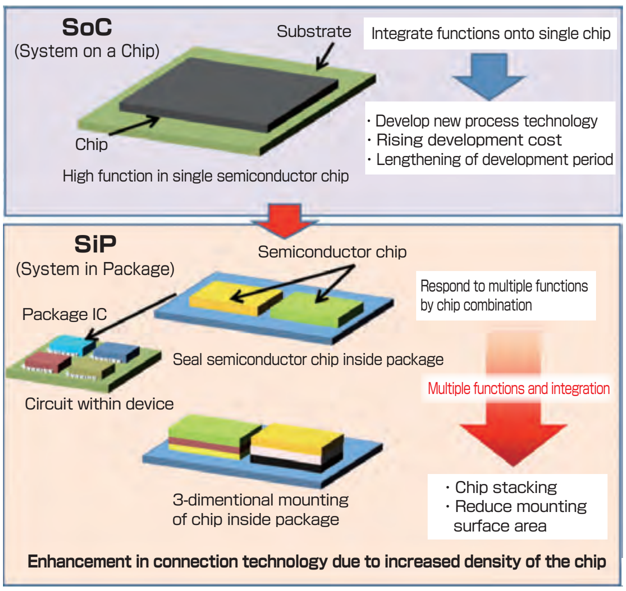

Fig. 1 Flow of high-density integration of IC chips to achieve multiple functions

the wide-ranging design rule from semiconductor chips to printed circuit boards (PCB). In μCP nano-imprinting, fine structures can be fabricated easily by transferring the mold plate to the resin substrate, and new developments are possible. In screen printing, the desired wiring pattern can be created by printing the conductive paste onto the PCB substrate using a screen. Screen printing is used as surface mounting technology[2]. Since these process technologies use masks or molds, the 3D mounting on uneven substrate is extremely difficult.

On the other hand, in the maskless process MIPTEC, the pattern can be changed easily simply by rewriting the program. Since the metal film wires formed by electroless plating are transferred by ablation with YAG or YVO4 laser to create three dimensional patterns, it is expected that this 3D mounting technology will allow high-diversity production necessary in creating structures such as 3D connectors. Another maskless process, the inkjet printing technology that is being developed in the organic electronics technology field[5] is using ink, in which the conducting nanosize metal particles are dispersed, to form the desired pattern by applying the necessary amounts in the pattern areas. The inkjet printing allows formation of patterns on uneven substrates. Moreover, recently, it has become possible with this technology to form wirings stably at about 50 μm in width and this make this process suitable for the application to 3D mounting technology.

A comparison of the characteristics of the process technology and the technological elements are shown in Fig. 3. The photolithography technology, which is the most practical process technology at this point, was developed heavily due to the important advantages offered by of fine-sizing, high throughput, and high yield. The mounting technologies were developed utilizing the characteristics of μCP nano-imprinting technology for its fine-sizing capability, the screen printing for its high throughput, and MIPTEC for

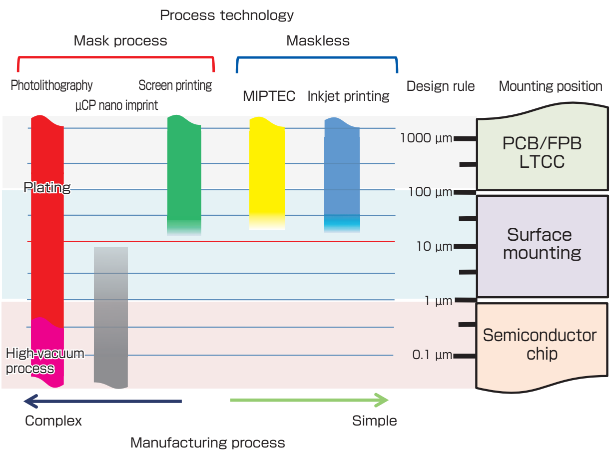

Fig. 2 Wire width corresponding to mounting position and wiring technology

its high-diversity capability and the superiority of maskless process.

In the same time, inkjet printing has other important advantages such as high-diversity, low cost, and energy and resource savings that are unseen in other process technologies, and it shows the potential to become the core of minimal manufacturing. However, there are technological issues that must be overcome, such as the low throughput needed to realize high productivity and low yield.

3 Technological issues and the selection of methods to solve them

3.1 Wet-spreading of ink that causes decreased wire formation speed

In the inkjet printing technology for wire formation, the wires are formed by connecting the dots, and the process factors are different from the home-use inkjet technology in which the dots are placed at even intervals. Specifically, the state-of-dot connection changes and the form of wiring pattern is greatly affected by factors such as the wire forming speed and ejecting frequency, ink viscosity and surface tension, and wet-spreading of ink onto the substrate.

In the conventional inkjet printing technology, the ink that lands on the substrate spread in the planar direction, the width of the wire spread further than the diameter of the droplet even with controlled surface tension, ink viscosity, or the wetness of the substrate. For example, under the conditions of stage speed 100 mm/s and ejecting frequency of 30 kHz, when the droplet with a diameter of 15 μm lands onto a substrate at contact angle of about 60°, the wire width will expand to about 50 μm or several times larger than the droplet diameter[6]. To achieve fine wiring of about 10~20 μm of width, it is necessary to reduce the droplet size to 10 μm or less.

This means that when the wire resistance is kept constant, or when the ink supply per unit length of wire is kept constant yet maintaining the throughput, the ejecting frequency depends by factor of 3 on the reduced droplet diameter.

	Functionality		Productivity		Production cost		Environmental friendliness	
	Fine-sizing	High diversity	High throughput	Large surface area	Manufacturing cost	Reduced manufacturing procedure	Energy and resource savings	High yield
Photolithography technology	◎	×	◎	△	×	×	×	◎
μCP nano-imprinting	○	△	△	×	△	△	△	△
Screen printing	△	△	◎	△	○	○	○	○
MIPTEC	△	○	○	○	△	△	△	○
Inkjet printing	△	◎	×	◎	◎	○	◎	×

Fig. 3 Wiring technology and characteristics of the technological elements

However, as the ejecting frequency of the inkjet head is increased, the meniscus (boundary between the ink and air) formed at the nozzle orifice vibrates during discharge making the continous discharge very unstable. Moreover, problems such as unstable discharge at various vibration modes occur due to the pressurization and decompression of the ink in the injector of the inkjet head. Therefore, it is necessary to simultaneously optimize the various parameters such as the droplet diameter, orifice diameter, volume change of the actuator, and physical properties of the ink (surface tension, viscosity, etc.). In the current inkjet technology, it is extremely difficult to significantly increase the ejecting frequency to several ten kHz without altering the pattern formation[7].

In the conventional inkjet wiring technology, the fine-sizing of the wires and the throughput have a trade-off relationship, and, to overcome this, a breakthrough in the technology to control the wet-spread after the droplet lands on the substrate was needed.

3.2 Conventional methods for controlling the wet-spread

Our research was also focused to control the wet-spreading of ink that lands on the substrate, which is an essential issue of inkjet printing technology. Summarized below are the methods for controlling the wet-spreading of ink in the R&Ds so far, and why the throughput cannot be further improved by further optimizations of these methods(Fig. 4).

1) Reduction of resistivity by improvements of ink
Before considering the methods to control the wet-spreading of ink, it may be possible to decrease the wire resistance by replacing the ink material with one with lower resistivity. However, it is clear that the ink resistivity cannot be lowered below the resistivity of the metals contained in the ink. Specifically, the resistivity of the currently commercially-available nanoparticle silver ink is 2−5 x 10^{-6} Ω·cm, which is higher than the 1.6 x 10^{-6} Ω·cm of silver metal. The room for reducing resistivity by improvements in ink material is relatively small. Therefore, we did not set the reduction of wire resistance through ink improvement as our development approach.

2) Use of ink with high viscosity; decreased diameter of droplets
When high viscosity ink is used, as mentioned before, there are reductions of the ejecting frequency or decreased throughput, because of the meniscus issue and the vibration mode that inhibits the stable discharge. There is also the problem of nozzle getting clogged easily. By reducing the nozzle diameter in order to reduce the droplet size decreased throughput cannot be avoided and the possibility of nozzle clogging increases.

3) Substrate surface treatment to control the wet-spreading after landing
Although the method of substrate surface treatment may possibly control the wet-spreading of ink while reducing the width of wire, the surface treatment agent may reduce the adhesiveness of the ink and wire. For example, when the wire is formed using the aqueous-solvent conducting ink on a flexible substrate such as water-repellent polyimide, the adhesiveness may be greately affected by the surface treatment[8]. To avoid this and to increase the adhesiveness of ink, patterning is done on the hydrophilic and hydrophobic surfaces using a mask, and then applying the ink only to the hydrophilic surface[9]. However, this causes an increase in the manufacturing process steps and the total improvement of throughput cannot be achieved.

4) Increased drying speed of ink by heating the substrate
When the substrate is heated, there are serious problems such as the nozzle drying due to the heat radiation from the substrate which causes clogging, and cracks and gaps are formed in the wire as bumping occurs when the ink lands on the substrate. Therefore, this method has no good practical applications.

The fine-sizing of the wire width by controlling the wet-spreading of ink and the achievement of high throughput of the wiring process were at a trade-off relationship. This was a technological issue that could not be overcome with conventional technology.

3.3 Ink drying method using the laser energy

To realize both the fine-sizing of the wire width and high throughput that were in trade-off relationship, we developed a process technology from a totally new approach. As the method to control the wet-spreading of ink, we did not select the methods that were extensions of conventional solutions such as the use of high viscosity ink, small nozzle bore, or substrate surface treatment, but we selected the method of providing energy assistance to the discharged droplet to

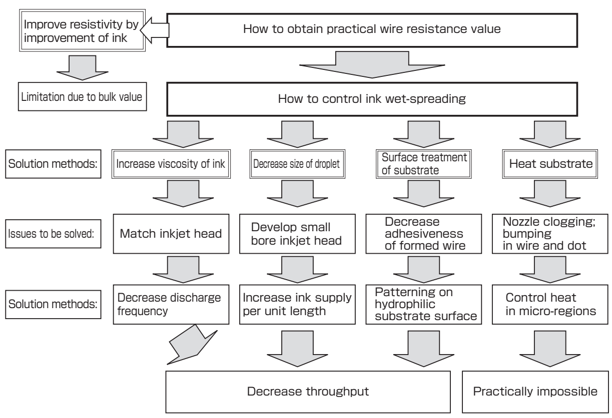

Fig. 4 Conventional methods to control the ink wet-spreading and the effect finally obtained

increase the drying speed.

As a method of injecting the energy directly into the discharged droplet without drying the nozzle or causing bumping, we devised a simple method in which drying is promoted by focusing the laser to the droplet and controlling the wet-spreading of ink (laser-assisted inkjet technology).

The laser-assisted inkjet technology is a method where the ink solvent is evaporated and dried instantly by heat energy, as the focused laser beam is irradiated onto the droplet and the substrate at the same time the droplet discharged from the inkjet head lands on the glass substrate.

Through the local assistance by laser energy, it was possible to reduce the nozzle clogging and damage to the substrate and to control of wet-spreading of ink through drying and higher viscosity.

In this research, the droplet of about 25 μm ~ 50 μm diameter was discharged from the single head, and the area around the discharged droplet was irradiated using the carbon gas laser with wavelength of 10.6 μm at continuous wave (CW) mode to form the wires.

3.4 Objective of the technological development and its aim

In the wire forming technology using the inkjet, to reduce the wire resistance, it is necessary to control the wet-spreading and increase the wire thickness, or in other words, to improve the aspect ratio of the wire. Therefore, to solve both the high throughput and wire resistance reduction, we wanted to establish a process technology that enables formation of wire with high aspect ratio without recoating (Fig. 6).

In the wire forming technology using the inkjet, the setting of the diameter of the discharged droplet is important. In the conventional inkjet technology, when the generally used droplet of 20 μm is used for wire forming, the ink spreads out, and the width of the formed wire would be about 30~50 μm even with substrate surface treatment[2]. Since recoating is necessary to reduce the wire resistance, the total time required to complete the patterning process is relatively high not only because of repeating coting process but also because of the waiting time necessary for the ink to dry before the next layer can be applied.

If wire formation is done at droplet diameter of 10 μm or less[10], the contribution of the surface area per unit volume increases according to the decreased size of the droplet[9], and the evaporation speed increases non-linearly during the flight of the droplet discharged from the inkjet head, making possible the control of the wet-spreading of the landed ink on the substrate surface and the wire formation of several μm or less width can be realized. But, because of the thin thickness of the wire, recoating must be performed several times to reduce the wire resistance, and this decreased the throughput.

To overcome the limitation of the conventional technology, the objective of laser-assisted inkjet technology was set to maintain the high throughput while realizing the wire width of 10 μm or less that was considered impossible with conventional technology.

The technological issue set was to reduce the wire width to smaller than the discharged droplet size by promoting drying with energy assistance, for droplets of about 25 μm ~ 50 μm in diameter. If the droplet size can be increased, the current inkjet head can be used, long-term stability and reliability can be obtained, the effect of airflow is reduced since the kinetic energy of the droplet increases, and the precision of the flying droplet landing on the substrate is increased. Moreover, by improving the landing precision, it would

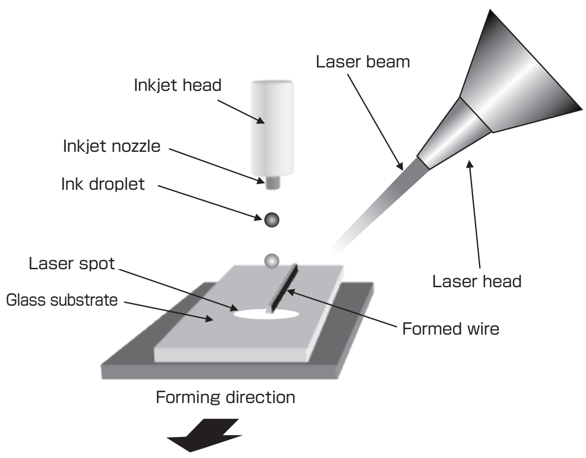

Fig. 5 Wire formation method by laser-assisted inkjet technology

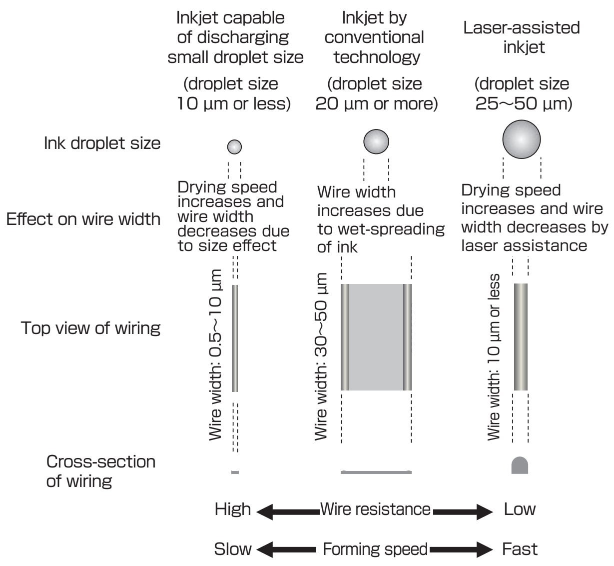

Fig. 6 Droplet size and wiring pattern targeted in the laser-assisted inkjet

become possible to widen the distance between the substrate and nozzle, and this will enable formation on materials with large step structures.

The technological issues of the conventional industrial inkjet technology were organized and the essential issues were extracted, to set the direction, technological issues, and objectives to be achieved for the laser-assisted inkjet technology.

4 Effect of the laser-assisted inkjet technology

4.1 Achievement of high aspect ratio of wire by laser assistance

Figure 7 shows the results of the formation on non-surface treated glass plate to study the effect of laser assistance on the wire width, to form fine wire with high aspect ratio.

When the formation was conducted under conditions of droplet diameter size of 25 μm, ejecting frequency of 3 kHz, and stage speed of 60 cm/min, the wires formed by the laser-assisted inkjet technology have a width of 10μm and a thickness of 11 μm. Compared to the wire forming without laser assistance, the wire width decreased from 230 μm to10 μm, or 1/20 time less, and the wire thickness increased from 0.8 μm to 10 μm, or about 12.5 times more. An extremely large improvement was observed.

Figure 8 shows the 3D configuration obtained by laser microscope. The wire formed by laser assistance was very different from the wire formed by conventional inkjet printing. The uneven wire formations such as the coffee stain phenomenon where the grooves are formed on both sides of the wire[9][11] and the bulge phenomenon where the wire width bulges out in some places[12] were not seen, and the wire had an even, smooth surface with a “semi-cylinder structure”.

It was possible by this approach to form a wire with high aspect ratio of 1 that is much higher than in che case of using the conventional inkjet method. Moreover, a wire with width smaller than the droplet diameter could be formed on untreated substrate surface using our approach.

In the conventional technology, even if the substrate surface treatment was done, wire thickness of about 290 nm[6] was the limit for one coating for a wire with width of 10 μm formed on the substrate with contact angle of 90°. Therefore, assuming the resistivity of the conductor at 2.0 μΩ·cm, the resistance per 1 cm of formed wire would be about 70 Ω/cm for wire formed with conventional technology with surface treatment. But the actual resistance value was about 6 Ω/cm for a wire obtained onto an untreated surface using laser assistance. The improvement observed in the wire resistance is over 10 times that of the conventional approach when laser assistance is used.

To get the same wire resistance by concentional inkjet methods, 13 or more recoatings are necessary. The potential for dramatic improvement of throughput by using laser assistance can be easely deduced from this comparison.

Moreover, since high precision in positioning and landing were required for recoating, laser-assisted method may solve these issues also.

4.2 Electric property of the wire

To develop the laser-assisted inkjet technology as the surface mounting technology specifically for the wires on the IC chip, we investigated the properties for the high frequency transmission line of the formed wire. The high frequency transmission property of the wire is affected greatly by the cross-sectional form and the precision of pattern. Therefore, the pattern of the coplanar transmission line, where the central conductor and ground conductor are arranged on the

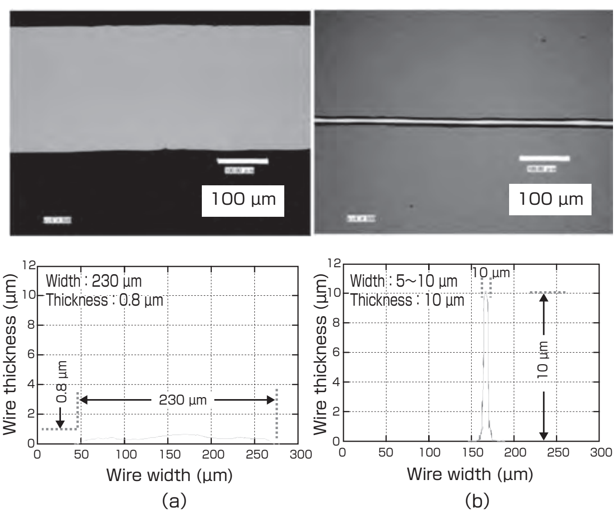

Fig. 7 Effect of laser assistance on wire width
(a) Without laser assistance (b) With laser assistance

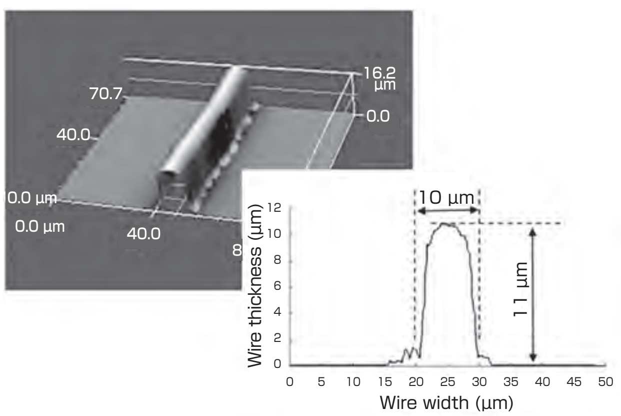

Fig. 8 3D configuration and cross-section of the wire formed by laser-assisted inkjet technology

same plane, was formed using only the laser-assisted inkjet technology and the high frequency transmission property was measured.

When the transmission line and the package were considered by the parameter measurement of the transmission property (S21) and the reflection property (S11) in the high frequency region using the Thru-Reflect-Line (TRL) calibration method by the network analyzer, it was possible to accurately observe which frequency could be used.

Figure 9 shows the results of the experiment and the simulation of high frequency transmission property to 1 GHz ~ 40 GHz, for the rectangular wire with resistivity of 3 x 10^{-6} Ω·cm, length of 4 mm, and width of 30 µm. In the conventional inkjet wire formation, the high frequency transmission of the wire was difficult because the wires had dot configuration. However, in the wire formation by the laser-assisted inkjet technology, the theoretical calculation values and the actual values matched well, and the wire capable of high frequency transmission is easy to be realized.

From the results of S11, slight discrepancies between the transmission gain of the calculated and experimental values was seen as the frequency increased. This is thought to be because the disorder on the wiring side of the coplanar transmission line pattern fabricated by the laser-assisted inkjet technology that may be affecting the impedance matching of the electromagnetic field. On the other hand, from the results of S21, good transmission property was obtained in the wire formation by the laser-assisted inkjet technology, since it was possible to transmit signals up to 40 GHz, and the attenuation was small up to about 10 GHz.

From the above results, the possibility of high-speed transmission, which was considered difficult by inter-chip connection and wire bonding in the 3D mounting, was shown to be possible for the high frequency region at about 10 GHz using the laser-assisted inkjet technology.

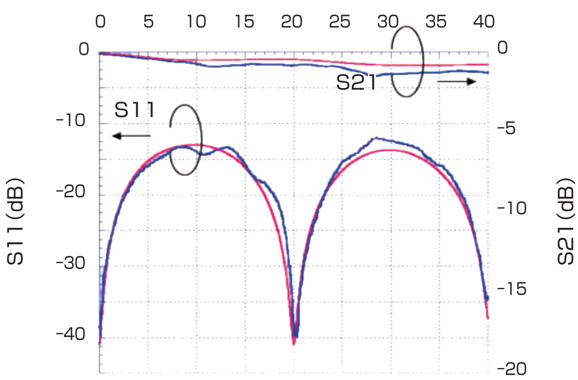

Fig. 9 High frequency transmission property of the formed wire
(<40 GHz; blue - actual value; pink - theoretical calculation value))

4.3 Overcoming the step structures

To check the possibility of formation to uneven surface and the control of the wet-spreading of ink on the rough-surface substrate with the laser-assisted inkjet technology, the wires were formed on a glass substrate ground in concave form with depth of about 200 µm. Figure 10 shows the electron microscope image of the wire pattern formed on the stepped, rough-surface substrate. When laser assistance was not used and the substrate surface was very rough, the formed pattern was spread out significantly due to the capillary force in the in-plane direction of the unevenness on the substrate surface. Conduction was not obtained when the wire resistance was measured on both ends of the grinding groove.

On the other hand, with laser assistance, there was no effect of the rough substrate surface, wire was formed having the same width in the stepped area, and conduction was obtained when the wire resistance was measured on both ends of the grinding groove. From these results, it was shown that the laser-assisted inkjet technology could be applied to the wire between the substrates with different wetness or lateral connection without using bump or fine through-via for the connection between IC chips.

4.4 Improvement of adhesiveness of the wire by rough-surface substrate

The wire was formed by the laser-assisted inkjet technology on the mirror-surface and rough-surface substrates, and the adhesiveness of the wire was checked by the peeling test using cellophane tape, as indicated by the peeling test for plating (JISH8504). Figure 11 shows the results of the tape peeling test on the mirror-surface and rough-surface substrates.

As a result, the wire on the mirror-surface substrate adhered to the tape, and the entire wiring peeled off the substrate. On the other hand, the wire on the rough-surface substrate did not peel off with the adhesiveness of the cellophane tape. From this result, it was indicated that the adhesiveness with the substrate could be increased if roughening treatment is applied to the substrate surface, due to the physical anchoring effect.

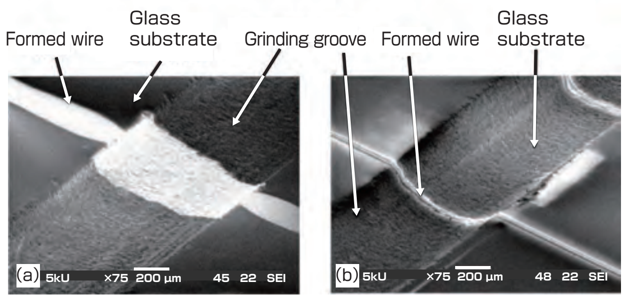

Fig. 10 Wiring on stepped structure and rough-surface substrate
(a) Without laser assistance (b) With laser assistance

However, the method for quantitatively measuring the adhesiveness of fine wiring with thickness and width of tens of μm has not been established, and new development is necessary to evaluate the adhesive strength of the wires.

5 Technological potential of the laser-assisted inkjet and its future prospect

In this paper, the possible solution to the problems that were considered difficult with conventional inkjet printing technology was indicated by using the laser-assisted inkjet technology in the wiring process for the diverse-type variable-volume production of electronic devices.

By setting and solving the technological issue of controlling the wet-spreading of ink, it was shown that the improvement of inkjet printing technology throughput and low wire resistance were possible. By controlling the wet-spreading of ink using the laser-assisted inkjet technology, the possibility of handling high frequency transmission needed for 3D mounting, wire formation on nonplanar substrate, and wire formation onto flexible substrate becomes a reality.

The positioning and possibility of the laser-assisted inkjet as a mounting technology are as follows:
(1) Achieving high frequency for the IC chip: fabrication of high frequency transmission line and good high frequency property at 1 GHz ~ 40 GHz
Possibility of high frequency transmission without shortening the distance of wiring between elements
(2) 3D wiring technology: capable of wiring onto uneven, stepped, and rough-surface substrate
Simplification of electric connection as well as flip chip mounting
(3) Durability of wiring: improved adhesiveness of the wiring
Applicability to the wiring of device that must be environment-resistant

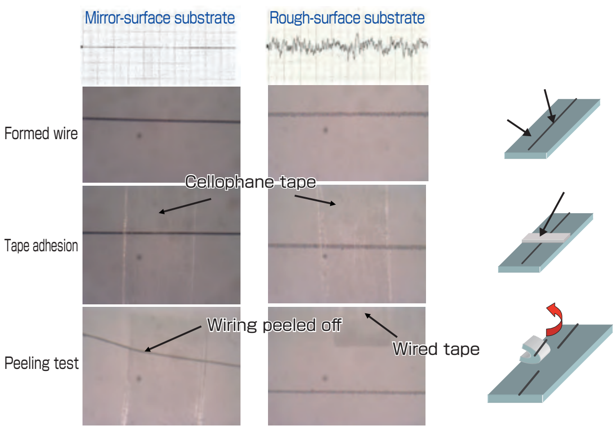

Fig. 11 Tape peeling test for wires on mirror-surface and rough-surface substrates

It is necessary to solve several other technological issues to establish this technology as a practical 3D mounting technology based on these results. It is also important to clarify the basic mechanism of the laser-assisted inkjet method and the phenomenon of gaining high aspect for the wire.

This means it is necessary to conduct a dual development into *Type 1 Basic Research* and *Product Realization Research*, using the *Type 2 Basic Research* as the entrance.

The principles of the mechanism by which wire with width less than the droplet diameter can be formed and the phenomenon by which high aspect ratio is obtained are not clarified, and to further improve the performance, the basic research to clarify the phenomena or *Type 1 Basic Research* is necessary.

On the other hand, to greatly minimize the time needed for practical application, the technological development for multiple functions and increased yield should be the central issue of the increased production efficiency, which is an area that is not a stronghold of the inkjet printing, and can be positioned as the *Product Realization Research*.

As the technological issue to improve the production efficiency, the advancement of multiple nozzle and post-annealing process technology are necessary. As technological issues of multiple functions, the development of functional ink, understanding of applicability of various substrate materials, and control of forming conditions are needed.

The technological development issues from *Type 1 Basic Research* to *Product Realization Research* become varied with the progress of R&D. Of course, there are limits in terms of human and monetary resources to engage in practical technology for a single research institute like AIST. It is mandatory to effectively appeal the technological concept of the results from the *Type 2 Basic Research*, and to continue the industry-academia-government collaboration to integrate the researchers and engineers of various fields.

Through such development of R&D, we wish to take the laser-assisted inkjet technology toward practical use and to establish it as the core technology of minimal manufacturing.

6 Summary and future prospect

This paper is a report of the R&D process of the laser-assisted inkjet technology, which is a development of the wiring technology using inkjet printing and has the potential to become the core technology for practical high-diversity variable-volume production. Comparison with other wiring technologies currently in practice, extraction of issues for high-diversity variable-volume production, selection of the solution method, and research results and positioning of the results are summarized. The issues that may become important in the future and the flow of the technological development are described.

In the future, we wish to develop additional multiple functions, to enable custom-made production that instantly provides function demanded by the user, to expand the market, and to create a new market for electronic device with new functions. By increasing the throughput of the laser-assisted inkjet technology, we plan to develop a technology that can handle devices with large surface areas that could not be handled with the conventional inkjet printing technology.

Acknowledgements

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References

[1] J. Akedo, S. Nakano, J. H. Park, S. Baba and K. Ashida: Aerosol deposition method - For production of high performance micro device with low cost and low energy consumption, *Synthesiology*, 1 (2), 130-138 (2008) (in Japanese) *Synthesiology English edition* 1 (2), 121-130(2008)).

[2] K. Suganuma and H. Tanaami: *Purinttedo Erekutoronikusu Gijutsu (Printed Electronics Technology)*, Kogyo Chosakai Publishing (2009) (in Japanese).

[3] J. Kolbe, A. Arp, F. Calderone, E. M. Meyer, W. Meyer, H. Schaefer and M. Stuve: Inkjettable conductive adhesive for use in microelectronics and microsystems technology, *Microelectronics Reliability*, 47, 331-334 (2007).

[4] New Energy and Industrial Technology Development Organization: *Seimitsu Buzai Seikeiyo Zairyo Sosei Kako Purosesu Gijutsu Ni Kansuru Chosa Seika Hokokusho (Report on the Survey of the Manufacturing and Processing Technology for Precision Member Forming Materials)*(2005) (in Japanese).

[5] H. Sirringhaus, T. Kawase, R. H. Friend, T. Shimoda, M. Inbasekaran, W. Wu and E. P. Woo: High-resolution inkjet printing of all-polymer transistor circuits, *Science*, 290 (5499), 2123-2126 (2000).

[6] P. J. Smith, D. Y. Shin, J. E. Stringer, B. Derby and N. Reis: Direct ink-jet printing and low temperature conversion of conductive silver patterns, *J. Mater. Sci.*, 41, 4153-4158 (2006).

[7] K. Takahashi: *Inkujetto Purinta No Oyo To Zairyo II (Application of Inkjet Printer and Material II)*, CMC Publishing (2007) (in Japanese).

[8] Konica Minolta Holdings, Inc.: Conducting film pattern and formation method of the conducting film pattern (Doden maku patan oyobi doden maku patan no keisei hoho), Patent Publication No. 2010-182775 (2009) (in Japanese).

[9] K. Morii and T. Shimoda: Film formation by inkjet: behavior of inkjet droplets, *Hyomen Kagaku (Journal of the Surface Science Society of Japan)*, 24 (2), 90-97 (2003) (in Japanese).

[10] K. Murata, J. Matsumoto, A. Tezuka, Y. Matsuba and H. Yokoyama: Super-fine ink-jet printing: toward the minimal manufacturing system, *Microsyst. Technol.*, 12, 2-7 (2005).

[11] R. D. Deegan, O. Bakajin, T. F. Dupont, G. Huber, S. R. Nagel and T. A. Witten: Capillary flow as the cause of ring stains from dried liquid drops, *Nature*, 389, 827- 829 (1997).

[12] P. C. Duineveld: The stability of ink-jet printed lines of liquid with zero receding contact angle on a homogeneous substrate, *J. Fluid Mechanics*, 477, 175-200 (2003).

Authors

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Discussions with Reviewers

1 Overall comment

Comment (Yasuo Hasegawa, Energy Technology Research Institute, AIST)

I think the developed technology is excellent, but to make this paper suitable for Synthesiology, please revise the following two points.

2 Clear statement of the technological issues

Comment (Yasuo Hasegawa)

For the titles of the subchapters, please revise them so the technological issues to be overcome can be readily seen.

Answer (Akito Endo)

In response to your comment, I revised the text so that the summary of the subchapters became the titles of the subchapters.

3 Solution to the ejecting frequency

Comment (Yasuo Hasegawa)

You indicate the issue of ejecting frequency, but can you describe how, after all, the authors solved the issue?

Answer (Akito Endo)

Until now, to reduce the width and the resistance of the formed wire, we reduced the size of the discharged droplet and reduced the ink supply per unit length, or in other words, we tried to increase the ejecting frequency of the inkjet. However, since we could increase the ink supply per unit length by forming the wire with small width using large droplets, we were able to solve the problem without greatly increasing the ejecting frequency.

4 Comparison with the conventional approaches

Comment (Yasuo Hasegawa)

For the conventional approaches compared with this research, please explain logically why those approaches were not appropriate, what kind of breakthroughs were necessary, and how you solved the problems. I think it will be easier to understand if you itemize the problems of high viscosity ink.

Answer (Akito Endo)

The following four methods are efforts to even out the wiring pattern and to reduce the wire resistance:

(1) Decrease resistivity of ink → limit of low resistivity

(2) Discharge high viscosity ink and reduce size of droplet → nozzle clogging and limit of ejecting frequency

(3) Formation of even pattern through surface treatment → reduced throughput by making the process complicated

(4) Increase drying speed by heating → breaks in wire due to bumping caused by rapid drying

1 and 2 greatly affect the narrowing of the wire width, and 3 and 4 the formation of even patterns. There were issues that were difficult to solve in using the inkjet as a practical process technology.

These four methods were not ways to deal with the essential issues of drying droplets in the process where the droplet discharged by the inkjet wet-spread at the moment it landed and dried. From the viewpoint of improving throughput, we set our topic as the control of wet-spreading of the droplet. As a result, we used the idea of locally applying the heat energy necessary for drying to the ink droplet by laser irradiation. This enabled the formation of wire with high aspect ratio with width smaller than the droplet diameter, without greatly increasing the ejecting frequency and with large droplet diameter, by optimizing the drying speed.

5 Size of droplet and value of the wire width

Comment (Yasuo Hasegawa)

Please indicate what were the droplet size and wire width in the conventional inkjet method. Since this is related to the development goal set in this research, please state them clearly.

Answer (Akito Endo)

The droplet size used in the conventional industrial inkjet method was about 15 μm (1.8 pl) ~ 40 μm (33.5 pl) in diameter. Therefore, the wire width was about 30 μm ~ 50 μm since it became larger than the droplet size, and the thickness was thought to be limited to several tens nm to several hundreds nm. When recoating was done several times to thicken the wire to about several μm, bulges occurred and formation of even wires was difficult.

6 Reason for setting the droplet size

Comment (Yasuo Hasegawa)

Please state clearly the logic of setting the droplet size. Did you decide on the droplet size after setting the target thickness from the target wire width and the target resistivity when it was formed?

Answer (Akito Endo)

In the conventional inkjet technology, the discharge of droplets of 10 μm or less was difficult. Therefore, the target values we set were wire width 10 μm or less and forming speed of several mm/sec to several tens mm/sec per nozzle. As technological issue needed to achieve the goal, it was necessary to form the wire width smaller than the droplet diameter. Therefore, we set the droplet diameter at 10 μm or more.

Formation of research strategy and synthetic research evaluation based on the strategy

— Toward research program evaluation as a creative activity —

Naoto Kobayashi[1]*, Osamu Nakamura[2] and Kenta Ooi[3]

[Translation from *Synthesiology*, Vol.4, No.1, p.11-25 (2011)]

Formation of research strategy, and synthetic research evaluation based on the proposed strategy have been considered. The importance of a setup of targets and a scenario of the research program to achieve the targets as a part of strategy formation, and the importance of research evaluation consistent with the research strategy are emphasized. Research evaluation should be performed in three aspects – the research progress, the research depth and the research phase. In the individual evaluation aspect, comparison of the research performance with the research strategy framework is essential and synthetic evaluation appropriately composed of deductive inference, inductive inference and abductive inference[Term 1] is recommended. To make the final integrated evaluation, the synthetic method is very crucial. Examples of research unit evaluation at AIST, and the research strategy formation and evaluation of public research organizations in Nagasaki prefecture are compared with the synthetic evaluation method. The method is thought to be a creative activity that can contribute to extract the value of research and accelerate the future evolution of research programs.

Keywords : Research strategy formation, research program construction, synthetic research evaluation, abductive inference, reflection and chain of evaluation, logic model

1 Introduction

In the 21st century, the environment where the earth and human community reside is subject to more pressure than in the 20th century. For the humankind to survive into the future, there are many issues to be solved by science and technology. Therefore, humankind needs a strategic approach in terms of how to promote science and technology. The evaluation of research and development (R&D) is extremely important when performing the R&D along a research strategy. Particularly, the evaluation must be performed to make the comparison with the research strategy, and to adequately present the significance and direction of the R&D being based on analysis and integration. Such research evaluation may spread further than the assumption made in the strategy, and has the potential of making the evaluation into a creative activity. Therefore, it is beneficial to propose a synthetic methodology for evaluation. It will be greatly useful if such evaluation method can be used to link the technology to an innovation.

As the social significance of R&D increases, the work on strategy is becoming active in various countries. The “Energy Innovation Hub”[Note 1][1] that shows the strategic direction of the R&D on future energy in the United States, the “Construction of the knowledge-based European Economic Society” at the Lisbon Strategy[Note 2][2], and the “New Growth Strategy” in Japan[Note3][3] are examples. However, the “research strategy study” that provides the academic foundation of research strategy has not been established, and that is a major issue of research and its evaluation.

In the past researches on research evaluation, the application of the “logic model”[Term 2] that indicates the logical sequence of input, output, outcome, and impact that were used for program evaluation for nearly 20 years has become active, and recently research on the method of performing evaluation according to the logic model has been conducted[4][5]. This has been effective as the evaluation method for research programs conducted through public grants in the United States and Canada, and is an excellent method because it clarifies the external logical structure that surrounds research. However, it does not evaluate the content of the research. On the other hand, peer review and bibliometric methods are available as means to evaluate the research itself. The former is a method in which the peers, or the experts of the research field, evaluate the contents and results of the research, while the latter is an evaluation through measurable values such as the number of papers, citations, or patents. In many cases these methods are combined to perform the actual evaluation[6][7]. However, research on the reaseach evaluation from the basic perspective of how to watch the research has not been so far sufficiently performed.

In this paper, we present the outline of the thoughts on how to synthesize research evaluation, starting from the perspective of properties of research, and the formation of research strategy and the logical construct of the elements

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related to the research evaluation based on such strategy. Particularly, the "synthetic research evaluation" is important in evaluating the essence of research and in advancing the research, regardless of whether a research is basic or applied, or analytic or synthetic.

2 Properties of research

Research is thought to possess "intrinsic properties". These properties include: 1) novelty, 2) originality, 3) logical completeness, and 4) influence. 1) Novelty is to add new academic findings not limited to a certain academic field, and 2) originality is that the research itself provides unique findings and introduces new theses. Research that gives totally new explanation to a known phenomenon may be low in novelty but is high in originality. 3) Logical completeness means that the research is a complete expression upon accumulation of solid logic. 4) Influence expresses the strength of the effect to the external field. It includes influences that affect the discipline itself, and those that affect other disciplines (these are effects on the academic field); and the influences that affect society. The latter influence will be called "practical properties".

The *Type 1 Basic Research*[Term 3] proposed by Yoshikawa is basic research that produces new knowledge in a certain discipline, and the influence is mainly contained within the discipline. *Type 2 Basic Research* (and the *Product Realization Research*) is research with practical properties that affect society, but both can be discussed within the same intrinsic property[8][9]. However, these two types of basic researches are not always clearly separated, and the elements of both can be found within a research project. Also, there is research where the influence of the intrinsic properties may stay within a discipline for a short period, but may become socially influential after some time. For example, it is well known that the various spatial and temporal compensations are done in devices that receive signals from the GPS (Global Positioning System) satellites, and this is based on the theories of special and general theory of relativity presented by Albert Einstein at the beginning of the 20th century.

3 Research strategy and research program

3.1 Significance of the research strategy and its formation

By defining strategy as a "way in which an objective is set; various elements such as people, resource, time, and information are allotted appropriately; and these are organically combined and activated in order to make the whole system function properly", the research strategy can be defined as "the strategy deployed to set and achieve the objective of research and its influence".

In forming the research strategy, it is desirable to set the specific research program for achieving the goal of the strategy, as well as the targets, scenario to attain the targets, and the targets for the individual research project that comprise the research program. The research program, according to Hirasawa, can be defined as "the unit of execution, development, and management of the policy that is structuralized and logically constructed, linking the policy and the research project[6]". Here, a research program will be defined widely as the "unit of research development that is structuralized and logically constructed to link the objective of the research strategy and the research project". Therefore, the research program may be also applied in the *Type 1 Basic Research* such as the experimental elementary particle study.

To what extent the targets and the scenario of the research program are set must be agreed upon by the research promotion group and the research sponsor (state or society in case of public research), and a preliminary contract should be signed. It is also important to incorporate a review process of the research strategy during the progress of the research program.

Also, assuming unforeseen circumstances that may occur in the research progress, some degree of redundancy should be included in the contract. The scenario must include several options and flexibility in schedule. Even in *Type 1 Basic Research* that is research within a discipline, for example, the research strategy can be formed and the potentials of the results may be cosmic and the influences may last for a long term. Even if a result different from the major assumption is obtained, the value of the research strategy will be determined based on how much it contributed in increasing the scientific knowledge of the discipline.

One example is given. The main objective of the Kamiokande, for which Dr. Masatoshi Koshiba received the Noble Prize in Physics in 2002, was to prove the proton decay by detecting the collision of the neutrinos that were released in proton decay. However, Koshiba *et al.* fortuitously detected, for the first time in the world, the neutrino produced by the supernova explosion that occurred in the Large Magellanic Cloud with the Kamiokande in February 1987. This demonstrated the correctness of the theoretical model of supernova explosion, and the era of neutrino astronomy started. While Koshiba had initially indicated the possibility of observing the neutrinos from space, the proton decay has not been observed even in the succeeding Super Kamiokande. As this example indicates, it is normal in science that an expected result is not necessarily obtained. However, the research strategy, in which a neutrino detector was made with a tank with 3,000 ton of pure water and 1,000 photomultiplier tubes under the Kamioka Mine, turned out to be very significant because it added new knowledge to physics[10].

In forming the research strategy, it is necessary to organize the crucial issues structurally into global issues that affect the wide-ranging field over long-term, social or domain issues that are mid-term issues for a nation, region, or an academic discipline, and the research programs that are conducted in relatively short-term in some specific field.

An example of the global issues is the “realization of a society with sustainable development”. It is possible to consider a layer structure containing various issues within this subject. Four issues of sustainability – “environment, energy, and natural resource”, “human, organism, and food”, “society, economy, and industry”, and “information, culture, and education” – are identified as shown in Fig. 1. In these layers, the subject of sustainability changes from natural to artificial as it moves from the lower to the upper layer. The items in the lower layers need urgent attention, but an integrated effort must be made to cover all layers in the national, social, and international policies.

What is important in forming the research strategy is to clarify the individual social issues that are reflected in the real world, to define and to break them down into research programs and individual research projects, and then to visualize their relationships. Figure 2 shows an example. The four points of sustainability are given as global issues, and the examples of related social issues and research programs are also shown. This method is a top-down or deductive method. The reason why it is called “deductive” is because the items that are assumptions of the strategy, such as the preservation of environment (realization of low-carbon society) in the context of the aforementioned sustainable society, can be deployed by the social agreement. However, complete deductive inference is not possible, and abduction[11]-[13] will always be in action[Note 4].

On the other hand, in the formation of the research strategy, there is also the bottom-up strategy formation from experience, findings, and future vision of the researchers in the specific research field. For example, if it is possible to develop optical switch devices with ultra-low energy consumption, and an optical path communication network using these devices, the power consumption of the current Internet can be reduced by three orders, and a scenario that can make a great contribution to the realization of a low-carbon society can be written[14]. While this is one of the elemental technologies, the research program can be based on the realization of a group of elemental technologies. Although this can be called the inductive strategic formation where the main proposition is formed from the individual facts and certain logical inferences, this also includes the inference by abduction. That is because several hypotheses are necessary to create a specific system by bundling the current technologies. The abductive research strategy formation is necessary as the juncture of deductive top-down synthesis and inductive bottom-up synthesis.

3.2 Synthesis of the research program

For the synthesis of the research program, it is necessary to consider on which domain the center of the research should be set within the academic framework. To solve the global and human issues (for example, industrial development and environment), it is impossible to rely on a single discipline, and we must muster knowledge of various fields including those of humanities and social sciences. Therefore, the domain will have a wide research field. In setting the research program, it is necessary to indicate the target of the research program set by the research strategy and the specific scenario to achieve the target. A roadmap is such a presentation along with the milestones that should be achieved along the time axis. It is necessary to set the individual research projects that comprise the research program α, as shown in Fig. 3. In this case, the program is composed of a group of research projects (A, B, and C) that are topics of the several research domains.

4 Structure of the research evaluation

4.1 On research evaluation

In considering the research evaluation, ideally it should help the researchers and the research advancement, and, on the other hand, it should be used as an effective method to obtain

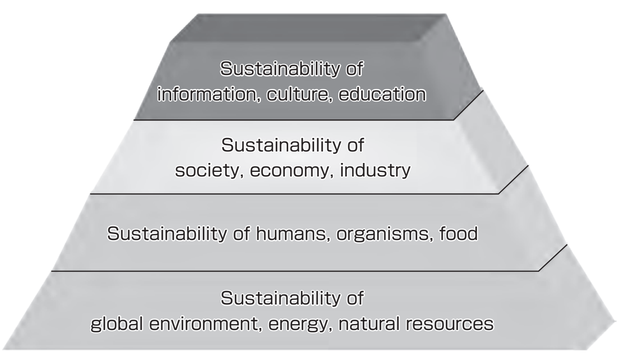

Fig. 1 Layer structure of sustainable development

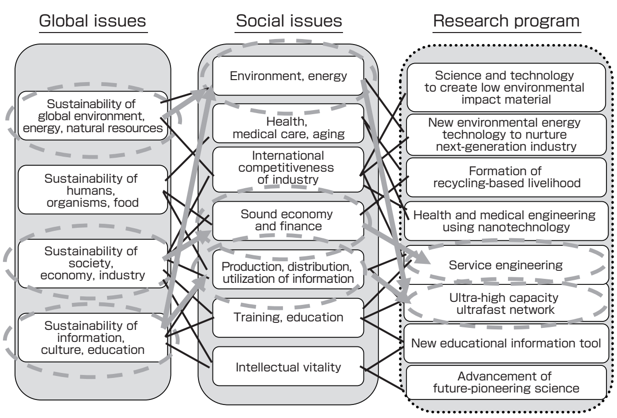

Fig. 2 Example of strategy formation

the understanding and cooperation of society, by making the "value" of the research visible in society even if it is basic research. The research evaluation should be performed based on the following way of thinking.

(1) As the basic thinking of the research evaluation method: 1) whether it is basic research, applied research, or experimental development[Term 4 [15]] or *Type 1 Basic Research*, *Type 2 Basic Research*, or *Product Realization Research*[8][9], the research and the evaluation should be done under one integrated way of thinking; 2) the research evaluation should be based on a contract [in which the purpose of the research is written as the strategy and scenario and shared by the parties (research fund provider, research group, and research evaluator), and the evaluation should be performed accordingly]; and 3) the evaluator and the evaluated should cooperate on the same plane. Also, (2) the aim of the research evaluation should be: 1) to bring out the value of the research; 2) to push the research forward; 3) to be the source of motivation for the researchers and their group; and 4) to be accountable to the sponsors and stakeholders.

The following is an explanation of the "synthetic evaluation", after due consideration of the characteristic of the research evaluation. The "synthetic evaluation" can be defined as the evaluation method that synthesizes the comprehensive evaluation of the research by clarifying the properties of the various aspects of research evaluation (this is called elemental evaluation) and by clearly positioning their relationship structurally. For the methods of research evaluation, refer to the comprehensively written article by Ohtani[16].

4.2 Research program/project and its evaluation

For the evaluation of R&D, it is necessary to understand the characteristics of the evaluation at each stage of the research. The main ones are: 1) appraisal, 2) process evaluation, 3) output evaluation, 4) program evaluation, and 5) outcome evaluation. Figure 4 shows what kind of evaluation and feedback are done in the series of R&D processes based on the strategy, from the strategy formation, construction/execution of program, creation of output, achievement of program, and creation of direct outcome. This series of processes is almost the same as the program evaluation method known as the ROAMEF[Term 5 [6][16]].

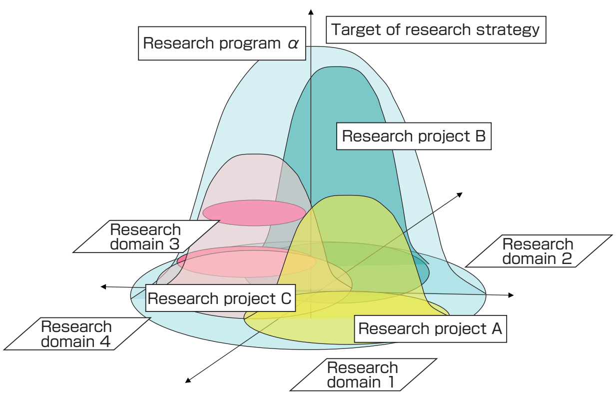

Fig. 3 Research projects that comprise the research program and their properties

In performing the research evaluation, the appraisal based on foresight is particularly important. In the appraisal, the adequacy of the research development scenario and the research program based on the strategy, the plan and content of each research project in accordance with the research program, and the system, resource, time, place and others for the execution are considered carefully. Particularly, it is important to clarify the aim of the research program, and to clarify the dynamic relationship among the plans, resources, expected outputs of several research projects included in the research program, and how the individual research projects interact with each other (sharing and utilization of the project results).

For the appraisal, it is necessary to perform an inductive and abductive evaluation to determine the strategy along a highly probable inference. One example is, when creating a research strategy for reduced greenhouse gas, low-cost production, and high export competitiveness by developing a new technology using a certain organic material. While it can be inductively estimated that the potential for realization is high, judging from the current material and device performance, there is a counterargument that the durability is an issue. Then, it is possible to perform the appraisal of the strategy based on the inference of the hypothesis that the durability can be dramatically improved by developing a technology to avoid contact with moisture and oxygen.

On the other hand, the flexibility of the scenario to respond appropriately to the changes in the situation will be important. However, achieving both the strictness and flexibility of the strategy and scenario may not be easy, and how to embed such flexibility is one of the issues.

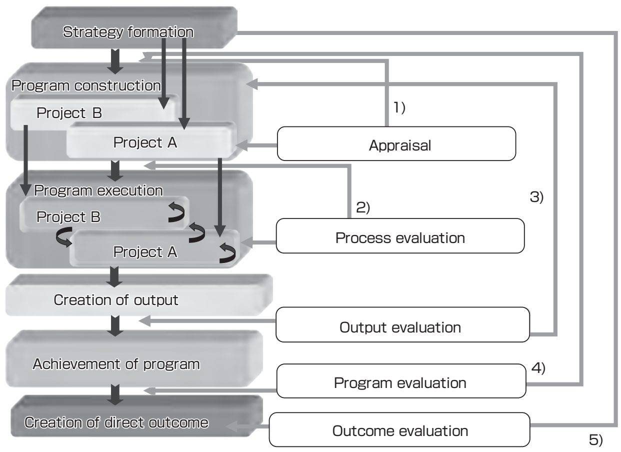

Fig. 4 Evaluation during the process from strategy formation to outcome

In the process evaluation, it is necessary to have a dynamic response such as feedback where the correction is made if there are problems and the recommendation to collaborate with other projects, along with checking the progress of the individual project. In the output evaluation, how the results obtained by the achievement of the program compare with the initial program target is checked. Here, the peer review that will be explained later is important in the *Type 1 Basic Research*, while the evaluation by the experts and stakeholders will be important when the main topic is social effect.

In program evaluation, the target of the research program set in the strategy and the execution of the scenario are investigated. In direct outcome evaluation, the direct outcome produced when the output of the research program is handed to the external party is compared with the target of the strategy. However, the creation of the direct outcome normally takes time after the completion of the program.

The feedback loop (FBL) is important in the evaluation process. In the FBL1, the issues extracted in the appraisals are fed back and reflected in the program construction. FBL2 is one of the PDCA (plan-do-check-act) cycles[Term 6] at the project level during the program execution. Here, the progress check at the individual project level is reflected in the course adjustment of the project and review of the invested resource. FBL3 and 4 are loops where the contents of the program evaluation and the output evaluation are reflected in the program formation in the next step. FBL5 is the process that uses the direct outcome evaluation in the adjustment of the research strategy and the formation of new strategies.

The research project has a simpler structure or function compared to the research program. Therefore, the research objectives, methods, results, and the expected outcomes are bound within a small range, and the above evaluation process can be applied since they possess a fractal structure upon the research program. However, the research project is positioned as an element of the research program, and the appraisal can be simplified.

4.3 Synthetic research evaluation and its application

4.3.1 Overview diagram

Figure 5 shows the overview diagram of research and evaluation for the execution of the research program based on the research strategy formulation. First, the research evaluation is considered analytically by breaking it down into elemental evaluations.

The X-axis is time that shows the progress of the research. Here, the process from program building to output creation will be simplified, and a research program will be composed of three blocks of plan, process, and results. The evaluation along this line mainly determines whether the research progressed according to the process assumed by the strategy, in terms of plan, process, and results. Here, the evaluation will certainly be on the content of the research, but even more so on whether management was done for the effective progress of the research. Not only is it necessary to deductively determine along the rule of the agreed strategy, but it is also necessary to conduct evaluation that encourages various trials and devising. The appropriate evaluators in this case will be the peers and experts with experience in research progress, and it is particularly desirable to have someone experienced as a research program leader.

The Y-axis shows the depth of research. The depth of research in terms of results means the quality of 1) novelty, 2) originality, 3) logical completeness, and 4) influence, which are the four properties of research explained in chapter 2. For the plan and process, they are the density and the vastness of the prospect of the plan for which high expectation is expected and the progress of the research that may lead to important results. Here, the evaluators must be peers in the same discipline or in multiple disciplines. Different evaluators are needed for each step for the Z-axis (phase) that will be explained below. In the case of the pure basic research phase, a good evaluator is a peer within the same discipline, but as the phase approaches the outlet to society, experts of industry and journalism will be necessary. The influence will be the scale of social effect and the potential for having such effect.

The Z-axis shows the phase of research. Phase is an index that shows where the research is positioned from the basic research to the social exit. For example, the research can be categorized into basic research, applied research, and experimental development[15], or can be categorized as the aforementioned *Type 1 Basic Research*, *Type 2 Basic Research*, and *Product Realization Research*. The evaluator must have knowledge about the content of the research and the significance of the strategy for each phase, and must be able to consider the potential for realizing the outcome. With the evaluation of this axis the results alone are not evaluated, but the results and the processes for arriving there, as well as the road to utilization of the results expected in the future are

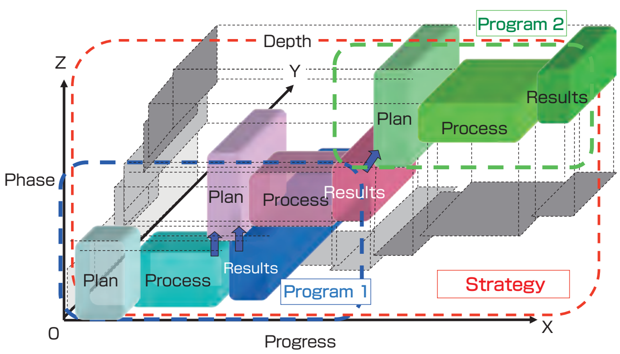

Fig. 5 Overview diagram of the synthetic research evaluation along with strategy formation and research program execution

also evaluated. In that sense, the basis of evaluation would be the targets and scenario set down in the strategy and the roadmap that specify them, and the evaluation would be the significance of the results in each phase (*Type 1 Basic Research*, *Type 2 Basic Research*, and *Product Realization Research*). In the case where the influence of the result stays within one or several disciplines, the influence is in the lowest level of the Z-axis. In this case, it is evaluated according to the depth axis by the peers. In summary, this overview shows the axes of the elemental evaluations, and the relationships of various elemental values in the synthetic evaluation are positioned structurally.

On the other hand, the positioning of the research becomes clear by applying the mode of the R&D. Figure 6 shows the phase-time-space arrangement composed of the XYZ axes of R&D. To synthetically link the evaluation of each axis to the final evaluation, it is necessary to refer to the primary strategy. In the formation stage of the strategy, it is important to clearly state which part of the phase-time-space the result was intended to cover. The three-dimensional structure shown as the transparent block in Fig. 6 is the estimate diagram of the result of research program considered in the strategy. This estimate is obtained as a result of the deductive, inductive, and abductive inferences as mentioned before. On the other hand, in the same diagram, the solid blocks in various colors indicate the actual results of research. The comparison between the transparent and the solid blocks can be linked to the final evaluation.

4.3.2 Actual practice of synthetic research evaluation

The evaluation at the individual evaluation axis is conducted through comparison with the target and scenario indicated by the strategy for that axis. For the progress evaluation at the X-axis, the evaluation index will be how the progress of the research matches or departs from the schedule intended and planned strategically. For example, if there is a departure from the plan within the expected time schedule, and if acceleration is necessary through the “selection and concentration” of research resources or by narrowing down the product through management, the abductive process

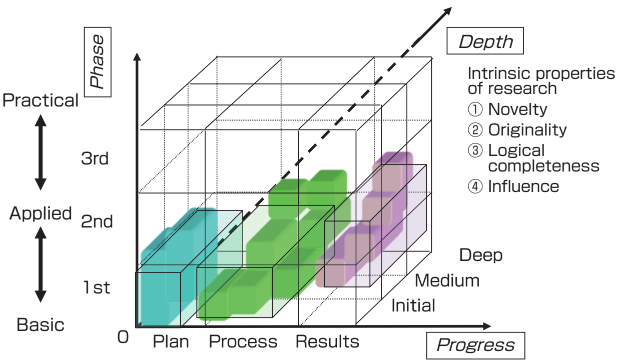

Fig. 6 Conceptual diagram of the research evaluation synthesis

is required in the sense that the effects must be estimated abductively.

For the depth of research in the Y-axis, the intrinsic properties of the research are evaluated, while the inductive decision based on the knowledge and experience of the peers plays a major role for the individual elements. In general, the “excellence” of the research will be determined, and abductive inference is necessary. Of the intrinsic properties of the research, novelty, originality, and logical completeness can be evaluated fairly objectively by peers, while the influence of the research depends largely on the evaluator’s abductive inference or imagination. This is because the evaluation of the intrinsic value of research is determined only after the evaluator performs the abductive inference including thinking about the influence.

In many cases of research, serendipity or unforeseen results may play a major role. This is not foreseen in the strategic plan, and it is extremely high in 1) novelty and 4) influence, among the four properties of research stated in chapter 2. The evaluation of such results may be high as they often surpass the planned range in terms of the depth of research.

For the evaluation axis of the research phase in the Z-axis, the evaluation index will be the social effect (in case of *Type 1 Basic Research*, it is the impact in the academic field, and this overlaps with the Y-axis evaluation), and further abductive inference and evaluation are necessary. That is because the social influence requires values that are accepted by society in addition to the intrinsic values of the science and technology research. It can be said that for this determination, there are more abductive elements than in the evaluation of progress (X-axis) or depth (Y-axis) of the research.

For the overall synthetic evaluation, it is necessary to comprehensively understand the elemental evaluations as mentioned above, and then synthesize the integrated evaluation. In that case, as mentioned earlier, the deductive inference that depends on the logical conclusion, the inductive inference that derives the conclusion from several specific examples, as well as abduction must be utilized, and the combination of the inferences to investigate the potential of the value of the results is important.

4.3.3 Integrated research evaluation

In conducting the synthetic evaluation, it is important for the research promoting group and the evaluators, to consider the property of research, share common understanding of the strategy and result index including the goal to be achieved, engage in deep discussion on the results and how the research should progress, check the target indicated in the strategy and distance from the actual results, and finally abductively discuss and investigate the significance and the effect of the research program execution. This entire process can be considered the "research evaluation = abduction and its expression". This is closely related to the research that is a creative activity, and research evaluation can be considered to be part of this creative endeavor.

To apply the synthetic evaluation to actual evaluation, some devising is necessary. This must be designed upon agreement by the three parties consisting of the research promotion group, research fund provider, and the research evaluator. While the proposal of the paper was not directly applied, a general evaluation was conducted in the example of "Evaluation from the viewpoint of outcome" that was conducted during the Second Mid-term Research Goal Period (FY 2005~2009) at AIST, by introducing the elemental evaluation of management evaluation, output evaluation, and roadmap evaluation that could be thought to be related to progress (X-axis), depth (Y-axis), and phase (Z-axis)[17]. However, it was not necessarily an elemental evaluation by comparison with the strategy as proposed in this paper. There was a lack of deep discussion with the evaluators, and it was still in a developing stage as a synthetic research evaluation. Specifically, it is necessary to design a general evaluation system including the incorporation of the constructive, deep discussion between the research promotion group and the evaluators, in addition to the elemental evaluation and appropriate synthesis.

5 Example of the synthetic research evaluation

5.1 Characteristics and issues of the research evaluation at AIST

5.1.1 Evaluation from the viewpoint of outcome

In the Second Mid-term Research Goal Period (FY 2005~2009) at AIST, "Evaluation from the viewpoint of outcome" was performed upon proposal of the Research Evaluation Investigation Committee (Chairman Rei Hirasawa) in 2004, to focus on the perspective of contribution of the R&D activities to industry and society[17]. In the process of design, 1) the roadmap evaluation, 2) the output evaluation, and 3) the management evaluation were set as the three items of elemental evaluation. The major part of the synthetic evaluation of this paper is the idea based on this experience. As written in chapter 4, 1) the roadmap evaluation corresponds to the Z-axis (phase) evaluation, 2) the output evaluation to the Y-axis (depth) evaluation, and 3) the management evaluation to the X-axis (progress) evaluation. Figures 7 shows the example of the input, output, outcome, and impact in the R&D at AIST as shown as the logic model related to research strategy formation.

The research strategy at AIST is formed from both the top-down and the bottom-up viewpoints, as already mentioned[18]. The outcome is defined at the research unit considering the relationship with the strategy. Looking at the work at AIST from the viewpoint of outcome, of course, the main work is the R&D activity for the creation of advanced knowledge and technology, but the activity for outcome creation by providing the results to the external parties can also be positioned as important work. At AIST, the latter is called the innovation hub function[19], and an innovation hub strategy is established with the research strategy.

5.1.2 Specific examples

At AIST, the target to be achieved as the result of strategy formation is separated into seven items, and the R&D is conducted systematically by breaking down each target into the strategy target, strategic issues, and priority issues. The process from the strategic targets to the research unit issues is designed in a top-down style based on the external environmental factors such as the social demand and marketability, and on the internal factors such as the technological portfolio and strength of the core technology. On the other hand, the results expected from the R&D are designed in a bottom-up style, looking at the process from output to outcome in the R&D from the individual research issues.

As a specific example, the "Research of biomarkers for brain cell functional molecules", a topic of the Neuroscience Research Institute, AIST is explained. This research is characterized by the clarification of the molecular behavior of the ion channel, receptor, and intercellular cell-signaling molecules in neurological diseases, and the search and identification of the biomarkers that specifically recognize the functional proteins. The roadmap for this topic is shown in Fig. 8. The roadmap shows the chronological development of the technologies from the R&D conducted at AIST (search of the marker, functional evaluation, and sensing core technology), to the development of the diagnostic and prevention system of the cerebral disease (development of sensor, cerebral disease risk diagnosis technology) through collaboration with companies.

The Evaluation Committee of the Research Unit is composed of external members (about five people) from universities,

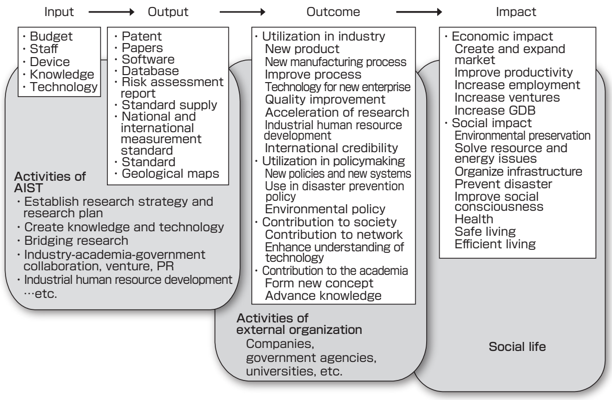

Fig. 7 Model of R&D and result diffusion at AIST

industries, and journalism, and internal members (about two chief evaluation officers from the Evaluation Department), to evaluate the roadmap and output, and the adequacy and appropriateness of the management. At the Evaluation Committee of FY 2008 (the fourth year of the five-year Second Mid-term Research Goal Period), there were positive comments for the roadmap such as "clear" and "shows advantages", and the research plan was judged to be appropriate. However, some members requested "clarification of the positioning in the overall roadmap" and "clarification of the milestone"[20]. For output, "discovery of new peptide through original molecular evolution technology", "results for the unique bioactive peptides such as ant and spider toxins", and "development of signaling substance receptor ligand sensor" were highly evaluated as new technologies that could be utilized for clinical application and as analysis tools for neurological function.

As other examples, the heads of research units including the Nanoarchitectonics Research Center and the Correlated Electron Research Center have reported that they obtained beneficial indications and guidance for the research unit activities from the evaluation from the viewpoint of outcome. The details are described in Reference [21]. In the former case, a clear scenario was written by focusing on the viewpoint of outcome, and the opinions of the evaluation committee members helped establish the strategic R&D plan. In the latter case, the task of forming a roadmap in *Type 1 Basic Research* helped to build the logical framework for the research progress, and it was deemed appropriate to set the "construction of new theory" as one of the outcomes. More beneficial results are expected through synthetic research evaluation in the future.

5.1.3 Phase evolution of the R&D and reflection of the synthetic research evaluation

Figure 9 shows the modeling of the above case from the perspective of phase evolution of the R&D. In practice, the R&Ds with different phases such as the "search of biomarker", "sensor development", and "application to diagnostic technology" progressed concurrently at different temporal development. The R&D topics can be modeled as the cycle of "accumulation of knowledge", "accumulation of elemental technologies", and "accumulation of product realization technology". The key technology linked the R&Ds of different phases, and the quality of this technology greatly influenced the level of R&Ds that developed in the new phase. For the movement between the phases, the fusion of technology through collaboration with the external parties (external knowledge, elemental technology, use of product realization technology, etc.) became the important management items in outcome creation.

In the evaluation from the viewpoint of outcome, it is necessary to aptly grasp the overall picture of the R&D and the result, and to have an integrated evaluation of the results with different qualities. It is also important to perform evaluation from the perspective of the adequacy and effectiveness of the overall composition of the R&D, as well as the effectiveness of the management to smoothly turn the R&D cycle of different phases.

In the evaluation at AIST as shown above, the synthetic research evaluation is being employed as a result, but there are still issues in the research evaluation based on the research strategy which is one of the major characteristics. Particularly, to evaluate the R&Ds at AIST in general, it is necessary to have a fine formation of the research strategy and the synthetic evaluation based on the comparison with the strategy. The issues that must be solved include: 1) the clarification of the final goal of the research strategy and the scenario to get to the goal, and the clarification and the evaluation axis (XYZ axes) based on the comparison; 2) the matching of the evaluation from the bottom-up perspective (inductive evaluation from the viewpoint of outcome for the result) and the evaluation from the top-down perspective (setting of the topic from target to the issue and the deductive evaluation of the roadmap); 3) the clarification of the correlation between the different phases; and 4) the clarification of the evaluation method on the phase axis (Z-axis) considering the characteristics of the research (such as basic, industrial application, policy, etc.). These are related

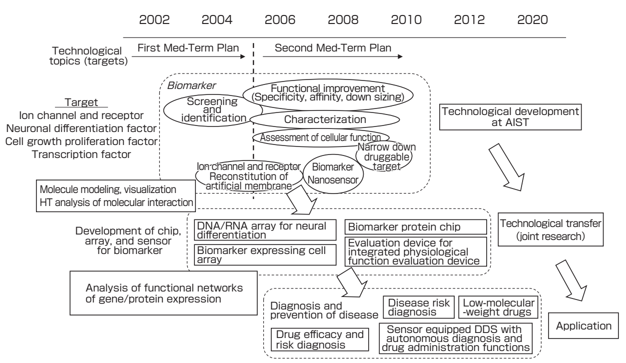

Fig. 8 Roadmap for the research of biomarker for brain cell functional molecule

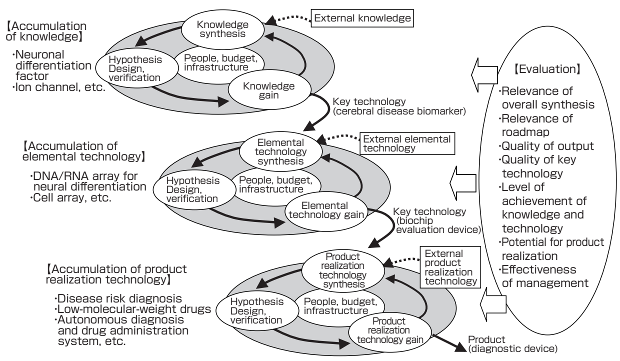

Fig. 9 Phase evolution of R&D and reflection of synthetic evaluation

to the issues of research strategy formation, composition and execution of the research program, and the elemental and synthetic evaluations, described above, and they should be fine-tuned for the evaluation of the research units for the Third Term[22].

5.2 Example of Nagasaki prefecture- Strategy formation and evaluation of the promotion of science and technology for local revitalization

5.2.1 Strategic vision and logic model

The public research institutes in the local government play a role in the important missions to promote the regional industry, and have unique issues as well as common issues shared with the R&D conducted by the government, universities, and companies. Here, an example of the research strategy formation and evaluation of the public R&D of the Nagasaki Prefectural Government, in which one of the authors (*i.e.* Nakamura) was involved, will be presented.

The companies and product districts of Nagasaki suffer from various issues such as population decline and low income. As the recovery from the global economic crisis triggered by the Lehman Shock in 2008 is slow, it is necessary to utilize the unique local resources unseen elsewhere to win the fierce competition and to build a sustainable society. Therefore, it is mandatory that the research institutes quickly capture the social needs, and consider them in the selection of the R&D topics. To do so, it is necessary to build strategic visions, set the clear goals, and to write the scenario for achieving them. Here, the case of promotion of strategic R&D[23] applying the logic model[4] will be introduced. The main point to employ the logic model is to set the strategic R&D in order to produce the results that can be accepted by the customers. The strategic R&D scenario to create the outcome must be completed through the series of tasks mentioned above[24].

5.2.2 Mission and strategy formation of the Science and Technology Promotion Bureau of Nagasaki Prefectural Government[25]

(1) The role of prefectural research institutes

The Science and Technology Promotion Bureau of Nagasaki Prefectural Government is an organization that governs the five research institutes: Institute for Environmental Research and Public Health, Industrial Technology Center, Ceramic Research Center, Institute of Fisheries, and the Agricultural and Forestry Technical Development Center[26]. The missions of the Promotion Bureau are 1) to nurture competitive and strong industry, and 2) to realize a safe and comfortable life through the application of science and technology, hence to build an energetic Nagasaki prefecture where people can live with dreams for the future. To do so, as the long-term outcome, the creation and aggregation of new industries in Nagasaki through the changes in the industrial structure are necessary. As elements, it is necessary to develop policies to create new businesses and new industries, strengthen the existing industries by utilizing the local resources, increase productivity of the prefectural industries, and expand employment. As the mid-term outcome, the current companies must take one step forward to advance into new fields, develop original products, establish the brand, and increase shares. As the short-term outcome, the companies must increase technological prowess, save energy and cost, and increase ability in marketing and design. The prefectural research institutes must collaborate with the universities and others to advance and increase precision of the core technologies, engage in R&D and technological supports for systemization, as well as provide technological development through interdisciplinary researches, marketing and design supports and others according to the needs of enterprises. The above items were organized through the logic model (Fig. 10) and this was shared with the related departments.

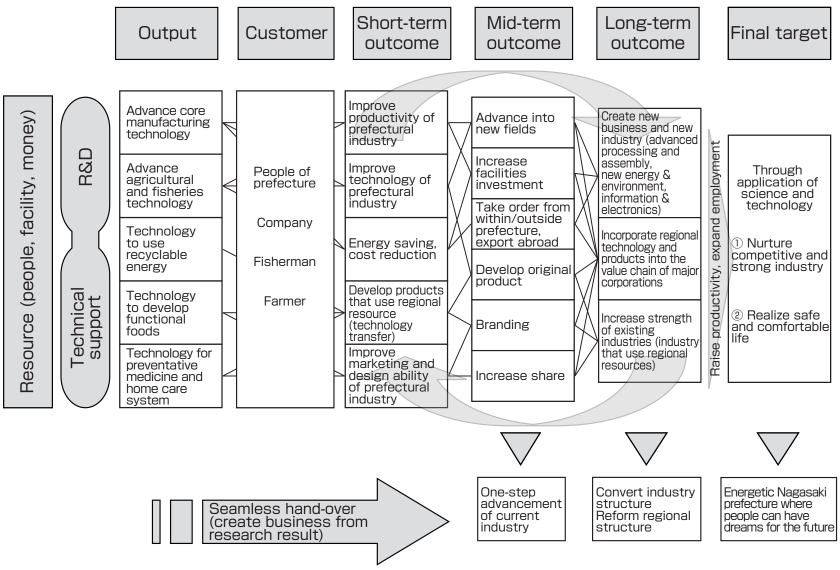

Fig. 10 Logic model for establishing how a research institute should function
(created by the Science and Technology Promotion Division, Nagasaki prefecture)

Using this diagram as the template, the application to the strategy formation at the Ceramics Research Center[27] will be explained below.

(2) Strategy formation at the Ceramics Research Center

The Ceramics Research Center of Nagasaki was established in Hasami-cho, Higashi-Sonogi-gun in 1930. Its mission is the development and promotion of the ceramics industry in Nagasaki. The Center works on the R&D of new materials and recycling of waste, the product development of new fields through fusion with new technology, and the advancement of the core manufacturing technology to support the ceramics industry. Of the logic models organized for the industrial supports of the ceramics field, inorganic material field, and the design field, the diagram for the ceramics field is shown (Fig. 11). In this logic model, the “Development of ceramics core technology and new products” is one program, and the research topics for individual output (for example, “technology for developing a new light-weight porcelain body”) correspond to the individual research projects. The mid- to long-term outcome corresponds to the mid- to long-term strategy.

The missions of the Ceramics Research Institute is the vitalization of the ceramics industry, and sets the mid- to long-term outcome to increase the brand power, to pioneer new markets through ceramic products with new functions, and to obtain domestic shares that beat the other product districts in the competition. As the short-term outcome, it is necessary to reduce production cost, develop high quality and high-value added products, develop new fields, develop products in response to changing lifestyles, and provide advanced supports. Figure 11 is a detailed summary that shows what is demanded as R&D outputs to be handed over to the customers in order to gain the short-term outcome. To produce such outputs, it is necessary to engage in the strategic R&D to develop the ceramics core technologies and new products, and to provide technological supports matching with the production sites.

5.2.3 Reflection of the research enterprise evaluation[28] and future issues

For the research enterprise evaluation at Nagasaki, the strategy formation for which the necessity is stated in this paper is just beginning, and the introduction of the thoughts of synthetic research evaluation is a future issue. Currently, the research enterprise evaluation by external committee members is conducted by the ordinance, to ensure researches that reflect the needs of the people and industry of Nagasaki with close observation of the market. This is also utilized for changing the thinking of the prefectural workers. As the evaluation scheme, for the individual research conducted by the research institutes of Nagasaki, the appraisal, interim, and ex-post evaluations are performed from the perspective of necessity, efficiency, and efficacy. The evaluation is done by the Research Evaluation Subcommittee (six external evaluators) set for each research institute, and the Research Enterprise Evaluation Committee (eight external evaluators) engage in the meta-evaluation (or evaluation of the evaluation itself) as the parent committee based on the reports from the subcommittees. In FY 2009, the logic model was started to be used to create an overview diagram of all projects handled by the research institutes. The positioning of each project based on the mission of each research institute, and the scenario of how the research result is handed over to the customers to form the outcome are clarified, whether the projects are progressing appropriately along the overall projects of the research institute are explained, and definite evaluations are obtained.

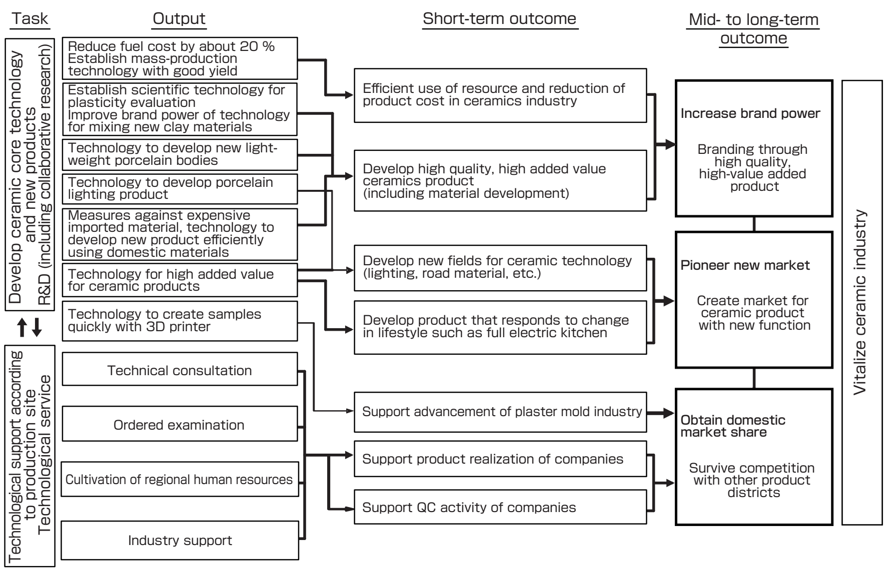

Fig. 11 Logic model for the strategy formation of the Ceramic Research Center
(created by the Ceramic Research Center of Nagasaki)

The evaluation results of the Research Enterprise Evaluation Committee are fed back to the research institutes and used to improve the projects, and are utilized in the discussions for the management of the specific policies indicated in the "Visions of the Promotion of Science and Technology in Nagasaki", proposal of new policies for the promotion of science and technology, and the proposal of strategic promotion fields.

Excavating the hidden needs from wide-ranging fields and creating new technologies that the market needs will lead to long-term and continued economic effects, and may lead to more expansion of job opportunities. For this purpose, it is necessary to maintain strong collaboration with the related departments, and to engage in interdisciplinary strategic R&D by drawing a scenario to achieve the goal. To organize the role and the future image of the R&D and technological supports by the research institutes, it is necessary to optimize the synthesis of the R&D to be undertaken by the research institutes as programs, and to continue the synthetic research evaluation from the perspective of whether the programs are based on a long-term strategy.

6 Reflection and linkage of the synthetic evaluation

One of the greatest responsibilities of the synthetic research evaluation based on the strategy formation is the reflection of the evaluation results. At AIST, the research unit evaluation is performed every two years as mentioned before, and the evaluations are performed for the purpose of (1) encouragement of research in the research units, (2) feedback to the management of AIST, and (3) execution of accountability to external and internal sectors. It is important that the evaluation results are reflected effectively.

Particularly in reflecting the appraisal, the evaluation must be utilized for the optimization of the resources, environment, and conditions necessary for the R&D when establishing research units and starting projects, and in some cases, the targets must be totally revised.

For the research evaluation during the progress, it is important to carry over that evaluation at that point to the next step. To do so, it is important to establish the methodology for rotating the PDCA model, and the most desirable situation is that the evaluation is fed back to the strategy spirally and is carried on to the formation of a new strategy. Moreover, in advancing the R&D, it is necessary to consider where the results are handed over and outcomes are directly produced.

As an issue of research evaluation, it is necessary to have an optimal overall strategic system in which the chain of PDCA from the project to the policy level is utilized effectively by each other. The PDCA cycle with insufficient linkage cannot be considered a functioning strategic research evaluation. For a public research institute, it is important that the evaluation is always linked as a chain from the evaluation of the institute level of whether it fulfills the function expected of the government including the mission and the resource invested, to whether the government (or local government) has a policy to utilize it effectively, all the way to the policy level of whether it is positioned clearly in the innovation policy[28].

7 Conclusion

In this paper, focus was placed on the formation of the research strategy based on the intrinsic properties of research and the R&D program to realize the strategy, and the research evaluation was viewed from the aspects of strategy formation and the synthetic evaluation based on the strategy. In the research evaluation until now, appraisal, interim, ex-post, and follow-up evaluations were performed, and the elements of the synthetic evaluation discussed in this paper had been incorporated. What should be emphasized here are: 1) in the research evaluation, the research strategy is extremely important, and the evaluation by comparison with the strategy should be set as the basic; 2) evaluation from the three aspects - progress, depth, and phase of the research - is necessary; and 3) a synthetic evaluation that summarized these ideas by taking abductive inference is important.

Figure 12 shows the summary of the intrinsic properties of the research, formation of the research strategy, and the synthetic research evaluation based on them that were discussed in this paper, and the aim of research evaluation. The research strategy shows the targets to be achieved by the R&D and the scenario. By conducting a synthetic research

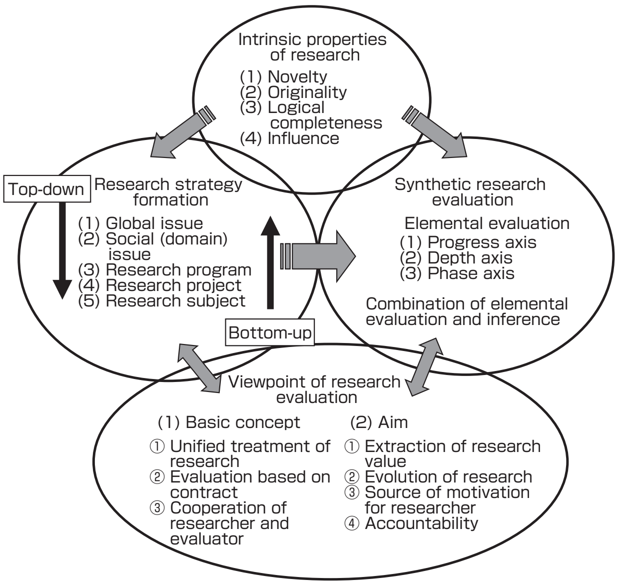

Fig. 12 Research strategy formation and synthetic research evaluation considering the intrinsic properties of research

evaluation based on them, the extraction of the value of research, the evolution of research, the source of motivation for the researchers, and the fulfillment of accountability can be performed effectively.

It would be very significant if the research program evolves through the research strategy formation and the synthetic evaluation proposed in this paper, and then heads toward a new development.

Acknowledgements

To perform this research and to write this paper, we have received great support from the staff of the Evaluation Department, AIST. The central concept of this research is based upon the knowledge and experience in the research unit evaluation performed by the Evaluation Department over nine years, since AIST was reorganized as an independent administrative agency, after the integration of the former Agency of Industrial Science and Technology. We are deeply grateful to Dr. Hiroyuki Yoshikawa, former President of AIST (currently Grand Emeritus Advisor, AIST; Director-General of The Center for Research and Development Strategy, Japan Science and Technology Agency), who provided valuable insight on abduction and synthetic evaluation as well as continuous support. We are also thankful to the staff of the Science and Technology Promotion Bureau of Nagasaki Prefectural Government and the Ceramics Research Center of Nagasaki who created the logic model for the role of public research institutes in Nagasaki prefecture etc..

Notes

Note 1) This project supports the series of activities for the research, development, and practical implementation of clean energy, led by Secretary Steven Chu of the U.S. Department of Energy in December 2009.

Note 2) This strategy was set for the establishment of Framework Program 7 (FP7), an R&D program for the entire EU started in 2007. It was declared at the Council of European Union at Lisbon in 2000.

Note 3) The strategy (basic policy) of Japan was approved by the Cabinet in June 2010. The policy emphasizes green innovation and life innovation as the growth field in which the strength of Japan can be applied.

Note 4) Deduction derives the result (this fruit is delicious) from the rule (an apple is delicious) and the fact (this fruit is an apple). Induction derives the rule (an apple is delicious) from the fact (this fruit is an apple) and the result (this fruit is delicious). Abduction is a method to infer the fact (this fruit is an apple) from the rule (an apple is delicious) and the result (this fruit is delicious). While the deductive inference has a logical structure not dependent on the content, the inductive inference has logic based on several specifics and experiences. Abduction is weaker in logic, and therefore various limitations are set in the conditions by which inferences are made. Yet unlike induction and deduction, abduction is a method with great inference potential. Historically, the discovery of the universal gravitation by Sir Isaac Newton and the elliptical orbit of heavenly bodies by Johannes Kepler are considered typical examples of abduction[11].

Terminologies

Term 1. Deduction, induction, and abduction: Deduction or deductive inference is “to logically derive the true conclusion from the true assumption only through inference without considering the content of inference”. Induction or inductive inference is “to derive a general proposition or law from individual specific facts”. On the other hand, abduction or abductive inference is the third way of inference proposed by an American philosopher C. S. Peirce (1839~1914)[11]-[13], and it is “to derive the individual fact from a certain result and the proposition or law that may cause that result”.

Term 2. Logic model: The logic model is a tool developed to visualize the scenario that is an important element in the strategy formation, to clarify the logical linkage by which the research program achieves its goal. It is employed when the American agencies apply for financing to the Office of Management and Budget (OMB). To write the scenario, an issue is broken down into resource, R&D, output, customer, short-term outcome, mid-term outcome, and long-term outcome. Then, starting from the long-term outcome of the program, the direct outcome that will be produced when the customer receives the result of the R&D is clarified, and the target of the R&D must be spelled out. The logic model is a tool to summarize this process into one big picture[4][5][23][24].

Term 3. *Type 1 Basic Research*, *Type 2 Basic Research*, *Product Realization Research*: According to the definition by Hiroyuki Yoshikawa, *Type 1 Basic Research* is the research to analyze the unknown phenomenon through observation, experiment, and theoretical calculation to establish universal principles and theories. *Type 2 Basic Research* is the research to realize a social value by integrating the knowledge of multiple disciplines, and it also includes research that derives a generalized methodology. *Product Realization Research* is a research that uses the result and knowledge obtained from *Type 1 Basic Research* and *Type 2 Basic Research* and the actual experience to realize the use of the new technology in society[8][9].

Term 4. Basic research, applied research, experimental development: According to the definition of OECD, basic research is an “experimental or theoretical work undertaken primarily to acquire new knowledge of the underlying foundations of phenomena and observable facts, without any particular application or use in view”. Applied research is an “original investigation undertaken in order to acquire new knowledge. It is, however, directed primarily towards a specific practical aim or objective”. Experimental development is the “systematic work, drawing on existing knowledge gained from research and/or practical experience, that is directed to producing new materials, products or devices; to installing new processes, systems and services; or to improving substantially those already produced or installed”[15].

Term 5. ROAMEF: Acronym for R (rationale), O (objective), A (appraisal), M (monitoring), E (evaluation), and F (feedback, or review of the cycle)[16].

Term 6. PDCA cycle: A kind of management cycle proposed in the 1950s by Walter A. Shewhart and W. Edwards Deming (U.S.A). It is an acronym for P (plan), D (do), C (check), and A (act). When one cycle is completed, the final “act” is linked to the “plan” of the next cycle so the project will improve spirally. The PDCA cycle can be implemented for a small group or for the entire organization. Ideally, the individual PDCA cycles should link to the higher PDCA cycle[24][28].

References

[1] U.S. Department of Energy website: http://www.energy.gov/hubs/index.htm

[2] European Commission FP7 website: http://ec.europa.eu/research/fp7/index_en.cfm

[3] http://www.kantei.go.jp/jp/sinseichousenryaku/sinseichou01.pdf (in Japanese)

[4] J. A. McLaughlin and G. B. Jordan: Logic models: A tool for telling your programs performance story, *Evaluation and Program Planning*, 22 (1), 65-72 (1999).

[5] G. B. Jordan: A theory-based logic model for innovation policy and evaluation, *Research Evaluation*, 19 (4), 263-273 (2010).

[6] R. Hirasawa: Hyoka kenkyu no sokatsu (Summary of evaluation research), *Material for the 3rd MEXT Mutual Training Session for Policy Evaluation FY 2008* (2009) (in Japanese).

[7] AIST Evaluation Department: *Heisei 17 Nendo Kenkyu Yunitto Hyoka Hokokusho (FY 2005 Research Unit Evaluation Report)* (2005) (in Japanese).

[8] H. Yoshikawa: *Honkaku Kenkyu (Full Research)*, The University of Tokyo Press (2009) (in Japanese).

[9] H. Yoshikawa: A journal for *Type 2 Basic Research*, *Synthesiology*, 1(1), 1-6 (2008).

[10] M. Koshiba: *Nyutorino Tentai Butsurigaku Nyumon (Introduction to Neutrino Astrophysics)*, Kodansha (2002) (in Japanese).

[11] Y. Yonemori: *Pasu No Kigogaku (Symbology of Peirce)*, Keiso Shobo, 173-200 (1981) (in Japanese).

[12] H. Yoshikawa: *Kagakusha No Atarashii Yakuwari (New Role of Scientists)*, Iwanami Shoten, 13-29 (2002) (in Japanese).

[13] Y. Yonemori: *Abudakushon (Abduction)*, Keiso Shobo (2007) (in Japanese).

[14] H. Ishikawa: Technologies for all-optical path routing toward huge capacity and low power consumption networks, *International Symposium on Ultra-high Capacity Optical Communication and Related Optical Signal Processing and Devices*, Sept. (2010).

[15] *OECD Frascati Manual*, Sixth edition (2002).

[16] R. Ohtani: “Science for society” and evaluation of research and technology development, *Synthesiology*, 3 (1), 264-274 (2010) (English version available).

[17] N. Kobayashi: Sangyo gijutsu sogo kenkyusho ni okeru autokamu e no shiten karano senryaku teki kenkyu hyoka to sangakukan renkei e no kadai (Strategic Research Evaluation in AIST from the Perspective of Outcomes and Its Critical Issues for Industry-Academia Collaboration), *Journal of the Japan Society for Intellectual Production*, 4 (1), 14-24 (2007) (in Japanese).

[18] AIST: *Dai Niki Kenkyu Senryaku (Second Term Research Strategy)*, (2005) (2006) (2007) (2008) (2009) (in Japanese).

[19] AIST: *Sansoken No Keiei To Senryaku (Management and Strategy at AIST)* (2005) (in Japanese).

[20] AIST Evaluation Department: *Heisei 20 Nendo Kenkyu Yunitto Hyoka Hokokusho (FY 2008 Research Unit Evaluation Report)* (2008) (in Japanese).

[21] O. Nakamura, S. Ito, K. Matsuzaki, H. Adachi, T. Kado and S. Oka: Using roadmaps for evaluating strategic research and development: Lessons from Japan’s Institute for Advanced Industrial Science and Technology, *Research Evaluation*, 17 (4), 265-271 (2008).

[22] AIST Evaluation Department: *Dai Niki Chuki Mokuhyou Kikan Kenkyu Yunitto Hyoka Hokokusho (Second Medium Term Target Period Research Unit Evaluation Report)* (2010) (in Japanese).

[23] O. Nakamura: Imakoso senryaku teki puranningu ni motozuku kenkyu kaihatsu o!- rojikku moderu no katsuyo- (R&D based on strategic planning now! – Use of logic model), *Letter from Industrial Technology Center of Nagasaki Challenge*, 145, Prefatory Note (2009) (in Japanese).

[24] O. Nakamura: R&D evaluation, *Kenkyujo Keiei (Research Institute Management)* (K. Kurata and K. Kawajiri, eds.), Kogyo Chosakai Publishing, 311-336 (2010) (in Japanese).

[25] Science and Technology Promotion Bureau, Nagasaki Prefecture: http://www.pref.nagasaki.jp/kagaku/ (in Japanese)

[26] O. Nakamura, S. Iwai, K. Nishimura and N. Inada: Chiiki kasseika o mezashita nagasaki ban kagaku gijutsu shinko no jitsurei to kosatsu (Case of Nagasaki’s promotion of science and technology for regional vitalization), *Collection of Lectures, 24th Annual Academic Conference, The Japan Society for Science Policy and Research Management*, 442-445 (2009) (in Japanese).

[27] Ceramic Research Center of Nagasaki: http://www.pref.nagasaki.jp/yogyo/index.php (in Japanese)

[28] O. Nakamura, O. Nakamura, M. Takagi, T. Sawada, S. Kosaka, M. Koyanagi, I. Matsunaga, K. Mizuno and N. Kobayashi: Strategic evaluation of research and development in a Japan’s public research institute, *New Directions for Evaluation*, 118, 25-36 (2008).

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Discussions with Reviewers

1 Synthetic evaluation versus analytic evaluation

Question (Motoyuki Akamatsu, Human Technology Research Institute, AIST)

When we use the term "synthetic evaluation", we think of "analytic evaluation" as its antonym. For example, when you break things down in elements as in Fig. 6, it seems you are doing analytical evaluation. What is the characteristic of synthetic evaluation when seen from the stance of synthetic versus analytic?

Answer (Naoto Kobayashi)

As you indicated, evaluation by breaking down into elements as shown in Fig. 6 can certainly be called analytic evaluation. Particularly, the elemental evaluation (progress, depth, and phase) in this paper corresponds to the analytic evaluation. For example, in the depth evaluation, the evaluation performed along novelty, originality, logical completeness, and influence is an analytical process. On the other hand, the characteristic of synthetic evaluation is to take the result of such analytical evaluation, and 1) to synthesize along the direction shown in the strategy (what did the strategy emphasize to begin with?), and 2) to form a progressive evaluation through deep discussion (here, abductive inference is important) between the evaluator and evaluated side.

2 Abduction in synthetic evaluation

Comment (Motoyuki Akamatsu)

You state that abduction is important in research strategy formation, and that abduction is necessary when selection and concentration are required in an evaluation. I see that abduction becomes most important in strategy formation. However, I don't think there has ever been a good discussion on this subject. I imagine that the readers won't understand how abduction or hypothesis forming is done, so I think they can understand better if you describe what kind of hypotheses are made for the strategy formation using a specific example. Also, you state that abductive inference is necessary in the evaluation for the depth of research in the Y-axis, but what do you mean specifically?

Answer (Naoto Kobayashi)

Thank you very much for pointing out the central tenet of this paper. The abduction or hypothesis forming needed in the strategy formation is not a factual hypothesis, but is a hypothesis of what "ought to be". The issue depends on how to form such a hypothesis. We added the description of how abduction is actually done. We also added the description of abduction using a specific example. Also, for the evaluation of the depth of research in the Y-axis, we added the explanations in places where abductive inferences are required.

3 Timing of when the evaluator should step in

Question (Kazunori Nakamura, Biomedical Research Institute, AIST)

The appraisal is important in the research evaluation based on research strategy formation, Does the evaluator need to be involved from the process of research strategy formation?

Answer (Naoto Kobayashi)

Basically, since the strategy formation and research evaluation are inextricably associated with each other, the evaluator should ideally be involved from the time of research strategy formation. However, the viewpoints of research strategy formation and evaluation are slightly different, and it is not desirable for the same entity to execute the P and C of the PDCA cycle. Therefore, I think only some members should overlap in the committees for research strategy formation and research evaluation.

4 Feedback in evaluation

Comment (Motoyuki Akamatsu)

In subchapter 4.2, you discuss the importance of feedback, and I think everyone will agree. However, if the feedback is provided offline in writing, I think you loose the opportunity for abduction based on the discussion between the research executant and the evaluator. If possible, please include a discussion on how this feedback should be done.

Also, a program is expected to run for five to seven years, and I imagine that the feedback loop is in the order of five years. In general, I don't think it is easy to reflect the result of a review from five years ago in the current program. That is because in a program of five to seven year scale, it is difficult to determine whether the objective was finally achieved immediately after the completion of the program, and the immediate feedback to the next step is difficult.

Answer (Naoto Kobayashi)

As you indicate, the evaluator and the research promoting group should not be antagonistic, but they should "walk side by side". Since the act of research is a repetition of abduction and validation, a feedback without the discussion on abduction loses its meaning.

For the feedback cycle, as you indicate, it is difficult to evaluate a program unless about three years have passed after completion. However, when the R&D, technological development, and system development are done in society, they inevitably become contiguous due to the social demand. Specifically, the FP7 framework in Europe is a seven-year (2007~2013) program. An intermediate evaluation was conducted in autumn 2010, and the appraisal of the FP8 (2013~2019), the next framework, will be started in 2011 based on this evaluation. In practice, the programs are sequential and the feedbacks are done in extremely short span of time.

5 Evaluation of the research program and evaluation of the research project

Comment (Kazunori Nakamura)

In order to apply this research evaluation method, it is necessary to apply synthetic research evaluation in the process of strategy formation of the research program. Therefore, I don't think it is readily applicable to a general research project that has not passed through this process.

Answer (Naoto Kobayashi)

A research project has, in a sense, a simple structure compared to a research program. There, the research objective, method, results, and expected outcome are contained in a small area, but has a fractal structure to the research program. For example, it is possible to apply the evaluation using the aforementioned three aspects (1) progress, (2) depth, and (3) phase, and it is also possible to apply the evaluation method that synthesizes the three. However, the execution of a research project is positioned as one element of the research program within the research strategy, and the appraisal of the research strategy can be simplified.

6 Verification of the case of research evaluation

Comment (Motoyuki Akamatsu)

Since this is a paper on research evaluation, it is desirable if you present an evaluation of an actual research. If there are reviews and discussions from the members of the evaluating committee, Evaluation Department, and the evaluated entity, the paper itself will become abductive and interesting.

Answer (Kenta Ooi)

In the *Second Medium Term Target Period Research Unit Evaluation Report* published in May 2010, the comments by the external evaluation committee members, the research unit heads, and the coordinators were analyzed, the characteristics and issues of the evaluation system in the Second Term were summarized, and the improvement points were organized. For the evaluation system, there were many who highly evaluated the current system, such as the "evaluation from the external evaluation committee members" and the "introduction of the viewpoint of outcome taking into account the exit to industry and society". On the other hand, many issues that must be improved were pointed out, for example, the "need for flexibility in handling of various types of R&D such as the bottom-up research or the long-term research", the "reduction of evaluation load", and "further utilization of the evaluation results". Being aware of these improvement issues, the evaluation from the viewpoint of outcome will be continued for the Third Term evaluation system, and efforts will be made to raise the immediacy of effect. It is not even 10 years since the research evaluation started at AIST. As you indicated, it is important to make improvements based on the verification of hypotheses, toward a better evaluation system.

For specific examples at AIST in this paper, we discuss the issues of the evaluation system currently used at AIST from the perspective of an ideal synthetic evaluation based on the research strategy. To actually apply the synthetic evaluation system, I think it is necessary to design the system as a whole including the strategic research advancement, rather than cutting out the evaluation system only. I think it is necessary to conduct the modeling and the hypothesis verification for the AIST system in a larger framework.

7 Logic model and synthetic research evaluation

Comment (Kazunori Nakamura)

The example of Nagasaki prefecture is described as a case where the logic model was applied to advance the strategic R&D, and the Research Evaluation Subcommittee and the Research Enterprise Evaluation Committee were held utilizing the logic model. I think you should clarify the basic differences between the evaluation based on the logic model in this case and the synthetic research evaluation described in this paper.

Answer (Osamu Nakamura)

It was presented as one of the examples of "R&D evaluation that seemed to have incorporated the thinking of synthetic research evaluation by trial-and-error", and so there is no basic difference.

As mentioned in this paper, the mission of the Science and Technology Promotion Bureau of Nagasaki Prefectural Government is to contribute to create energetic Nagasaki prefecture where people can live with dreams for the future by utilizing science and technology. To evaluate whether the research institutes quickly recognize the needs of the local companies and product districts, and set the research topics that can achieve the demanded results, we asked to review all the running projects and summarize them into the logic model at first. That is because the application of the logic model is effective to clarify the strategic logic of the scenario.

Each evaluation committee checked the positioning of each research topic based on the logic model, evaluated whether the strategic R&D were conducted according to the mission of each research institute, checked whether the structure of the overall projects was strategic, and checked whether the program was a strategic program. They also evaluated whether the individual project had a long-term vision, had clear targets, and whether it was producing adequate results toward the targets. However, this attempt has just started, and so it is necessary to evolve the strategic evaluation system.

8 Specific content of the integrated evaluation

Comment (Motoyuki Akamatsu)

You write that synthetic evaluation is to "integrate" the evaluations, but I think it is hard to understand because there is no example on what exactly is integrated evaluation. Do you add the three axes, or do you evaluate by changing the weight of other axes? Please provide a specific example.

Answer (Naoto Kobayashi)

This indeed is the pillar of the evaluation design. In the case of AIST, various things were done such as weights were added or averages were taken, and this is where the evaluation organization can become creative. Considering this point, the following description was added to "4.3.3 Integrated research evaluation".

"In conducting the synthetic evaluation, it is important for the research promoting group and the evaluators, to consider the property of research, share common understanding of the strategy and result index including the goal to be achieved, engage in deep discussion on the result and how the research should progress, check the target indicated in the strategy and distance from the actual result, and finally abductively discuss and investigate the significance and the effect of the research program execution. This entire process can be considered the "research evaluation = abduction and its expression." This is closely related to the research that is a creative activity, and research evaluation can be considered to be part of this creative endeavor.

… Specifically, it is necessary to design a general evaluation system including the incorporation of the constructive, deep discussion between the research promotion group and the evaluators, in addition to the elemental evaluation and appropriate synthesis."

9 Conclusion

Comment (Motoyuki Akamatsu)

For research evaluation, you give as requirements: (1) unification under *Type 1*, *Type 2*, and *Product Realization*, (2) to be based on a contract, (3) the evaluator and evaluated to stand on the same ground, (4) value of research to be brought out, (5) research to evolve, (6) to be the source of motivation, and (7) accountability. Can you please describe in the conclusion, how these and the research strategy formation and synthetic evaluation discussed from chapter 3 are connected. I think the strategy formation satisfies (1)~(3) and (7), and (4)~(6) can be realized by synthetic evaluation. I think the paper would become organized and comprehensive if you have a summary that shows the relationships among the four intrinsic properties of the research, seven points of research evaluation, research strategy formation, and synthetic evaluation, and diagrams to explain them.

Answer (Naoto Kobayashi)

Thank you for indicating a very important point. We added Fig. 12 at the end, and also added the following description: "Figure 12 shows the summary of the intrinsic properties of the research, formation of the research strategy, and the synthetic research evaluation based on them that were discussed in this paper, and the aim of research evaluation. The research strategy shows the targets to be achieved by the R&D and the scenario. By conducting a synthetic research evaluation based on them, the extraction of the value of research, the evolution of research, the source of motivation for the researchers, and the fulfillment of accountability can be performed effectively."

Development and release of a spectral database for organic compounds

— Key to the continual services and success of a large-scale database —

Takeshi Saito * and Shinichi Kinugasa

[Translation from *Synthesiology*, Vol.4, No.1, p.26-35 (2011)]

The research activities of spectral database for organic compounds (SDBS) in AIST started in 1982. Since then, many parts of research activities have changed while the other parts have remained unchanged for almost 30 years. The unchanged parts since the start of this project are the two principles that the spectral data with high authenticity should be compiled in the database as the standard data and that several kinds of different spectra should be compiled for each compound, and the concept that compounds used commonly in industry and society are objects of compilation. On the other hand, the computer system used for database management and the ways for data release has changed completely over time. After the data have come to be opened to the public through the Internet, we have started to take considerations of comments, requests and indications from users. SDBS has had innumerable Internet accesses from many researchers, engineers, educators and students from all over the world. In this paper, the total framework, the structure of the database, the method for its data compilation and the ways to release the data to the public are described with analysis and clues of long time continuance and success of SDBS activities.

Keywords : Spectrum, database, nuclear magnetic resonance, infrared, mass, chemical information, web

1 Introduction

The reliable analysis of chemical substances is required not only in industry but also in various situations in society. The nuclear magnetic resonance (NMR), the infrared (IR) and the mass spectroscopy (MS) give powerful and essential information in the identification of an organic compound. The measurements and the analyses of spectra need to be performed whenever a new chemical is developed, unknown materials are analyzed or chemicals are identified.

In general, identification of a material from spectra by comparing and matching with those obtained as a standard spectral data is one of the most reliable methods. Since this approach has been used in a variety of applications, the role of such standard data and their database is important. Spectral database system for organic compounds, i.e. SDBS, of the National Institute of Advanced Industrial Science and Technology (AIST) was started in 1982 as a project of the former Agency of Industrial Science and Technology. Since the start of this database project, two basic concepts of 1) collection of standard spectral data that are reliable and 2) compilation of more than two kinds of spectra for each compound have been maintained. In other words, its basic concepts are acquisition of as many as six spectral data of MS, ^{13}C NMR, ^{1}H NMR, IR, Raman and electron spin resonance (ESR) spectra for a compound by ourselves (AIST), and management and maintenance of the associated chemical information for the compound[1].

During almost 30 years of the database activity, collection of Raman and ESR spectra have been discontinued. Currently, activities on four kinds of spectral data of MS, IR, ^{1}H NMR, and ^{13}C NMR have been continued along with the management of compound information, and these spectral data and chemical information are disclosed to the public[2].

In 1997, we started to release the database contents to the public through the Web[3] by a project of the former Agency of Industrial Science and Technology[4]. The total number of compounds and spectra disclosed as of April, 2010 is about 33,000 and about 100,000, respectively. Figure 1 shows the number and fraction of each spectrum. The main users of the present spectral database are those who access through the Web. Since the database has been disclosed to the public through the Internet, it has had many accesses. The average number of page views per day during the last three years exceeds 100,000 times, which is exceptionally high

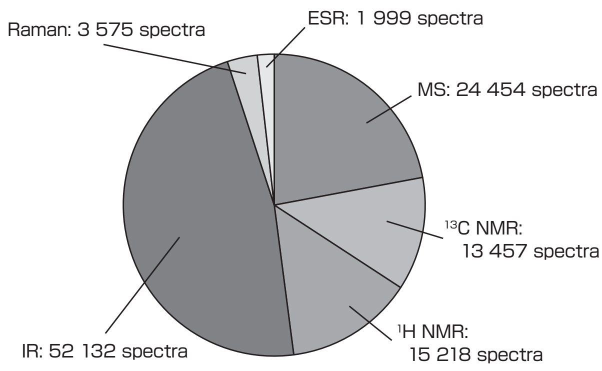

Fig. 1 Fractions and the number of spectra open to the public by the spectral database for organic compounds (SDBS) of AIST as of April, 2010

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among databases open through the Web by the "Research Information DataBase (RIO-DB)" that is operated by AIST. The total number of page views since the database was disclosed to the public exceeded 300 million at the end of fiscal year 2009. The transitions of the number of accesses to the database and the number of spectra compiled to the database per fiscal year are indicated in Figs. 2 and 3, respectively. The number of accesses has been increasing every year in the last ten years because of a remarkable expansion of the usage of the Internet and the recognition of this database among Internet users. Requests for using our spectral data for textbooks[5], reference books[6], and as materials for examination problems, etc. come often from users; there are users who point out mistakes found in our database as well.

Figure 4 shows the scenario of the development of this database. This figure indicates a list of various elements which compose this database, relationships between each of the elements and the main characteristics of the database such as the basic structure, completeness, reliability and usability. Important elements for the operation of this database are shown here. A method of how respective elements have been integrated to this spectral database is described in the following chapters.

2 Structure of database

2.1 Importance of basic structure of database

This database has taken a structure that allows two or more kinds of spectra to be accessed for each compound. In order to achieve such a structure, this database was designed and built as seven independent databases: a compound database, which has been called a compound dictionary, and six different spectral databases. All of them were integrated mainly under the compound dictionary as shown in Fig. 5.

To do this work smoothly, several kinds of management numbers were prepared. These are a bottle number which is given to a unique bottle of a chemical reagent, a spectral management number which is assigned to each individual spectrum, a spectral code which is only given to the spectrum which is compiled in the database, and an SDBS compound number (called SDBS number within our databasing group)

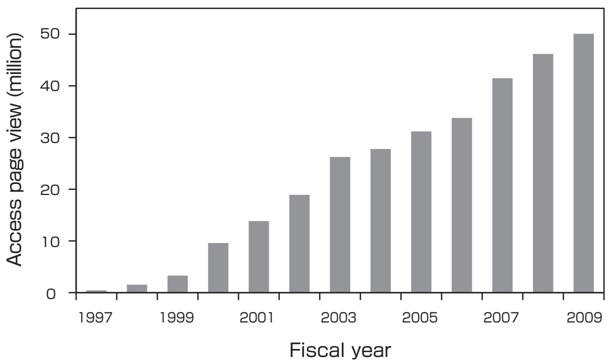

Fig. 2 Yearly transition of the number of access page views since opening to the Web of the spectral database for organic compounds (SDBS) of AIST

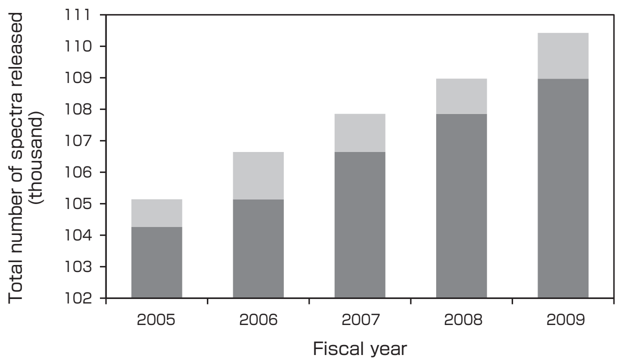

Fig. 3 Transition of the number of spectrum open to the public for the last five years for the spectral database for organic compounds (SDBS) of AIST

New spectral data released each fiscal year are shown in faint color.

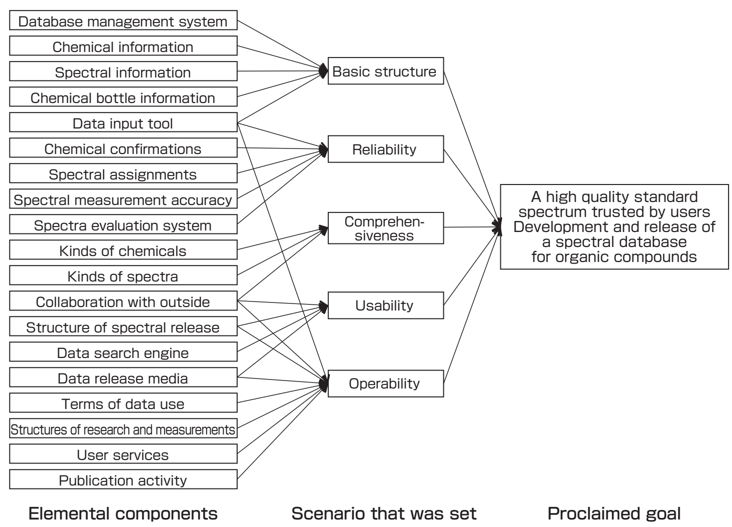

Fig. 4 A scenario of a construction of database and data release to the public for the spectral database for organic compounds (SDBS)

which is a unique number for each chemical identity. The spectral code for each kind of MS, IR, ^{13}C NMR and ^{1}H NMR spectrum has been managed individually. Thus the database for a single kind of spectrum and chemical information can be separated as an independent database. Compound and spectral information corresponding to these numbers are managed as relational databases independently, and these numbers made our work proceed smoothly.

In particular, adopting the SDBS compound number that is a unique identification to a compound is a characteristic of this database. This number is not just a management number of the compounds. This number enables the compound dictionary to be independent from a spectrum database. As a result, the flexibility of changing the compound dictionary was maintained. Thus operation of useful compound information has been possible up to now. The founders of this database had had rich experiences in constructing databases while in the gas chromatographic data committee, the infrared data committee, and the NMR data subcommittee during the era of the former Agency of Industrial Science and Technology. Based on such experiences, the SDBS compound number was adopted to this database and made the database functional for some 30 years after it was established.

In principle, all compounds have been obtained and their spectral data have been acquired by ourselves. The unique bottle number was assigned to each chemical bottle obtained. An SDBS compound number was assigned to each compound. Each sample identified in a bottle had been carefully checked for avoiding assignment of two or more different SDBS compound numbers to an identical chemical compound. This number was assigned only when the sample was evaluated as a new chemical compound in

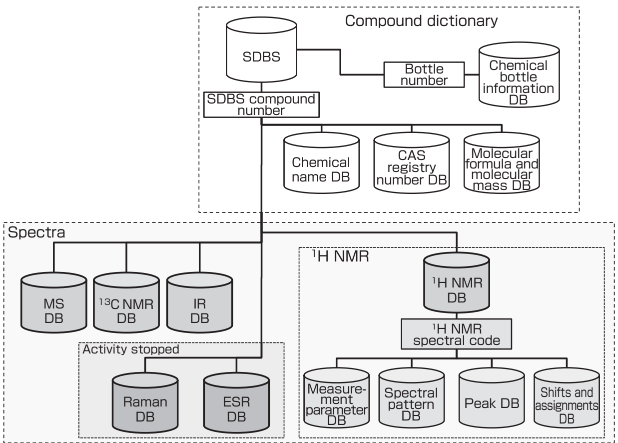

Fig. 5 Structure of the spectral database for organic compounds (SDBS)
SDBS in this figure contains information of the SDBS compound number that is the unique number for each compound, the number of elements for the compound, and other information. The structure of ^{1}H NMR database is shown on behalf of each spectral database. All information is correlated to the SDBS compound number via a relational database.

the database. This work might not have been a tough task in the early days of this database, however, as time passed, the task became more difficult. In the past few years, we encountered questions and problems in the checking process. The assignment of a SDBS compound number to a unique chemical became a more complex task and required longer time compared to the early days. This is because compound structures and thus their names have become more complex, and the number of compiled compounds has become large extending to some 30,000 different chemical compounds. For solving this problem, first we collected as much information of a chemical compound as possible, then individual information was searched through our compound database. Deeper consideration by several chemists was made only for those compounds with possibilities of having already been compiled. This enabled us to spend more time to acquire and evaluate the spectral data. As a result, the problem of assigning different SDBS compound number to two or more identical compounds has occurred less frequently and full supervision by chemists has become unnecessary. In recent years, SDBS compound assignment process has become smooth.

2.2 Decision of the database operation and renewal of the database platform

The operation of this database was started with a mainframe computer in the1980’s. The choice of such a computer made sense because the first Japanese Windows computer, NEC PC-9800, was just released about the same time. However, operation of this mainframe computer (FACOM MSP) ended in March 1999 due to the decision by the former Agency of Industrial Science and Technology. It was needed to decide whether activity of the database would be continued with another mainframe computer or a personal computer (PC), or terminated altogether. At that point, we decided to continue our activities and to adopt Windows PC, and a new data input tool was developed on the PC[7]. With much of the computer software, it was difficult to shift platforms from MS-DOS to Windows computers, and the majority of the system had to be rebuilt. This database, however, was successfully and completely transferred to a different platform of its operation. If we had remained with the mainframe computer at that time, our system might have been in trouble in adopting many tools for assisting data input to the database system. The data collection and handling became greatly easy by adopting Windows PC as a platform for the data management.

3 Selection of data to be collected

3.1 Strategy for selecting compounds

This database was designed as a useful tool for compound identification. Data collections were mainly focused on spectral data of commercial reagents that were frequently used by many people. Figure 1 shows the number of spectral data released through the Web. There are many more spectra that had not been released to the public. The total number of bottles of chemical reagents exceeds 39,000.

Among these, more than 10,000 reagents have been offered free of charge by Tokyo Chemical Industry Co. Ltd., from which the most abundant chemicals have been supplied. Therefore, although the selection of chemical reagents partially has followed this company's policy in development of reagents, it has indirectly reflected our user's needs. In the development of a new material by chemical synthesis or other methods at research and development departments, a starting material is in many cases a commercial chemical reagent. Thus, the support we have been given by the company has been valuable to us.

Since 2001, our strategy for a spectral collection has focused on pesticides and deleterious substances. Collection of much spectral information on regulated chemicals is an important function of public research institutes like AIST. Thus the number of spectra collected for such substances has been slowly increasing. Recently, the concern for the safety of food has been increasing, which enhances the need for such information. It is important that our strategy focus on collecting the spectral data of pesticides and regulatory chemicals.

3.2 Selection of visual data form (digital data)

The most important decision for the selection of data format was made at the early stage of this database. Although it is not surprising now, this database chose to collect all spectral information in digital coordination format on a computer since the activity was started. In the 1970's, spectral information was collected more often in a data book format. Although it was recognized that the handling of spectral data would become easier by making them digital, limitation of the computer memory prevented this. Due to the limitation of the computer, digitization of the data often resulted in the loss of information. As a result, the analog data format recorded on paper was still the majority[1] at that time. For example, NMR data was composed of several tens of thousand points of data. Digitalizing such data about thirty years ago must have been a big decision because of the limitations in disk and memory capacity. An achievement of such a system would have been extremely difficult if there had been no mainframe computer operated at the former Agency of Industrial Science and Technology at that time. Under this condition, management of the spectral database required not only to concentrate on accumulating spectral data, but also to find a creative way to minimize the data points. This system was the world's first ^{1}H NMR spectral database with digital coordinate data of a collected spectrum[8]. We adopted compression of data size by collecting data which represented only peak areas. For the ^{13}C NMR, values of peak positions, their intensities and their peak width at half high were recorded. From these data, all spectra were reconstructed with the assumption of all peaks as the Lorenz function. For the IR and Raman, coordinate data of the spectral points were collected. For the MS, the mass numbers and the signal intensities were collected. For ESR, each point of spectral data was digitalized. Some of the data was reconstructed from paper data by using a curve reader. ^{1}H NMR has a capability of spectrum simulation by using chemical shifts and spin-spin couplings[9]. After AIST was established, all digital data including the peaks and noise have been collected for ^{13}C NMR and ^{1}H NMR. Users can recognize the strength of the peak signal compared to the noise level. In 1997, this database became disclosed to the public through the Web by the former Agency of Industrial Science and Technology. If all the data were not collected digitally, there would have been problems for converting old analog data, and many data might have had to be recollected.

3.3 Balance between quality and quantity of data; stick to the high quality data

The spectral database consists of data acquired, evaluated and compiled in our institute with some exceptions in ESR and ^{1}H NMR spectra. This is the most reliable way to keep the quality of the spectral data. This makes quality of the data reliable. However, on the contrary, the number of accumulated spectral data has become limited. To cover a wide variety of data is one of the important elements of a database. How we balance the two different concepts for the data collection, i.e. quantity and quality of spectral data makes for serious argument. Our first decision was to take a strategy of collecting reliable standard data. On this basis, the quantity of the data would be increased as a result of data accumulation over a long period of time.

The criteria for keeping quality and reliability of spectral data and for accumulation of data were established. For example, tetramethylsilane (TMS) was not only used as a chemical shift standard for NMR spectra but also its line width was used for a criterion of spectrum resolution. When the peak resolution of the TMS peak was sharper than the criterion, the resolution of the spectrum was determined well even if the resolution of the peak from a compound showed poor resolution. This was considered as the nature of the compound giving such a spectrum, and not caused by the bad experimental condition. For IR, no interference noise, no water peaks, or no surge in baseline were the criteria. A criterion for each spectral data evaluation was established by respective researchers in charge of the spectrum.

3.4 Policy of data registration

This database only compiles unique spectral data. In other words, when several spectra for a compound have been acquired with identical conditions, only the spectrum of the best quality is compiled and released to the public. For MS, a direct sample injection method was adopted for the measurement. Therefore, each compound had a unique measurement condition. Only the best quality MS spectrum was compiled for a molecule. For IR, different conditions of measurement such as KBr plate method and Nujor method for a solid sample was adopted. In such cases, spectra with the best quality and reliability in each condition were compiled. For ^{13}C NMR, ^{1}H nucleus was decoupled from the spectrum which made the spectrum simple singlet peak for each carbon for most of the cases. Only one ^{13}C NMR spectrum was compiled for a compound.

For ^{1}H NMR, a resonance peak pattern depends on the resonance frequency. This makes spectral pattern for a given sample solution to be also dependent on resonance frequency. Many ^{1}H NMR were acquired at resonance frequency of 90 MHz at the beginning of this database activity. When a molecule had a complex structure and it was hard to make chemical shift assignment at this frequency, a higher frequency of 400 MHz, which simplified spectral patterns, was also adopted for such a molecule. Simulation of spectral pattern was also important. This database had a capability of simulating spectrum observed at different resonance frequencies. For fulfilling this capability, chemical shifts and spin-spin coupling constants for a molecule were also compiled in the database independent of spectral patterns.

For ^{1}H and ^{13}C NMR, chemical shift assignments were compiled in addition to the information above. Especially for ^{1}H NMR, since the resonance peak pattern depends on resonance frequency, it was indispensable to provide a universal property of chemical shift assignments. If there was no such data compiled in this database, two ^{1}H NMR spectrum obtained at different resonance frequencies cannot be compared. The chemical shifts and their assignments were the most valuable information for the ^{1}H NMR spectral database.

Information on a chemical compound was compiled as much as possible. It is usual that the more complex the structure of a compound is, the more chemical names or abbreviations are assigned to it. We thought that it was beneficial for users of this database if they could easily find a compound with various names, and therefore, much chemical information was compiled encyclopaedically.

3.5 Kinds of spectra collected

In the early days, six kinds of spectra were collected. Currently, four out of the six kinds are still actively collected (Fig. 5). The spectra used in analysis in the 1980's were not limited to those six kinds of spectra. Spectra such as ultra violet-visible spectral data were not incorporated in this database. The selection of the six spectra for this database is thought to have depended on instrumentations and researchers in our institute at that time. The reasons for the decision to terminate the activities of Raman and ESR spectra were not only based on the instrumentation and the researcher issues but also on the then supposed relatively low potential demands from users of the database. However, the demand for Raman spectral data has now expanded academically and in industry. Based on this point, this database may not cover enough to respond to the user's needs. On the other hand, MS, ^{13}C NMR, ^{1}H NMR, and IR have had huge demands from the 1980's up to the present days. After this database was released to the public, the demands of users can be evaluated by the number of accesses to spectral data (Fig. 2).

4 Policy of data release to the public

4.1 Releasing data on the Web

In 1997, spectral data of MS, ^{13}C NMR, and ^{1}H NMR was released from the website of AIST, and IR and ESR followed a year later[10]. Currently, six kinds of spectral data, including Raman spectra, are opened to the public through the Web. When our data were opened to the public for the first time, people had started to use web browsers such as NCSA Mosaic and Netscape. Although more and more people started to use the Web, the internet line was slow and functions of the browsers were insufficient compared to the current situation. Therefore, it was important to display the information efficiently on the Web. As a result, we decided to use GIF image format for displaying spectral patterns and structures of molecules which placed the least load on the internet line. The speed of the web access has increased rapidly in Japan, and therefore, it may not be applicable to other particular parts of the world. Therefore, this format is still kept in our system.

Another reason to use the GIF format is to protect the data. In other words, image display format can prevent illegal loss of coordinate data or intellectual property of our database. It is easy to reproduce a high resolution spectrum using digital data. On the contrary, it is not possible to create spectral data with higher resolution than the original image when it is reconstructed from the image. We have had several experiences of systematic data download activities for taking all or at least the majority of our data. The protection plan that we took worked for preventing the coordinate data to be inappropriately taken. In the future, with sufficient protection against illegal accesses, spectral expansion functions based on the coordination data can be provided on the Web.

We chose English for information on the Web. This choice was possible because the collected compound names were in English. The other information, or the spectral data, did not depend on any languages. At present, when users access with the Japanese setting computers, the database gives frame information in Japanese.

To increase the users' convenience, links to other databases disclosed on the Web have been created for the information that cannot be maintained by ourselves. Since 2006, the links to online catalog of Tokyo Chemical Industry Co., Ltd.,[11] and Chemical Materials Link Center operated by Japan Science and Technology Agency[12] have been maintained. Components, such as a search system for Japanese compound names and chemical structures which have not been covered by us, have been supplemented by the links.

One of the advantages of data release by the Web is its easiness of data management in a lump. It became possible to provide all users with equal services at a time by updating data in the database server. A feature different from other researches is the fact that the comments from the users come directly to us through the Web.

Before the data was opened to the public through the Web, an online access was possible since 1989[13] and the databases were sold in a CD-ROM medium with both data and their search engine from 1991[14]. It was only specific users of some tens of domestic users that were able to use this CD-ROM medium. In this format of distribution, contents could be stored for a long time. However, it was limited to the data collected up to the point the CD-ROM was created. Updating data contents and renewal of data managing software were difficult for all the users. Moreover, the service was offered to limited users who owned the CD-ROM. However, having enabled search and display of data by CD-ROM that operated on MS-DOS, it provided an opportunity of exercise for the present format of data release through the Web. This was similar to the pioneering works before the development of this database that helped to create the appropriate design of the database. Opening to the public with CD-ROM might have been an important project for opening this database to the public through the Web.

4.2 The analysis of users and the role as public resources

For the analysis of the database users, an access log in the fiscal year 2009 was analyzed and classified by country identification codes. Figure 6 indicates the data. Of more than 50 million page views, accesses from domestic users were about 14 %. The most accesses came from the North America region. The domains that cannot be assigned to specific regions such as ".net" and ".com" were classified independently. Focusing on the accesses from Japan, shown in Fig. 7, the most accesses came from the users of ".ac.jp" or those accesses from academic institutes, and the accesses from ".ne.jp", or network providers and ".co.jp" or general enterprises follow the academic users. Users accessed through the ".ac.jp" and ".ne.jp" domains have intense seasonal variations in the number of accesses. The accesses of March and August were less than half of June when there were the most accesses. On the other hand, roughly the same level of accesses came from the ".co.jp" domain throughout the year. The seasonal dependency of access was thought to be caused by summer break and the end of the scholastic year of students. The access tendency of users through the network providers resembles that of academic institutes. Therefore, the majority of users accessed through the ".ne.jp" were suggested to be also students; the database has been used by many students.

This database is used by various users, and it is one of the public resources that a public research organization such as AIST provides. In general, database compiles much information, and demonstrates its strength by retrieving necessary information efficiently. Many resources and much time are needed for the development and maintenance of such a database, and this database is not an exception. The database users may become limited if we ask the users for the equivalent amount of the development and maintenance costs. This database takes a role of giving various people who are in industry as well as those just starting to learn the usage of spectral data an opportunity by showing it as free accessible

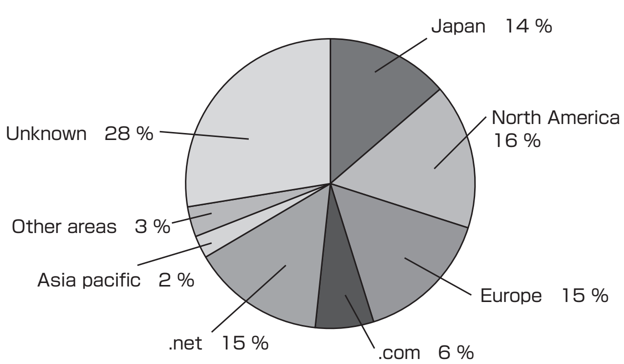

Fig. 6 Fractions of regional domains of users who accessed this database in the fiscal year 2009
Domains ".com" and ".net" are counted independently of the unplaceable domains. The unknown indicates users whose access domains cannot be specified, for instance, those who accessed to the database with only IP addresses.

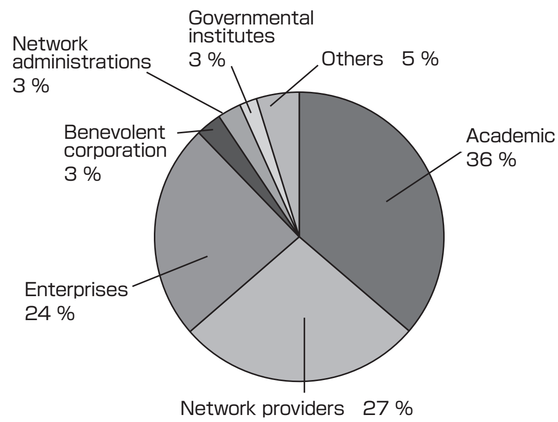

Fig. 7 Fractions of domestic domain of users who accessed this database in the fiscal year 2009
Domains of academics, network providers etc., enterprises, benevolent corporations etc., network administrations, and governmental institutes correspond to ".ac.jp", ".ne.jp", ".co.jp", ".or.jp", ".ad.jp", and ".go.jp", respectively. Other ".jp" domains are added up as "others".

public goods. Many companies can also use our spectral information in their chemical analysis without constructing their own database. The cost of the chemical analysis is, in this way, reduced. This database plays the role as an intellectual foundation that supports industry. This database has also been used by both domestic and international users for educational purposes widely for understanding the use of the spectrum. 36 % of accesses from the domestic users comes from academic sites, and there are many requests for using spectral data in text books and materials for training. From these facts, this database contributes greatly to the whole society.

4.3 Correspondence to comments from the users

We have received many comments from users by e-mail. While most of the research activities are evaluated by their research publications, this database is directly evaluated by the Web users from all over the world. Comments from the users are one of the outcomes of their database evaluation. We think it is important to catch the comments with sincerity and to use them in order to ascertain the direction and further development of the database.

The comments are classified into applications for permission to use the spectra in other materials, and technical questions. Many e-mails of appreciation of our work are delivered, which encourages us.

Examples of the technical indications are incorrect assignments of an NMR spectrum and problems related to its acquisition condition. When a comment indicating our mistakes in spectral data is received, we re-evaluate the data closely at once. When we cannot make a judgment at this point, we may acquire the spectrum of the compound again. The data will be corrected when we come to the conclusion that the user's comment is correct after our evaluations. When we reach a conclusion that our data is correct, the data will be kept disclosed. In the mean time, we explain our decision and reasons for the conclusion to the user. When needed, we obtain the compound for re-evaluation. However, when this is not possible, the data may be withdrawn.

We accept applications for the permission to use the GIF spectral data released in the Web in other materials as much as possible. We think each comment is an indication of the high quality of the data that has been disclosed in this database. We think it is important to maintain a system that can correspond to such a comment promptly.

From the analysis of the data access log, we have already indicated that we receive many accesses from educational sites. Inquiry concerning a spectrum, especially for ^{1}H NMR, of a compound that frequently appears in a textbook is sometimes received. ^{1}H NMR spectrum of such a compound is often acquired at 90 MHz. It is necessary to replace such a spectrum to one acquired at 400 MHz which is suited to the current state.

5 Summaries

Since the beginning of its construction in 1982, this spectral database of organic compound of AIST has so far undergone three generation changes of researchers. Researchers involved in the first generation had started up and made the direction of this database. Those in the second generation released the spectral data to the public through the Web, and completed a prototype of the data management system on a personal computer. Correspondence to the small letters that could not be used on the mainframe computer were started. Problems in notations of compound names, molecular formula, and others were solved.

We are the third generation researchers. Our activities started with the reorganization of our research organization from the National Institute of Materials and Chemical Research of the Agency of Industrial Science and Technology to AIST in 2001. Instrumentations for MS, NMR and IR were renewed. The staff in charge of each spectrum who used to work separately at different places worked together at one site with a staff member who had been maintaining the compound dictionary. With this environment, confirmation and discussion of spectral data and information of dictionary contents could easily be performed when a doubt in a spectral data occurred. An internal data management system, which has a capability of creating data for disclosure, was developed to maintain spectral data and chemical information. Functionalities such as the search engine have been expanded in the Web page. By releasing the data through the Web, academic users have increased, and the users are not limited to industry which had been our primary users. We need to consider development of a new policy of data collection. One of the examples is a spectrum especially the update of ^{1}H NMR information.

It is needless to say that the activity of the database does not work without a researcher who seriously works on it. In addition, continuous activity has been possible because of support from the organization to the researcher. This database has been supported by many users through the Web. Such a demand enabled us to receive support from inside the institute. The fact that the researcher and the organization have become the two wheels is one of the reasons for long term activities of this database. It is not easy to keep releasing highly reliable information to the database with limited resources. In NMR spectral activities, we have collected reliable information effectively by acquiring spectral data soon after its sample preparation to avoid the sample degradations, adopting automated spectral acquisition system, and acquiring two dimensional spectra and obtaining ^{1}H and ^{13}C skeleton of a molecule to increase accuracy of spectral assignments. Final data evaluation is performed by the researcher. When an automatic and more efficient evaluation method could be established, it would become the next big conversion point for this database.

6 Acknowledgements

Many staff members have contributed to the development of Spectral Database for Organic Compounds (SDBS) since its activity started. We want to express our gratitude to the people who have contributed to this database.

References

[1] O. Yamamoto, K. Someno, N. Wasada, J. Hiraishi, K. Hayamizu, K. Tanabe, T. Tamaru and M. Yanagisawa: An integrated spectral data base system including IR, MS, ^{1}H-NMR, ^{13}C-NMR, ESR and raman spectra, *Anal. Sci.*, 4, 233-239 (1988).
[2] T. Saito: Yuki kagobutsu no supekutoru detabesu (Spectral database for organic compounds), *Sansoken Today*, 7 (1), 36-37 (2007) (in Japanese).
[3] http://riodb01.ibase.aist.go.jp/sdbs/ (As of April 1, 2011)
[4] http://riodb.ibase.aist.go.jp/index.html (As of April 1, 2011)
[5] S. C. Chen: *Fragmentation and Interpretation of Mass Spectra*, China Medical University, Taiwan (2010).
[6] K. Ogawa, K. Sakakibara and S. Murata: *Kisokara Manabu Yuki Kagobutsu No Supekutoru Kaiseki*, Tokyo Kagaku Dojin, Tokyo (2008) (in Japanese).
[7] K. Hayamizu: An input tool by a personal computer for the NMR Spectral Database (SDBS-NMR), *J. Comp. Aid. Chem.*, 2, 1-10 (2001).
[8] O. Yamamoto, K. Hayamizu and M. Yanagisawa: Construction of proton nuclear magnetic resonance database system with full spectral patterns, *Anal. Sci.*, 4, 347-352 (1988).
[9] O. Yamamoto, K. Hayamizu and M. Yanagisawa: Construction of proton nuclear magnetic resonance parameter database system, *Anal. Sci.*, 4, 455-459 (1988).
[10] K. Hayamizu: Intanetto jo no supekutoru detabesu (SDBS) (Spectrum database (SDBS) on the Internet), *Busshitsuken NEWS*, 37, 3 (1995) (in Japanese).
[11] T. Nakamura: Kagaku busshitsu rinku center, samazamana kagaku busshitsu deta o wan sutoppude (Chemical substance link center, various chemical substances data by one stop), *CICSJ Bulletin*, 25 (4), 88 (2007) (in Japanese).
[12] T. Saito: Yuki kagobutsu no supekutoru detabesu *SDBS* (Spectral database for organic compounds), *CICSJ Bulletin*, 25 (4), 99-102 (2007) (in Japanese).
[13] K. Hiraizumi, N. Wasada, K. Tanabe, Y. Tamura, M. Yanagisawa and S. Ono: Kagobutsu supekutoru detabesu shisutemu (SDBS) no onrain sabisu (On-line service of compound spectrum database system (SDBS)), *Kagiken News*, 6 (1), 2 (1988) (in Japanese).
[14] K. Hayamizu, K. Tanabe, Y. Tamura, M. Yanagisawa and S. Ono: Kagobutsu supekutoru detabesu shisutemu (SDBS) no CD-ROM ban (CD-ROM version of compound spectrum database system (SDBS)), *Busshituken News*, 9, 6 (1994) (in Japanese).

Authors

Takeshi SAITO

Joined the National Institute of Materials and Chemical Research of the Agency of Industrial Science and Technology in 2000. Engaged in research for development and advancement of the Spectral Database for Organic Compounds (SDBS). Currently, member of the National Metrology Institute of Japan, AIST, where he has made extensive use of NMR in his research; he is a leader of SDBS project. Worked with a project conducted by the New Energy and Industrial Technology Development Organization (NEDO) on platform for measurement at nano-scale, focusing on measurement of particle diameter in liquid using NMR. Currently, working for improvement of precision and accuracy of quantitative analysis using NMR. Also works on the development of SI traceable reference materials using the NMR technique. Saito put together the overall of this paper.

Shinichi KINUGASA

Joined the National Chemical Laboratory for Industry, the Agency of Industrial Science and Technology in 1987. Section chief of the Polymer Standards Section at National Metrology Institute of Japan, AIST. Engaged in research on polymer characterization and development of polymer and nano-particle reference materials. Since 2001, in charge of IR spectrum of SDBS. Kinugasa also put together the overall of this paper with Saito.

Discussions with Reviewers

1 General evaluation

Comment (Shigeko Togashi, Evaluation Department, AIST)

The methodology of the database structure, the data accumulation, and the data release is described for the spectral database of organic compounds (SDBS) whose number of accesses from the outside is the most among the databases opened to the public by AIST, and the paper is considered a suitable research paper for this magazine.

Comment (Akira Ono, AIST)

The concept and processes of the database have been plainly brought together from the basic plan to the development, maintenance, and data release for a long-term project of 30 years. I think this research has brought about a suitable result for a public research organization like AIST in a wide research area covered from the *Type 2 Basic Research* to the *Product Realization Research*. Moreover, it can be said that the success in this project is shown by the enormous number of accesses from all over the world.

2 Analysis of access log and function as public goods

Comment (Shigeko Togashi)

Considerable user information should be obtained by analyzing access log of the database. The classifications of international or domestic users, of academic, public organizations, enterprises, or general users, etc. must have been recorded in the log. I think adding such classifications would be beneficial to the reader.

It is frequently emphasized in the paper that the database is "open to the public free of charge". I think releasing free useful information to the public that can be used widely as public goods is a crucial role for the public research institute. I think, as a paper of *Synthesiology*, it is beneficial if an independent chapter discussing these points is created.

Answer (Takeshi Saito)

About the access log, a figure which summarizes countries of accessing users and domains such as ".ac" and ".co" of domestic users is added.

We agree it is beneficial to discuss the topic of "open to the public free of charge". We created a subchapter, 4.2, and discussed the meaning of free services.

3 Persons and expenses for the database

Question (Akira Ono)

I would like to ask about the cost of development and data release of the spectral database for organic compounds of AIST. Would you estimate roughly costs and human resources spent in the development of hardware and software, sample purchases, acquisition of spectra, data maintenance and their quality control, and user support for the database, respectively?

Answer (Takeshi Saito)

Between years 2001 and 2007, the strategy of this database operations and development, and evaluation of the spectral data were charged to two researchers. Four contract staff were employed for acquisition of MS, IR and NMR spectrum data and maintaining chemical dictionary data. Each person was also responsible for maintaining the disclosing data. All the disclosure processes which opened the data through the Web, were maintained by the system engineers (SE) of the Research Information Data Base (RIO-DB) of AIST. Estimation of the total work load per year as a researcher was 0.25 person for the database system construction, 0.25 person for the spectral measurements, 0.8 person for the quality assurance, 0.25 person for the data maintenance and user support. Looking at the budget, 200,000 yen for constructing the database hardware, 1.5 million yen for the software construction, 250,000 yen for obtaining chemical compounds, 1.8 million yen for the consumable items and the maintenance of instrumentations, and 700,000 yen for the data maintenances were roughly spent each year. Besides this, we asked the SE to do much work, but we cannot estimate the cost of work done by them.

4 Balance of comprehensiveness, reliability and urgency

Question (Akira Ono)

(1) It has been described in this paper that it is important to make a balance between comprehensiveness and reliability of data for database construction. I understood that the primary objective of this database was to focus on compiling and offering standard spectral data to help identify compounds that were widely used. I also understood that you took a policy to limit information and measurements on compounds to the range which your group (AIST) could grasp and control. My understanding of this point was that you took a policy of taking the reliability of the data over the comprehensiveness so if the achievement of the comprehensiveness was postponed, it was considered unavoidable (or took a policy of "time would solve the problem of comprehensiveness"). Thirty years after the start of this activity, the database has reached a sufficient number of spectra (30,000 compounds). Is this a correct understanding?

(2) I think the spectral data for special compounds such as pesticides and deleterious substances are requested urgently by our society. It seems to me to be important to construct a spectral database for these and release the data to the public. Is there any organization in the world which releases such data? I would like to ask whether the current situation of such a database is satisfactory to the users.

(3) If it is not satisfactory, the current policy of AIST may not be speedy enough to cover a large number of spectra in a short period of time. I think spectral information of pesticides and deleterious substances need to be covered more comprehensively and rapidly even if you lose some reliability. I would like to ask how the authors think about this point.

Answer (Takeshi Saito)

(1) It is true that as a result of having given the priority to reliability over comprehensiveness, it was not possible to increase the quantity of data rapidly. As a result of having actively compiled the data for a long period of time, the database now contains more than 100,000 spectra from more than 30,000 compiled compounds. We think the compounds that are widely used have been covered by now.

When limiting it to NMR, increasing the data bulk and speeding up the data release had become difficult and the work load had almost reached the limit of capacity of our human resources and instrumentations. We not only acquired the spectra but also assigned them for data release. We think another reason obstructing comprehensiveness of spectral data other than NMR was budget that was too limited to collect enough compounds for the data acquisition.

(2) The mass spectral database of medicine, poison, pesticides, and contaminants is offered from the John Wiley & Sons Co. as a set of CD-ROM and a paper book format, and the IR spectral database of pesticides and environmental materials is offered from the Bio-Rad Co. I do not think a database of spectral data of compounds classified as deleterious substances exists because it is a classification based on Japanese law. We believe, although there is no such classifications, many databases cover such compounds in their data entry. However, as we think the situation is not satisfactory to the users, this database will keep collecting such spectral data.

(3) There is a limit in our current resources for compiling urgent data quicker just by cutting down the reliability of the spectrum. For achieving this, we think a project with priority on acquiring, evaluating and releasing the spectra of such compounds that have high urgency is useful. Another way to achieve this is to collect spectral data from people all over the world as an open data recruit system. To make this possible, we have to build up at least a standard spectral data format, data evaluation criterion, and data submission protocol for our database. With instructions covering our requirements, we should be able to collect spectral data with a certain quality much more quickly.

5 Digital data format and copyright

Question (Akira Ono)

I understood that all data were managed digitally in the development site while these were converted into analog format for the data open to the public so that the users from the Web were unable to access the digital data. Is this correctly understood?

The reason for a user not being able to access the digital data is because the spectral data acquired by AIST is copyrighted. When a third party requests to use the data, they have to pay a royalty. Is this correctly understood?

Answer (Takeshi Saito)

When the "digital data" in the question is "data consist of coordinate point information" and the "analog data" is a "GIF image data", then your indication is correct.

The main reason for the users not being able to reach the digital data format is not because of the rights or the royalties of copyright that we may receive but is for the protection of the copyright. This is based on the protection of SDBS from unjust imitations and of others making profit by using the imitated spectral information of SDBS. The digital data have high workability so reproduced materials from the data have a high commercial value. If most of the digitally compiled spectral data were copied by others, they can construct a spectral database similar to SDBS or may be able to create more valuable database from the data. This is a menace for SDBS. We think even if the copyright infringement is recognized and can be appealed in court, we must spend considerable time and effort on the suit. Large amount of data copy is a copyright infringement even if the data is in GIF format and may cause SDBS to be in a threatening situation. Therefore, user access from the Web is monitored all the time.

When a third party wants to use data in the digital or the image formats, the licensing from AIST is necessary. In the case where the party wants to sell the data, they have to pay a royalty to AIST. We think this is a different point from the copyright in disclosing the data in the Web. We are not allowed to name names because of secrecy agreements, but we have several experiences of offering a large amount of data at a time, and in each case we have received payments of royalties based on the contracts. In the case of IR spectra, we have a contract to offer data with royalty when we release new spectral data. We also have experience of offering GIF image data to a database operated in the United States of America.

6 Comparison with other spectral databases

Question (Akira Ono)

I think there are spectral databases besides this one in the world, especially, those distributing the digital spectral information to private companies with a fee operated by private companies. Would you introduce such databases, and instruct us of the differences in roles and characteristics from this database?

Answer (Takeshi Saito)

There are not many spectral databases that are open through the Web. When looking at such free databases opened to the public, the number is very limited. We have not encountered a free accessible spectral database with this many ^{1}H NMR spectral entries with their spectral patterns and chemical shift assignments.

One of the free accessible databases on the Web is NIST Chemistry WebBook (http://webbook.nist.gov/) operated by the National Institute of Standards and Technology, NIST. This database compiles a variety of physical chemistry data as well as spectral data. This database is similar to RIO-DB of AIST because most of the data compiled in the WebBook are based on the research products of NIST. Besides 15,000 MS and 16,000 IR spectra, the WebBook compiles other spectra like an ultraviolet-visible absorption spectrum and a terahertz spectrum. There is no need to install software to browse the data of the WebBook. Spectra and other information are compiled along with the compound information, which you can search. We do not have a list of compounds compiled in the WebBook, however, it is our presumption that many generally used chemical reagents are compiled. This database works much like our database that serves as that of a public organization. MS data was sold as NIST 08 Mass Spectral Library which was released in 2008. Many spectral data were obtained at National Institutes of Health (NIH) and United States Environmental Protection Agency (EPA) and were evaluated at NIST. The data can be purchased for use on an independent personal computer (PC). The number of data compiled in this database is about 220,000 spectra for 190,000 compounds, which is much more than those open through the Web. When we did collaborative research with NIST during our former Agency of Industrial Science and Technology era, many of our MS data were compiled in the NIST MS Library. These data must have been included in the NIST Mass Spectral Library. This data library can be searched with a fee with MS spectral patterns obtained by many kinds of MS spectral instruments.

SpecInfo releases data through the Web with access charge, and it consists of 90,000 ^{1}H NMR, 300,000 ^{13}C NMR, and many multinuclear NMR, IR and MS spectra. Data update does not seem to have been performed since 2006.

Looking at a domestic site, MassBank (http://www.massbank.jp/) which is a high resolution mass spectral database of metabolites is open free to the public. As of April 05, 2011, almost 31,000 spectra from 20 research institutes have been compiled. Target compounds are specified and limited to metabolites. Users of this database should download special software for this database, and install it on their computers. This software enables you to search, browse, display full and expanded spectrum, and register spectral data to the database. The database construction was initiated and has been supported by the project, “Integrated Database System for Metabolomics”, under the Institute for Bioinformatics Research and Development of Japan Science and Technology Agency since 2006. As our database started with a research project and had developed into a solid base of our activity, we look forward to seeing how MassBank will be developed after this project is finished.

Databases from Bio-Rad are using a non web platform. The database covers data of SpecInfo, NIST MS Spectral Library in addition to Sadtler spectral data. Our NMR spectral data are also compiled. This database is sold as a package of data and software for handling the data, “KnowItAll”, that needs to be installed on a computer. The compiled data are about 50,000 ^{1}H NMR, 430,000 ^{13}C NMR, 190,000 MS, 7000 Raman, and 230,000 IR spectra. Of our data, 13,000 and 11,000 ^{1}H and ^{13}C NMR spectra, respectively, are included. Users can use a spectral pattern for spectral search, search for mixtures, and more complicated searches can be performed with the software.

Sigma-Aldrich sells “Sigma-Aldrich Spectral Library” which has a total of more than 50,000 compounds of NMR, IR and Raman spectra. There are two formats of data on a computer and as a book.

When comparing a database operating on the Web and on an independent PC, there exist both advantages and disadvantages for each. For example, an advantage of the Web based database is instantaneousness. Our database can perform data addition and update easily; our database is updated twice every year to supply new data to our users. Many of the other databases introduced here do not seem to update their data that often. On the other hand, a database on the PC has better usability. For example, spectral pattern matching search can be done which many users find useful.

Challenge for the development of micro SOFC manufacturing technology

— Compact SOFC using innovative ceramics integration process —

Yoshinobu Fujishiro*, Toshio Suzuki, Toshiaki Yamaguchi, Koichi Hamamoto and Masanobu Awano

[Translation from *Synthesiology*, Vol.4, No.1, p.36-45 (2011)]

Realization of highly efficient SOFC (solid oxide fuel cell) modules, which are compact and capable of quick startup and shut-down operation, is strongly expected because it would be useful to solve environmental problems. In order to yield new outcomes in new energy production industry market, we have carried out continuous R&D directly linked with the original idea, trial production, and evaluation by using the ceramics integration manufacturing platform. In consequence, original, compact and high-power SOFC modules operable at low temperature have been realized by upgrading of function-structure integration technology. These are drawing attention as products of ingenious technology. This paper presents, in addition to industrial needs, approaches and methods in industry-academia-government collaborative research to overcome tasks toward productization.

Keywords : Ceramics processing, ceramic integration technology, energy conversion, fuel cell, micro SOFC, energy module

1 Introduction

The development of the technology for a low-carbon society by shifting from fossil fuel to clean energy is a global concern for humankind. As shown in the Japanese energy statistics, the demand and use of energy to support the social infrastructure are increasing every year. There is an increasing emphasis on technologies that do not use fossil fuels, such as the unused energy of waste heat as well as recyclable solar cells[1]. Particularly, the fuel cell technologies that enable the use of hydrogen energy is gaining attention as the energy management by electrochemical energy conversion that does not emit CO_2. The principle of the fuel cell technology was proposed by Sir William Robert Grove of the United Kingdom in 1893. With the advancement of electrodes that enable electrochemical reaction and technologies for ion-conducting electrolyte materials, the fuel cell technology was put to practice as the power generation technology, initially for plants in the beginning of the 20th century. The commercialization of home-use cogeneration and automobile generator is starting now. As more facilities will be powered by fuel cells, a drastic reduction in CO_2 emission by 5 million kW level cogeneration is expected by the year 2030[1].

In the development of fuel cell technology, various R&Ds using the electrolyte materials as core technology are being conducted actively as shown in Table 1. Currently, the developments are mainly for polymer electrolyte fuel cells (PEFC) that can be handled easily and solid oxide fuel cells (SOFC) that have high generation efficiency[2].

In the history of the development of materials for SOFC that used ceramic material, the developments were done for electrolyte materials such as zirconium (zirconium oxide) that employed the ion-conducting property of oxides at high temperature range, as well as the cermet electrode materials that combine the catalyst materials and various ceramic electrodes with mixed conductivity. The developments for manufacturing flat or cylindrical ceramic cells and for manufacturing module stacks were led by Japan[3]-[5]. Until now, the nickel electrodes were developed for temperature ranges of 700 °C or higher because the characteristic of SOFC is the utilization of direct reforming reaction of hydrocarbons at high temperature range, and high energy conversion can be achieved with fuels other than hydrogen. Therefore, compared to the low-temperature PEFC, in the conventional SOFC modules, it was necessary to increase the operation temperature and generation surface area by reducing the cell resistance to obtain high power generation. As the module increased in size due to increased generation surface area, a technological issue developed where rapid startups and shutdowns could not be repeated due to thermomechanical stress. On the other hand, since excess generation could be controlled by startup/shutdown depending on the power load, the realization of SOFC module that could be started up or shut down rapidly and was operable at low temperature was highly in demand[2]. If such flexible operation became possible by overcoming the technological issues of downsizing and lower generation temperature, the CO_2 emission could be reduced further. Also, if the operation temperature of the module were lowered, low-cost metal materials could be used.

In this paper, we describe our efforts in solving the various R&D issues that were presented as challenges for the

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Table 1 Types and characteristics of fuel cells

	Electrolyte material	Operating temperature	Characteristics	Generation efficiency
Solid oxide fuel cells (SOFC)	Oxide ion-conducting ceramics	500-1000 ℃ (point is achieving high performance at low temperature range)	Electrode resistance is low since it operates at high temperature, and the cell performance is high. Major improvement in efficiency is possible by altering the fuel quality by using waste heat. It is expected to be future dispersed power source.	40-70 %
Polymer electrolyte fuel cells (PEFC)	Proton-conducting polymer film	Room temperature ~ about 90 ℃	Easy to handle due to low operating temperature. Research is active for use at home, in automobiles, and in portable devices, and commercialization has been achieved in some fields.	~38 %
Molten carbonate fuel cells (MCFC)	Molten carbonate	600-700 ℃	Can be up-scaled easily. Biogas produced from garbage and wood can be used as fuel. Separation of CO_2 is possible.	45-60 %
Phosphoric acid fuel cells (PAFC)	Phosphoric acid	160-220 ℃	Developed for commercial use among fuel cells currently available. It has also been used for dispersed power source at plants.	35-42 %

Reference: J. Larmine and A. Dicks: *Fuel Cell Systems Explained*, Wiley (2003)
[H. Tsuchiya trans.: *Kaisetsu Nenryo Denchi Shisutemu*, Ohmsha (2004) (in Japanese)].

revolutionary micro SOFC manufacturing technology that uses the ceramic integration process technology.

2 Status of the development of energy module technology ~ Expectation of industry for compact fuel cells with high power density and operable at low temperature

As shown in Fig. 1, the industrial demand for highly efficient energy conversion at several W to several kW levels increased due to the diversified use of SOFC in various industries. The expectation is high for the compact SOFC technology that can be easily handled and is space-saving.

In order to promote the use by expanding the operating condition of SOFC as an electrochemical module made of ceramic material, it was essential to develop the micro SOFC technology that would allow rapid startup/shutdown with equivalent performance at lower temperature range of 650 °C or less compared to the conventional operating temperature (700 °C~1000 °C). The micro SOFC is a power generation technology for palm-top cells that is smaller in size compared to the conventional ones, and it enables compact module design that also is space saving. Therefore, we embarked on the micro SOFC technology development to solve the various technological issues. Figure 2 shows the advantages of the micro SOFC. In general, since the oxide ceramic material had smaller heat conductivity compared to metals, a steep temperature gradient occurred throughout the cell during temperature increase (particularly during rapid increase) when the volumes of integrated module and ceramic electrochemical cell increased, and this could cause the destruction of the cell or the module parts. One of the technological solutions was to employ a design that reduced the volume of the cell or the module parts to decrease the relative temperature gradient, as shown in Fig. 2. This reduced the startup energy, and allowed the temperature distribution of the SOFC to be easily controlled at the same time. As a result, high thermal shock resistance was obtained for the cell and the module. In planar cell module, since the generation density per volume of the unit decreased by reducing the cell volume, it was necessary to increase the performances such as the generation efficiency and power density. To do so, it was necessary to develop a new high integration manufacturing technology that could be mass produced and could increase the generation performance per volume, by increasing the electrode surface area and by controlling the unit structure such as the diameter using small tubular cell as shown in Fig. 2. Setting several W to several kW level as our output target, it was important to develop the construction technology of the module that fit within 1 L size even at 2 kW level that surpassed the performance of the PEFC. As the output power increased, the temperature control of the module became difficult. Therefore, the cell integration module technology that enabled low temperature operation and easy control of startup/shutdown was demanded.

The SOFC module is composed of dense oxide ion-conducting ceramics electrolyte, electrodes (anode and cathode) that enhance the electrochemical reaction, and

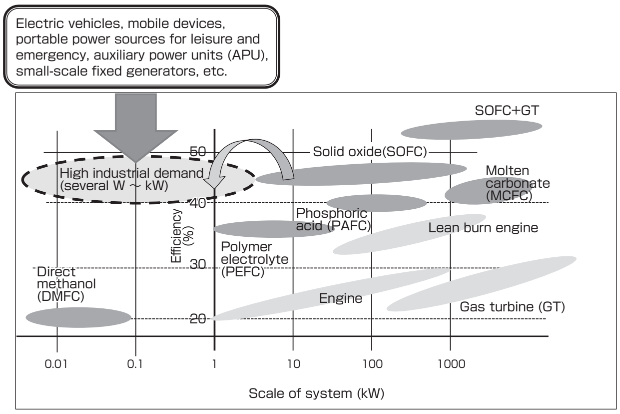

Fig. 1 Industrial development of micro SOFC

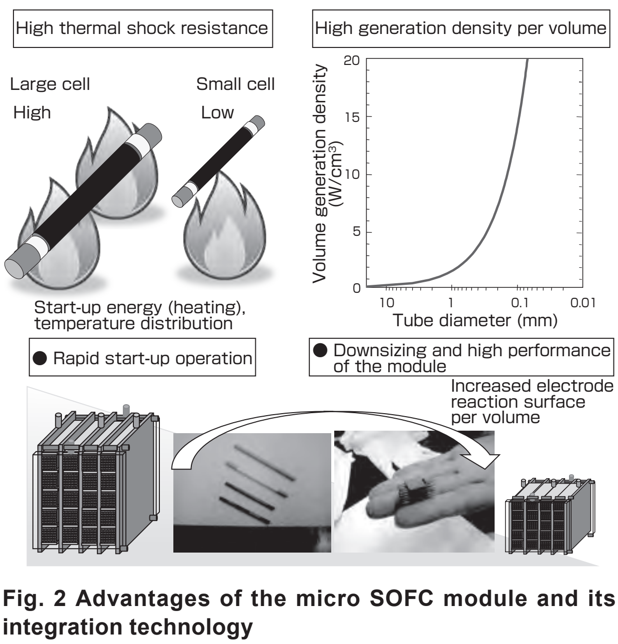

Fig. 2 Advantages of the micro SOFC module and its integration technology

fuel or oxygen (air). To create a unit structure of ordinary SOFC, the ceramic members are manufactured by forming the ceramic powder that exerts various functions into required shapes, by coating and laminating, and then firing. Therefore, according to the shape and size of the cell and integrated module, various ceramics manufacturing process technologies are employed. Moreover, since the cell and integrated modules are manufactured by multiple lamination of various functional materials with different thermal expansion, electric, and strength properties, the design of each material at nano-,micro- and macro-size levels and structural control in the fabrication process strongly affects the final power generation performance.

The challenge for the integrated module using the new micro SOFC was a difficulty of the ceramic manufacturing process technology, and it was necessary to return to the manufacturing of the cell and integrated module as ceramic parts. However, it would take too long a time to develop if we built the individual elemental technologies one at a time. It was necessary to conduct the development of ceramic parts with thermal management properties and ceramic material with electrochemical structure that increased the generation performance at low temperature, as well as the revolutionary manufacturing technology.

With such a background, the "center for the development of functional ceramic manufacturing technology" was established and the R&D was conducted under the "ceramic integration manufacturing process technology" of the "The Advanced Ceramic Reactor Development (subcontracted by NEDO, 2005-2010)" to realize the new product and to solve the issues of the highly integrated micro SOFC manufacturing technology[6][7].

As shown in Fig. 3, the PDCA of design-manufacture-analysis was conducted at the center for the development of functional ceramic manufacturing technology, and the core technology and the product realization technology were developed simultaneously. As a result, the open innovation system where the engineers and researchers of the ceramic manufacturing companies and user companies collaborated was established. As an output, it functioned as the opportunity to train industrial human resource where people could obtain academic degrees as well as produce research results. Specifically, for the development of highly integrated ceramic electrochemical module based on the new concept such as the realization of high-performance SOFC at low temperature, of integration, of high performance, and of mass production, the developments were done from the material selection and cell design (manufacturing design such as structure and size) to the prototype cell and module fabrication (structural control process in clay forming, coating, firing condition, etc.), the establishment of original evaluation and analysis technology for the new cell and module structure (thermal behavior, electrochemical property, generation property), and the general evaluation of the cell and module (improvements in structure and manufacturing process). These were discussed directly among the engineers and researchers of the manufacturer and user companies at the center. Proposals were made for the new process technology, the structural control technology upon discovery of a new phenomenon, and the utilization of new technology in industry. Through collaborations between the researchers and the corporate engineers, a flow was built toward the solution of issues for the new highly integrated module prototype and the development of materials and the elemental process technologies.

In the R&D at the center, the development of fine ceramic manufacturing process was done in collaboration with the ceramics industry in the Chubu region that has traditionally engaged in this industry. They helped build and accumulate the manufacturing technology. An optimal cycle of

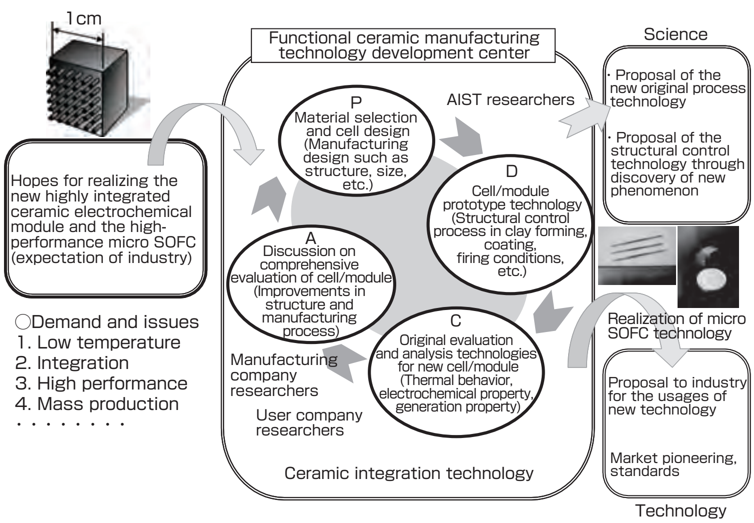

Fig. 3 R&D model for the new micro SOFC module manufacturing technology

prototype manufacture, evaluation, and analysis was set forth toward the mass production of high-performance fuel cell materials that used to be considered unsuitable for the forming technology. Moreover, since the investigation of the structural control that determined the optimal condition was done concurrently with prototype evaluation, the new high-performance micro SOFC and the highly integrated compact module manufacturing were developed in a short time.

3 Issues in manufacturing the micro SOFC for the high-efficiency compact energy module ~ Valley of death in product realization and the solution

For the micro SOFC and integrated module manufacturing technology that was not available before, it was necessary to develop the ceramic manufacturing process that could be mass produced industrially, the electrochemical design of the module of highly integrated micro SOFC, and the technologies for increasing performance. As a new manufacturing process technology under the concept of fusion of function and structure, we shall explain the manufacturing design in the R&D model of Fig. 3 and the development of new structure control process technology.

i) Highly integrated micro SOFC manufacturing and design technology

To increase the performance of the SOFC module, it was necessary to increase the electrode surface area per unit module volume, raise the degree of cell integration, and improve the mechanical strength. For the structure that fulfilled such requirements, it was advantageous to achieve high integration by both the bottom-up manufacturing where the unit cell members were combined and highly integrated, and the top-down manufacturing where the cell structure was built in later using the regularly arrayed micro-channel. To increase the performance of micro SOFC which made use of the conventional manufacturing technology of tubular SOFC, the bottom-up structure of development of the high integration of tubular SOFC was effective. On the other hand, to reduce the cost of module manufacturing and to achieve advanced cell integration structure, it was necessary to develop a new technology where the module with equivalent performance obtained in the bottom-up manufacturing was made by top-down manufacturing. In this R&D, considering the high performance and cost reduction, the R&Ds were conducted for the two types of module manufacturing technology including the tube integration module and the honeycomb micro SOFC.

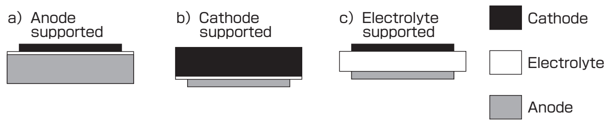

Fig. 4 Structure of various fuel cells

To bring out the advantages of high efficiency and high power density in SOFC power generation, we needed to consider the technologies to improve the reactive surface area of the electrode to enable effective progression of the electrochemical reaction of the supplied fuel, as well as the module structure that allowed the integration of current and gas flow. Ultimately, it was mandatory to select the manufacturing process technology in a form that could be mass-produced, as several cells were needed for high integration. For the reduction of cell resistance that enabled high performance at low temperature range, the support structures of the Anode, Cathode, and the electrolyte were crucial, as shown in Fig. 4. This was because the resistance became minimum in the cermet anode that was partially metalized by reduction. The tubular integrated body with high symmetry of stress distribution was superior to the planar structure as a unit structure that achieved the mechanical strength and also improved the relative surface area of the porous electrode by increasing the degree of integration.

As researches for similar microtube SOFC, there have been studies on rapid startup using the YSZ electrolyte supported SOFC at 2~5 mmφ level with high thermomechanical strength[8][9]. However, there were very few developments for the manufacturing technology for high performance such as achievements at low temperature range of 650 °C or less or the development of small integrated modules. Our challenge was to manufacture high-performance SOFC and integrated modules unseen before, and therefore, we investigated the manufacturing technology of the integrated modules composed of anode supported micro SOFC. Moreover, although there were only a small number of studies since the mechanical strength was low and forming was difficult, we developed the manufacturing process using ceria electrolytes with high oxide ion conductivity at low temperature.

As the technologies for manufacturing and design of the microtube SOFC and integrated module with fuel gas pores

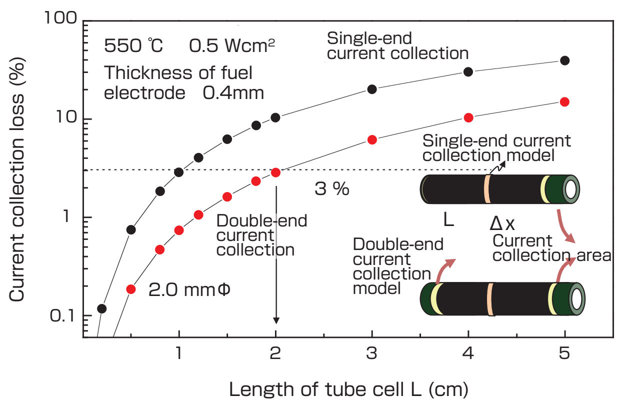

Fig. 5 Design model and the results of current collection loss calculation for the integration of the micro-tubular SOFC design technology

of 2 mmφ or less, the optimization of the cell form (thickness of electrolyte and electrode, optimal cell length, etc.) that affected the final module generation capacity was important. In the anode supported cell, because the electrode has the roles of reactive field in the three-phase boundary for the electrochemical reaction and of the collector of current generated in the reaction, its design greatly affected the generation performance of the cell and integrated module. Figure 5 shows the results of the different power collection methods and the cell form for achieving high performance in the Anode supported microtube SOFC and its integrated module. The results were used to design the length of the cell collector. The collection resistance increased when the long cell design was used to extend the electrode surface area of the single cell structure, and the power generation output decreased (current collection loss).

The design technology needed to manufacture the microtube SOFC with exterior diameter 2 mmφ (interior diameter 1.6 mmφ, electrode film thickness of 0.2 mm) is explained. Assuming the generation performance to be 0.5 W/cm^2 at 550 °C, the current collection loss in the equivalent circuit was calculated using the single-end and double-end current collection models. The relationship of the current collection loss arising from the current collection resistance factor and cell length is shown in Fig. 5. When the length whereby the current collection loss in power generation would be 3 % or less was calculated, it was found that the integrated module must be designed with cell length of 2.0 cm for double-end current collection and 1.0 cm for single-end current collection. This showed that it was necessary to increase the thickness of the double-end current collector and anode in order to increase the surface area of the generation electrode by increasing the cell length[10]. Conversely, since it was necessary to decrease the electrode thickness to increase the cell performance, the cell length optimization was important to improve the integrated module generation performance at low temperature. Under such design guidance, the integrated module manufacturing technology was developed by bottom-up design, and the mass-producible cell manufacturing was developed by improving the film coating technology and the forming precision in the extrusion technology[11]. As a result, the anode supported micro SOFC using the 2.0 mmφ ceria electrolyte achieved a high power density of 1.0 W/cm^2 at 570 °C[11]. Moreover, this high-performance cell (microtube cell) was combined to fabricate the module structure integrated inside porous ceramics, and the optimal cell arrangement within the module was studied by similar equivalent circuit simulation design. As shown in Fig. 6, by calculating the current collection loss in the integrated module model, it was found that the conductivity over 100 S/cm was required at cell interval of 1.0 mm for the current collector members (between cells). The 2 W level generation unit was realized where several microtube SOFC with 2.0 mmφ diameter was integrated in a space the size of a sugar cube. In this investigation, the design and manufacturing technology for the integrated module (cube module) with generation performance over 2 W/cm^3 at 550 °C was developed, and it became possible to fabricate various integrated module structures such as of the serial connection[12].

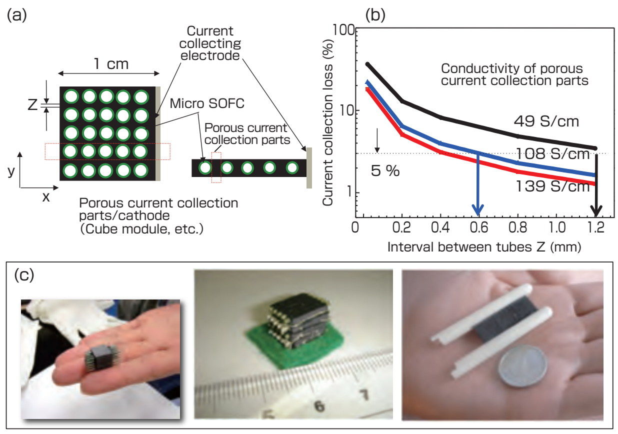

Fig. 6 Cube module design and the developed integrated module
a: Design model of integrated module
b: Result of current collection loss calculation at 650 °C
c: Example of developed module

ii) Cell structure control technology in the advanced coating process

In achieving high performance for the SOFC and integrated module, it was necessary to develop the manufacture process technology that could be applied to macro connections by creating the multilayer structure of different materials such as ceramics electrode and electrolytes based on the electrochemical structure design at nano to micro size. Moreover, it was necessary to develop a simple and mass-producible manufacturing technology such as wet coating that could effectively control the degree of cell integration without being influenced by the composition of base material on which the cells were arranged. For the manufacture of electrodes for the ceramics electrochemical device such as SOFC, new developments of the various cell forms, composition control, and layer structures were necessary, and both the coating technology with high degree of freedom to form functional ceramics and advanced 3D coating technology had to be established. The increased density and formation of the electrolyte film and the structural controllability in cell structure formation had to also be increased. To form the film structure necessary to increase performance, we embarked on the development of the manufacturing process technology that allowed even slurry coating in sub-millimeter 3D space, by advancing the new wet coating manufacturing process technology.

Figure 7 shows the characteristics of the various wet ceramics coating processes. For the wet paste coating on ceramic base material, the control technology for forming the dense electrolyte at single μm thickness was realized for the tubular cell using the dip-coating method[11]. In ordinary dip-coating method, the film formation on the exterior of the base material such as the tube was possible. However, when the electrochemical functional layer had to be formed on the interior wall of the microspace, application of an even coating on the whole surface was difficult, as the slurry would not penetrate deeply due to the balance of viscosity resistance and capillary force. The space could be filled with the slurry by flooding the interior by slurry aspiration method and then spewed out, but the film on the interior wall became thick and uneven, and the coat volume could not be controlled as the number of pinholes increased. To solve these coating process issues, a unique coating process called the slurry injection method was newly developed, where the external force that counteracted the capillary force was added to the coating paste, and the coating volume was controlled by forcefully moving the paste material[13]. With this new top-down manufacturing technology, it became possible to use the microspace in the honeycomb structures with regular 3D pinhole arrays of sub-millimeter diameter, and to form the even multilayer film with controlled film thickness. This method was important for the fabrication of the integrated module structure and for cost reduction by reducing the number of members. In the developed process, the even film coating could be formed on the substrate under the same control condition even in corner areas where the liquid tended to collect during the coating process. The controlled functional layer could be formed in the micropore with sub-millimeter diameter on the ceramics base material, using a simple coating process regardless of the shape of the pore. This developed process technology was adapted to the multilayer coating of the ceramic electrochemical structure of the electrolyte and electrode layers. By utilizing this process for the cell formation in the regular array structure with sub-millimeter diameter, the top-down manufacturing method allowed the fabrication of the electrode unit with regular array of pores in the sub-millimeter space by using the honeycomb extrusion technology, and then later forming the multilayer cell structure such as the dense electrolyte film and porous electrode by combining the coating technology.

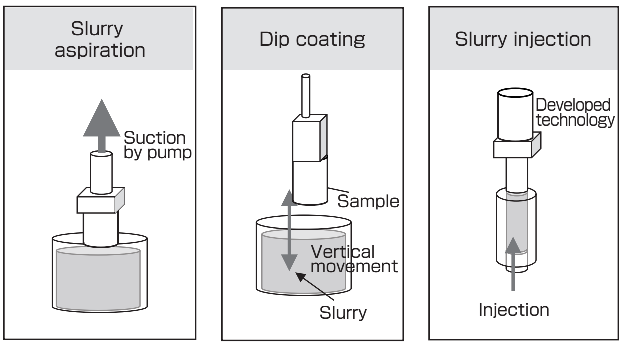

Fig. 7 Wet ceramic coating technology

Table 2 Technological indices for the developed micro SOFC technology

	Cell diameter (mmφ)	Electrolyte material	Start-up temperature (℃)	Power density (W/cm^2) at 0.7 V	Start-up speed (℃/min)
Developed micro SOFC technology	Exterior diameter: 0.8-2.0 (Interior diameter 0.4-1.6)	ScSZ, GDC	550 – 650	0.5 – 0.8* @ 650 ℃	65 – 217**
Korea Institute of Energy Research (Korea)	Exterior diameter: 10.0	YSZ	750	0.45	20
Adelan Ltd. (U.K.)	Exterior diameter: 2.0	YSZ	850	0.3	200

ScSZ : 10 mol% Scandia-stabilized zirconia, YSZ : 8 mol% Yttria-stabilized zirconia, GDC : 10 mol% Gadolinia doped ceria

Reference) Data updated based on V. Lawlor, S. Griesser, G. Buchinger, A. G. Olabi, S. Cordiner, D. Meissner: Review of the micro-tubular solid oxide fuel cell, Part I. Stack design issues and research activities, *Journal of Power Sources*, 193, 387-399 (2009).

* Data for 2.0 mmφ ScSZ electrolyte micro-tubular SOFC

** Demonstration data for honeycomb SOFC

Using this technology, the dense electrolyte with thickness 10 μm and the electrode with tens of μm thickness on the bulk body (40 cm^2/cm^3, relative surface area per volume about 20 times the conventional flat SOFC) where there were hundreds of spaces at 0.5-1.0 mm*φ* diameter were successfully formed, and the new honeycomb micro SOFC was developed[13].

The design-to-manufacturing process technology that was important for the integration of the micro SOFC module was built as the top-down and bottom-up manufacturing technologies, and the new manufacturing technology was presented for the 3D integrated structure in the ceramic electrochemical device manufacture.

4 Realization of the new low-temperature operable micro SOFC manufacturing technology through revolutionary ceramics manufacturing technology ~ Conversion to full-fledged integrated module

We could now fabricate an original unprecedented micro SOFC, based on the new high-performance micro SOFC design and manufacturing technology. As a result, high performance of the micro SOFC technology was achieved in the technical indices such as size, power, temperature reduction, short startup time, and others, as shown in Table 2[14].

To increase generation performance at the low temperature in micro SOFC, the reduction of the structural resistance factors such as the reaction dispersal and ohmic resistance of the cell and integrated module was essential. Much attention was devoted to the film forming technology of the electrolyte layer involved in the reduction of the resistance factors, the analysis of material contraction behaviors in the aforementioned slurry dip coating process, and the co-sintering of laminated material. We succeeded in forming a flawless solid electrolyte film with thickness of single μm in the cycle of the R&D model shown in Fig. 3. Also, the electrochemical reaction resistance and the reaction dispersal were confirmed in detail through the original evaluation and analysis of the micro SOFC prototype using the zirconia electrolyte (ScSZ: Scandia stabilized zirconia) at temperature lower than 650 °C for which there were few precedents. In the low temperature range, it was newly found that the resistance factors of the fuel cell changed according to the operation condition and contributed greatly to the increased generation performance. As shown in Fig. 8, by the optimization of the ceramics manufacturing process, high porosity surpassing 50 % was realized for the anode, and it was found that this greatly reduced the reaction resistance of generation at low temperature range. Figure 8b shows the relationship of the porosity of anode and the cell impedance resistance value at 600 °C. As shown in Fig. 8b, it was confirmed that the reduction resistance values represented as arcs decreased in relation to the increase of porosity of the anode. As a result, the output power performance surpassing 1 W/cm^2 was realized in the low temperature range of 600 °C, as shown in Fig. 8c. From the post-reaction observation of the electrode structure, it was thought that the reduced nickel became nano particles in the electrode structure with high porosity, a high dispersal structure was formed, and this led to the increased number of three-phase boundaries that provided the active sites[15]. For the realization of this technology, the major factor was that the ceramics companies and others were able to achieve high properties at the cell manufacture level through the extrusion and wet coating processes that enabled mass-production and cost reduction. By considering the manufacturing process technology that incorporated the PDCA cycle in the R&D model in Fig. 3, we were able to achieve the micro SOFC manufacturing technology at low temperature range of 600 °C with the same performance as the zirconia electrolyte SOFC with power density 1 W/cm^2 at 700−800 °C[16].

Attentions were drawn in Japan and from abroad to this highly integrated module of fingertip or palm size that was distinctly different from the conventional energy module. Through the manufacture and evaluation in collaboration with user companies, it was demonstrated that these cells could be used to manufacture integrated modules of several hundred W level and were capable of realizing efficiency surpassing 40 % as fuel cells[17]. The future issues will be the development of kW class modules using the integrated modules composed of the developed microtube SOFC, as well as the development of the low-cost manufacturing technology.

In the honeycomb micro SOFC development shown in Fig. 9a, it is necessary to create the electrochemical module of the integrated cell and to ensure the gas seal between the honeycomb SOFCs. As shown in Fig. 9b, a new integrated module technology was developed to handle rapid thermal history utilizing the thermomechanical property that was the stronghold of the honeycomb structure by forming the joint structure using the silver-silica paste as the interconnect. It became possible to manufacture an arbitrary serial structure unit by combining the highly integrated structure of several hundred cell/cm^3 using this SOFC module technology. Also, by utilizing the easily warming property of the micro SOFC structure that has high relative surface area and low relative heat capacity and by confirming the electromotive force and current value, as shown in Fig. 9c and 9d, we proposed the micro SOFC module manufacturing technology that could handle 3-5 minute rapid startup, which was one of the required technical issues[18]. Also, the output power performance per unit volume at 650 °C was 2.8 W/cm^3 or equivalent to the tubular integrated module, and high conversion efficiency could be expected for the SOFC. The

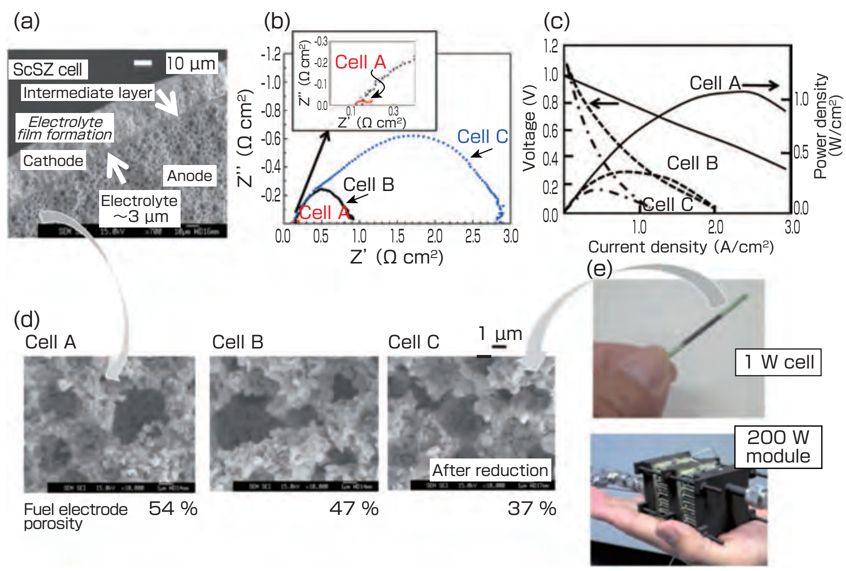

Fig. 8 Realization of zirconia low-temperature micro SOFC module
a: Photograph of cell cross section
b: Relationship of electrode porosity and electrode resistance (600 °C)
c: Generation performance (600 °C, humidified hydrogen)
d: Structure of developed porous fuel electrode
e: Example of developed cell and integrated module

development will continue for easily usable and inexpensive SOFC module utilizing the advantages of high cell integration and rapid startup of the honeycomb micro SOFC, and our aim will be the increased generation performance of the module through seeking solutions for issues such as low temperature.

The developed cell and integrated module technology was a unprecedented totally new ceramic integrated structure composed of small extruded members unseen before, and there were many comparisons with the conventional technology right from the start. Particularly, questions were raised concerning the generator density and generator module structure, that it may not be possible to create a generator module for practical use if the performance is merely the same as the current cells and integrated modules. On the other hand, the micro SOFC achieved the high power density of the same level as 800 °C in the low temperature range of 500−650 °C, and academically significant experimental results were accumulated since the strategic design ~ material and manufacture process technology ~ evaluation technology were rebuilt for the cell design and its realization. This technology realized the module structure for low temperature generation through electrical serial structure and sugar cube size 2 W/cm^3 module. The expectations for a readily usable, compact SOFC module are high.

5 Summary ~ Product realization and creation of a new market

In the future energy-related manufacturing industry, the micro SOFC and integrated module technology is an important technology that utilizes the advanced ceramic materials and manufacturing technology at the level of nano-micro-macro size for which Japan takes the lead. On the other hand, the SOFC technology is mainly geared for the fixed power generation facilities. Our micro SOFC manufacturing technology has cleared the low temperature, rapid startup, sufficient output power, and compact size that are necessary for the module for power generation, future automobiles, portable generator technology, and is geared for new innovations and product development. At this point, the generator module fabrication for several tens W to several hundreds W level have been demonstrated. Currently, the technological issues according to usage are being organized, and developments are done toward high performance with multiple fuel and module fabrication at kW level. It is also possible to propose the usages to industry taking advantage of the characteristics of the micro SOFC. One proposal is the range extender technology using the vehicle-mounted power generator and hybrid technology that uses the internal combustion engine to extend the cruise distance of the electric vehicle that is now being developed aggressively[19]. Our compact generator module can be used in the power source technology as the high-efficiency generator module that can achieve the energy conversion efficiency of 50 % or above (well-to-wheel) that surpasses the limits of the internal combustion engine[19]. The development of fuel cells that do not dependent on hydrogen infrastructure using the advantages of SOFC multiple fuel use is drawing attention. In the future, further improvements must be made for the rapid startup/shutdown properties and the reliability of performance with multiple fuel use, and the technical issues for the requirements of the mobile generator module must be extracted and solved. The development of a safe and low-cost module is an important subject in the future nanotechnology material and manufacture. The priority will be to deliver the easy-to-use, low-cost fuel cell technology to as many industrial fields as possible, for the efficient use of resource and energy and for the realization of a low-carbon society. To do so, it is necessary to continue the development in many industrial fields for the new micro SOFC and its integrated module for which our experience was accumulated by tackling the problems at the center for the development

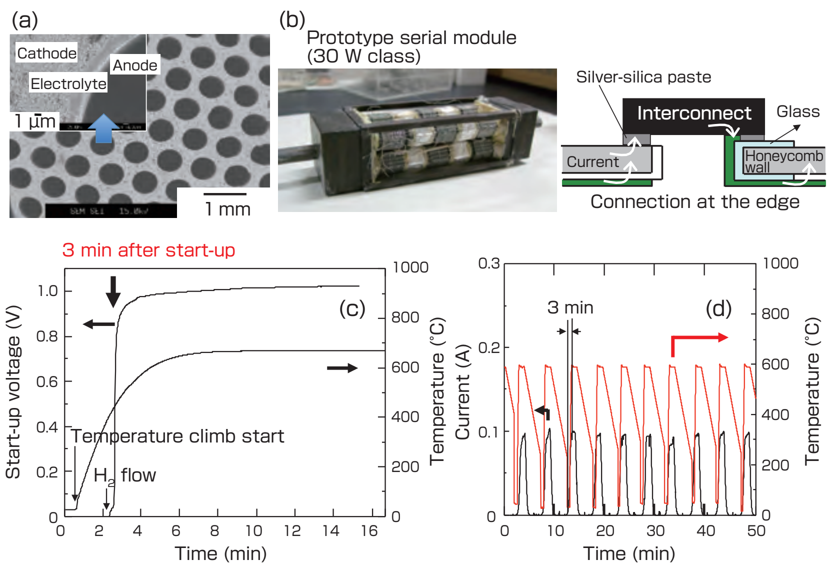

Fig. 9 Honeycomb-type micro SOFC module capable of rapid operation
a: Integrated cell with honeycomb structure
b: Example of prototype module and connecting structure
c, d: Rapid start-up and generation property through thermal history

of functional ceramics manufacturing technology. We aim for the development of an original technology that leads the world in ceramics manufacturing technology, including the standardization of the micro SOFC manufacturing technology.

Acknowledgements

This work is partly funded by the New Energy and Industrial Technology Development Organization (NEDO) through the "Ceramic Reactor Development" for the development of the micro SOFC manufacturing technology. We are also deeply thankful to the people of the collaborating companies, particularly the Fine Ceramics Research Association, NGK Spark Plug Co. Ltd., NGK Insulators, Ltd., and Toho Gas, Ltd.

References

[1] Advisory Committee for Energy and Natural Resources : *Choki Enerugi Juyo Mitoshi (Long-term Energy Demand Outlook)*, Agency for Natural Resources and Energy (2010) (in Japanese).
[2] J. Larmine and A. Dicks: *Fuel Cell Systems Explained*, Wiley (2003) [H. Tsuchiya trans.: *Kaisetsu Nenryo Denchi Shisutemu*, Ohmsha (2004) (in Japanese)].
[3] J. Weissbart and R. Ruka: A solid electrolyte fuel cell, *J. Electrochem. Soc.*, 109, 723-726 (1962).
[4] C. S. Tedmon, Jr., H. S. Spacil and S. P. Mitoff: Cathode materials and performance in high-temperature zirconia electrolyte fuel cells, *J. Electrochem. Soc.*, 116, 1170-1175 (1969).
[5] O. Yamamoto, Y. Takeda, R. Kanno and M. Noda: Perovskite-type oxides as oxygen electrodes for high temperature oxide fuel cells, *Solid State Ionics*, 22, 241-246 (1987).
[6] Y. Fujishiro, T. Suzuki, T. Yamaguchi, K. Hamamoto, Y. Funahashi, S. Shimizu and M. Awano: Development of high performance micro SOFCs and outline of advanced ceramic reactor project, *Ceramics Japan*, 44 (4), 308-312 (2009) (in Japanese).
[7] Y. Fujishiro, T. Suzuki, T. Yamaguchi, Y. Funahashi, S. Shimizu and M. Awano: Development of SOFC for low-temperature operation, *Nenryo Denchi (Fuel Cell)*, 9 (3), 83-87 (2009) (in Japanese).
[8] K. Kendall and M. Palin: A small solid oxide fuel cell demonstrator for microelectronic applications, *J. Power Sources*, 71, 268-270 (1998).
[9] K. Yashiro, N. Yamada, T. Kawada, J. Hong, A. Kaimai, Y. Nigara and J. Mizusaki: Demonstration and stack concept of quick startup / shutdown SOFC (qSOFC), *Electrochemistry*, 70, 958-960 (2002).
[10] T. Suzuki, T. Yamaguchi, Y. Fujishiro and M. Awano: Current collecting efficiency of microtube SOFCs, *J. Power Sources*, 163, 737-742 (2007).
[11] T. Suzuki, T. Yamaguchi, Y. Fujishiro and M. Awano: Fabrication and characterization of microtube SOFCs for operation in the intermediate temperature, *J. Power Sources*, 160, 73-77 (2006).
[12] T. Suzuki, Y. Funahashi, T. Yamaguchi, Y. Fujishiro and M. Awano: Development of cube-type SOFC stacks using anode-supported tubular cells, *J. Power Sources*, 175, 68-74 (2008).
[13] T. Yamaguchi, T. Suzuki, S. Shimizu, Y. Fujishiro and M. Awano: Examination of wet coating and co-sintering technologies for micro SOFCs fabrication, *J. Membr. Sci.*, 300, 45-50 (2007).
[14] V. Lawlor, S. Griessera, G. Buchingerd, A. G. Olabib, S. Cordinere and D. Meissnera: Review of the microtube solid oxide fuel cell Part I. Stack design issues and research activities, *J. Power Sources*, 193, 387-399 (2009).
[15] H. Iwai, N. Shikazono, T. Matsui, H. Teshima, M. Kishimoto, R. Kishida, D. Hayashi, K. Matsuzaki, D. Kanno, M. Saito, H. Muroyama, K. Eguchi, N. Kasagi and H. Yoshida: Quantification of SOFC anode microstructure based on dual beam FIB-SEM technique, *J. Power Sources*, 195 (4), 955-961 (2010).
[16] T. Suzuki, Z. Hasan, Y. Funahashi, T. Yamaguchi, Y. Fujishiro and M. Awano: Impact of anode microstructure on solid oxide fuel cells, *Science*, 325, 852-855 (2009).
[17] Joint Press Release of AIST, NGK Spark Plug Co. Ltd. and Toho Gas, Ltd.: Development of a compact fuel cell module that can be operated at low temperature through aggregation of the microtube SOFC (2009) (in Japanese). http://www.ngkntk.co.jp/news/2009/pdf/20090910b.pdf
[18] Low-temperature operable SOFC module, *Nikkei Electronics*, 24 (April 5, 2010) and *Nikkei Monozukuri*, 21 (April 2010) (in Japanese).
[19] K. Ikoma and H. Miwa: Development of SOFC system for automotive application at Nissan, *Nenryo Denchi (Fuel Cell)*, 10 (1), 70-74 (2010) (in Japanese).

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Discussions with Reviewers

1 Overall evaluation of the paper

Comment (Toshimi Shimizu, Deputy Director-General for Nanotechnology, Material, Manufacturing, AIST)

This paper is a description of the ideas, the prototype fabrication, and the evaluation results for the power generation module that is compact, has high output, and is highly efficient. It was realized by utilizing the original ceramic integration and manufacturing technology. It contributes greatly to solving the energy issues that are raising social concerns today, and I feel it is appropriate as a paper for *Synthesiology*.

However, in general, the logical construct and the expressions are like project reports or technical manuals. Therefore, while it can be understood by readers who are versed in fuel cells and related technologies, the text including the terminologies and figures is rather difficult for other readers. I think it will be a readable and fulfilling paper by improving the points indicated in the following discussions.

2 Basic positioning of the R&D

Comment (Hiroshi Tateishi, New Energy and Industrial Technology Development Organization)

The points and the flow of technological development are overall appropriately organized but the explanation of the strategy for R&D is weak as a paper of *Synthesiology*. I think the following three points are problems in terms of synthesis, so please consider revising them.

(1) I think there is a lack of explanation on what social significance this development has. If it is a development of the ceramic reactor the content can stand as is, but since you state specifically that it is a development of SOFC, you need to provide a corresponding explanation. The technological goal of realizing characteristics never seen in conventional SOFC is clear, but it is unclear what you wish to accomplish with the results to be obtained. You need to state that in the beginning: “There are A, B, and C that are applications that could not be handled by the conventional SOFC, and we set as our goal such-and-such performance and cost for the specs required.” In reality, the application tends to become visible later in the course of events, but in a paper you should state the objective of the development at the beginning.

(2) You set as the targets for SOFC, the low temperature operation and the speeding up of startup and shutdown. However, these issues are not directly related to the output capacity and aside from the required parameters, they are issues demanded in large-capacity devices as well. This means they are not issues limited to the capacity set as the target in this paper. The creation of a “micro-module” is clearly effective in solving these issues, but in this paper the establishment of the relationship between the above two issues and the output capacity is not sufficiently described. Does the micro-SOFC technology target only the 10~100 W class devices, or will it be extended to large-capacity devices in the long run? You may not be able to achieve this technologically at this point, but what is the strategy you have in mind? I don’t think you will be evaluated highly by electric power users if these points remain unclear.

(3) The relationship between the microtube module and the honeycomb module is not clearly stated in the paper. I think that tubular comes first then honeycomb appears in terms of chronology, but what are their characteristics, will they be used according to different uses in the future, or will you eventually settle on one structure for practical use? What are the future issues for the two structures? You need to explain these points.

Answer (Yoshinobu Fujishiro)

As social significance, when the highly efficient SOFC is used particularly in the homes, significant reduction in CO_2 emission will become possible if it can be operated by DDS (daily start and stop) according to the power load used. To do so, the realization of SOFC that is compact, of high performance, capable of rapid startup/shutdown, and that has high performance at low temperature to allow simple heat management is necessary. Until now, there was no technology to enhance the high performance or high integration by increasing the electrode surface area per volume and to address the issues of resistance of the ceramics material. The greatest significance of the research for the realization of high-performance, compact SOFC is that the ceramics integration technology developed by AIST was utilized to achieve the high integration and high performance at low temperature that were not possible before. We see the research strategy as the development and technological diffusion (through the presentation of readily-usable module) of the functional ceramics member manufacturing technology.

Specifically, we considered the following social significance and modified the text.

(1) We reconsidered the relationship of the issues of output

capacity and the solution by low temperature operation and speeding up the startup/shut-down.

The target is set for generation module, and we assumed the kW class module that is highly in demand as civilian power source. As the module capacity increases, the module volume increases and the exchange of heat rises. The technology to manufacture a module that can withstand low temperature and rapid startup/shutdown using the micro module SOFC will be effective from the aspect of solving the heat control issues.

We added the description of the target for developed output capacity and the thoughts on solutions by low temperature operation and startup/shut-down control.

(2) We reconsidered and modified the paper in response to your indication that the flow from microtube to honeycomb SOFC is unclear, and that there is a need for future issues.

3 Current situation, issues, and strategy for solution of the micro SOFC technology

Comment (Toshimi Shimizu)

I understand that there is importance in the development of compact, high-output, low-temperature fuel cells to meet the demands of industry and society from the descriptions in the first half of the paper. However, the main part or the development trend, comparison of performances, problems, and other things about the micro SOFC technology are not described. However, in the latter half of the paper, you abruptly bring out the comparison chart of performances, and conclude that you realized an original micro SOFC never seen before. The readers want to know the details of the table, and the strategy of this research and the synthesiology. I think the table should be utilized more effectively in the first part.

Answer (Yoshinobu Fujishiro)

As you indicate, we understood that the descriptions of development trends, comparison of performances, and problems of the micro SOFC technology are insufficient in the text, and also that the discussion of the research strategy for the solution is weak. On the other hand, the micro SOFC technology and its module development have not progressed very far in Japan and abroad among the various SOFC fields. It is not a generally major technological field, and the research is carried out with the advantage of AIST, and we think it is a field for which the technological development should be pushed by defining the issues. We wish to emphasize that, along the technological strategy road map, one of the solutions for the compact, high-output, low-temperature fuel cells is the realization of the micro SOFC module technology, and I hope the readers understand this. There is no technological index for micro SOFC, but we presented the comparison table to clarify the positioning of our technology and to show the world benchmark. For the above reason, we shall reconsider if it is necessary to review the synthesis. We added some description of the technological issues and explanation to emphasize that the technological issues for SOFC is the realization of low-cost, readily usable, high-output, and low-temperature fuel cells, and this is a strategy for the CO_2 reduction technology.

Comment (Hiroshi Tateishi)

This point is related to Discussion 2. In Table 2, there is no explanation of the technological indices shown here and I am unable to see how the technology shows “high performance”. Also, it is unclear whether the results shown in the table are the results of the microtube or those of the honeycomb integration.

Answer (Yoshinobu Fujishiro)

The technological indices are values achieved in microtube SOFC and honeycomb SOFC for the cell form, material, and operating temperature. For the generation density, since the anode thickness is thinner in honeycomb than in microtube SOFC, the maximum value is the value for microtube SOFC. We added the output density for honeycomb SOFC and included an explanation. The rapid startup (217 °C/min) in 3 min was demonstration data for honeycomb SOFC, and this will be stated in the note. Even with the microtube SOFC, startup can occur in a few minutes for a single cell, it is about 10 min (65 °C/min) at 200 W level by burner startup in the module.

"Monozukuri" (manufacturing) of Japan and synthesiology

[Translation from *Synthesiology*, Vol.4, No.1, p.46-51 (2011)]

New advantage must be added to Japanese manufacturing (monozukuri) for which Japan has held the leading position. To do so, it is necessary to build a new mechanism for research and development and innovation. We heard from the people who have led the Japanese manufacturing about the new strategy for monozukuri, the importance of synthesis, and the role of *Full Research* that AIST is trying to achieve.

***Synthesiology* Editorial Board**

Participants of the round-table talk

Hideki Nariai	Professor Emeritus, University of Tsukuba; and former President, Japan Nuclear Energy Safety Organization
Ayao Tsuge	President, Shibaura Institute of Technology; former Executive Member, Council for Science and Technology Policy; and former Executive Representative Director, Mitsubishi Heavy Industries, Ltd.
Akira Yabe	Vice-President, AIST (Editor, *Synthesiology*; Moderator)

Yabe

The main purpose of the journal, *Synthesiology*, is to appeal the importance of "synthesis in manufacturing" and to share the methodology of synthesis with all the people in the world.

For the result of an R&D to become practical, technological issues must be solved to overcome the "valley of death". Giving some examples, the R&D for super heat pump energy integration system was a national project, in which I was involved, to double the performance of the heat pump in about 10 years up to 1993. When the project was completed, the late Dr. Katayama of the Tokyo Institute of Technology said, "We have a wonderful racing car, but we still don't have a luxury commercial car". After that, dozen more years were required before the technology could be commercialized. This period was called the "valley of death", and it took over 10 years to improve both the economic feasibility and the performance, where various technologies were fortified and reinforced. Now, it has become widely utilized both in Japan and abroad. In the eco-energy city system, we developed the cold heat storage and transport system using the hydrate slurry, and it took six years until practical use. In the case of energy technology, economic feasibility is a major factor, and the six years was a period of challenge in economics. Another case is the automation of product inspection procedure of automobile, which was a project conducted jointly with a medium company. This automated inspection device employed the specular diffraction of the laser, and although the principle was set up in five years, it took seven years from the time we started to apply it to the automobile companies to actual practice. This was a challenge for reliability, durability, and achievement of high speed.

On the other hand, in the energy project called the New Sunshine and Moonlight Projects, there are many technologies that cannot find their way out of the valley of death. Therefore, I ask this question. Is there an effective method for overcoming the valley of death, and to what degree is the perspective of technology integration i.e. synthesis important in overcoming the valley of death? Also, which characteristic of the Japanese manufacturing should be emphasized to lead the world? I wish to open the discussion now.

Importance of synthesis in Monozukuri

Tsuge

"Japanese manufacturing or so called monozukuri that leads the world" is the creation of front-runner type innovation,

Dr. Ayao Tsuge

and we need both the ability to create the individual state-of-the-art science and technologies and the ability of integration for the large scale-complex socioeconomic system. The large scale-complex socioeconomic system is a giant sprawl of spatial, physical, social expanse, having complex interactions of the various elements within, and the performance and reliability affect society and economy significantly. It is exemplified by the social network of artifacts such as the Internet, the high-speed transportation systems, the nuclear power plant, and the space system. The creation of the life innovation and the green innovation launched in the 4th Science and Technology Basic Plan can be called the creation of the large scale-complex socioeconomic system. The proposition of the high added value manufacturing (monozukuri) that leads the world involves the interaction of the recognition science or the “research of the existing” and the design science or the “study of things that should exist”, as well as the integration of knowledge of these science and technologies. I think the importance of synthesiology lies here.

Yabe

The mega-complex socioeconomic system cannot be built without knowledge integration. Integration involves synthesis. Dr. Nariai, what is your view on this topic?

Nariai

I graduated from the Department of Mechanical Engineering of the university in 1962. In the classes at the time, importance was placed on the design and experiments, along with the four dynamics: mechanical, material, fluid, and thermal. In many classes, the actual mechanical systems were lectured. The core of the education at that time was to advance the technologies introduced from abroad since the Meiji Era, in a Japanese-manner. When designing or experimenting the rotating machines, we had to calculate the strength, vibration and thermal-fluid characteristics all by ourselves. They were synthetic classes.

In contrast, university education in the late 1960s began to emphasize the basic engineering. The universities were to teach the basics, and the companies were to train persons in the specialties after they became employed at the company. As a result, there was a diversification of the fields of specialty in university education. At the University of Tsukuba, the engineering field was established in 1977 under the new concept that emphasized design integration as well as basic engineering. In practice, however, not only education but also research at the university put emphasis on the basics.

Dr. Hideki Nariai

After the transition from the introduction of technology from abroad in the Meiji Era, to the self-development of technology, and now in the age of globalization, we must develop the technology with Japanese advantages. Therefore, synthesis is very important in such technological developments.

The characteristic of Japanese manufacturing is the presence of major companies that develop the devices and systems, and the small-medium companies that possess specific technologies to support them. In the 1960s when Japan started to take advantage of technology, excellent young people, known as the “golden eggs”, came from the countryside to the small-medium companies and contributed significantly to the formation of the technological foundation. By the 1980s, however, young people from the countryside became scarce. At the same time, the technology became sophisticated with the advancement of computerization and IT. Despite such difficulties, it was wonderful that the small-medium companies adopted new technology to adapt to the sophistication of Japanese manufacturing. Dr. Tsuge called such transfer of technology as “Japanese style techno-genome”. My current concern is: as industry globalizes with competition becoming increasingly fierce, is it possible to sustain the uniquely Japanese technological genetic information into the future? In any event, integration and synthesis of wide-ranging fields are important to reinforce the technological foundation of Japan.

Tsuge

I think there are two qualities of synthesis. One is the

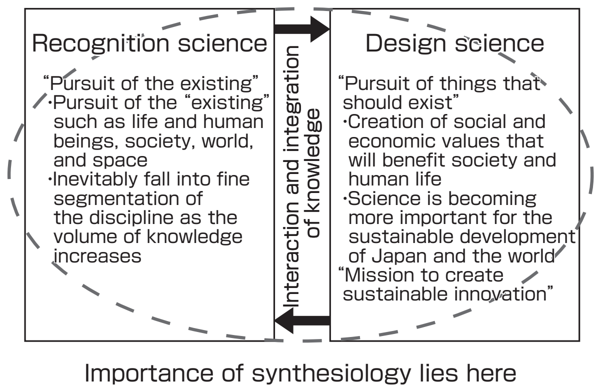


Fig. 1 Proposition of the high value added manufacturing (monozukuri) for leading the world in the “ability to create large scale-complex socioeconomic system”

"modular type architecture" where the world's leading state-of-the-art sciences and technologies are collected and connected through open innovation. And the other is the "integral type architecture" where socioeconomic values are generated by complex combination of the individual state-of-the-art science and technologies. Considering the process of creating the value including the time and collaboration of people-people and people-organization, I don't think we can simply call it the "age of open innovation".

The concept of "techno-genome" that denotes the genetic quality of technology is the terminology of Dr. Takemochi Ishii. When we were discussing the new opportunities for Japanese manufacturing as the developing countries are beginning to catch up, Dr. Ishii said, "There are technologies that can be transferred in a short time if you have money and guts, and there are those that require a long time to be transferred".

In organisms, it takes tens of thousands of years for the genome to change to adapt to the change in the environment. The time frame for technology is 10 or 20 years, but it tends to evolve like the genome over time. The Japanese manufacturing or monozukuri does not have to be so pessimistic as long as innovations in science and technology occur to maintain the 10 to 20 year lead, and by continuously making them part of the social values. This is the root of techno-genome.

On the generalized methodology for technological development to overcome the valley of death

Yabe

I think it is important to take advantage of the characteristic of Japanese manufacturing for the technological development to overcome the valley of death. How do you think about the methodologies? I think this is one of the characteristics of synthesis. How do you think about the characteristics of synthesis?

Tsuge

To overcome the valley of death in innovation process, I think the reconstruction of the innovation traction engine is one of the key solutions.

In the United States, the corporate central laboratories that functioned as the innovation traction engines collapsed over 10 years ago. The current traction engines are the combination of universities, venture companies surrounding the universities, and the venture capital that supports them. Education, R&D, and innovation work as three-in-one to germinate the seed. Then, when the early stage is completed, the major companies step in to invest and the innovation is kicked off. This engine structure is firmly established in the United States.

In Japan, the corporate central research centers have collapsed as well. The national research institutes, such as the labs of the Nippon Telegraph and Telephone (NTT) Corporation, were privatized, and the age of central labs ended. Although the R&D entities, some corporate labs, and universities are working hard, the abilities of knowledge creation and combination by these three kinds of research organizations are weak, and the collaboration between the higher education and R&D is fragile. Therefore, I think the general methodology for overcoming the valley of death in Japan is to strengthen the innovation pipeline network. The innovation process is nonlinear and probabilistic to the degree that one can say that "if he wasn't around or if this organization didn't do that, the innovation might have not occurred". Therefore, as a general method, it is necessary to strengthen the three-in-one collaboration of universities, R&D entities, and industry, and to build the three-in-one structure of the higher education, R&D, and innovation. It is important for the participants to be "under one roof" for education, R&D, and innovation. I think the Japanese-style innovation traction engine must be rebuilt from this perspective.

Yabe

Are you saying that there is insufficient interface function among the universities, companies, and the R&D entities, and to have this function under one roof is a requirement?

Tsuge

Yes. For example, there should be an emphasis on the flow or interface of values from universities to the R&D entities, or from the R&D entities to industry. To put it bluntly, it may not produce an academic paper, but it is vital to contribute to the socioeconomic value creation. To get the academia appreciate the fact that such activities are academically valuable; I think that is the mission of synthesiology. The students and researchers are not passionate about such things because they won't be recognized for doing them.

In industry, this accomplishment is recognized in the personnel evaluation. This individual combined the demand and potential of Business A and Laboratory B, and created the driving force for generating the new Product X. That is what the companies evaluate highly. Unless the academia recognizes this value on the academic table, I don't think the gap between industry and the academia will close.

Nariai

I still remember what a person from industry said a long time ago. He said "Say, that basic research need 1 effort and money, then, 10 times more effort and money are needed to make the actual product, and another 10 times more is needed to create a product that can sell". I felt that it was very difficult to create a selling product. The obstacles we faced on creating a product is, what we call, "the valley of death".

There are two valleys: one to actually create a product from the result of basic research, and the other to create a selling product. There is a difference between the two. The first valley involves the proper combination and integration of various kinds of findings, and the second valley requires wide-ranging integration of them so as to attain social acceptance.

Dr. Tsuge mentioned earlier that the collaboration of three-in-one is fragile in Japan, particularly the collaboration of universities with others. The research at universities had been only to search for the truth and the result was to be disclosed widely to the public. However, the corporated researches were limited. In the past 20 years, researches at universities shifted to what leads to produce an actual product, but still there are other problems, such as the barriers among the government agencies. I hope we can knock down the barriers and form good collaborations of three-in one.

Effective method for raising the level of synthesis

Yabe

I think the points of discussion will be how to knock down the barriers or how to deepen the collaboration. What are some of the effective methods for raising the level of synthesis?

Tsuge

To raise the level of synthesis, I think we need a major reformation of the current situation where the pipeline that binds the knowledge creation and the socioeconomic value creation is broken, as shown in Fig. 2. We must not forget the fusion with education or the human resource training policy. If the government decides to provide the place of fusion, strengthen vertical collaboration among the agencies, or to advance the innovation policy, the education policy must be incorporated. I think building such mechanism is very important. The “realization of a strong economy, strong finance, and strong social welfare” as proposed by the government must be sustainable. To strengthen the sustainable innovation creation, the three-in-one advancement of education, R&D, and innovation is essential. If the innovation traction engine with such structure is set forth, the level of synthesis will automatically rise.

Nariai

As effective methods for raising the level of synthesis, I suggest the “use of human network in the local areas”, the “tradition of technological development at companies”, and the “Japanese decent character of helping each other”.

As an example of the use of the human network in the local area, Tsukuba Science City is illustrated, where national research institutes and companies gathered in 1980. The researchers of heat transfer and thermal engineering gathered and started a study session in order to exchange information. It resulted not only in reports of the academic society, but also the publication of the book *Jisedai Gijutsu To Netsu (Next Generation Technology and Heat)*. Diverse researchers involved in basic research and in problem-

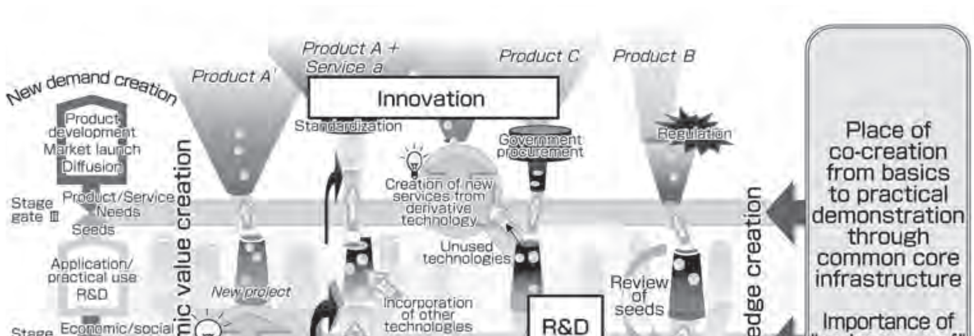


Fig. 2 Need for three-in-one promotion of education, research, and innovation

solving research got together, and the level of research was raised through these discussions at the study sessions. Now, the information technology has advanced, and there are other means for information exchange among researchers compared to 30 years ago. In the study sessions at Tsukuba, researchers could often see actual products at the study session and that was extremely useful to advance their studies. Thus, local human network can be utilized to raise the level of synthesis.

Yabe

People of universities, companies, and national research institutes gathered in Tsukuba to talk about the demand and potential, and how they were viewed by society. I think this is an example of being "under one roof" where the three parties gathered in one place. We are now building the "Tsukuba Innovation Arena", which is inspired by research associations. Gathering the universities, companies, and research institutes in one place is an excellent method for Japan.

Tsuge

I certainly think so. My view is that graduate students do not have to sit at the main table, but the professor may say, "Hey, there's an interesting session in the evening, so why don't you come along?" and the graduate students can participate. I wish to do that consciously. When I look back at my university years, Dr. Nariai was in the doctorate course and was studying in the engineering department. By participating in such study sessions, I could feel the energy and technologies that support society.

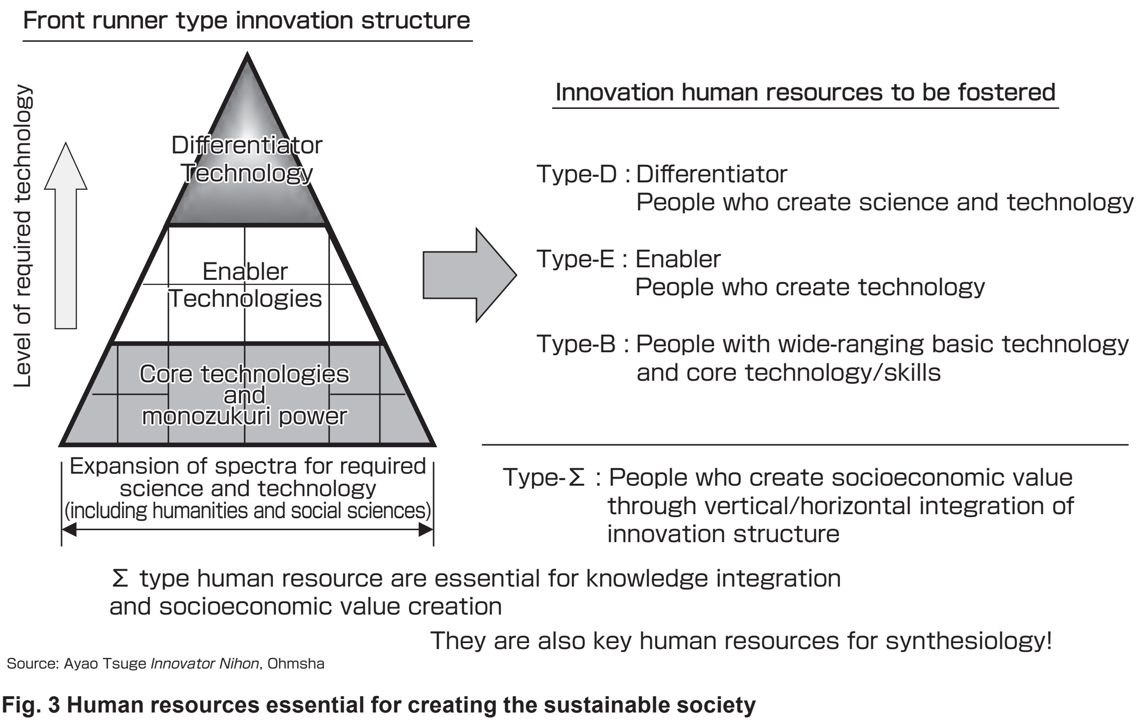
How synthesis can be utilized in creating a sustainable society

Yabe

You discussed that one of the effective methods to raise the level of synthesis is to establish a system where everyone can exchange information and share wisdom. Creating a "sustainable society" is extremely important for us. How can we incorporate the objective of sustainability into synthesis? Will that be at the individual or organizational level?

Tsuge

The important point in the methodology for building a sustainable society is to create a sustainable innovation traction engine structure. Furthermore, the "human resource education" is the most important. As shown in Fig. 3, there are roughly four types of human resources to propel the front-runner type innovation structure. One is Type D or the "differentiator" who creates the cutting edge of science and technology. This person may win the Nobel Prize. Type E is the "enabler" who creates the enabling technology. Type B or the "base" who truly supports the innovation structure and monozukuri tends to be forgotten, but this person has wide-ranging basic technology and possesses core technology and skills. I think a large part of engineering education is to nurture the Type B people. I fear what is forgotten in the current science and technology and the education policy is the so-called Type Σ. This is someone who works to create the socioeconomic values through vertical and horizontal integration of the innovation structure. Type Σ is the person who supports synthesiology and is crucial in building the sustainable society.



Source: Ayao Tsuge *Innovator Nihon*, Ohmsha

Fig. 3 Human resources essential for creating the sustainable society

Nariai

I consider establishing a sustainable society as making such a society utilize advanced science and technology sustainably. I have been involved in researches and regulations pertaining to the safety of nuclear power. The nuclear power plants were developed abroad, mainly in the United States. Japan imported the technology, and then manufactured, constructed, and operated the plants. The researchers studied hard and investigated carefully about how to protect the safety of the residents and the workers, even in case of any accidents. In the nuclear power plant, the heated fuel melts when the cooling water is depleted, which leads to the release of the radioactive materials. Therefore, the researchers conduct analyses and experiments for the extremely complex phenomena to prevent the fuel meltdown by injecting emergency cooling water when the water pipes are broken and the cooling water is depleted. The late Dr. Hideo Uchida has called such research as "the development of nuclear safety". Through the goal-oriented R&D, the research is conducted by mobilizing various knowledge to achieve an objective. The basic point is synthesis.

Regulatory science is proposed in the fields of food and drugs. It is the research involving risk evaluation, risk management, and risk communication which needs all related disciplines including humanities and social sciences. At this point, regulatory science belongs to the goal-oriented domain, rather than the domain of the conventional basic applied sciences. In nuclear power, the issues of risk evaluation, risk communication, and risk management including the role of the regulatory agencies are indicated. In order to gain social acceptance in society of advanced technology, the methodology or science to guarantee safety and security is necessary. I think the synthetic way of thinking is important.

Tsuge

Dr. Nariai's discussion that views including the humanities and social sciences are necessary for goal-oriented research is pointing to design science or the science for the pursuit of things that should exist, isn't it? I think it is necessary to understand design science when creating a sustainable society. Moreover, design science cannot exist without recognition science. Therefore, we must set up an education program for people with birds-eye-view that enables such collaboration, and the government should support it. Similar proposal was made in "Japan Perspective: Proposals from the Science Community" published by the Science Council of Japan in April 2010.

Yabe

How to get the importance of design science and synthesis accepted by society; I think this is a topic on which it is rather difficult to write a scientific paper.

Tsuge

To practice science and technology for society, it is necessary to nurture human resources for design science. That is to educate people with ability for bird's-eye-view, synthesis, and co-creation. That is why the evaluation standards are different in design science and recognition science. It is necessary to clarify each evaluation standard, and we must engage in activities that deepen the understanding of the Japanese people for "science and technology for society".

What can synthesis do for technological innovation?

Yabe

Because we want people to recognize the importance of design science, we use the word "social technology" or the technology at the contact point with society. Dr. Tsuge discussed earlier about the creation of technological innovations, such as green innovation and life innovation. What can synthesis accomplish, and what is expected of synthesiology?

Tsuge

Synthesiology is a foundational discipline that supports the creative power of the large scale-complex socioeconomic system, Japan's advantage in monozukuri, and the creativity of front-runner type innovation. At the same time, it is a practical science. I would like synthesiology to establish an academic evaluation standard, as well as play the part as a practical science on site.

I believe design science or synthesiology can provide academic meaning. That will be the academic evaluation standard, and for example, the standard for funding a project can be discussed in terms of whether it is valuable as design science. I think it is a challenge for the academia.

Yabe

Applying this to *Synthesiology*, what AIST has been stating as synthesiology must be organized from the viewpoint of design science and then transmitted further.

Dr. Akira Yabe

Nariai

When looking through *Synthesiology*, I felt AIST has done quite a few useful researches. It is important to think about the world of a globalized society and the developing countries, in order to grasp the social needs. The countries with certain technology will compete and the one with superior technology will win. To prepare for such competition, it is sometimes necessary to reform the conventional Japanese system and perhaps to change the consciousness of the Japanese people.

I heard the terminologies *Type 2 Basic Research* and *Full Research* for the first time, but I've always been concerned about technological development. As for my expectations for *Synthesiology*, I look forward to the new issues of the journal on this matter. AIST proposes an important methodology in today's advanced technological society. I hope this will spread to wide-ranging fields, not just within the researches at AIST. It will help train human resources to get the researchers to think widely and deeply about practical research, as Dr. Tsuge mentioned. The discussions are especially very valuable and interesting. This should be carried on so editors can be trained. I hope this will lead to the training of program managers and research coordinators in Japan.

Yabe

To bring out Japan's strength from synthesis and to point the direction the world should take; I think these are the important roles of synthesiology. The ideas transmitted as synthesiology must be organized and then re-organized from the perspective of design science. By transmitting the importance, we would like to lead the world. I think that is important for the future of Japan. Thank you very much.

(This round-table talk was held at AIST Akihabara Office in Chiyoda-ku, Tokyo on September 6, 2010.)

Profiles

Hideki NARIAI

Born in Tokyo in 1938. Graduated from the Department of Mechanical Engineering, Faculty of Engineering, the University of Tokyo in 1962. Completed the doctorate course at the Graduate School of Engineering, the University of Tokyo in 1967. Doctor of Engineering. Joined the Ship Research Institute, Ministry of Transport in April 1967 as a researcher, then became the Senior Researcher. Assistant Professor of Structural Engineering System, University of Tsukuba in April 1980; Professor in November 1987; retired in March 2002 as Professor Emeritus. Chairman, Atomic Energy Society of Japan from 2002 to 2003. President, Japan Nuclear Energy Safety Organization from October 2003 to March 2009; Special Adviser from April 2009 to March 2010. Collaborating Member of the Japan Council for Science. Specialties are thermal engineering and nuclear safety.

Ayao TSUGE

Born in Tokyo in 1943. Graduated from the Faculty of Engineering, the University of Tokyo in 1967. Completed the doctorate course at the Graduate School of Engineering, the University of Tokyo in 1973. Doctor of Engineering. Completed AMP 101 at the Harvard Business School in 1987. Joined Mitsubishi Heavy Industries, Ltd. in 1969, and engaged in the R&D for nuclear power generation. Manager of Nuclear Power Research Promotion; Director of Takasago Research & Development Center; Director and General Manager of Technological Headquarters; and Executive Director of Technological Headquarters. Executive Member, Council for Science and Technology Policy, Cabinet Office in January 2005. Special Adviser, Mitsubishi Heavy Industries, Ltd. in January 2007. President of Shibaura Institute of Technology in December 2007. Member, Japan Council for Science; and Vice Chairman, Engineering Academy of Japan.

Synthesiology Workshop

Methodology of technology integration toward establishing an open innovation hub

[Translation from *Synthesiology*, Vol.4, No.1, p.52-58 (2011)]

The Synthesiology Workshop was held in October 2010 as part of the lecture series for the “AIST Open Lab” organized by the National Institute of Advanced Industrial Science and Technology (AIST). This is a report of this workshop.
In this workshop, an attempt was made to categorize the academic papers published in *Synthesiology* into various types of synthetic research. Ways to promote innovation were discussed with the industrial researchers who have been engaging in synthetic R&D and have produced successful results.

***Synthesiology* Editorial Board**

[Opening Address]

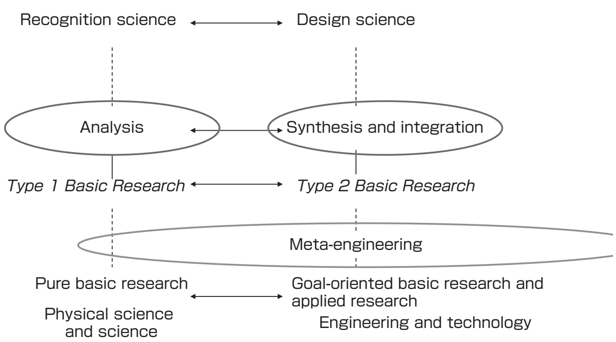
Akira Ono (Editor-in-Chief, *Synthesiology*, AIST)

The international competition for innovation is becoming fierce. While there are heated discussions about “open innovation” and “collaboration among industry, academia, and government” here in Japan, I think it is important to understand the situation as a whole, to engage in discussions on what are the mindset, objectives, and shared area among researchers and engineers, in order for the academia such as universities, public research institutes like AIST, and the industries to understand each other and deepen collaboration despite our differences.

Overlooking the method of research in science and technology, the traditional science started in 17th century Europe, and has been successful by employing reductionism. The success continues to the present, but many people are beginning to realize that reductionism alone will not solve complex problems of environment, energy, and safety. There have been several proposals for new scientific methodologies that do not rely on reductionism. For example, if we consider recognition science to be the traditional science, why don’t we have design science as a new science? When handling complex problems, don’t we need approaches of synthesis and integration where we are not grounded in a single technological field? At AIST, we have the contrast of *Type 1 Basic Research* versus *Type 2 Basic Research*. There are also contrasts of pure basic research versus goal-oriented basic research or applied research, and also science versus engineering, as well as science versus technology.

Compared to the traditional scientific methodology, we paid very little attention to the methodologies and approaches for the new science, even though we are practicing such research on a daily basis. Or, each scientist may have an accumulation of know-how, but these are not shared as assets

Research method for science and technology



of society and cannot be handed down to others. Those are our understanding of the issue. I think the objective of *Synthesiology* will serve as a point of discussion.

Today, under the title "Methodology of technological integration for the open innovation", we invited several people with broad views and rich experiences. I hope we have a deep discussion on the new scientific methodology.

[Presentation]
Categorization of synthetic research for the creation of innovation

Naoto Kobayashi (Senior Executive Editor, *Synthesiology*; Waseda University; former AIST member)

Synthesiology is a journal for papers that emphasize the objective and scenario of the social technology that leads a research result to product realization and its social diffusion. If these papers could promote the practice of *Full Research* and accelerate innovations, *Synthesiology* will play a major role as an academic journal. While the creation of innovation is not easy, it would be beneficial if we can get a glimpse of the integration methodology that may lead to innovation. Therefore, the Synthetic Methodology Working Group of the *Synthesiology* Editorial Board has reviewed 50 papers among the 60 papers published from Vol. 1 No. 1 to Vol. 3 No. 2. The papers were comprised of: 8 papers in environment and energy field; 9 in life science (biotechnology) field; 6 in life science (human technology) field; 10 in information technology and electronics field, and nanotechnology, materials and manufacturing field; 12 in metrology and measurement science field; and 5 in geological survey and applied field geosciences field. I have previously proposed the (1) "Aufheben" type (two opposing topics are integrated to create a new concept), the (2) Breakthrough type (marginal technology elements are combined with major essential technology element to develop integrated technology), and the (3) Strategic selection type (technology elements are strategically selected and synthesized). These concepts were used as examples for the basic types of synthesis method.

Overall, the papers of *Synthesiology* were found to be interdisciplinary, but we have also discerned characteristics for each field. The (1) environment and energy field mainly involved the "strategic selective + breakthrough types", where the topics are selected strategically as the clear social demands are broken down, a main technology is generated from the key elemental technologies, breakthrough occurs with the combination of the main and marginal technologies, and an integrated technology is born.

The characteristic methodology for the (2) life science (biotechnology) field is the spiral development. For example, in bioinformatics, after a core technology is synthesized, this leads to the hop-step-jump phases of the next development, and this Full Research loops up to the "hop" of the next stage. The biotech industries have higher uncertainties than other fields, where one may not know whether a product is usable unless it is realized as a product, and it is important to bring the product to realization however small. The spiral manner in which the processes of *Type 1 Basic Research*, *Type 2 Basic Research*, and *Product Realization Research* spiral upward is the characteristic of the field. Moreover, in the (3) life science (human life) field, as represented by the paper on the development of eyeglass frame to match an individual, its characteristic is to create a system for providing a product based on customer satisfaction by integrating the technology elements, categorizing the core technologies, and by seeking new findings.

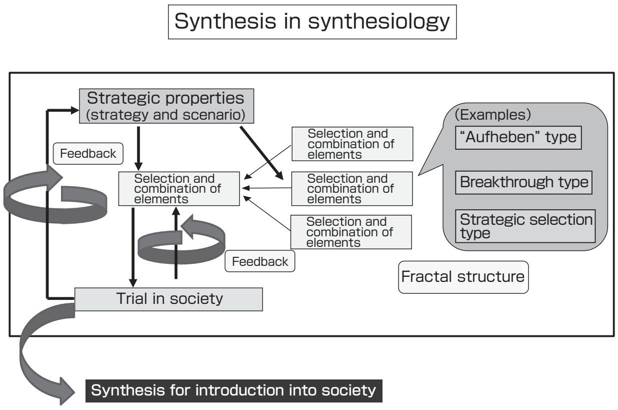
In the (4) information technology and electronics field, the creation of nonvolatile electronics using the spintronics technology was very typical. It could be called a tandem breakthrough type, where there are two consecutive breakthrough technologies including the development of the new material and device and the development of the mass production technology that is crucial for practical use and product realization. In the (5) nanotechnology, materials, and manufacturing field, the mass synthesis of organic nanotube is one of the good examples. While this is a seed-driven breakthrough type, the characteristic is that the mass production was attained by extremely detailed molecular design and the integrated technology, and the practical use has been sought by pioneering the use of the product jointly with various companies.

In the (6) metrology and measurement science field, there is the mission of establishing the national standard and providing traceability to the International System of Units (SI), guaranteeing the international equivalency of the standard using a measurement method recognized internationally, and building a traceability system that reaches the far corners of society through standard provision. The technological development can be called the "strategic selection type S (standard)". Its characteristics are that the goal is clear, and the technology elements necessary for its achievement are selected and synthesized. Finally, papers in the (7) geological survey and applied field geosciences field can overall be called the "integrated strategic type", but they include several types such as the individual strategic type and the individual strategic and field fusion type. There are also those that transform from the breakthrough type to the fusion type as the types change and develop over time. The research may progress according to the shifting social demands, the geological phenomena are often understood as complex systems, and the interactions tend to take place in a spiral structure.

Lastly upon the analysis of the 50 papers, we extracted the issues for the synthesis method. First is the “synthesis method in *Synthesiology*” (see figure). There is the process of strategy and scenario → selection and combination of elements → testing in society, but it was found that another important factor is the “feedback”. The examples of selection and combination of the elements can be categorized into the aforementioned “aufheben”, breakthrough, and strategic selection types.

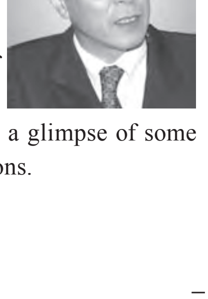
Second is the “property of the research field and synthesis”. In the fields such as physics, chemistry, mechanics, device technology, and metrology, the elemental technologies are clearly defined and the synthesis method is relatively simple. There are also complex systems such as environment, energy, and geology. Then, there are complex interactive systems such as biotechnology, human technology, and information technology, where the synthesis method changes and the complexity increases.

Finally, the “introduction into society” is our main issue. To introduce a research result into society, a social action that is independent of and collateral to the technological development enters into the factor, as well as the addition of values such as emotional aspect and need of an impressive concept, aside from the function. It may also be necessary to promote autonomous synthesis by sowing the seeds of elements while giving up short-term profit. Not only is it a matter of technology, but it will be also important to respond to the feedbacks from society. I propose such issues for our discussion.



[Panel discussion]

Motoyuki Akamatsu (Senior Editor, *Synthesiology*, AIST)



The objective of *Synthesiology* is to publish papers that describe the synthetic researches conducted according to the scenarios that outline the process of creating the technology that will be used in society. Therefore, I hope we may get a glimpse of some synthesis methodology to create innovations.

We shall hear from Dr. Kobayashi who proposed the issue, Dr. Suzuki who promotes the idea of meta-engineering at the Engineering Academy of Japan, Mr. Kitayama who has experience in the R&D of optical network, and Mr. Ito who will explain the history of the car navigation system. Then, I would like the participants to discuss the synthesis methodology for introducing the products into society.

Proposal of meta-engineering

Hiroshi Suzuki (Technology Executive, GE Energy; Chair of the Task Force for Committee on Technology Policy, Engineering Academy of Japan)

The Engineering Academy of Japan is a group of leading engineers and was established to contribute to the advancement of engineering and technological sciences in Japan. I am leading a study group there and proposing an idea of “Meta-Engineering”. Recently, I feel that the definition of engineering has been fixed as seeking optimal answers only within a given condition or constraints. Here I find two problems. The first problem is that this condition is regarded as a given and irremovable. The second one pertains to optimization process. Optimization falls into global optimization and partial optimization. I feel that people tend to fall into local optimization that would not lead to a radical solution. Assuming that these two bottlenecks might prevent the sequential occurrence of innovation in Japan, our group was determined to review “Engineering” and named this concept “Meta-Engineering”.

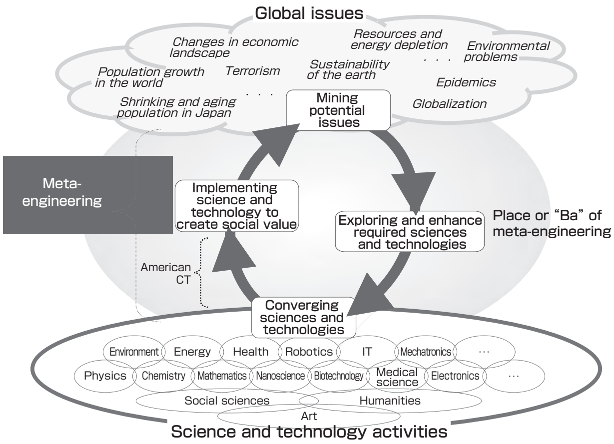
When people seek an optimal answer within a given condition, they might focus only on “How”, but “What” should come before “How”----this inspired me to get the idea of “Meta-Engineering”. Some people say that we should make innovation happen taking full advantage of Japanese manufacturing, and the word “manufacturing” makes most people think about “how we make things”. However, what is important is “what we make” and “why we make it” in the background.

In line with the implementation of the Third-stage Basic Plan for Science and Technology, we see some visible results in science and technology. Each individual result is respectable, but it is hard to think of the innovations that have recently happened in Japan. A single respectable technology or science comes out in Japan, but is not converted---this is the impression that I have.

I use the word “meta-engineering” for the Japanese word *komponteki* engineering or down-at-the-root engineering.

Getting back to the basics of Engineering, we firstly think about an issue. We might have seized visible issues, or issues at hand, but there might be more radical and invisible issues behind them. These issues should be our targets. It is important to see them from a bird's eye point of view in efficiently implementing science and technology on the issues.

First, pick up a potential issue and consider what kind of technology and science are necessary. Then, investigate if any of the existing technology or science would be useful in addressing the issue. Since the recent issues are more complex and difficult, it may be hard to solve the issues in a single science and technology field. So, science and technologies converge, and social values are created by implementing them in the real world. And then, a new issue will emerge, and we go through the same process to create the next social value. I think that the dynamic and spiral process is a key driving force for innovation.



Passive optical network and fiber to the home

Tadayoshi Kitayama (President&CEO, Mitsubishi Precision Co., Ltd.; former Vice President of Communication Systems Business Division, Mitsubishi Electric Corporation)

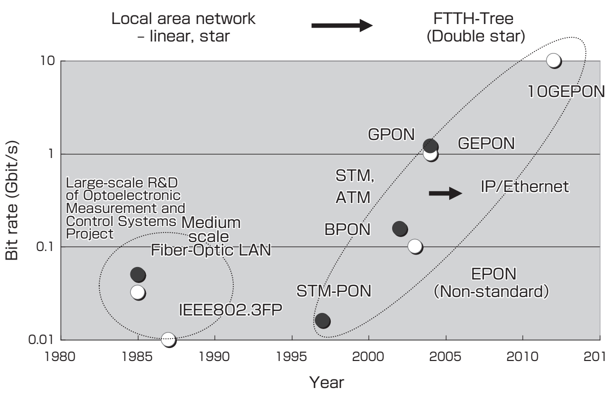
I think many of you are already using the Internet through optical fibers connected between your home and a telephone company office or an internet provider site. This fiber optic access system is called "fiber to the home (FTTH)". FTTH system is composed of optical fibers, optical couplers to tap optical signals from a central office, and terminals. This network configuration is called passive optical network (PON). We first conceived PON in the1980, and it took more than 20 years for it to materialize. We got a hint from satellite communication that was composed of the geostationary satellite and earth stations. In the Large-scale R&D of Optoelectronic Measurement and Control Systems Project administrated by the Agency of Industrial Science and Technology of the Ministry of International Trade and Industry, the primary data network consists of loop-configured passive fiber-optic transmission system equipped with optical couplers, burst mode optical transceivers, TDMA processors for N:N communication and interface adaptors for data-terminal equipment were developed(1980-1985). The star configured passive optical networks were also adapted to Ethernet-base fiber optic local area networks in 1987. In the 1990s, the star configured passive optical networks were chosen as a network topology of FTTH because of its cost effectiveness and upgradability in the future.

In the development of FTTH, there were two candidates of multiple access methods of PON, One is the asynchronous transfer mode (ATM) which was the ITU-T telecommunication standard that efficiently multiplexes telephone and Internet services. The second is the Ethernet-base random access method which is the IEEE standard and popular interface of computer communication systems. In Japan, the Ethernet was chosen because it would become a more familiar and less expensive interface than ATM. By Voice over IP technology, Telephone services are easily multiplexed with Internet services. The transmission bit rate is 1 Gbit/s and will be going up to 10 Gbit/s to multiplex wider services like video communication services.

It took about 25 years to get here. Why did it take 25 years? We had to wait for the innovation of optical and electrical devices. Standardization of PON needed to be established. The Internet demand had to grow and communication carriers had to change business models from telephone services to internet access services.

The continuous technical innovation of PON for over 25 years could not be handled by a single company. The seed sowing of the technology was supported by the government as I described. Challenges to commercialize fiber-optic Ethernet were carried out through cooperation between a communication carrier and system vendors. FTTH standardization and its development were strongly promoted by a communication carrier. But it was the open collaboration with system LSI vendors, optical component vendors and equipment vendors to speed up the development and reduce the burden on individual vendors that enabled short term development and commercialization of PON base FTTH.

Development of passive optical network



In the future, as the scale of required resources for new technologies development will increase, technological seed sowing led or supported by government will be more important than now. In commercialization stage, open collaborations will be effective and inevitable.

The case of car navigation and route guidance system

Hajime Ito (Former Managing Director, Yazaki Meter Co., Ltd.; former General Manager Body Engineering Division, Toyota Motor Corporation)

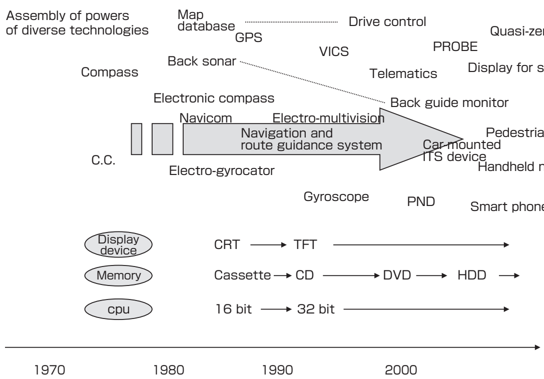
The precursor of navigation was the celestial navigation using a marine sextant and the radio navigation for aircrafts. In thinking about measuring one's present location and which way to go, these are highly important technologies in the development of automotive navigation.

There is 30 years of history in automotive navigation and route guidance system. The early automotive navigation was dead reckoning, where the "present location" was entered and the direction sensor was used to determine how one could reach the destination by following the directions. It is surprising that the three Japanese automobile manufacturers came up with similar technologies and products at the same time around 1980. The companies were searching high and low for various technologies, and realized that they could do certain things using certain technologies, and started to create similar things at once. I have been involved in design for about 20 years, and I repeatedly experienced the situation where similar products appear within a span of a year. I think "corporate competition" is the keyword. In the latter half of the 1970s, various government agencies including the Ministry of International Trade and Industry conducted research on some of the functions of the current navigation. Navigation appeared in 1980 as the crystallization of various technologies including display, memory, microprocessor, and others. Since then, the product power of car navigation increased, it became multifunctional, and became an essential product for cars. For the device to be installed in the car, it had to be incorporated in the design of the automobile, and the automobile companies began to install it as standard equipment.

In the technological field, navigation is considered as a field of intelligent transport system (ITS). The team developing the ITS and the team standardizing it are working side by side, to develop the product, standardize, and to advance it as the world standard. The ITS Promotion Council is a Japanese organization to discuss ITS among government, academia, and industry. The activities are done under the supervision of this organization, and the manufacturers are not working individually. This is an important point.

For human factors, the HARDIE guideline was created in Europe, but Japan had made many navigation systems after 1980, and the guideline of the Japan Automobile Manufacturers Association (JAMA) became the basic guideline of the world standard or the human factor requirements. For example, one cannot set the destination while driving, the map display disappears when one enters the community road, the prefectural roads are shown preferentially in the route guide, or one cannot watch TV while driving. These conditions created in Japan became the world requirements, then became the requirements considered by the ISO, and as a result, became the guideline of the Ministry of Land, Infrastructure and Transport. Since the navigation is not a prerequisite for driving, it is placed some distance from the center of driver's vision, yet it is placed in a fairly visible place to prevent accidents if the driver looks at it while driving. I described the display requirements earlier, and the manufacturers must, of course, follow the requirements, but they must provide added value to their products in other areas. It will eventually become safe to view it while driving and be useful to the driver. That will be the future automotive navigation product.

Evolution tree of automotive navigation



[General discussion]
What is the difference between the "what" in the 80s and the present "what"?

Kobayashi

Dr. Suzuki has mentioned in meta-engineering, that the most important thing in taking the bird's eye view is "what to do". The Large-scale R&D of Optoelectronic Measurement and Control Systems Project had been underway at around 1980, but what is the difference between the situation at that time and the current "what"?

Suzuki

"What" arises from "why it is necessary". In the history of electrical engineering, I analyzed how the technology was born from a certain social background and social demand. The air conditioner was first used for cooling only, but with the development of the inverter and heat pump, it became usable for both cooling and heating. Currently, there are concerns for health and human factors. We must spend our effort on learning the social background of what the society needs, what is important in our daily lives, and "how" to make the "what". However, recently we've been neglecting that and we seem to be thinking only about the "how", and I hope we can get back to basics.

Akamatsu
Is the "what" in optics to realize large volumes of communication at once?

Kitayama
In the early stage, loop or ring configured optical fiber communication systems were introduced to computer controlled manufacturing plants because of their high electromagnetic immunity. As the number of computers and terminals increased, loop or ring configured optical networks needed higher bit rate, larger number of communication nodes and cost for the system soared. We thought downsizing and reducing the cost of the communication nodes were necessary to construct a larger area optical network. We thought PON and multiple accesses scheme would be the most promising architecture for FTTH.

Ito
The 1980s was when motorization exploded. It was a time when roads were not organized and the road signs were all messed up. The available maps were crude. It was an era when many problems could be solved through technology that allowed one to find out where he/she was and which way he/she was heading. At present, navigation and route guidance system is one of the instruments on a car, and it has several functions. However, I do not think that it is important to just think of safety and environment, nor do I think that navigation has been perfected. I think there is room for research in route guidance that matches the human perception, is ergonomically sound, and allows reduction of traffic jams.

Was the government support for the R&D project effective?

Akamatsu
When the automotive navigation was realized, can I assume that the government support for the R&D project was effective?

Ito
I think yes. Back then, I think there was antagonism among the government agencies, but there was a good and close relationship for the ITS field, and the Cabinet Office supervised the activities. ITS Japan played the role of linking the private companies, government, and the academia. There are participations of 180 private companies. These companies cannot do what they want. The entire thing must be coordinated to set the key competitive areas. I think we are in such a situation.

Kitayama
In trunk line communication systems, it was very clear that by introducing higher bit rate optical transmission technologies, the cost of communication would remarkably reduce. But the market was not so big compared with access network. While many people thought that high-speed optical communication technologies would be available even in access networks in the future, nobody conceived to develop optical access network by themselves because many breakthroughs would be necessary, especially about passive networking and cost reduction. Large-scale R&D of Optoelectronic Measurement and Control Systems Project had an important role to trigger the optical network technology development.

Suzuki
Exploring an invisible issue, identifying necessary science and technologies, converging these science and technologies if necessary and creating social value by implementation cannot be all done by one person or one organization. Therefore, it is necessary to consider how to make a "place or "Ba" of Meta-Engineering" or an ecosystem where various companies can participate. In this case, I think the national project made a significant contribution.

Ito
I think it is true that everything went fine because of the cooperation from the government organizations, and it will continue to be so. Now, for example, VICS is the information obtained from the police vehicle detectors. Since tests have just begun for the probe that collects information from the vehicles on the road for the next-generation traffic jam information, there must be cooperation with such organizations. Another point is that the Japanese navigation is based on maps, but the Ministry of Internal Affairs and Communication and the Ministry of Land, Infrastructure and Transport claim that using the map just for navigation display is wasteful. I hope we can discuss such things in the "place".

Kitayama
Before, system manufacturers had to develop the semiconductor process, optical devices and ASICs and software by themselves. Recently, the developing period has become short and the scale of development has become large. There is a limit on resources or risks a company can manage. I think to win the competition in commercialization, good cooperation in an open environment is very important. Not only large companies, but also venture companies need to cooperate with each other. In an open environment, it is essential to build a trusting relationship, and to cooperate to run the project until an achievement is made.

Ways of selecting and combining the successful elements and universalizing them

Audience

I think the discussion is drifting into the particulars. The selection and combination of the elements of the "synthesis in *Synthesiology*" discussed by Dr. Kobayashi is very important. You talk about aufheben, breakthrough, and strategic selection types, but which would survive? In the Theory of Inventive Problem Solving (TRIZ), or as Dr. Kikuya Ichikawa who wrote the *Sozo Kogaku (Creative Engineering)* says, there is a pattern in the evolution of technology, and those that do not follow the pattern fail. I want *Synthesiology* to mark out the thought process toward success. Since we are doing things in a bottom-up style, I've been a bit concerned. I think we can start from a hypothesis.

Kobayashi

Our goal was to get there, but currently we don't have enough accumulation of case studies. There is interpretation involved in the consideration for synthesizing technology, and I think hypothesis is included in the selection and combination. Also, it could be seen from the analysis so far that the cycle must be turned until the final implementation in society.

Suzuki

In *Synthesiology* Vol. 1 No. 2, the interview of Professor Richard Lester by Dr. Kobayashi was very interesting. Professor Lester mentions that not only analysis but also interpretation is important in "innovation". Innovations occur as many things are adeptly interpreted, but he also says that innovation does not occur by interpreting alone. Innovation must be made by striking the balance of analytical and interpretive areas. I think this is where *Synthesiology* can be powerful, and I am hopeful.

Ono

I think the comment from the audience presents a lofty ideal. We also purport the ideal, but *Synthesiology* as a journal is rather a framework or forum for discussion and presentation of opinions. There are two objectives with *Synthesiology*. One is that while pure basic research has been established as the methodology for science, we do not know what exactly constitutes originality for the applied and integrated research, and there is no method for seeing whether a certain result is true. I think *Synthesiology* is a forum to address such issues. That is the first objective. The second objective is for people in various technological fields to present and exchange strategies and integration methods. People can show each other what has not been established with an integrated research or discipline, and seek solutions in a bottom-up style. *Synthesiology* provides chances for such discussions, so please submit papers of your thoughts. It's like an advertisement for the journal, but that is what we would like to do.

To create an environment for thinking about "why" and to overcome the barriers

Audience

Many people indicate the problem of education as the cause of not being able to think "why". After World War II, the Japanese were educated to work hard on the problems that were laid before their eyes. That was fine during the era of catching up (to the United States and Europe), but that does not work now. What should we do?

Another point; considering the "why", I think to get a breakthrough, we must do things by trial and error, but if one wants to do something in Japan today, there is always some barrier or regulation. There are so many things that can be learned from failure, but we can never say "I failed". Do you have any suggestions for overcoming such barriers?

Suzuki

If there were answers to those questions, I would certainly like to hear them. There is a book by Mark Stefik called *Breakthrough*. I translated it. Stefik states "the researches we need now are 'radical researches'". The basic research until now was a study of a given research subject, the solution was sought, and one thought of how to overcome a barrier when he/she encountered it. In application research, when one came against a barrier when attempting to realize something, the product was completed by taking a different method that bypassed the barrier. In radical research, if one encounters a problem, the problem is studied as a subject, and the knowledge will expand although the research subject may change. I think it is necessary to solve the problem by introducing other technologies and fields as well as social technology.

As for the suggestion for overcoming a barrier when considering the "why", it is perhaps a bad habit of the Japanese to enter from the "how". I think *Synthesiology* will be an interesting place or "Ba" that may provide a chance to see the "why" once again. I hope people will take advantage of this place.

Akamatsu

We are thinking of various methodologies for utilizing research in society, and are working to establish synthesiology as one of the ways. Please continue to support our efforts.

Editorial Policy

Synthesiology Editorial Board

Objective of the journal

The objective of *Synthesiology* is to publish papers that address the integration of scientific knowledge or how to combine individual elemental technologies and scientific findings to enable the utilization in society of research and development efforts. The authors of the papers are researchers and engineers, and the papers are documents that describe, using "scientific words", the process and the product of research which tries to introduce the results of research to society. In conventional academic journals, papers describe scientific findings and technological results as facts (i.e. factual knowledge), but in *Synthesiology*, papers are the description of "the knowledge of what ought to be done" to make use of the findings and results for society. Our aim is to establish methodology for utilizing scientific research result and to seek general principles for this activity by accumulating this knowledge in a journal form. Also, we hope that the readers of *Synthesiology* will obtain ways and directions to transfer their research results to society.

Content of paper

The content of the research paper should be the description of the result and the process of research and development aimed to be delivered to society. The paper should state the goal of research, and what values the goal will create for society (Items 1 and 2, described in the Table). Then, the process (the scenario) of how to select the elemental technologies, necessary to achieve the goal, how to integrate them, should be described. There should also be a description of what new elemental technologies are required to solve a certain social issue, and how these technologies are selected and integrated (Item 3). We expect that the contents will reveal specific knowledge only available to researchers actually involved in the research. That is, rather than describing the combination of elemental technologies as consequences, the description should include the reasons why the elemental technologies are selected, and the reasons why new methods are introduced (Item 4). For example, the reasons may be: because the manufacturing method in the laboratory was insufficient for industrial application; applicability was not broad enough to stimulate sufficient user demand rather than improved accuracy; or because there are limits due to current regulations. The academic details of the individual elemental technology should be provided by citing published papers, and only the important points can be described. There should be description of how these elemental technologies are related to each other, what are the problems that must be resolved in the integration process, and how they are solved (Item 5). Finally, there should be descriptions of how closely the goals are achieved by the products and the results obtained in research and development, and what subjects are left to be accomplished in the future (Item 6).

Subject of research and development

Since the journal aims to seek methodology for utilizing the products of research and development, there are no limitations on the field of research and development. Rather, the aim is to discover general principles regardless of field, by gathering papers on wide-ranging fields of science and technology. Therefore, it is necessary for authors to offer description that can be understood by researchers who are not specialists, but the content should be of sufficient quality that is acceptable to fellow researchers.

Research and development are not limited to those areas for which the products have already been introduced into society, but research and development conducted for the purpose of future delivery to society should also be included.

For innovations that have been introduced to society, commercial success is not a requirement. Notwithstanding there should be descriptions of the process of how the technologies are integrated taking into account the introduction to society, rather than describing merely the practical realization process.

Peer review

There shall be a peer review process for *Synthesiology*, as in other conventional academic journals. However, peer review process of *Synthesiology* is different from other journals. While conventional academic journals emphasize evidential matters such as correctness of proof or the reproducibility of results, this journal emphasizes the rationality of integration of elemental technologies, the clarity of criteria for selecting elemental technologies, and overall efficacy and adequacy (peer review criteria is described in the Table).

In general, the quality of papers published in academic journals is determined by a peer review process. The peer review of this journal evaluates whether the process and rationale necessary for introducing the product of research and development to society are described sufficiently well.

In other words, the role of the peer reviewers is to see whether the facts necessary to be known to understand the process of introducing the research finding to society are written out; peer reviewers will judge the adequacy of the description of what readers want to know as reader representatives.

In ordinary academic journals, peer reviewers are anonymous for reasons of fairness and the process is kept secret. That is because fairness is considered important in maintaining the quality in established academic journals that describe factual knowledge. On the other hand, the format, content, manner of text, and criteria have not been established for papers that describe the knowledge of “what ought to be done.” Therefore, the peer review process for this journal will not be kept secret but will be open. Important discussions pertaining to the content of a paper, may arise in the process of exchanges with the peer reviewers and they will also be published. Moreover, the vision or desires of the author that cannot be included in the main text will be presented in the exchanges. The quality of the journal will be guaranteed by making the peer review process transparent and by disclosing the review process that leads to publication.

Disclosure of the peer review process is expected to indicate what points authors should focus upon when they contribute to this journal. The names of peer reviewers will be published since the papers are completed by the joint effort of the authors and reviewers in the establishment of the new paper format for *Synthesiology*.

References

As mentioned before, the description of individual elemental technology should be presented as citation of papers published in other academic journals. Also, for elemental technologies that are comprehensively combined, papers that describe advantages and disadvantages of each elemental technology can be used as references. After many papers are accumulated through this journal, authors are recommended to cite papers published in this journal that present similar procedure about the selection of elemental technologies and the introduction to society. This will contribute in establishing a general principle of methodology.

Types of articles published

Synthesiology should be composed of general overviews such as opening statements, research papers, and editorials. The Editorial Board, in principle, should commission overviews. Research papers are description of content and the process of research and development conducted by the researchers themselves, and will be published after the peer review process is complete. Editorials are expository articles for science and technology that aim to increase utilization by society, and can be any content that will be useful to readers of *Synthesiology*. Overviews and editorials will be examined by the Editorial Board as to whether their content is suitable for the journal. Entries of research papers and editorials are accepted from Japan and overseas. Manuscripts may be written in Japanese or English.

Required items and peer review criteria (January 2008)

	Item	Requirement	Peer Review Criteria
1	Research goal	Describe research goal (“product” or researcher’s vision).	Research goal is described clearly.
2	Relationship of research goal and the society	Describe relationship of research goal and the society, or its value for the society.	Relationship of research goal and the society is rationally described.
3	Scenario	Describe the scenario or hypothesis to achieve research goal with “scientific words”.	Scenario or hypothesis is rationally described.
4	Selection of elemental technology(ies)	Describe the elemental technology(ies) selected to achieve the research goal. Also describe why the particular elemental technology(ies) was/were selected.	Elemental technology(ies) is/are clearly described. Reason for selecting the elemental technology(ies) is rationally described.
5	Relationship and integration of elemental technologies	Describe how the selected elemental technologies are related to each other, and how the research goal was achieved by composing and integrating the elements, with “scientific words”.	Mutual relationship and integration of elemental technologies are rationally described with “scientific words”.
6	Evaluation of result and future development	Provide self-evaluation on the degree of achievement of research goal. Indicate future research development based on the presented research.	Degree of achievement of research goal and future research direction are objectively and rationally described.
7	Originality	Do not describe the same content published previously in other research papers.	There is no description of the same content published in other research papers.

Instructions for Authors

Synthesiology Editorial Board
Established December 26, 2007
Revised June 18, 2008
Revised October 24, 2008
Revised March 23, 2009
Revised August 5, 2010

1 Types of contributions

Research papers or editorials and manuscripts to the "Readers' Forum" should be submitted to the Editorial Board. After receiving the manuscript, if the editorial board judges it necessary, the reviewers may give an interview to the author(s) in person or by phone to clarify points in addition to the exchange of the reviewers' reports.

2 Qualification of contributors

There are no limitations regarding author affiliation or discipline as long as the content of the submitted article meets the editorial policy of *Synthesiology*, except authorship should be clearly stated. (It should be clearly stated that all authors have made essential contributions to the paper.)

3 Manuscripts

3.1 General

3.1.1 Articles may be submitted in Japanese or English. Accepted articles will be published in *Synthesiology* (ISSN 1882-6229) in the language they were submitted. All articles will also be published in *Synthesiology - English edition* (ISSN 1883-0978). The English edition will be distributed throughout the world approximately four months after the original *Synthesiology* issue is published. Articles written in English will be published in English in both the original *Synthesiology* as well as the English edition. Authors who write articles for *Synthesiology* in Japanese will be asked to provide English translations for the English edition of the journal within 2 months after the original edition is published.
3.1.2 Research papers should comply with the structure and format stated below, and editorials should also comply with the same structure and format except subtitles and abstracts are unnecessary. Manuscripts for "Readers' Forum" shall be comments on or impressions of articles in *Synthesiology*, or beneficial information for the readers, and should be written in a free style of no more than 1,200 words. Editorials and manuscripts for "Readers' Forum" will be reviewed by the Editorial Board prior to being approved for publication.
3.1.3 Research papers should only be original papers (new literary work).
3.1.4 Research papers should comply with various guidelines of research ethics.

3.2 Structure

3.2.1 The manuscript should include a title (including subtitle), abstract, the name(s) of author(s), institution/contact, main text, and keywords (about 5 words).
3.2.2 Title, abstract, name of author(s), keywords, and institution/contact shall be provided in Japanese and English.
3.2.3 The manuscript shall be prepared using word processors or similar devices, and printed on A4-size portrait (vertical) sheets of paper. The length of the manuscript shall be, about 6 printed pages including figures, tables, and photographs.
3.2.4 Research papers and editorials shall have front covers and the category of the articles (research paper or editorial) shall be stated clearly on the cover sheets.
3.2.5 The title should be about 10-20 Japanese characters (5-10 English words), and readily understandable for a diverse readership background. Research papers shall have subtitles of about 15-25 Japanese characters (7-15 English words) to help recognition by specialists.
3.2.6 The abstract should include the thoughts behind the integration of technological elements and the reason for their selection as well as the scenario for utilizing the research results in society.
3.2.7 The abstract should be 300 Japanese characters or less (125 English words). The Japanese abstract may be omitted in the English edition.
3.2.8 The main text should be about 9,000 Japanese characters (3,400 English words).
3.2.9 The article submitted should be accompanied by profiles of all authors, of about 200 Japanese characters (75 English words) for each author. The essential contribution of each author to the paper should also be included. Confirm that all persons who have made essential contributions to the paper are included.
3.2.10 Discussion with reviewers regarding the research paper content shall be done openly with names of reviewers disclosed, and the Editorial Board will edit the highlights of the review process to about 3,000 Japanese characters (1,200 English words) or a maximum of 2 pages. The edited discussion will be attached to the main body of the paper as part of the article.

3.2.11 If there are reprinted figures, graphs or citations from other papers, prior permission for citation must be obtained and should be clearly stated in the paper, and the sources should be listed in the reference list. A copy of the permission should be sent to the Publishing Secretariat. All verbatim quotations should be placed in quotation marks or marked clearly within the paper.

3.3 Format

3.3.1 The headings for chapters should be 1, 2, 3…, for subchapters, 1.1, 1.2, 1.3…, for sections, 1.1.1, 1.1.2, 1.1.3.
3.3.2 The text should be in formal style. The chapters, subchapters, and sections should be enumerated. There should be one line space before each paragraph.
3.3.3 Figures, tables, and photographs should be enumerated. They should each have a title and an explanation (about 20-40 Japanese characters or 10-20 English words), and their positions in the text should be clearly indicated.
3.3.4 For figures, clear originals that can be used for printing or image files (resolution 350 dpi or higher) should be submitted. In principle, the final print will be 15 cm × 15 cm or smaller, in black and white.
3.3.5 For photographs, clear prints (color accepted) or image files should be submitted. Image files should specify file types: tiff, jpeg, pdf, etc. explicitly (resolution 350 dpi or higher). In principle, the final print will be 7.2 cm × 7.2 cm or smaller, in black and white.
3.3.6 References should be listed in order of citation in the main text.

Journal – [No.] Author(s): Title of article, *Title of journal* (italic), Volume(Issue), Starting page-Ending page (Year of publication).

Book – [No.] Author(s): *Title of book* (italic), Starting page-Ending page, Publisher, Place of Publication (Year of publication).

4 Submission

One printed copy or electronic file of manuscript with a checklist attached should be submitted to the following address:

Synthesiology Editorial Board
c/o Website and Publication Office, Public Relations Department, National Institute of Advanced Industrial Science and Technology (AIST)
Tsukuba Central 2, 1-1-1 Umezono, Tsukuba 305-8568
E-mail: synthesiology@m.aist.go.jp

The submitted article will not be returned.

5 Proofreading

Proofreading by author(s) of articles after typesetting is complete will be done once. In principle, only correction of printing errors are allowed in the proofreading stage.

6 Responsibility

The author(s) will be solely responsible for the content of the contributed article.

7 Copyright

The copyright of the articles published in "*Synthesiology*" and "*Synthesiology English edition*" shall belong to the National Institute of Advanced Industrial Science and Technology (AIST).

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Letter from the editor

While all the research results published in this issue are original and are geared toward practical application, they are subjected to different interpretations when viewed from the perspective of how a technology evolves and becomes established as a new technology, or how to overcome the valley of death in the course of taking the technological development to practical use.

From the perspective of the evolution of technology, in the "Development of laser-assisted inkjet printing technology", the laser-assisted method, which is a new surface treatment method, is devised and established as the ultra-fine wiring technology through demonstration experiments, based on the experience of the successful R&D of aerosol deposition method. It is offered as the solution for reliability that is a major issue in the advancement of inkjet technology, as well as the differentiating factor from the conventional technologies. In the "Challenge for the development of micro SOFC manufacturing technology", the compact-size of fuel cells is achieved and demonstrated through the idea of highly applicable ceramic integration process. It is a case where the technology moves forward through fusion of different technologies, and is an excellent example of how the technology evolves.

"Spectral database system for organic compounds" is an example of an R&D whereby the valley of death is overcome by maintaining close relationship with society and by spending effort on social acceptance. The process by which the database would eventually become widely used is a general process of acceptance in society, and the paper is a fine example that analyzes the methodology of that process.

In the "Formation of research strategy and synthetic research evaluation based on the strategy", the importance of having a goal for the research program and the scenario to attain the goal as part of the strategy formation is emphasized. It is also stated that for evaluating the research, it is important to have a synthetic evaluation method that combines the elemental evaluations based on the inference through deduction, induction, and hypothesis formation, while comparing them with the research strategy. Overall, it points to the importance of strategy and its evaluation to overcome the valley of death.

There are two discussions on the general methodology for overcoming the valley of death. "Methodology for technological integration for open innovation hub" discusses how the evolution of technology may lead to innovation from the side of technological potentials, while "Japanese manufacturing and synthesiology" discusses the promotion of design science by strengthening the competitive power, the system for increasing the level of synthesis, and the establishment of the outlet toward the circulating society, from the standpoint of society as an outlet of social technology. The two articles are discussed from opposing stances; the evolution of technological development that is the entrance to the valley of death; and the establishment of the social technology at its exit. Here are the two sides of the general discussion for overcoming the valley of death. I think the importance in organizing the discussion for the synthesis methodology to overcome the valley of death will be reackowledged in the future.

Editor
Akira Yabe

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