Utilization of Combinatorial Method and High Throughput Experimentation for Development of Heterogeneous Catalysts

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(Received December 12, 2005)

The combinatorial method and high throughput experimentation have been applied to catalysis development in the last decade. Here we describe equipment for catalyst preparation, catalysis evaluation and product analysis with a gas sensor system. High throughput experimentation using these devices has allowed us to optimize catalyst composition with stochastic methods such as the genetic algorithm. The improvement of propane selective oxidation catalysis is described. High throughput experimentation allowed the construction of a database for elemental reactions. We have developed novel catalysts for ethanol steam-reforming catalysts and a dimethyl ether steam-reforming catalyst by combining good catalysts for each elemental reaction. Our new concept of "Materiomics" is introduced as a promising method for material science based on combinatorial technology.

Keywords
Combinatorial method, High throughput experimentation, Materiomics, Heterogeneous catalyst

1. Introduction

The success of combinatorial technology in pharmaceutical chemistry and industry in the early 90s encouraged material scientists to apply the technology to their research field[1]. Some researchers in the catalysis field also tried to apply it to catalysis development[2,3]. At the early stage, high throughput screening technologies were often reported because catalysis evaluation is often a bottleneck to catalysis development. For example, an IR-thermograph was developed to evaluate simple combustion catalysts by the detection of reaction heat[4]. At the same time, miniaturization and parallelization of catalyst preparation was developed and can be divided into two types: solution-based catalyst preparation such as the sol-gel process[5,6], and a monolithic catalyst support such as a pellet[7]. Although some improvements are still required for both catalysis evaluation and preparation, the basic hardware technologies for combinatorial catalysis had been developed by 2000[8].

Although high throughput screening technology is useful to examine many catalysts in a short time, how to accelerate catalyst development remained an important problem with this technology. In 2000, Wolf et al. reported the utilization of an evolutionary approach for the optimization of metal oxide compositions composed of 8 metals suitable for the oxidative dehydrogenation of propane[9]. The algorithm is effective to identify a composition meeting the requirements. On the other hand, data mining technology is also attracting researchers based on the utilization of an artificial neural network for extracting specific "knowledge" from a lot of information achieved by high throughput experimentation[10]. Utilization of combinatorial or high throughput screening technology with artificial intelligence seems to be promising for the acceleration of catalysis development.

Here we describe our results on the study of high throughput experimentation and combinatorial catalysis since 1999. First, we developed a fast screening technology with a gas sensor system. The sensor system can evaluate not only simple reactions like CO oxidation but also the oxidative hydrogenation of ethane and the selective oxidation of propane[10]. The potential of the gas sensor system is presented for the evaluation of selective oxidation or ammoxidation of benzene[11]. We then developed catalyst preparation equipment such as a powder dispenser and a reaction controller which simply parallelized conventional methods for conventional materials. We can prepare a catalyst library with various powder supports by impregnation, deposition-precipitation, etc., and evaluate the catalysis with a conventional L-type fixed bed flow-type reactor[12]. In order to iden-
tify novel catalysts with our method of high throughput screening, two different methods were examined. The first method is the utilization of a genetic algorithm with a designed 1st generation for the catalysis improvement of propane selective oxidation\(^1\). We found that the number of experiments can be effectively reduced by the addition of chemical knowledge to the experimental design. The second method is catalyst design with reference to a database on-demand\(^14\). The catalysts for steam reforming of dimethyl ether or ethanol were designed utilizing the database of their elemental reactions\(^14\)–\(^16\). Finally, we introduced a novel research concept of "Materiomics" based on combinatorial methodology and analytical technologies including theoretical science\(^14\).

2. Equipment for High Throughput Experimentation

2.1. Gas Sensor System for High Throughput Screening of Heterogeneous Catalysts

High throughput analysis is often the most important technology for the success of combinatorial catalysis. Researchers in the catalysis field are interested in both catalytic activity and product distribution so that catalysis evaluation should be performed by quantification of all educts and products, or at least the desirable product. For the quantification of each product, several different technologies have been developed. Senkan developed a REMPI (resonance enhanced multi photon ionization) detector for the evaluation of the hydrogenation of 1-hexene\(^18\). Cong et al. used a q-mass spectrometer for product quantification in the oxidative dehydrogenation of ethane\(^19\). Snively and Lauterbach have developed a parallel FT-IR (Fourier transform infrared spectroscopy) with 2-D detectors\(^20\). Dye utilization is also a possible technology reported for NO\(_2\) detection\(^21\). We have developed gas sensor systems mainly using semiconductor gas sensors which are small, inexpensive and usually highly sensitive\(^10\)–\(^11\). A problem of the gas sensor system remains the poor selectivity originating from its relatively simple working mechanism; the surface of the semiconductor is covered with oxygen supplied from the air under atmospheric conditions. The oxygen molecules or atoms withdraw electrons from the semiconductor. When the semiconductor is exposed to certain chemicals, the oxygen atoms are consumed by the combustion of the chemicals. As a result, combustion leads to release of the electrons withdrawn by the oxygen and changes the resistance of the semiconductor. The selectivity of the sensor can be improved by the addition of sensitized materials such as oxidation catalysts to control the depth of oxidation of each product on the semiconductor surface.

Odor discrimination with a gas sensor system is an important research field for various purposes such as food processing. We used a gas sensor system developed for odor discrimination for the evaluation of selective alkane oxidation catalysis because the desired products such as alcohol and aldehyde have specific odors. On the other hand, the educts of lower alkanes, and byproducts of CO and CO\(_2\) do not have an odor. Figure 1 indicates the sensitivity of the odor gas sensors toward various chemicals. The sensor elements are highly sensitive toward aldehydes, alcohols, and ketones, but are insensitive to propane, CO and CO\(_2\). Also the output from gas sensors increases in proportion to the concentration of oxygenated compounds. These properties are suitable for the detection and quantification of the products formed by alkane selective oxidation.

![Figure 1](image-url)
**Figure 2** compares the quantification results of a gas sensor system with those using gas chromatography in propane selective oxidation. The gas sensor system consists of an odor gas sensor, a potentiometric CO sensor and NDIR (nondispersive infrared) CO₂ gas sensors. From their output, each concentration in the effluent can be easily calculated. The absolute values of these concentrations are not so accurate; however, a rough estimation of product selectivity was possible. Two minutes was sufficient for the quantification. In contrast, we needed more than 40 min for each analysis by conventional gas chromatography.

**Table 1** summarizes the reaction system validated with the gas sensor system by our group. Although some educts were not odorless, the difference in sensitivity of the gas sensors enables the quantification of products.

The smaller size of the gas sensor elements allowed parallel setting in a limited space. **Figure 3** shows the five gas sensors for the evaluation of CO oxidation catalysis. The size was only 2 cm × 2 cm for each element. The rapid response of the CO gas sensor allowed real-time monitoring of CO concentration in the effluent. An oscillation phenomenon on Rh/SlO₂ was observed as indicated in **Fig. 4**.

### 2.2. Catalysts Preparation and Reactor System

Catalysis often depends on the preparation method. Catalysts cannot always be prepared with the sol-gel method or a monolithic support. Powder supports are

![Five Parallel Catalytic Combustion Type Sensors for the Evaluation of CO Oxidation Catalysis](image)

**Figure 3**  Five Parallel Catalytic Combustion Type Sensors for the Evaluation of CO Oxidation Catalysis

### Table 1 Reaction Systems Suitable for Evaluation by the Odor Gas Sensor System

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Educt</th>
<th>Product</th>
<th>Comments</th>
<th>ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>oxidative</td>
<td>ethane</td>
<td>ethylene</td>
<td>Not suitable for systems involving aldehyde or ketone compound</td>
<td>10)</td>
</tr>
<tr>
<td>dehydrogenation</td>
<td>propane</td>
<td>propylene</td>
<td></td>
<td>*</td>
</tr>
<tr>
<td>selective oxidation</td>
<td>methane</td>
<td>formaldehyde, methanol</td>
<td>Hard to determine selectivity for oxygenated products</td>
<td>*</td>
</tr>
<tr>
<td></td>
<td>ethane</td>
<td>acetaldehyde, acetic acid, ethanol</td>
<td>Hard to determine selectivity for oxygenated products</td>
<td>*</td>
</tr>
<tr>
<td>ammonoxidation</td>
<td>benzene, ammonia</td>
<td>aniline</td>
<td>Evaluated with standard gas</td>
<td>11)</td>
</tr>
<tr>
<td>alkylation</td>
<td>benzene, propane, propylene</td>
<td>cumene</td>
<td>Poor selectivity (only active catalysts can be evaluated)</td>
<td>11)</td>
</tr>
</tbody>
</table>

* unpublished result.
often used for conventional catalyst preparations. **Figure 5** shows the powder dispensing machine built in-house\textsuperscript{13}. The machine consists of four parts: an X-Y robot for transferring a tube holder onto the balance, a balance, two powder containers with a mesh filter inside and a computer for programming the required weight of powder. The X-Y robot transfers the holder on the balance. After the holder sits on the balance, support powder in a container filtered by vibration is dropped into the tube up to the weight programmed. By changing the vibration frequency and mesh size, we can use various powders with different properties. Usually a certain amount of powder can be weighed within 2 min. The tubes containing the support powder are arranged in a parallel magnetic stirrer placed on the stage of a liquid pipetting machine delivering precursor solutions for impregnation or ion exchange.

For catalysis measurement, the catalytic material is often placed in an L-type fixed bed flow-type reactor made of quartz\textsuperscript{16}. Usually a large space is required for keeping the samples. Also, it is not easy to recover all the samples after reaction so that the reactors must be washed thoroughly every time. These are trivial problems for usual experimentation; but not for combinatorial catalysis which treats many candidates at the same time. For ease in the sample treatment, a tiny cartridge tube with ground glass joint and a holder were developed as shown in **Fig. 6**. By keeping the catalyst in the glass cartridge, as many as fifty samples can be stored in a small box measuring 7 cm × 14 cm and the same catalyst used repeatedly without loss in weight.

The reaction controller shown in **Fig. 7** holds five reactors and can control the reaction gas composition, flow rate, reaction time, and reaction temperatures for each catalyst and analytical tools such as a gas chromatograph\textsuperscript{15,22}. Depending on the reaction conditions, we can usually perform more than 100 reaction runs per day with the controller.

### 3. Optimization of Additives with Genetic Algorithm: Selective Oxidation Catalyst for Propane

A genetic algorithm is a kind of artificial intelligence for optimizing a system with the survival-of-fittest rule\textsuperscript{23}. The algorithm is stochastic and has multiple starting points. The optimization proceeds with the repetitive operations of crossover and mutation which imitate the behavior of genes in nature. The algorithm can be used to solve mathematical problems with a computer because it requires examination of less hope-
ful candidates. High throughput experimentation technology allows us to examine such candidates in the real experimental system.

Application of the genetic algorithm for the optimization of catalyst compositions was first reported by Wolf et al. Since then, many groups have used the algorithm for investigating a new catalytic system. Maiert et al. added an operation for a "combination" suitable for producing a complex system easily. We also improved two points of the reported genetic algorithm for the optimization of our catalysts; how to generate the 1st generation and how to treat the concentration of each additive. Usually compositions of the 1st generation are determined at random. However, the diversity in composition of the 1st generation affects the optimization speed. When a 1st generation composed of few elements is used, many mutations are required for searching all the combinatorial space. A 1st generation containing a wide variety of elements can save investigation time due to the coverage of a large part of the combinatorial space. When considering the coding of elements in materials, we noticed that the concentration information for each element can be coded although the genetic algorithm usually treats the code consisting of 0 and 1 corresponding to "absence" and "presence," respectively. We can set several or more levels in the element concentration and put in a code corresponding to "concentration" instead of that expressing "presence." It is important to modify the optimization methodology for catalyst development.

The loading amount of an additive element is an important parameter to determine the structure of the catalyst supports. For example, an isolated structure included in a support metal oxide is often observed at very low loading. Full coverage of the support surface is expected only at high loading. Based on these two ideas, we optimized the combination of 7 different additives at 3 levels of concentration to improve the catalysis of Fe/SiO2 in the selective oxidation of propane. For a selective oxidation catalyst, the control of the redox property of an active site seems to be important for controlling the reactivity of bound oxygen or the substrate. Combinatorial selection of elements from the following seven, Cs⁺, Cu²⁺, Zn²⁺, Co²⁺, Ga³⁺, Zr⁴⁺ and Nb⁵⁺ with various atomic charges or redox properties, were added to Fe/SiO2. Here we limited the available loading amount of each corresponding metal oxide to three levels of 0.1, 1 or 5 wt% on the basis of the correlation between the metal oxide structure and its catalysis. The expected structure at each concentration is shown in Fig. 8.

Scheme 1 shows how to determine the combinations of loading chemical species onto Fe/SiO2 at the 1st generation. At first, three elements were picked from the 7 elements for mounting on Fe/SiO2, and then their loadings were independently determined by three random digits. Three was selected for the number of mounting elements because this number seems to be sufficient to cover all 21 chemical species produced by the combinations of the 7 elements and 3 loadings when the number of catalytic materials is 20 at each generation. Actually, all 21 species were found in the 20 cat-

The device controls gas composition, gas flow rate, reaction temperature, reaction time, sampling interval, etc. Fig. 7 Reaction Controller for Five Catalysts Assembled by BEL Japan

Fig. 7 Reaction Controller for Five Catalysts Assembled by BEL Japan

Fig. 8 Three Typical Structures of Metal Oxides on Silica Surface Depending on the Loading Amount

alalytic materials of the 1st generation. Such a large diversity of chemical species at the initial stage of an optimization is important to avoid trapping at a local maximum.

The optimization procedure used here was the same as the usual operations in the genetic algorithm based on “crossover” and “mutation.” After preparing the catalysts following the composition in Scheme 1, catalysis measurements for propane oxidation were performed. For the 2nd generation, 10 parents were selected from the catalysts in the 1st generation according to the evaluation of the selectivity for desired products at 5% propane conversion. The operation was repeated up to the 5th generation. When we saw the composition of added metal oxide at the 4th and 5th generations, we could identify the most suitable chemical species for catalysis improvement. No catalyst included any kind of copper species. On the other hand, Ga$_{0.1}$ (isolated) appeared in 12 materials in the 4th generation. Also, it was obvious that bulk Cs$_2$O (1% or 5%) was the most effective species for the improvement of the selectivity of Fe/SiO$_2$. The positive effect of cesium addition was already known in the selective oxidation of ethane or propane over M/SiO$_2$ (M – Fe, V)$_{25}$~28. As for other species, isolated Zn$^{2+}$ seemed to be effective if combined with Cs$_2$O. In order to elucidate the effect of these species, bulk Cs$_2$O, isolated Ga$^{3+}$ and isolated Zn$^{2+}$ in different compositions supported on Fe/SiO$_2$ were examined for selective oxidation. A total of twenty-seven combinations were examined for further optimization with concentration levels of 0.05, 0.1 and 0.2% for Ga$^{3+}$ and Zn$^{2+}$ and levels of 1, 3 and 5% for cesium oxide. As a result, we found that the best selectivity of 49.5% in 5% propane conversion was obtained by the addition of Cs$_2$Ga$_{0.5}$Zn$_{0.2}$ and Cs$_2$Ga$_{0.5}$Zn$_{0.2}$ to Fe/SiO$_2$. By using the genetic algorithm with modification for the production of the 1st generation and treatment of the concentration information for each element, we succeeded in improving the catalysis of Fe/SiO$_2$ for the selective oxidation of propane.

4. Catalyst Design Referring to the Database Constructed on Demand

High throughput screening of a material library designed by the combinatorial concept is a powerful tool to achieve a database including quantitative information on demand. When we design a new catalyst, we collect information in the literature not only on the target reaction but also on its elemental reactions. Sometimes we find that the reaction conditions are not the same in terms of reaction temperatures, space velocities, gas composition, etc. The construction of the database on the target reaction and its elemental reactions is useful for rational design of a novel catalyst for the target re-
action because we can combine superior catalysts for each reaction step. Based on this concept, steam-reforming catalysts for ethanol and dimethyl ether were developed. The steam-reforming catalyst is expected to be important to supply hydrogen for the fuel cell as a portable power generator. At present, methanol is the most promising candidate for the source of portable hydrogen because methanol steam-reforming proceeds at low temperature. However, methanol is highly toxic so that when we choose the source from a safety point of view, the best candidates are less toxic chemicals such as ethanol and dimethyl ether (DME) whose steam-reforming catalysts are less studied. We developed novel catalysts for these reactions with the construction of a database on the target reactions and their elemental reactions.

4.1. Development of Ethanol Steam-reforming Catalyst Referring to the Database on Demand

Hydrogen production from a renewable source is an important technology for a hydrogen-based society. Ethanol is a renewable resource because it can be produced by fermentation of biomass. At present, methanol is regarded as the most promising candidate for a portable hydrogen source because its steam-reforming proceeds under mild conditions; however, from a safety point of view, methanol is highly toxic so that it is not suitable for portable use. Ethanol is less toxic but its steam-reforming requires a higher temperature because ethanol has a C–C bond which is more stable than a C–H bond.

A catalyst library consisting of precious metals loaded on various metal oxides was examined for ethanol steam-reforming. Precious metals and metal oxides were selected from Pt, Pd, Ir, Rh and Ru and from Al2O3, ZrO2, TiO2, La2O3, SiO2, Ta2O5, CeO2, WO3, Nb2O5, SnO2, MnO2, and V2O5, respectively. The atomic ratio of precious metals to the metals in the oxide support was 1% for each catalyst. The reaction was performed from 200 to 400°C at intervals of 50°C with SV = 20,000 ml·g⁻¹·h⁻¹. The reaction gas consisting of 1% ethanol and 3% H2O in Ar was allowed to flow over each catalyst for 5 min before product analysis.

Figure 9 shows the correlation between ethanol conversion and H2 yield for each analysis. The open circles in Fig. 9 indicate high hydrogen yielding catalysts with hydrogen yield higher than 1.96%. These catalysts provided the top 10% hydrogen yields. The H2 yield depends not only on ethanol conversion but also on the catalyst and reaction temperature. For the catalysts indicated by open circles in Fig. 9, product distributions were examined, and selectivity for C2H4 or CH3CHO was found to be very low. Also, as shown in Fig. 10, the catalysts yielding high C2H4 (>0.114%) or high CH3CHO (>0.265%) provided a limited yield of hydrogen. These results are quite reasonable when we consider the reaction route of ethanol steam-reforming.

There are three routes for the 1st step of ethanol reforming. The first route is dehydration to provide C2H4, the second route is dehydrogenation to provide acetaldehyde, and the third route is homolytic scission to produce radical species. Ethylene steam-reforming is not easy at the reaction temperatures, which leads to a low hydrogen yield. Acetaldehyde formation is desirable for a higher hydrogen yield if the catalyst is active for steam-reforming of acetaldehyde. The catalysts selective for acetaldehyde formation are less active for the steam-reforming of acetaldehyde.

Figure 11 shows the comparisons of hydrogen yield for CH3CHO steam-reforming and ethanol steam-reforming. Rh/CeO2 shows the highest activity for steam-reforming of CH3CHO. On the other hand, Rh/CeO2 shows only limited activity for ethanol steam-reforming. If acetaldehyde is selectively formed from ethanol as the first step over Rh/CeO2, a high hydrogen yield could be achieved over Rh/CeO2.

To induce the high potential of Rh/CeO2 for ethanol steam-reforming, we searched for a selective catalyst to provide acetaldehyde from ethanol at these temperatures. We examined 14 metal oxides, 12 metal oxides used as support and CuO and Ga2O3, for ethanol decomposition. SnO2 showed a high activity for the reaction. SnO2 on Rh/CeO2 catalyst was examined for ethanol steam-reforming. Figure 12 shows the H2 yield of SnO2 + Rh/CeO2 catalysts compared with other Rh-loaded catalysts. The reaction was performed at 300 and 350°C. Even at a temperature as low as 300°C, the hydrogen yield was 2.9%, which is higher than that of 2.8% at Rh/CeO2 without SnO2 at 400°C. We succeeded in achieving a novel catalyst for ethanol steam-

![Fig. 9](image-url) Correlation between Ethanol Conversion and Hydrogen Yields for a Series of Catalysts at Reaction Temperatures from 200 to 400°C at 50°C Intervals

reforming with the fact database for ethanol steam-reforming, CH₃CHO steam-reforming, ethanol decomposition on-demand.

4.2. Development of DME Steam-reforming

Catalyst Referring to the Database on Demand

DME is also a promising candidate as a source of portable hydrogen because it becomes liquid at as low as 6 atm, and no vaporization unit is necessary, in contrast to the steam-reforming of alcohols, before the reaction due to its low boiling point of −25°C. Also, the toxicity level is similar to that of liquid petroleum gas so that DME is suitable for a portable hydrogen source. Figure 13 (a) shows the hydrogen concentration in the effluent from DME steam-reforming at 200°C. The highest hydrogen concentration of 1.1% was achieved over Pt/Al₂O₃. The superior catalysis of Pt/Al₂O₃ has been already reported by a few research groups. The acidic property of Al₂O₃ accelerates the hydrolysis of DME which is believed to be the rate-determining step of the reaction.

Catalysis highly depends on the supports. In the series of Pt catalysts, Al₂O₃, TiO₂ and ZrO₂ seem to be suitable supports for the reaction. Among Rh-loaded catalysts, TiO₂, ZrO₂ are suitable supports and Al₂O₃ and SiO₂ are suitable for Pd. There seem to be two types of reaction mechanisms. The first one is the reaction via methanol formation by hydrolysis following

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Fig. 10 Correlation between Ethanol Conversions and Hydrogen Yield of Catalysts Forming C₂H₄ or CH₃CHO at High Yield

Fig. 11 Comparisons of Hydrogen Yield in CH₃CHO Steam-reforming with the Ethanol Steam-reforming over a Series of Catalysts at 400°C
reforming. The second one is the direct reforming of DME without formation of methanol. The reaction over a Rh-loaded catalyst proceeds without the formation of methanol because a Rh-loaded catalyst usually shows a high activity for steam-reforming of hydrocarbons. A Pd-loaded catalyst is known to be a less active catalyst for the steam-reforming of hydrocarbons than Rh. The reaction over Pd-loaded catalysts proceeds by the formation of methanol. The reaction over a Pt-loaded catalyst includes two mechanisms.

**Figure 13 (b)** shows the hydrogen concentration in the effluent from methanol steam-reforming at 140°C. The highest methanol concentration was obtained over Pd/MnO₂. No apparent trend in support effect and loaded precious metals was observed. The highest activity of Pd/MnO₂ was obtained accidentally.

A new catalyst for DME steam-reforming was developed by combining a suitable support for DME steam-reforming and the best catalyst for methanol steam-reforming. **Figure 14** shows the hydrogen yield for the reaction over Pd/MnO₂ physically mixed with Al₂O₃, TiO₂, and ZrO₂ which are suitable supports for DME steam-reforming compared with the results of Pt/Al₂O₃ and Pd/MnO₂ at different temperatures. The ratio of Pd/MnO₂ to each metal oxide is 1 : 1. A higher hydrogen concentration was observed over these physically mixed systems at high temperature although the hydrogen conversion was lower over Pd/MnO₂ + Al₂O₃ than over Pt/Al₂O₃ at temperatures less than 250°C. This is due to the low activity of Al₂O₃ for DME hydrolysis. The hydrolysis activity of Al₂O₃ was dramatically enhanced by the loading of Pt. At temperatures higher than 300°C, the activity of Pd/MnO₂ + Al₂O₃ was higher than that of Pt/Al₂O₃ when the mixed Al₂O₃ shows certain activity. In fact, mixing of Pd/MnO₂ with Pt/Al₂O₃ showed higher activity even at low temperature (data not shown). A novel DME steam-reforming catalyst was successfully obtained by the combination of Pd/MnO₂ suitable for methanol steam-reforming with a...
suitable catalyst for DME hydrolysis on the basis of the constructed database for the elemental reactions of DME steam-reforming.

5. "Materiomics" Based on High Throughput Experimentation with Analytical and Theoretical Science

The ultimate goal of functional materials research is to achieve "knowledge" on how to design materials with adequate performance. "Materials informatics" treats a huge number of experimental results for extracting "knowledge" by data mining techniques. A similar concept of "Materials informatics" has already been established in biological studies as "Bioinformatics." "Bioinformatics" treats a huge amount of information achieved by an "-omics" study such as proteomics. Proteomics is defined as the total research of all proteins in a cell. It concerns not only the structural and functional features of each protein but also how the proteins interact with each other for maintaining life. "Materiomics" is the equivalent study in the materials research field. Materials showing high performance are and will often be found in a complex system as the result of interaction among several or more chemical species. "Materiomics" will identify the species being investigated by an analysis tool such as electron microscopy and investigate the effect of interaction between the species on materials function and how the species combine by various techniques such as spectroscopic methods and theoretical methods. "Material informatics" can be established by "Materiomics."

In the case of a catalyst study, "Materiomics" is also required. Because the catalytic reaction proceeds on a material surface, investigation of the surface structural features of each catalyst is indispensable to establish the relationship between surface structure and catalysis. Theoretical calculation is a powerful technology to compensate for the lack of electron microscope observations and to correlate catalysis and structural features because catalysis depends on the bulk properties of materials which are sometimes difficult to measure. The construction of a database consisting of catalysis data, structural analysis data and theoretical calculations data is one of the promising methods of collaborative research. A similar framework can be applicable to many research fields of materials. "Materiomics" will provide a database useful and suitable for data mining and knowledge extraction by "Material informatics."

The difference between a biological study and a materials study seems to be the presence of a desirable research target. The research target in biology is usually provided apriori, whereas the target of material research is usually a required characteristic of materials. High throughput experimentation and combinatorial technology are suitable for both creating a novel material in a complex system and constructing a systematic database for the study of interactions between chemical species. "Materiomics" accelerates our understanding of the correlation between materials function and interactions between chemical species.

Acknowledgment

The authors would like to thank New Cosmos Electric Co., Ltd., for the study of gas sensor utilization. The authors acknowledge the Taiyo Corp. for the design and manufacturing of the powder dispensing instrument and Bel Japan Inc. for the robust instruments for rapid catalysis measurement.

References


要 旨

コンビナトリアル手法および迅速実験手法を用いた固体触媒開発

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筆者らは、コンビナトリアル手法を固体触媒開発へ応用するための手段・手法について、主に金属触媒を具体制例とし
て取り上げ研究を行ってきた。本報では、触媒調製、評価に必
要な各種実験装置、それらを利用した触媒探索手法の紹介、今
後展望について述べる。迅速実験手法を用いることにより、
これまで実際の材料探索には用いられてなかった確率的探索
手法を用いた組成最適化が可能となった。本手法を用いた触媒
組成最適化の実例として、プロパン選択性酸化触媒を取り上げた。

また、システムとしてのデータベースがオンデマンドで得られ
るため、それらのデータベースを利用した新たな触媒設計手法
も可能となった。実例として、メタノール水蒸気改質触媒なら
びにエタノール改質触媒を取り上げた。さらに、今後の展開と
して、コンビ手法と計算科学を含めた解析的手法の組合せが中
心的役割を果たす「マテリオミクス」の概念についても紹介す
る。

………………以上略………………