Process Informatics of High-Entropy Alloy for Automotive Catalysis

Azusa Kamiyama[1], Kohei Kusada[2,3], Hiromasa Kaneko[4], Megumi Mukoyoshi[2],
Masafumi Sakota[1], Hiroto Tsuchiya[1], Atsushi Furukawa[1], Hiroshi Kitagawa[2] and Hitoshi Mikami[1*]
[1]*Honda R&D Co., Ltd., Innovative Research Excellence, 4630 Shimotakanezawa, Haga-machi, Haga-gun, Tochigi, Japan.*
[2]*Kyoto University, Division of Chemistry, Kitashirakawa-Oiwakecho, Sakyo-ku, Kyoto, Japan*
[2]*Kyoto University, The Hakubi Center for Advanced Research, Kitashirakawa-Oiwakecho, Sakyo-ku, Kyoto, Japan*
[4]*Meiji University, Department of Applied Chemistry, 1-1-1 Higashi-Mita, Tama-ku, Kawasaki, Kanagawa, Japan*
**hitoshi_mikami@jp.honda*

Significance and Relevance

We successfully developed a material screening method and explored High-Entropy Alloy (HEA) catalysts which show higher activity for exhausted gas purification than Pd mono-metal catalyst from huge search space. This method is based on high-throughput screening and direct inverse analysis and optimizes the elemental species, composition, and synthesis conditions for the catalyst with high catalytic activity and durability. By using this method, the search efficiency was increased by 200 times compared to conventional methods.

Preferred and 2nd choice for the topic: Automotive and stationary emission control and Air cleaning and combustion
Preferred presentation: Poster

Introduction and Motivations

Automotive catalysts are essential for creating eco-friendly automobiles. Much effort has been devoted to enhancing their performance and reducing their costs by selecting metals and support materials. Recently, HEA nanoparticles have attracted much attention due to unique properties which do not appear in the bulk.[1] Therefore, we expected that HEA can dramatically improve the performance of automotive catalysts. However, it is challenging to search HEA catalysts by using traditional search methods which rely on the researcher's experience, intuition, and good luck, due to an enormous number of combinations and compositions of elemental species, and synthesis conditions. In this study, we conducted process informatics to obtain HEA catalysts with high catalytic activity for exhaust gas purification catalysts.

Results and Discussion

The process informatics platform was developed as shown in Figure 1(a). The catalysts were synthesized by the automatic flow reactor based on a homemade flow reactor[3], and their activities were evaluated by a high-throughput screening (HTS) which can perform not only evaluation but also durability testing and pre-treatment for reduction. Results of evaluation were used for direct inverse analysis which can directly predict x values by putting target y values into the GMR model to obtain some recipes with a high possibility to achieve the target of activity performance.[2] Approximately 80 samples were synthesized and analyzed each week, totaling approximately 1,500 samples evaluated over one year. Figure 1(b) shows the performance results of predicted HEA catalysts with fixed elemental species and varying synthesis conditions. These results show that their catalytic performance varies with different synthesis conditions, suggesting the importance of investigating not only materials but also the synthesis conditions. Detailed results of our study and future plans toward the product development will be discussed in the presentation.

(a) (b)

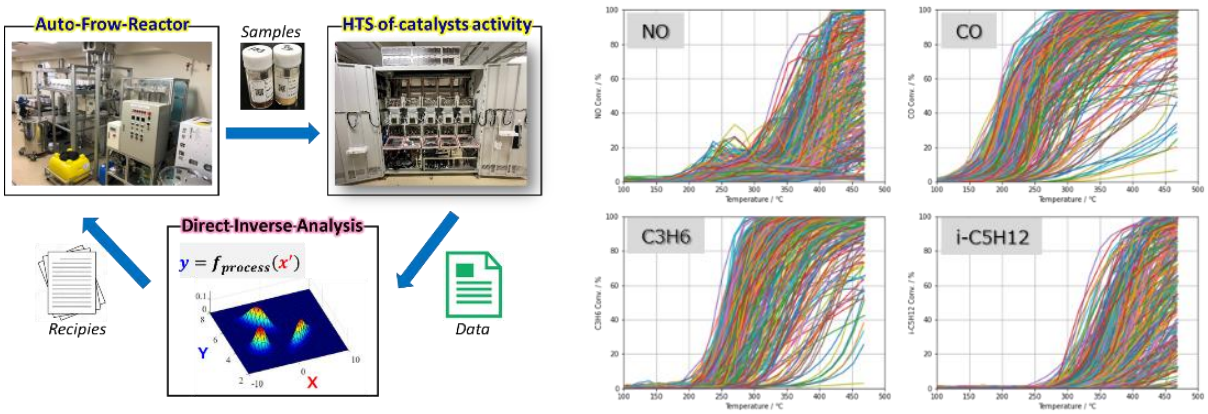

Figure 1 (a) Process informatics platform and (b) results of high-throughput screening of HEA with fixed the elemental species and different synthesis conditions.

References

1. K. Kusada etal., Angew. Chem. Int. Ed., **2022**, 61, e202209616.
2. H. Kaneko, Chemom. *Intell. Lab. Syst.*, **2021**, 208, 104226.
3. K. Kusada etal., *J. Phys. Chem. C*, **2021**, 125, 458.

Acknowledgements

The authors are grateful thank to Prof. M. Koyama's group at Shinshu University for their kind advice on computational chemistry, to Prof. Masaaki Haneda at Nagoya Institute of Technology for infrared spectroscopy, and to Prof. Murakami's group at Kyushu University for TEM measurements.