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Title	ハイスループット実験と遺伝的アルゴリズムを組み合わせたコンビナトリアル材料探索法の確立
Author(s)	瀧本，健
Citation	
Issue Date	2023-03
Type	Thesis or Dissertation
Text version	ETD
URL	http://hdl.handle.net/10119/18434
Rights	
Description	Supervisor:谷池 俊明，先端科学技術研究科，博士

JAPAN ADVANCED INSTITUTE OF SCIENCE AND TECHNOLOGY

Japan Advanced Institute of Science and Technology

Abstract

Ken Takimoto (2020025)

Most of the chemical reactions in the world are composed of several elementary reactions. Therefore, even if one element is controlled, other elements will affect it, making it difficult to achieve the desired control. For this reason, it is common practice to add multiple elements for control, and this makes material design multidimensional. However, because the interactions between elements in multidimensional material design are very complex, material development to date has mainly been a trial-and-error approach based on intuition and experience. In this dissertation, combinatorial materials exploration, which combines materials informatics (MI) and high-throughput experimentation (HTE), leads to a new design guideline for materials. The main research results are as follows:

In **Chapter 2**, a high-throughput experimental protocol was established for yellowing inhibition of transparent plastics on the basis of solution film casting on microplates and ultraviolet/visible spectroscopic evaluation using a microplate reader. The combination of this protocol with a genetic algorithm (GA) enabled a large-scale exploration for stabilizer formulations. Furthermore, the obtained data were analyzed and validated based on decision tree classification and force-directed graphs. As a result, we succeeded in deriving a formulation design guideline that it is important to formulate as many mutually complementary and synergistic stabilizers as possible.

In **Chapter 3**, HTE instrument and GA were studied in combination. Catalyst design for low-temperature pyrochemical reforming of methane was investigated. The vast amount of data generated by the high-throughput experiments was subjected to various data science techniques to obtain guidelines for catalyst design and process optimization. Catalyst exploration revealed that the combination of elements belonging to different families, mainly Ni and Pd, has a synergistic effect on catalytic performance. Visualization using force-directed graphs also revealed that it is important to include as many synergistic elements as possible in the design of high-performance catalysts.

In summary, the two verifications achieved a large-scale combinatorial search. In addition, it was found that it is very important to select and coexist elements that establish synergistic effects with each other in the multidimensional material design for chemical reaction control. In conclusion, this study has demonstrated a new methodology for multidisciplinary material design through “Realization of multidimensional exploration”, ”Discovery of new combinations” and “Derivation of design guidelines”.

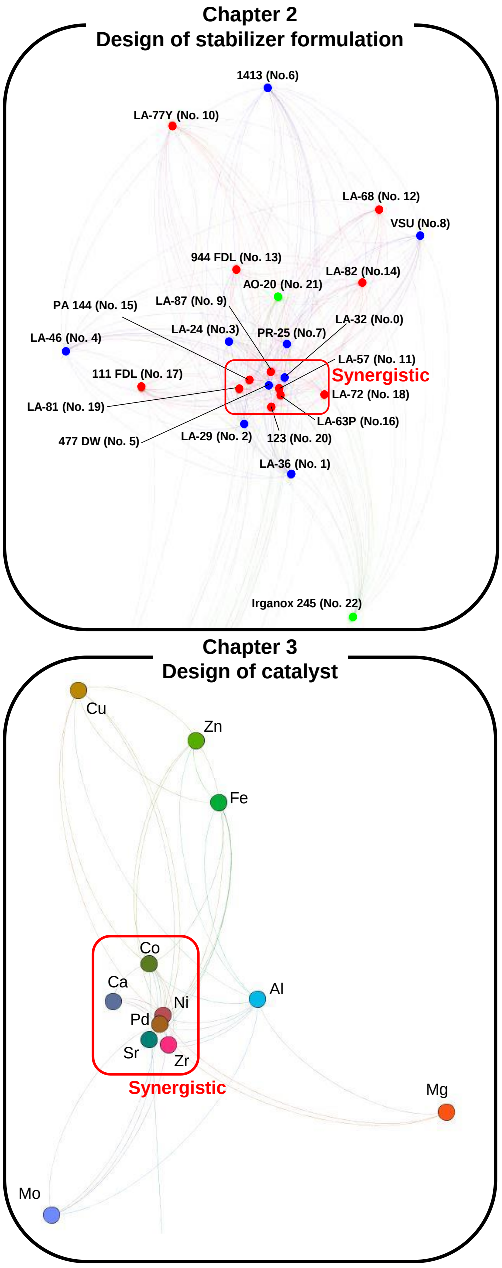

Fig. 1. Materials design guidelines in this dissertation.

Keywords: combinatorial materials exploration, materials informatics, high-throughput experimentation, photo degradation, dry-reforming reaction