所望の材料の作製条件を予測する人工知能モデルに関する研究

Research on Artificial Intelligence Models for Predicting Process Conditions of Desired Materials

金子弘昌

Hiromasa Kaneko

明治大学理工学部応用化学科

Department of Applied Chemistry, School of Science and Technology, Meiji University

This study proposes a machine-learning framework for material and process design based on direct inverse analysis (DIA). Conventional data-driven design relies on repetitive forward predictions or pseudo-inverse approaches, in which a large number of virtual conditions (X) are generated and evaluated to identify those that produce desired properties (Y). Such methods are inefficient and limited in exploring high-dimensional design spaces. In contrast, the proposed DIA approach enables the direct prediction of experimental or synthesis conditions from target material properties, allowing efficient exploration and optimization of design parameters.

The method employs Gaussian mixture regression (GMR) to model the joint probability distribution of X (e.g., synthesis temperature, composition ratio, pressure, or reaction time) and y (e.g., conductivity, mechanical strength, or optical property). By applying Bayes' theorem, the posterior probability p(X|Y) is calculated to estimate the most probable synthesis or processing conditions that yield the desired properties. To ensure accuracy and robustness, the framework integrates design of experiments for initial data acquisition, regression and classification models for predictive modeling, and cross-validation–based reliability evaluation.

The proposed method was validated through several material systems, successfully predicting process parameters that achieve the target physical and chemical characteristics. The results demonstrated that DIA can efficiently guide experimental design, achieving high prediction accuracy even with limited data.

In addition, a complementary study introduced an outlier-classification index ("ICO-likeness") to distinguish between consistent and inconsistent outliers, improving the reliability of datasets used in machine learning models.

Overall, the proposed DIA enables efficient and interpretable optimization of complex processes, reducing computational cost by an order of magnitude compared with conventional pseudo-inverse design. This framework represents a shift from forward-only simulation toward data-driven, autonomous design of processes and materials, and it provides a foundation for future integration with robotic experimentation and AI-assisted material discovery.