Autonomous experiments for thin films and solid materials
- Theorists can confirm their predictions using this system -

Taro Hitosugi[1,2]

[1] Department of Chemistry, School of Science, The University of Tokyo, Japan
[2] School of Materials and Chemical Technology, Institute of Science Tokyo, Japan
hitosugi@g.ecc.u-tokyo.ac.jp

Integrating machine learning and robotics into established research methodologies can significantly accelerate materials science research. Many studies have already demonstrated the potential of autonomous (self-driving) experiments in materials science [1, 2]. The rapid advancement of digital technologies is changing the way we conduct research.

Here, we discuss the status and prospects of data- and robot-driven materials research using autonomous experiments. We have developed an autonomous experimental system for thin-film materials. We constructed a system that automates sample handling, thin-film deposition, optimization of growth conditions, and data management. By using Bayesian optimization in conjunction with robots, our approach facilitates high-throughput experiments and generates comprehensive datasets that cover many aspects of materials (X-ray diffraction, Raman spectroscopy, scanning electron microscopy, optical transmittance measurement, electronic conductivity measurement). We tuned the hyperparameter for Bayesian optimization using the domain knowledge of chemistry; the number of trials to reach the global optimum is reduced.

The system demonstrated the synthesis and optimization of the electrical resistance in Nb-doped TiO_2 thin films [5]. Moreover, this autonomous approach has enabled the discovery of new ionic conductors [6]. We discuss the potential impact of this technology in accelerating materials science research, particularly in solid materials.

I wish theorists would use this system to confirm their predictions quickly.

References
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