Machine Learning-Driven Optimization of Blocking Force in Photomechanical Crystals

([1]*Graduate School of Advanced Science and Engineering, Waseda University*, [2]*Center for Data Science, Waseda University*) ○Kazuki Ishizaki,[1] Toru Asahi,[1] Takuya Taniguchi[2]

Keywords: Blocking force; Photomechanical crystals; Machine learning; Bayesian optimization; LASSO regression

Photomechanical crystals deform upon light irradiation, making them attractive as lightweight and remotely controllable actuators. In the practical application of actuator materials, not only the mode of deformation but also the output force, such as blocking force, are important properties. Since the blocking force depends on the crystal properties and experimental conditions, exploring the optimal conditions from a vast parameter space is necessary. In this study, we employed two types of machine learning for molecular design and experimental optimizations, focusing on salicylideneamine molecules (Figure 1a). First, the LASSO regression was used for the molecular design of photomechanical crystals with different Young's moduli. Crystals of several compounds were prepared based on the molecular design, creating a material pool with varying Young's moduli and crystal sizes. Then, we used Bayesian optimization for efficient sampling from the material pool to maximize the blocking force.

Based on LASSO regression, we synthesized 10 salicylideneamine molecules and fabricated the crystals of them. After preparing the material pool, we explored the optimal conditions. First of all, the crystal was selected randomly, and measured blocking force F_{max} under UV light. F_{max} is defined as the maximum blocking force minus the initial load (Figure 1b). Then, the crystal was irradiated from both top and bottom, and the larger force value was adopted. In addition, four other light intensities were tested, followed by the same procedure with another crystal under five different intensities. Using these 10 data as the initial dataset, Bayesian optimization was performed. Blocking force was measured under a total of 110 conditions, including the initial dataset (Figure 1c). The optimal condition achieved a maximum blocking force of 37 mN, surpassing the previous reported value.

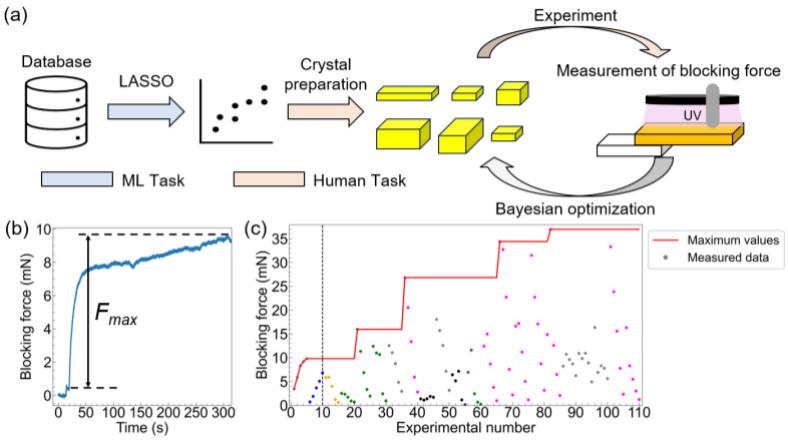

Figure 1. (a) Research workflow, (b) Definition of blocking force, (c) Progression of blocking force through experiments.