SELF-DRIVING LAB OF PHOTOPOLYMER SYNTHESIS AND MECHANICAL TESTING FOR EXPEDITED MATERIALS DISCOVERY

SUMMARY

Material discovery has gained significant research attention in recent years as it has the potential to revolutionize the development of new materials for targeted applications. However, material discovery typically relies on hundreds and thousands of experiments. Self-driving labs (SDLs) have been intensively researched in recent years as they can leverage autonomous high-throughput experimentation and characterization to enable efficient materials discovery. They can effectively replace a human researcher by working with machine learning algorithms as the “brain” and with robots for dexterous actions. In a common scenario, an SDL will create samples, test, and collect data. Then it will use an active learning algorithm to update the design for the next experiment. After many iterations, the design space will begin to fill and the algorithm will learn the relationship between factors and responses, enabling the discovery of an optimized material without human intervention. In an SDL, automated machines, systems, and sensors must be created to interface with the computer and robots to perform specific research tasks, such as material synthesis and sample testing/characterization. Although many SDLs have been developed in recent years, no SDL has been made for the discovery of 3D printable photopolymers with targeted mechanical properties.

This work has developed three important components of SDLs for synthesizing and testing photopolymers. The first component prepares photopolymer inks using a robotic arm, closed-loop liquid dispensing system for monomers/crosslinkers, and powder dispenser for photoinitiators. The second component cures photopolymer inks with a custom rheological sensor to determine time, temperature, and speed of curing. The third and final component automatically performs tensile tests on tensile bars made from the previous photopolymer inks using a robotic arm, force sensor, and automated clamp for grasping the samples. Simultaneously, the tensile testing system utilizes cameras for anomaly detection with machine learning, and digital image correlation for detecting sample dimensions. There is also automated data processing and property extraction with an algorithm that calculates and stores material properties including modulus of elasticity, elongation, and tensile strength. The three components can precisely create mixed photopolymer inks with desired concentrations of monomers, estimate curing properties for determining printability, and reliably provide mechanical properties, respectively. This work paves the way for more efficient materials discovery for photopolymer-based 3D printing.