AI4X – Accelerate Conference 2026, Singapore, 16–19 June 2026

A Self-Driving Lab for Novel Energy Material Discovery

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1. Introduction

After having been used successfully in pharmaceutical research for many years [1], self-driving labs (SDLs) have recently been employed in materials research for energy applications. Prominent examples include efforts in battery research [2] and perovskite photovoltaics [3]. Alkali-metal chalcogenides including sulphur-based perovskites like $BaZrS_3$ are a large class of materials with significant potential in energy applications, such as in batteries and solar cells. As semiconductors, they are highly sensitive to synthesis conditions, and their study involves the exploration of a significant parameter-space involving compositions, temperatures and pressures [4]. With these challenges in mind, an SDL capable of rapidly performing autonomous and sequential synthesis and characterization experiments is highly suitable for their study. To ensure high material quality, it is necessary to go beyond the common solution-process based SDL paradigm and implement an SDL based on multi-stage vacuum processing. This is a challenge in itself but an important direction for automated materials discovery. To address this, our group is constructing an SDL utilizing automated physical vapour deposition (PVD) and sulfurization stages for synthesis of chalcogenides. Material characterization will be performed in-line using hyperspectral imaging. All sample transfers will be autonomously performed using a robotic arm. This setup is designed to rapidly map the physico-chemical space for materials formation, identify phase diagrams, defect-property relationships and discover the domains of process conditions for formation of high-performance materials.

2. Methods

2.1 Material synthesis

A magnetron sputter with six sources is used for PVD. The system employs machine learning to determine co-deposition process for a given target composition [5]. A compositional gradient is achieved by keeping the sample orientation fixed during deposition, and is also automatically learned during process development. After sputtering, the substrate is transferred through an argon-atmosphere glovebox using a robotic arm. Sulfurization is completed using an RTP and hydrogen sulfide gas. Thanks to the compositional gradient in the metal film, the final sample features a corresponding variation in chalcogenide materials, allowing for each sample to constitute a materials library.

2.2 Material characterization

After synthesis, the sample is scanned with a hyperspectral imager with 281 colour channels. The resulting spectral resolution lets each pixel contain an entire visible-light spectrum, with reflection and transmission images being combined to generate absorption spectra and obtain insight in optoelectronic properties at each pixel. Through this method, material data can be collected in-line with synthesis and resolved against the known composition distribution of the library, resulting in dense datasets and increasing lab throughput.

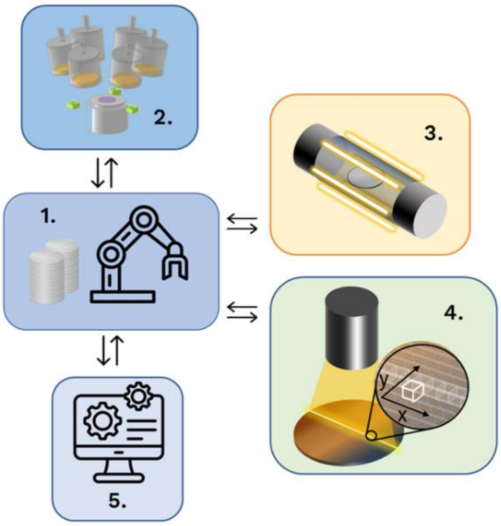

Fig. 1: Process outline: **1.** Robot arm and substrates in inert-atmosphere glovebox, **2.** Magnetron sputtering, **3.** RTP in reactive gas, **4.** Hyperspectral imaging, **5.** Automatic control system

3. Discussion

Key discussion points to be presented at the conference include the following: (1) the engineering, tooling and process control challenges of automating multistage PVD; which is an emerging need that is pushing the SDL field into new territory; (2) the scientific demands of SDL-based materials exploration – i.e., knowledge generation as opposed to simply building surrogate models; (3) general paradigms for SDL systems capable of exploring the broad chemical space of inorganic materials.

References

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