Development of a benchtop self-driving laboratory for electrocatalyst deposition and evaluation

Shigeru Kobayashi[1] Atsuki Shibuya[1] Keisuke Obata[1] Yumie Miura[1] Ryo Tamura[2] Kazuhiro Takanabe[1] Taro Hitosugi[1]

[1][The University of Tokyo, 113-0033 Tokyo, Japan] [2][National Institute for Materials Science, 305-0044 Ibaraki, Japan]

Correspondence to: [Shigeru Kobayashi] kobayashi-shigeru@g.ecc.u-tokyo.ac.jp

1. Introduction

Green hydrogen production via water electrolysis is a key technology for sustainable energy. However, developing cost-effective systems requires breakthroughs in the efficiency and durability of earth-abundant electrocatalysts. Traditional electrocatalyst development is hindered by the vast chemical space of their chemical species and synthesis conditions. Therefore, an efficient experimental approach is essential to accelerate the discovery of high-performance electrocatalytic materials.

In this study, we present a compact benchtop self-driving laboratory (SDL) that automates the entire experimental cycle, including the electrodeposition of catalyst films, electrochemical evaluation of catalytic activities, and autonomous decision-making regarding experimental conditions (Fig. 1). From the perspective of SDL development, implementing such an SDL system on a benchtop scale that is accessible and adaptable to standard laboratory environments involves significant challenges in robust hardware design and software orchestration.

2. Methodology

2.1 Hardware system integration

The system integrates a collaborative robot (COBOTTA, DENSO WAVE) for handling substrate mesh electrodes, a switching delivery pump system (DP-11, FLOM) for precise liquid dosing, four peristaltic pumps for rough and high-volume tasks such as electrolyte supply and washing, and a potentiostat/galvanostat (SP-150e, Bio-Logic SAS) for electrochemical measurements. The entire experimental system is compact, with a total footprint of approximately 700 mm × 700 mm, allowing it to be contained within a standard fume hood. To enable catalytic activity evaluation at elevated temperatures (e.g., 80 °C), custom reaction vessels and holders were designed with the following two critical implementations.

- *3D printed labware*: We printed the vessel caps with ports for electrode and liquid tube insertion, as well as vessel/mesh electrode holders using ABS resin. ABS was selected for its thermal stability (up to 100 °C) and ease of printing via fused deposition molding.
- *Liquid handling*: High-viscosity or concentrated solutions often lead to unexpected mixing and salt formation, causing fluidic clogging. We separated the liquid delivery pumps and channels for acidic and basic solutions based on their required dosing precision. Additionally, a robust cleaning protocol was implemented using a dead volume flush with air and deionized water between each deposition cycle to ensure experimental reproducibility.

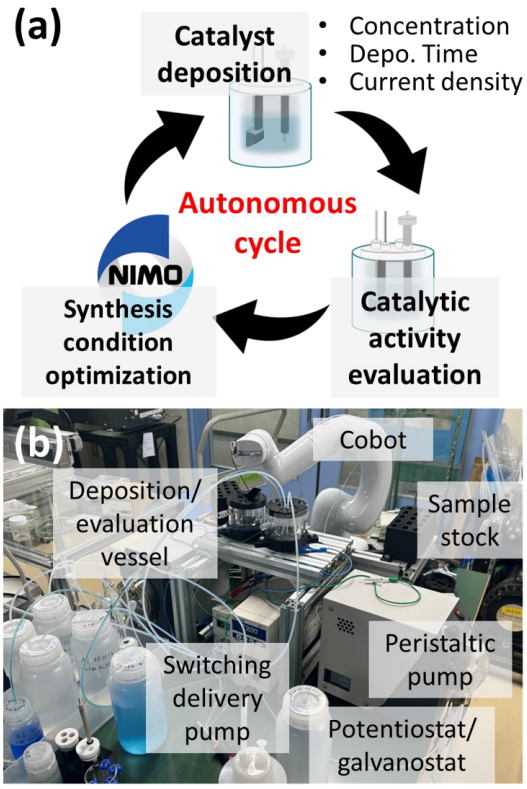

Fig. 1: (a) Schematic of autonomous cycle for high performance catalyst exploration. (b) Photograph of the developed benchtop self-driving laboratory for electrocatalyst film deposition and catalytic activity evaluation.

2.2 Hardware control programming and AI-driven optimization

The hardware control architecture is fully modularized using python3-based codes for the flexible integration of hardware components [1]. The synthesis parameters and robotic coordinates were managed using structured JSON files. The autonomous decision-making protocol and orchestration are powered by the NIMO framework [2]. The following optimization algorithms were implemented to explore the electrocatalyst:

- BLOX algorithm [3]: Initial synthesis condition filling to map the global landscape of the parameter space.
- PHYSBO algorithm [4]: Bayesian optimization, using a Gaussian process to predict the best synthesis conditions to minimize the overpotential (η) during operation.

2.3 Related work

Several SDLs for catalyst exploration have been reported over the past five years. For instance, Bennett et al. developed modular platforms for the discovery of homogeneous catalysts and ligands using flow reactors [5]. Compact systems, such as PANDA or autoRDE-film, focus on high-reproducibility characterization of electrodeposited polymer films or dried catalyst inks but are often limited to ambient-temperature operations [6,7].

Our system stands out because of its benchtop and modularized integration, which is capable of using practical mesh electrodes and high temperature experiments (80 °C). Moreover, while previous studies have relied on a single optimization algorithm [8], the system can implement a flexible strategy to navigate the complex chemical spaces in electrocatalyst discovery.

3. System stability evaluation

The developed SDL demonstrated highly stable and reproducible electrochemical operations (Fig. 2). The system successfully automates the entire sequence, including the electrodeposition process for Cu-based catalyst on carbon paper support (Fig. 2(a)), the subsequent evaluation of the double layer capacitance, and electrochemical impedance spectroscopy (Fig. 2(b)). A key achievement of this platform is the reliable robotic handling and force-controlled gripping of the electrodes. The stability of voltage profile and low and continuous impedance indicates that the COBOTTA arm provides precise and repeatable electrode positioning, which is critical for maintaining a stable measurement environment. These results confirm that the system is a powerful tool for the autonomous discovery and synthetic optimization of electrodeposited materials for electrochemical systems.

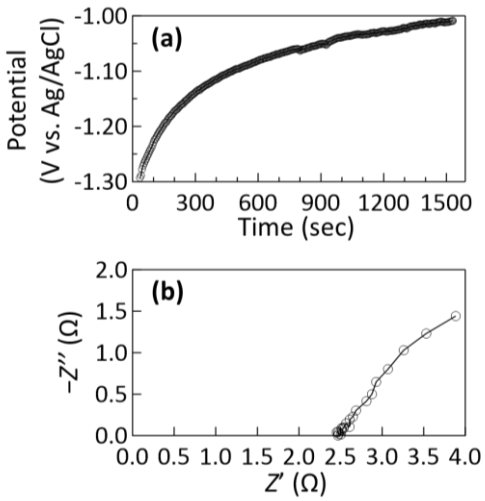

Fig.2: (a) Potential profile during electrodeposition of copper electrocatalyst at a current density of 0.2 Acm^{-2}. (b) Nyquist plot obtained from electrochemical impedance spectra under hydrogen evolution reaction condition.

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