Autonomous exploration of new alloy chemistries using a Material Acceleration Platform (MAP)

Ozlem Ozcan, Mert Ozan, Ahmad Rashid Hazem, Matthias Dimper, Julia Witt
Federal Institute for Materials Research and Testing (BAM)
Unter den Eichen 87 12205 Berlin, Germany
ahmad-rashid.hazem@bam.de

The discovery and commercialization of novel corrosion-resistant alloys via conventional methods and manual experimentation is inherently slow and costly. Recent international efforts have concentrated on the development of self-driving laboratories, termed Material Acceleration Platforms (MAPs)[1]. These MAPs integrate material synthesis, characterization, and testing modules into automated workflows, leveraging artificial intelligence (AI) for efficient and autonomous experiment design, property prediction, and data analysis.

We have developed a MAP (Figure 1.) tailored for both corrosion and electrocatalysis research, automating diverse liquid handling operations, electrochemical testing, and data evaluation. The test results are processed through a machine learning (ML)-based backend. The electrochemistry module workflows are configured for the electrodeposition of various alloys, followed by multi-technique electrochemical corrosion testing and/or electrocatalytic screening. The platform iteratively adjusts deposition parameters based on test outcomes in a continuous and autonomous loop until the predefined objectives are achieved.

In this project, the MAP was employed to design new multi-principal element alloys (MPEAs) as corrosion-resistant electrode materials for H_2O and CO_2 electrolysis and as active cathode materials for NO_3 reduction reaction. Each campaign can encompass up to 144 experimental runs. From each successful campaign, leads and additional randomly selected materials are advanced to upscaling, either through larger-scale electrodeposition or as bulk ingots produced via arc-melting. These samples undergo detailed chemical and electrochemical characterization using advanced surface analysis techniques to validate the MAP-based optimization outcomes. The presentation will detail the design and construction phases of our MAP, its constituent modules, and workflows. Furthermore, we will present our findings from the FeNi-X MPEA system.

References

[1] A S. P. Stier, C. Kreisbeck, H. Ihssen, M. A. Popp, J. Hauch, K. Malek, M. Reynaud, T. P. M. Goumans, J. Carlsson, I. Todorov, L. Gold, A. Räder, W. Wenzel, S. T. Bandesha, P. Jacques, F. Garcia-Moreno, O. Arcelus, P. Friederich, S. Clark, M. Maglione, A. Laukkanen, I. E. Castelli, J. Carrasco, M. C. Cabanas, H. S. Stein, O. Ozcan, D. Elbert, K. Reuter, C. Scheurer, M. Demura, S. S. Han, T. Vegge, S. Nakamae, M. Fabrizio, and M. Kozdras, Advanced Materials 36 (2024) e2407791.

Figures

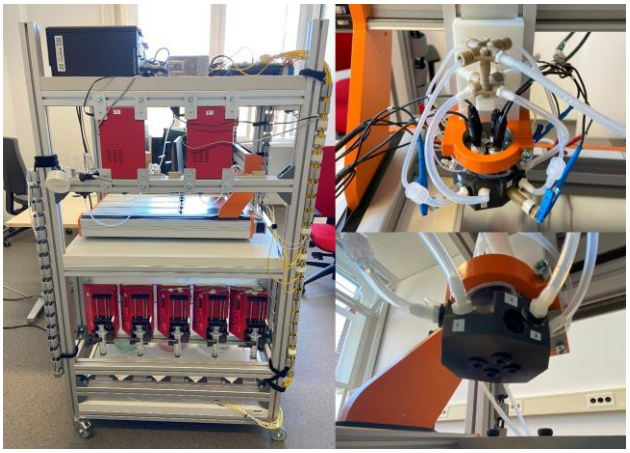

Figure 1. (left) The electrochemistry MAP is structured into three levels: the lowest level houses the pumps and electrolytes; the middle level contains the electrochemistry setup; and the top level accommodates the electronics and potentiostats. The electrochemistry module (right) includes four cells for simultaneous measurements. During each run, three cells are dedicated to electrodeposition, with two of these cells subsequently tested for corrosion or electrocatalytic properties to ensure reproducibility. The third coated area is dried post-electrodeposition and rinsing with deionized (DI) water for further chemical analysis outside the MAP. The fourth cell undergoes identical testing procedures on the bare substrate, without any thin film deposition, serving as a reference measurement to monitor potential changes in substrate surface chemistry over extended campaigns.