Weather forecasting technique speeds up electrocatalyst degradation predictions

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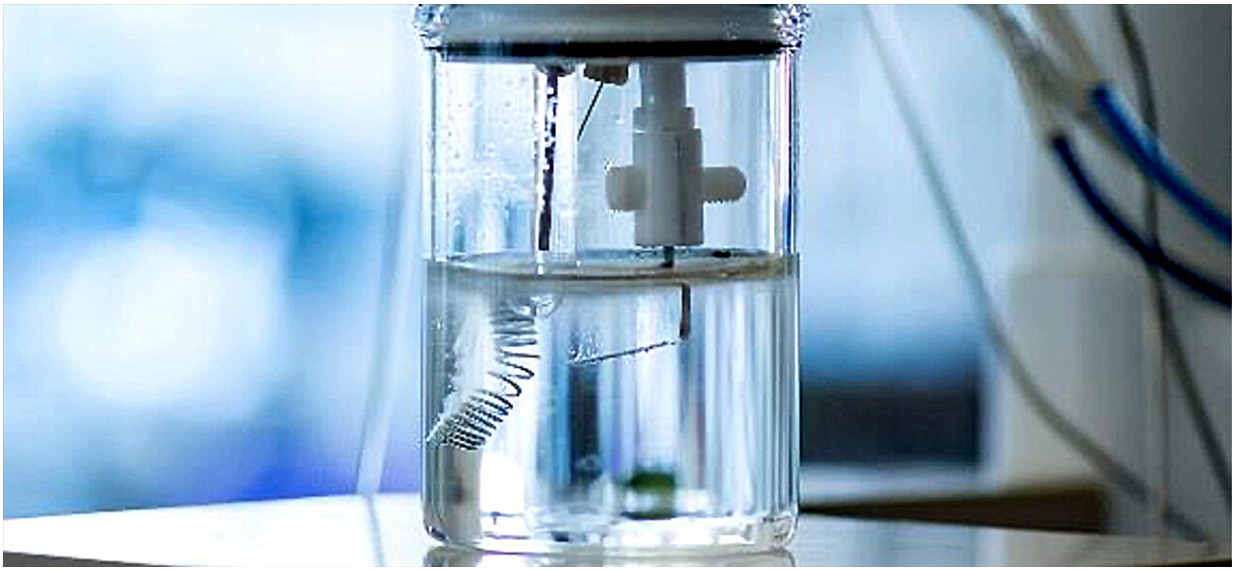

Water electrolysis in action. The double-bent plate at the center served as the electrode material used for electrocatalyst degradation testing in this research. Credit: Ken Sakaushi, National Institute for Materials Science

A NIMS research team has developed an approach capable of accurately and rapidly predicting the degradation behavior of electrocatalysts used in water electrolyzers by employing data assimilation—a method commonly employed in weather forecasting.

After analyzing only 300 hours of experimental data, this approach

accurately predicted the degradation of an electrocatalytic material occurring after approximately 900 hours of water electrolysis. This approach is able to accelerate and simplify the comparison of degradation properties among various electrocatalytic materials, potentially facilitating investigations into their degradation mechanisms and expediting the development of more efficient, economical and durable electrocatalytic materials.

The work is published in the journal *ACS Energy Letters*.

A society can become more sustainable by promoting the use of green hydrogen as a major energy source. Achieving this aim would require the widespread installation of water electrolyzers that produce green hydrogen, which is a fuel without carbon dioxide emissions. Developing durable electrocatalysts is crucial for improving the efficiency and lifetime of water electrolyzers.

However, evaluating the durability of potentially promising electrocatalysts typically takes thousands of hours—sometimes tens of thousands—raising a strong demand for the development of techniques that can more rapidly, accurately and reliably assess the degradation properties of electrocatalysts.

This NIMS research team recently integrated data assimilation into their mathematical model for predicting the degradation behavior of electrocatalysts. Data assimilation is a method applied to various fields—including weather forecasting—in which observed data is combined with numerical models to improve the accuracy of predictions. It optimizes parameters by iteratively fitting theoretical prediction curves to experimental data as new observations become available, accounting for uncertainties in the data.

The team constructed a simple mathematical model to simulate the

degradation process of electrocatalysts, considering surface dissolution and other mechanisms. The accuracy of this degradation prediction model was first validated by confirming its fit to the degradation data collected during the initial hours of a water electrolysis experiment.

Subsequently, the team tested its accuracy using data assimilation on long-term experimental data (approximately 900 hours). They found that only the initial 300 hours of data were needed to accurately predict the degradation behavior of the electrocatalyst specimens at 900 hours, with a margin of error of just 4%.

In future research, the team aims to further enhance the technique by refining the algorithm, enabling it to accurately predict electrocatalyst degradation using data collected over even shorter experimental periods. The team also plans to advance efforts to clarify electrocatalyst degradation mechanisms.

These initiatives are expected to facilitate the development of higher-performance electrocatalysts and support carbon neutrality efforts by increasing hydrogen production through the more widespread adoption of water electrolyzers.

More information: Miao Wang et al, Accelerated Electrocatalyst Degradation Testing by Accurate and Robust Forecasting of Multidimensional Kinetic Model with Bayesian Data Assimilation, *ACS Energy Letters* (2024). DOI: 10.1021/acsenergylett.4c02868

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electrocatalyst-degradation.html