Feature extraction of microwave annealed hematite photoanodes using the factor analysis of machine learning model

([1]*Chuo University*) ○Kaori Matsuzawa,[1] Yuya Nagai,[1] Kenji Katayama[1]
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In recent years, fossil fuel resources have been depleted, and photoelectrochemical water splitting reactions using sunlight are attracting attention as a new energy source. Hematite(α-Fe_2O_3), a photocatalyst, is inexpensive, abundant on earth, and responds to visible light. Therefore, hematite is a promising photoanode for photoelectrochemical water splitting cells. In a conventional fabrication of hematite photoanode, one of the issues was reproducibility of performance and formation of inactive samples with a certain ratio. On the other hand, we have introduced the microwave annealing method to reduce the annealing time and improving reproducibility. We found that all the samples showed photoelectrochemical (PEC) performance higher than a threshold (photocurrent density > 0.05 mA/cm^2). In this study, we identified the physical/chemical factors that cause the differences with the conventional preparation method by using the machine learning (ML) and its model analysis.

We prepared 54 samples using a conventional method and 36 samples using the microwave annealing method. In ML, an SVM model was constructed using the XRD peak intensities and electrochemical parameters obtained for the samples as input data (X) and the photocurrent at 1.23 V (*vs.* RHE) as output data (Y). From the Shapley additive explanation (SHAP) analysis of the constructed ML model, three important factors in the analytical data for the PEC performance were determined. In Figure, the contribution of the selected factors to the PEC performance was plotted. (The color indicates the amplitude of the feature values for each sample and the horizontal value corresponds to the contribution to the PEC performance.) The maker type indicates the annealing method (microwave and conventional furnace). The distribution was clearly divided in R3 (interfacial resistance) and XRD peak4 (FTO) depending on the annealing methods. Then, the two factors were controlled by the annealing devices. It was suggested that the surface conditions of hematite and FTO were affected by the annealing, resulting in the PEC performance.

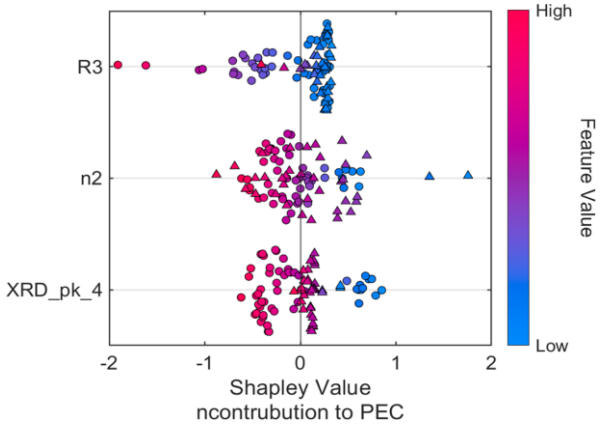

Figure SHAP analysis result for determination of the PEC performance. ○: general furnace, △: microwave furnace.