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Outline

This doctoral thesis entitled “Utilizing machine learning and robots for the development of fuel cells” is composed of seven chapters in total. This study paves the way for establishing an automatic system with machine learning to accelerate materials research in fuel cells.

In Chapter 1, the current application of polymer electrolyte fuel cells (PEFC) is introduced, and the author explains the technical difficulty in reducing contact resistance at the interface of the gas diffusion layer (GDL) and stainless-steel separator in the PEFC cell stack. To overcome this problem, the author focuses on anatase $Ti_{1-x}Nb_xO_2$ (TNO) protective layers due to their electrically conductive and corrosion-resistive properties. Since there is no report on applying TNO to the protective layer, optimizing TNO fabrication processes to reduce contact resistance is necessary. In this study, the author demonstrates a new approach utilizing machine learning and robots to reduce contact resistance.

In Chapter 2, the experimental details of the mist chemical vapor deposition (mist CVD), which is utilized for anatase TNO thin film deposition in this research. Then, the measurements of thin-film characterization and contact resistance are described.

In Chapter 3, the results of the deposition of conductive anatase TNO thin films using mist CVD are shown. The author manually tunes the conditions of solution (Nb concentration in solution and type of solvent) and deposition (flow rates of carrier gas and dilution gas, deposition temperature, T_{depo}, and post-deposition annealing temperature, T_{PDA}), and achieves the contact resistance of 3.4 $m\Omega \cdot cm^2$. In particular, the author finds that contact resistance is sensitive to T_{depo} and T_{PDA}.

In Chapter 4, for applications of Bayesian optimization to the efficient optimization of contact resistance, appropriate hyperparameters for Bayesian optimization (BO) under 2D and 3D synthesis conditions are simulated to minimize the number of trials. The model functions with three different process windows are set to mimic actual 2D and 3D thin-film synthesis. According to the simulation results, the author determines the optimum hyperparameters of BO.

In Chapter 5, the automatic experiment system composed of mist CVD and the contact resistance measurement is constructed. All the apparatuses are integrated and controlled from the computer. In addition, the BO algorithm is introduced to the automatic system so that contact resistance can be efficiently reduced as a function of T_{depo} and T_{PDA}. As a result, the author achieves the contact resistance of 2.2 $m\Omega \cdot cm^2$, which is the lowest value to date.

In Chapter 6, the effect of T_{depo} and T_{PDA} on contact resistance is studied. The increase of T_{depo} and T_{PDA} promotes TNO crystallization, suggesting a decrease in resistivity and contact resistance. In contrast, the contact resistance increases up to T_{depo} = 600°C due to the incorporation of carbon from the thermal decomposition of the solvent. Thus, optimizing T_{depo} and T_{PDA} is the key to controlling the contact resistances.

In Chapter 7, the author summarizes and concludes this work. The author provides a progressive example of applications of machine learning and robots to fuel-cell research through the fabrication of TNO protective layer coating onto stainless steel separators using mist CVD.

To sum up, this thesis provides a new approach utilizing machine learning and robots to facilitate research in fuel cells. The author deserves to receive a Doctor of Engineering from the Tokyo Institute of Technology.