Digital Twin-Driven Innovations in SOFC Electrode Virtual Engineering

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This study establishes a digital twin-based virtual laboratory environment to innovatively improve the manufacturing process of electrode materials, which are key components of Solid Oxide Fuel Cells (SOFCs). Operating at high temperatures, SOFCs are recognized as a next-generation energy technology due to their high energy efficiency and versatility in using various fuels [1]. As the performance of electrode materials significantly influences the overall efficiency of SOFCs[2], this research utilizes digital twin technology and artificial intelligence (AI) to explore optimal manufacturing conditions, aiming to enhance the accuracy and efficiency of the process [3].

The major manufacturing processes for SOFC electrode materials primarily consist of selecting cell configuration and components, a combining process (ball milling), a coating process, and a sintering process [4,5].

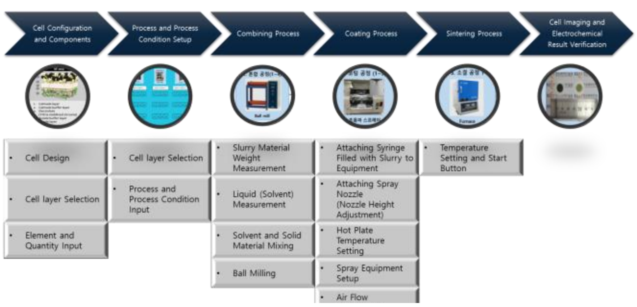

Figure 1. SOFC key processes and virtualization implementation processes

Specifically, in this project, digital twin technology was used to virtually implement each key process as shown in Figure 1. Firstly, during the cell composition phase, users selected material combinations such as the cathode layer, cathode buffer layer, and electrolyte layer, simulating the weight and temperature of the materials. Secondly, in the mixing process, ball milling was employed to achieve uniform mixing and fine particle size adjustment, optimizing mixing speed and duration to enhance material quality. Thirdly, in the coating process, a spray device was utilized to form coatings of uniform and precise thickness, with detailed management of nozzle height and pressure to improve coating quality. Fourthly, the sintering process involved heat treating the materials at high temperatures to increase the mechanical strength and durability of the electrode materials. Lastly, a process for verifying results within the virtual laboratory environment was added to enable the evaluation of the material properties of the final product as shown in Figure 2, reflecting the variables from the previous processes. The results that can be verified in our virtual laboratory are listed below:

- Dispersion Stability: The ability of particles to remain evenly dispersed in a medium.
- Electrode Thickness: The measure of thickness of electrode.
- Electrode Thickness Uniformity: Consistency of electrode thickness across a surface.
- Polarization Resistance: Resistance of an electrode to changes in polarization.
- Ohmic Resistance: The inherent resistance of the electrode material to electrical flow.
- Maximum Power Density: The highest amount of power output per unit volume from a device.
- Initiation Potential: The voltage at which an electrode begins to actively participate in a reaction.

Figure 2. Verification of material properties of the final product in a virtual environment

In this study, artificial intelligence (AI) models are developed using lifecycle data from the entire SOFC manufacturing process. The dataset includes information on raw materials (e.g., La, Sr, Fe, Mn, O), composition (mol%), processing conditions (e.g., zirconia content, chamber humidity and temperature, sintering temperature and duration), and the physical properties of each layer involved in cell fabrication. The deep neural network (DNN) model demonstrated high predictive performance with an R-square of 0.89 and RMSE of 0.03, and was integrated into a virtual reality (VR) environment.

Within the VR platform, an API enables users to input materials, compositions, processing conditions, and measurement environments. The AI model then predicts corresponding material properties, such as dispersion stability from the ball milling process, electrode thickness and uniformity from the coating process, and initiation potential, ohmic resistance, polarization resistance, and maximum power density from the sintering process. Furthermore, a real-time interaction environment was established by integrating the AI model with a digital twin system via APIs. This allows process data to be transmitted to the AI model, and the predicted results to be immediately returned to the digital twin system. Through this framework, researchers can efficiently evaluate various process conditions, significantly reducing time and cost in actual manufacturing. The developed digital twin virtual laboratory is designed to be user-friendly and accessible, supporting not only research applications but also educational purposes.

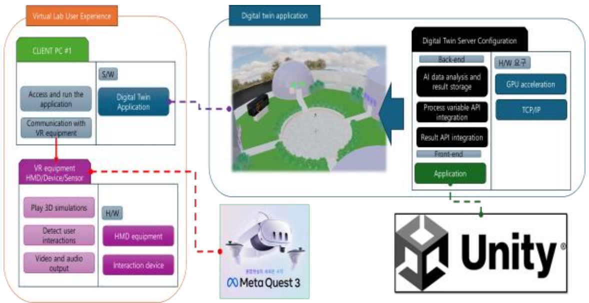

Figure 3. Virtual laboratory environment framework

The main framework of this system , as shown as Figure 3, is based on real-time interaction between client PCs and VR equipment such as the Meta Quest 3[6], with the virtual environment constructed using Unity3D[7]. On the client PC, the digital twin application collects and processes sensor data and user input from the VR device. Additionally, the system executes simulated 3D processes within the virtual laboratory environment based on user interactions and visualizes results in real-time.
On the digital twin server side, collected data is analyzed and processed in real-time to optimize the current state of the process, and these results are integrated back into the VR application. This structure allows users to intuitively understand and manipulate processes within a virtual laboratory environment, with all data processing and interactions occurring seamlessly through real-time communication between the VR equipment and the server.

In conclusion, this study proposes a methodology and system that significantly enhances the efficiency and performance of the SOFC electrode material manufacturing process by integrating digital twin and AI technologies. The developed methodologies are applied in two main ways. First, virtual experimental training is provided within the digital twin environment, enabling researchers to practice and optimize experimental procedures in advance. This has improved the quality and stability of actual laboratory experiments, leading to more consistent product performance. Second, the VR environment allows researchers to simulate and predict experimental outcomes based on complete lifecycle data before conducting real experiments. By configuring material compositions and process conditions virtually and reviewing the AI model's predictions in advance, researchers can more efficiently design experiments and accelerate the development of materials with the desired properties. Specially, this approach is expected to contribute to the advancement of next-generation SOFC material development technologies.

Future research will focus on expanding the diversity of experimental data to improve the generalizability of the AI models to a wider range of SOFC types and material systems. In addition, establishing a rigorous validation framework will be essential to ensure the physical accuracy of the digital twin simulations when compared to real-world experimental results. Improving the usability and scalability of the integrated platform especially for small- and medium-scale manufacturing environments will also be an important direction. These efforts aim to strengthen the practical applicability of the proposed system and accelerate its deployment in real-world manufacturing settings.

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