論　文　要　旨
Thesis Abstract

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主論文題名　（Title）

Three-dimensional numerical analysis of transport phenomena in a Positive-Electrolyte-Negative assembly of a Solid Oxide Fuel Cell

内容の要旨　（Abstract）

In this dissertation, a three-dimensional, microstructure-scale model of a Solid Oxide Fuel Cell Positive-Electrolyte-Negative assembly is constructed, validated and applied to a series of research problems. Empirical relationships from open literature are used to compute the material conductivities and exchange current densities for a number of anodic and cathodic materials. Butler-Volmer model is implemented to compute local reaction rates. Cylindrical Pore Interpolation Model is used to solve mass transport equations in transitional regime, accounting for both the free-molecule, and the continuum-flow diffusion phenomena. The model equations are discretized using the Finite Volume Method, and solved using the Successive Over-Relaxation method with local linearization. The computational domain is based on digital reconstructions of electrode microstructure, obtained using the Focused Ion Beam Scanning Electron Microscopy nanotomographic technique. The methods are implemented in an in-house numerical code written from scratch in C++. The model is validated against empirical data from a commercial Solid Oxide Fuel Cell stack. Additionally, simulations at different operation parameters are performed, and the impact of microstructure inhomogeneities is assessed, along with the effects of cross-electrolyte phenomena in thin-electrolyte cells. The model is applied to explain unusual results of a long term operation experiment, in which stack performance enhancement, rather than deterioration was observed. The decrease of pore tortuosity due to microstructure evolution was identified as the cause.

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