GeoDict
The Digital Material Laboratory

"Solid Oxide Fuel Cells" Simulations vs. Experiments

Ni-8YSZ as the Anode of SOFCs: How Simulated and Experimental Parameters Meet Each Other?

Solid-oxide fuel cells (SOFCs) are a type of electrochemical conversion device that generates electricity by oxidizing a fuel in the presence of oxygen. These fuel cells use a solid oxide material as the electrolyte and typically operate at very high temperatures, ranging from 600 to 1000 °C. SOFCs offer high power efficiency, long-term stability, fuel flexibility, low emissions, and relatively low cost, making them suitable for a wide range of applications, including auxiliary power units in vehicles and stationary power generation.

To evaluate the capabilities of GeoDict in simulating SOFC components, we developed a model of the anode (Ni-8YSZ) and calculated several key parameters, including thermal and electrical conductivities, Young's modulus, and the thermal expansion coefficient. The simulated results were then compared with experimental data.

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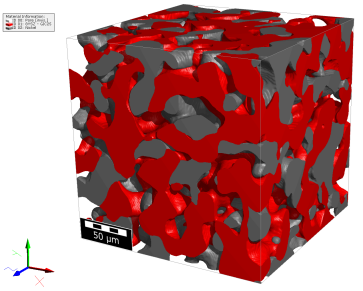
Structure Information



"The modelled structure"

- Domain size of the structure: 200×200×200 voxel
- Voxel size: 1 µm
- SVF of 8YSZ (8 mol% yttria-stabilized zirconia): 36%
- SVF of Ni (nickel): 24%
- The ratio of 8YSZ:Ni is 1.5:1
- Porosity of the model: 40%
- The materials Ni and 8YSZ are selected from the GeoDict's default Material Database
- The experimental values of Ni-8YSZ are taken from the literatures (cited in References)

GeoDict modules that are used in this study

GeoApp

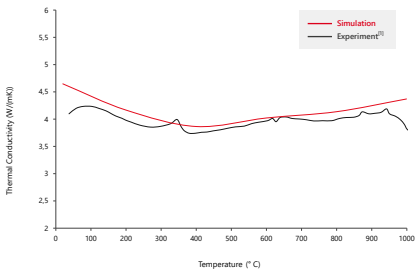
- Fuel Cell and Electrolyser (to generate the structure of Ni-8YSZ)

GeoDict Modules

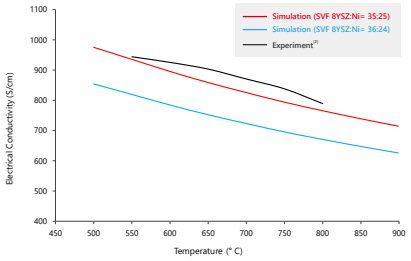
- ConductoDict (to compute Thermal & Electrical Conductivities)
- ElastoDict (to compute Young's Modulus and Thermal Expansion Coefficient)

ConductoDict Simulations Results

Thermal Conductivity



Electrical Conductivity



Notes for ConductoDict results

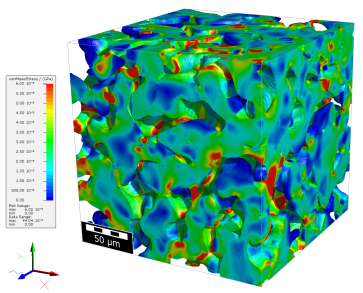
Thermal Conductivity

- The simulated and experimental values are in excellent agreement.

Electrical Conductivity

- The simulated and experimental values are in good agreement.
- The Electrical Conductivity strongly depends on the ratio of the components.

ElastoDict Simulations Results



"Visualized von Mises stress result of a confined thermal expansion simulation (Temperature Change: 1 K)"

Young's Modulus (GPa)		Thermal Expansion Coefficient (K^{-1})	
Simulation[a]	Experimental	Simulation	Experimental
50±6	59[1] 51[3]	10.71×10-6	10.3±0.3×10-6[4] 10.52×10-6[1,b]

[a] All of the results are reported at room temperature, unless otherwise stated.
[b] at 50 °C.

Notes for ElastoDict results

Young's Modulus

- In the "Stiffness Mode", the Stiffness Tensor is selected
- The value is reported based on an isotropic structure

Thermal Expansion Coefficient

- The calculated value is very close to the experimental values from two different references.

GeoDict's powerful modules, coupled with its accurate material database, provide the possibility of reliable simulations

A Ni-8YSZ anode structure for SOFCs was created by combining Ni and 8YSZ components using the GeoApp in Fuel Cells and Electrolyser. Subsequently, key parameters such as thermal and electrical conductivities, Young's modulus, and thermal expansion coefficient were calculated using the ConductoDict and ElastoDict modules of GeoDict. The results showed very good agreement between the simulated values and the reported experimental data.

GeoDict offers the flexibility to adjust various simulation parameters, including material composition, ratio, porosity, simulation temperature, and segment size, among others. As a result, it is a highly efficient and versatile tool for designing and modeling materials with diverse characteristics tailored to real-world systems.

References:

[1] M. Radovic, E. Lara-Curzio, R. M. Trejo, H. Wang, W. D. Porter, Thermophysical Properties of YSZ and Ni-YSZ as a Function of Temperature and Porosity In book: Advances in Solid Oxide Fuel Cells II: Ceramic Engineering and Science Proceedings, edited by N. P. Bansal, A. Wereszczak, E. Lara-Curzio, John Wiley & Sons, USA, 2006, pp. 79–85.

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[3] S. Biswas, T. Nithyanantham, N. T. Saraswathi, S. Bandopadhyay, J. Mater. Sci. 2009, 44, 778–785.

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