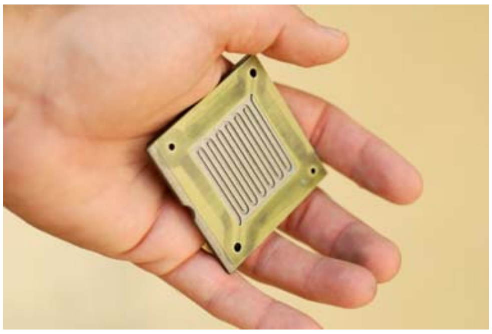
Nanoscale Reaction Models in Solid Oxide Fuel Cells

Reaction models on fuel cells can be established based on detailed orientation / phase map analysis

Solid oxide fuel cell (SOFC) technology is a promising energy conversion option at a time when efficient solutions are sought. During the electrochemical reaction of a fuel with an oxidant gas (usually air) at an operation temperature of ~ 800°C, SOFCs cogenerate heat and electricity with high efficiency: Electric efficiencies close to 60% are obtained now with a SOFC alone. When coupled with a micro gas turbine (SOFC-GT), these can increase up to 70%. Advantages of SOFCs also include flexibility of fuel use (e.g. CO, H_2, CH_4), delocalization of energy conversion, and reduction of pollutants such as NO_x and SO_x.



Hydrogen Fuel Cell component

A SOFC is composed of three main components: an anode, an electrolyte and a cathode. The standard design is based on the use of a porous ceramic-metal (cermet) composite anode made of yttria (Y_2O_3)-stabilized zirconia (YSZ) and Ni .

The anode acts as a fuel oxidation catalyst, hydrocarbon reforming catalyst, current collector and often as a mechanical supporting layer of the whole fuel cell. NiO particles are sintered with YSZ and then reduced by the fuel to metallic Ni during the first operation of the cell. During service life, minimum 5 years at ~ 800 °C, the anode runs on fuel and Ni is kept in its reduced state.

In this project, environmental transmission electron microscopy (ETEM) is used to understand the reaction mechanisms and the structural evolution of the as-sintered NiO-YSZ anode during reduction. A thin window, which is prepared using a dual beam FIB/SEM, is reduced inside the ETEM in a total pressure of 1.3 mbar of H_2. NiO reduction is observed to start at the grain boundaries with the YSZ phase. Pores form within the NiO grains to accommodate the volume shrinkage linked to the removal of oxygen. A post mortem analysis using ASTAR orientation imaging allows monitoring of the crystallographic changes induced by reduction at nm scale. It can be seen that the reduced Ni grains maintain the same orientation as the initial NiO grains, while the YSZ phase is left unchanged by the reaction. Based on these observations, reaction models can be established.

The challenge: Monitoring crystallographic changes after reduction of fuel cell: orientation / phase of two different phases with details of 1 nm

Solution: ASTAR technique coupled with precession electron diffraction

Crystal Structure

Y_2O_3: Cubic, $Ia\bar{3}$, a = 10.58 Å
NiO: Cubic, $Fm\bar{3}m$, a= 4.168 Å
Ni: Cubic, $Fm\bar{3}m$, a = 3.52 Å

Experimental Data

TEM type: Jeol 2200 FS
Map resolution: 1 nm
Scanned area: 4 x 4 µm

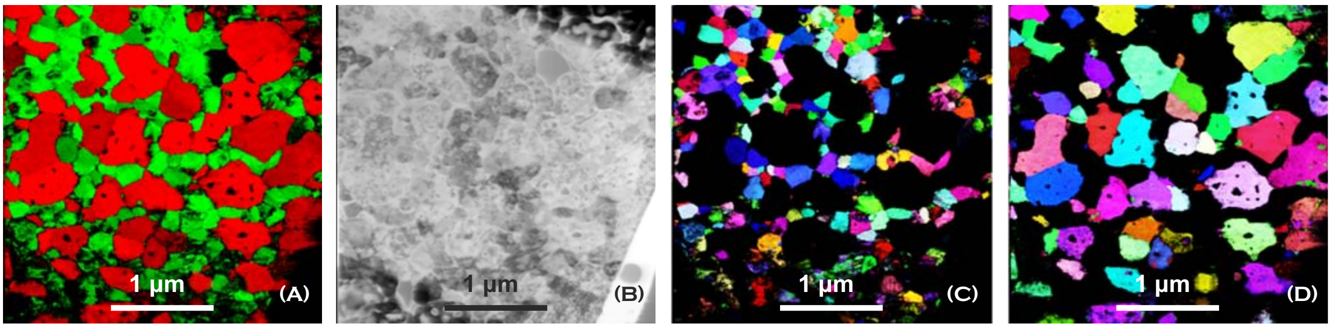


figure 1

(A) ASTAR phase map where both NiO phase (red) and YSZ phase (green) can be seen
(B) same area TEM bright field image
(C) ASTAR orientation mapping for NiO phase and (D) ASTAR orientation map for YSZ phase.

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