

Structural evolution and stability of Au-Mo-Ni/GDC cermets under reducing/operating conditions: Characterization with in-situ CH₄-XRD and in-situ H₂-XPS

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Abstract

Solid oxide fuel cells (SOFCs) have grown in recognition as a viable technology able to convert chemical energy directly into electricity, with higher efficiencies than conventional thermal engines. Direct feeding of the SOFCs anode with hydrocarbons from fossil or renewable sources, appears more attractive compared to the use of hydrogen as a fuel. The addition of mixed oxide-ion/electron conductors, like gadolinium-doped ceria (GDC), to commonly used nickel-based anodes is a well-known strategy that significantly enhances the performance of the SOFCs. [1, 4]. However, the reaction mechanisms and possible structural formations of Ni/GDC (either modified with Au – Mo, as well as not modified) anodes have not been fully explained yet, especially under the operating conditions of the cell. One example of the occurring processes has been recently reported and it was shown that during the reduction of a cell, comprising Au-NiO/GDC as anode, the deposited gold nano-particles dissolve into nickel to the formation of a bimetallic Ni-Au solid solution [2, 3]. The latter process has been further studied with *in-situ* H₂-XPS measurements and some of the results are presented in the present study. It is suggested that Au nano-particles are subjected to sintering from the high calcination temperature, during the cells' fabrication. The latter effect makes their detection with XPS difficult, when the cells are in their oxidized form. However, this does not affect significantly the stability of Au because under H₂ reducing conditions there is gradual formation of the surface Ni-Au solid solution [2, 3]. Furthermore, Ni/GDC and Au-Mo-Ni/GDC have been examined with *in-situ* HT-XRD measurements, under H₂ reducing conditions (isothermally and temperature programmed) and under CH₄/N₂ feed. Specifically in the latter type of measurements, the cermets were originally reduced with 5 vol.% H₂/N₂ and subsequently the feed was changed to 1 vol.% CH₄/N₂. The *in-situ* HT-XRD CH₄/N₂ experiments showed several structural changes, depending on the examined cermet. The key findings comprise: (i) differentiations on the amount of deposited carbon and on the interacting crystal phases, where Ni/GDC is highly vulnerable and (ii) possible detection of the formed Ni-Au structure.

Acknowledgments

This work has been carried out within the framework of **ROBANODE** (245355) and **T-CELL** (298300) projects (Joint Technology Initiative-Collaborative Project), which are financially supported by the **European Union** and the **FCH-JU**.

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