Accepted Manuscript

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PII: S0013-4686(18)31081-8

DOI: 10.1016/j.electacta.2018.05.058

Reference: EA 31844

To appear in: *Electrochimica Acta*

Received Date: 3 July 2017

Revised Date: 30 April 2018

Accepted Date: 7 May 2018

Please cite this article as: A.N. Tabish, H.C. Patel, J. Schoonman, P.V. Aravind, A detailed look into hydrogen electrochemical oxidation on ceria anodes, *Electrochimica Acta* (2018), doi: 10.1016/j.electacta.2018.05.058.

A detailed look into hydrogen electrochemical oxidation on ceria anodes

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Abstract

Using the Nernst-Planck-Poisson model and a detailed reaction mechanism, we studied the hydrogen electrochemical oxidation on a ceria anode. Resistances caused by surface kinetics, and bulk transport of oxide-ion vacancies and electrons are computed individually to identify the dominant resistive process. The effect of operating conditions like temperature and gas-phase composition on the polarization resistance is evaluated and compared with the experimental data obtained by Electrochemical Impedance Spectroscopy (EIS). The rate-determining step is found to be the charge-transfer reaction in which hydrogen adsorbs at the surface oxide ions and forms hydroxyls along with the charge-transfer to adjacent cerium ions. Based on the rate-determining step, the exchange-current density is also calculated and validated with the experimental data.

Keywords: pattern anodes, SOFC, ceria, NPP model, elementary kinetics

1. Introduction

Ceria is one of the extensively studied mixed ionic and electronic conducting (MIEC) material and inherits outstanding redox properties [1]. It is widely used as a three-way catalyst in automotive industry as well as a promoter for water-gas shift conversion, thermochemical water splitting, and various other catalytic reactions [2]. In the recent years, ceria has gained a considerable attention as an SOFC anode material due to its ability of oxidizing carbon containing fuels [3, 4] and extended electrochemically active area. Doping ceria with trivalent elements like gadolinium and samarium enhances the oxygen vacancy concentration and

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