Origin of electrolyte dopant dependent sulfur poisoning of SOFC anodes

Zeng, Zhenhua; Björketun, Mårten; Ebbesen, Sune Dalgaard; Mogensen, Mogens Bjerg; Rossmeisl, Jan

Published in:
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY

Publication date:
2013

Document Version
Publisher's PDF, also known as Version of record

Link back to DTU Orbit

Citation (APA):
Origin of electrolyte-dopant dependent sulfur poisoning of SOFC anodes

ZhenHua Zeng1,2, zheng@purdue.edu, Mårten E. Björketun7, Sune Ebbesen3, Mogens B. Mogensen3, Jan Rossmeisl8. (1) School of Chemical Engineering, Purdue University, West Lafayette, Indiana 47906, United States, (2) Department of Physics, Technical University of Denmark, Kgs. Lyngby, Denmark, (3) Department of Energy Conversion and Storage, Technical University of Denmark, Roskilde, Denmark

The mechanisms governing the sulfur poisoning of the triple phase boundary (TPB) of Ni-XSZ (X2O3 stabilized zirconia) anodes have been investigated using density functional theory. Calculated sulfur adsorption energies reveal a clear correlation between the size of the cation dopant X3+ and the sulfur tolerance of the Ni-XSZ anode; the smaller the ionic radius, the higher the sulfur tolerance. The mechanistic study shows that the size of X3+ strongly influences XSZ's surface energy, which in turn determines the adhesion of Ni to XSZ. The Ni-XSZ interaction has a direct impact on the Ni-S interaction and on the relative stability of reconstructed and pristine Ni(100) facets at the TPB. Together, these two effects control the sulfur adsorption on the Ni atoms at the TPB. The established relations explain experimentally observed dopant-dependent anode performances and provide a blueprint for future search for and preparation of highly sulfur tolerant anodes.

Figure 1 Sulfur adsorption energy on Ni-XSZ, relative to the corresponding value on a Ni(111) terrace, plotted versus the ionic radius of X3+. HCP11 and Hollow14 are adsorption sites on reconstructed and pristine Ni(100) facets, respectively. The dotted line indicates the ionic radius of Zr4+.

Reference
ZhenHua Zeng, Mårten E. Björketun, Sune Ebbesen, Mogens B. Mogensen and Jan Rossmeisl, Phys. Chem. Chem. Phys., DOI:10.1039/C3CP51099A.