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A DFT Interfacial Study of a Bimetallic Glassy Carbon Supported Electrocatalyst

The hybrid sulphur (HyS) cycle[1] has shown potential to be a viable hydrogen producing process via the electro-oxidation of aqueous SO_2. The process makes use of a platinum electrocatalyst. Hence research conducted by Falch [2], into reducing the amount of Pt in the catalyst was done at the North-West University. They achieved promising results by vapour deposition of Pt onto a glassy carbon (GC) substrate, to produce a thin-film metal electrocatalyst. GC is an excellent material for use as an electrocatalyst substrate due to its high conductivity, low resistance, and low reactivity towards acids and bases.[3] The pure thin-film catalysts performed well but had one limitation, namely the delamination of the metal from the GC support. Hence, Falch, et al. [4] tried different bimetallic combinations and surface treatments to solve the delamination problem. It was found that the bimetallic catalyst, Pt_3Pd_2 annealed at 800℃, had significantly less delamination, and performed similarly to the pure Pt catalyst. The increased adhesion was not easily explained using normal analytical techniques, which gave rise to the need to use molecular modelling to investigate the interfacial characteristics of the bimetallic catalysts on a GC substrate. The GC and bimetallic models were constructed and optimised independently before the interfacial study was conducted. It was found that the atoms in close proximity to the surface defects would migrate towards one another after relaxation. These results indicate that the defects in the GC surface play an important role in the adhesion of the layers. The defects in the GC act as a binding site. Additionally, it was observed the specific metal above the binding site affected the strength of the bond. These bonds were analysed using a few different techniques, namely, work of adhesion [5], Mulliken charge transfer and d-band centre shift. These values were calculated for each model, and used to describe variations in the bonding between the different metallic and GC surfaces. It was concluded that the addition of a second metal overall increased adhesion characteristics between the metal layer and GC, with the molecular models supporting the experimental observations made. All the calculations were done with the CASTEP [5] module of Material Studios software by BIOVIA. This study would not have been possible without the national supercomputing cluster Lengau at the Centre for High Performance Computing (CHPC).

[1] W. A. Summers, M. R. Buckner, M. B. Gorensek, in GLOBAL 2005, Citeseer, Tsukuba, Japan, 2005.
[2] A. Falch, North-West University (South Africa) (Potchefstroom), 2016.
[3] a) L. A. Pesin, Review: Structure and properties of glass-like carbon, Journal of Materials Science, 2002, 37, 1-28;b) P. J. F. Harris, Fullerene-related structure of commercial glassy carbons, Philosophical Magazine, 2004, 84, 3159-3167.
[4] A. Falch, V. Lates, R. J. Kriek, Combinatorial Plasma Sputtering of Pt_xPd_y Thin Film Electrocatalysts for Aqueous SO2 Electro-oxidation, Electrocatalysis, 2015, 6, 322-330.
[5] S. J. Clark, M. D. Segall, C. J. Pickard, P. J. Hasnip, M. I. Probert, K. Refson, M. C. Payne, First principles methods using CASTEP, Zeitschrift für Kristallographie-Crystalline Materials, 2005, 220, 567-570.

Student?

Yes

Supervisor name

Prof CGCE van Sittert

Supervisor email

cornie.vansittert@nwu.ac.za

Primary author: MEERHOLZ, Kyle (North-West University)

Co-authors: VAN SITTERT, Cornie (North-West University); FALCH, Anzel (North-West University)

Presenter: MEERHOLZ, Kyle (North-West University)

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