THE THEORETICAL DESCRIPTION FOR BOROHYDRIDE CoO(OH)-ASSISTED BOROHYDRIDE ELECTROOXIDATION IN FUEL CELLS

Volodymyr V. Tkach[1,2], José Inácio Ferrão da Paiva Martins[2], Sílvio C. de Oliveira[3], Petro I. Yagodynets[1], Zholt O. Kormosh[4], Lucina V. dos Reis[5], Jarem R. Garcia[6]

[1] Chernivtsi National University, 58000, Kotsyubyns´ky Str. 2, Chernivtsi, Ukraine
[2] Faculdade de Engenharia da Universidade do Porto, 4200-465, Rua Dr. Roberto Frias, s/n, Porto, Portugal
[3] Universidade Federal de Mato Grosso do Sul, Av. Sen. Felinto. Müller, 1555, C/P. 549, 79074-460, Campo Grande, MS, Brazil
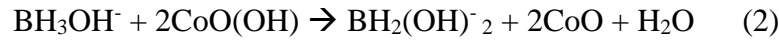[4] Eastern European National University, 43000, Voli Ave., 13, Lutsk, Ukraine
[5] Universidade de Trás-os-Montes e Alto Douro, Quinta de Prados, 5001-801, Folhadela, Vila Real, Portugal
[6] Universidade Estadual de Ponta Grossa, Campus de Uvaranas, Av. Gal. Carlos Cavalcanti, 4748, 84030-900, Ponta Grossa, PR, Brazil

Borohydride ion, alongside with other borane derivatives, is one of the most popular fuel cells anolytes. It is a coordination compound, formed by the borane molecule and hydride ion. It is characterized by highly expressed reducing properties in either inorganic or organic reactions, ceding, in both cases, the hydride anion.

In fuel cells, the borohydride may undergo either direct or gradual oxidation, and cobalt (III) oxyhydroxide may be easily used as an electrode modifier, capable to catalyze the borohydride gradual oxidation:

$$BH_4^- + 2CoO(OH) \rightarrow BH_3OH^- + 2CoO + H_2O \qquad (1)$$
$$BH_3OH^- + 2CoO(OH) \rightarrow BH_2(OH)^-_2 + 2CoO + H_2O \qquad (2)$$

etc. The global oxidation reaction will be thereby exposed as:

$$BH_4^- + 8CoO(OH) \rightarrow BO_2^- + 8CoO + 6H_2O \qquad (3)$$
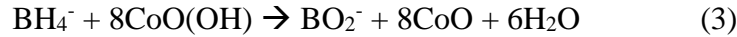
As both borohydride oxidation and cobalt (III) oxyhydroxide synthesis tend to be accompanied by the oscillatory behavior, the goal of our work is to describe theoretically the behavior of this system. Taking into account the reaction sequence and limiting the modeling on the global reaction on the first stage and hydroxyborohydride total oxidation, we describe the system behavior by the trivariant system:

$$\begin{cases} \frac{db}{dt} = \frac{2}{\delta}\left(\frac{\Delta}{\delta}(b_0 - b) - r_1 - r_3\right) \\ \frac{db*}{dt} = \frac{2}{\delta}(r_1 - r_{21}) \\ \frac{dc}{dt} = \frac{1}{C}(r_1 + r_3 + r_{21} - r_O) \end{cases} \qquad (4)$$

The analysis of the model confirms that the oscillatory behavior in this system is caused by the influence of both chemical and electrochemical stages on double electric layer. Nevertheless, cobalt (III) oxyhydroxide may be efficient electrode modifier for borohydride oxidation.