Transition metal nitrides in ammonia production: Challenges and Possible Solutions

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Protonic Ceramic electrochemical devices can have an important role in the decarbonation of industrial chemicals, in line with current European green directives that aim to reduce CO_2 emissions by the development of new C-neutral technologies for industries and processes[1].

The most common protonic ceramic electrolyte materials are those of alkaline earth doped cerates, zirconates and their solid solutions, due to their high proton conductivity and low activation energy. Typically these are materials of the perovskite structure, with the best perfoming containing basic A-site elements such as barium, e.g. $BaZrO_3$-$BaCeO_3$, with minor B-site acceptor doping by rare earth elements, such as Y,Gd.

The current presentation will discuss ongoing studies performed in the University of Aveiro, Portugal, that aim to eletrochemically synthesise NH_3 directly from H_2O and N_2, with the input of renewable electricity, by the use of such Proton Ceramic Electrolyser Cells (PCECs), using these electrolyte materials, Fig.1.

Ammonia (NH_3) is a key chemical that is produced as a precursor in a range of products that are vital to society, such as fertilizers and medicines. Nevertheless, the current Haber-Bosch process produces ammonia from nitrogen and hydrogen at high pressures (100-300bar) in the temperature range 300-550ºC [2,3], with a very high energy consumption, low equilibrium conversion (10-15%) and with the production of ~300 million metric tons of CO_2 per year due to its reliance on hydrogen produced from natural gas [2,3].

New green concepts for NH_3 production, are, therefore, urgently needed, such as that of Fig.1.

In our work we will highlight the possible use of oxynitride materials as electrocatalytically active electrodes for these devices, focusing on their potential advantages, as well as their limitations and key challenges for successful implementation..

Work will describe, the preparation of the oxy(nitride) materials, their stability, their compositional tailoring and their processing to form potential electrodes, Fig.2. This, includes the chemical compatiblity of the oxynitride materials and the aforementioned proton ceramic eletrolytes. Further discussion will assess how modification of the composition of the oxynitrides by control of synthesis conditions can effect their subsequent properties. From this basis, preliminary results of the performace of these materials as potential catalysts for NH_3 formation will be presented.

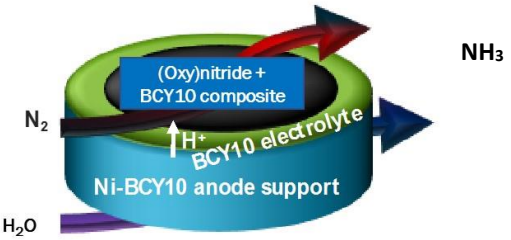

Figure 1. Schematic electrochemical NH_3 production using a PCEC.

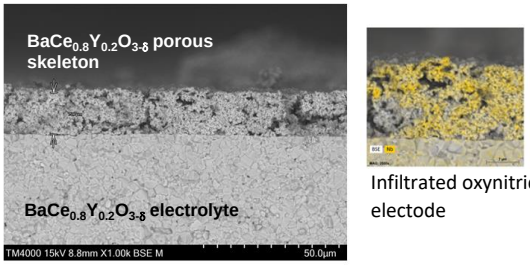

Figure 2. SEM micrographs of an oxynitride electrocatalyst deposited on a proton ceramic substrate.

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