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Modeling of platinum oxides formation and reduction: a performance model for O₂ reduction reaction

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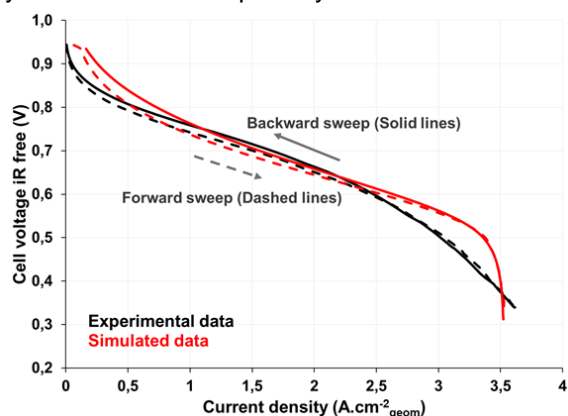
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Despite many improvements, PEMFC systems still suffer technological limitations, such as their initial cost and overall durability in real life operation, which prevents widespread industrial deployment. Some of these limitations can be overcome by combining experiments and modeling to characterize and better understand the behaviour of the carbon-supported platinum (Pt/C) electrocatalyst, its utilization/effectiveness in PEMFC catalyst layers and to be able to predict the performance and durability of PEMFC. This should help making the most relevant choices to accelerate the development processes of PEMFC.

In this work, physico-chemical and electrochemical measurements are performed from the scale of the raw Pt/C materials up to the complete catalyst layer, to gather as much information as possible on the catalytic layer micro-structure and its operating properties. Coupling experiments in classic RDE and in PEMFC differential-single cell (1.8 cm² under high reactant stoichiometry) enables to fully characterize the electrochemical properties and behaviour of our materials. During experimental performance measurements, reversible performance gains/losses can be observed. This behaviour is often ascribed to variable hydration state of the ionomer in the catalyst layer and the bulk membrane and also to the evolution of platinum surface states due to oxides partial formation/reduction.

In parallel; several models have been developed to simulate one or combined mechanisms leading to the performance¹ and degradation of cell components^{2,3}. Based on our experimental work and data sets, the behaviour of the Pt/C electrocatalysts has been studied in order to introduce new electrocatalytic features and especially the Pt surface oxide formation and reduction which is linked to Pt surface



state as well as Pt 'bulk' oxide formation via chemical place exchange reaction. This preliminary step was then further developed into a complete performance model for the O₂ reduction reaction at the cathode to better describe the physical and electrochemical phenomenon involved in catalyst layers during fuel cell operation. With this new description, the position of the main adsorption/desorption peaks monitored by CV under inert atmosphere and the hysteresis phenomenon on the polarization plot during real fuel cell operation are well captured by the simulation compared to experiment keeping complete physical meaning.

Keywords: Performance model, Hysteresis phenomenon, Reversible degradation, Modeling, Fuel cell.

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