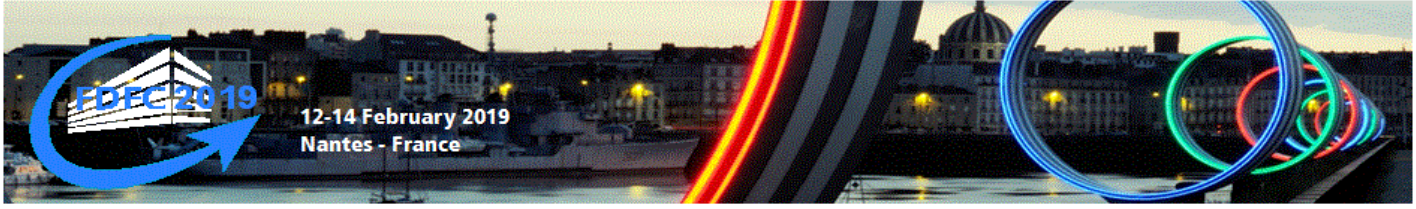

Physical modeling of catalyst degradation in PEMFC: simulation of particle growth and platinum band formation under AST and real operation

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Catalyst degradation at the cathode is one of the main causes of performance loss in PEMFC. Typically platinum or platinum alloy nanoparticles are used as catalyst. Small particle sizes ensure high electrochemical active surface area (ECSA) at low platinum loading. However, these small particles are also more prone to platinum dissolution, requiring a compromise between performance and durability. Dissolution can lead to Ostwald ripening as well as to platinum band formation. In both cases the ECSA and therefore the cell performance will decrease. The dissolution kinetics is related to the platinum oxide formation and reduction and strongly depends on the operating conditions.

Here, we present a physical model for the catalyst degradation which includes a platinum oxide model, platinum dissolution, Ostwald ripening and platinum band formation. The platinum oxide model is validated with dedicated CV measurement to determine the oxide evolution kinetics. The platinum oxide coverage affects the dissolution kinetics via the oxide dependent surface tension. In addition platinum oxide reduction can also cause platinum dissolution. The produced platinum ions can move within the ionomer of the catalyst layer where precipitation on larger platinum particles leads to Ostwald ripening. This is described by a balance equation for the local particle size distribution. Alternatively, the platinum ions can move into the membrane where they can react with hydrogen to form the platinum band.

We couple the developed degradation model with a PEMFC single cell model in our modeling framework NEOPARD-X [1] to simulate the catalyst degradation during various degradation tests, including AST, long-term degradation tests and dynamic driving cycles. ECSA evolution and particle size distributions obtained from TEM are used for model validation. Stressors and spatial distribution of the catalyst degradation are investigated.

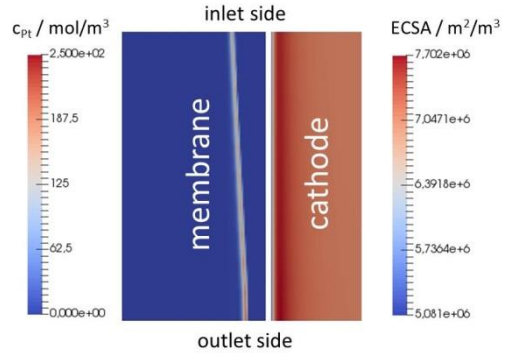

Figure 1: Simulated platinum band formation and ECSA distribution after 2000h of operation at 0.2A/cm²

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