Kinetic Monte Carlo simulation of the Yttria Stabilized Zirconia (YSZ) fuel cell

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A Kinetic Monte Carlo (KMC) model is developed to simulate non-symmetrically the cathode side of a Yttria Stabilized Zirconia (YSZ) fuel cell, in order to translate experimental, and ultimately theoretical rates into an atomistic model of the fuel cell\textsuperscript{1}. The KMC model consists of a set of several electrochemical reaction rates, adopted from experiments and first-principles calculations. The KMC simulations are used to model these simultaneously occurring events, to determine potential limitations in cathode/YSZ performance. The focus of this work is ionic current density ($J$), studied as a function of various physical parameters: oxygen partial pressure ($P_{O_2}$), external applied bias voltage ($V_{ext}$), temperature ($T$), dopant concentration (mol \% $Y_2O_3$), relative permittivity ($\varepsilon$) of YSZ, and geometrical features of the YSZ electrolyte. This simple model can be used as a baseline to translate elementary chemical reaction rates into atomistic simulations of working solid oxide fuel cell cathodes, pertinent to the complete set of experimental operating conditions.

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