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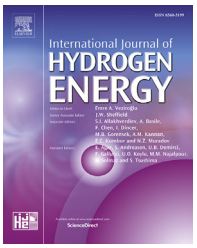

Study on electrochemical and mass transfer coupling characteristics of proton exchange membrane (PEM) fuel cell based on a fin-like electrode surface

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ABSTRACT

Proton exchange membrane (PEM) Fuel cells are widely used because of its environmental protection and high efficiency. In the present study, a novel fin-like structure of the electrode surface is investigated by establishing the theoretical model and numerical simulating. For this purpose, the influence of different fin spacing and pressure boost on the performance of the PEM fuel cell is analyzed by numerical simulation. Results show that increasing pressure of cathode or both side experiences greater performance improvement compared to the other cases, and the maximum values of power density during both conditions is founding for fin density 1/1, followed by fin density 1/12, then last the basic model. Furthermore, the analysis shows that increasing CL surface area combined with cathode pressurization is the best strategy for fuel cell performance optimization. The fin structure under the condition of cathode pressurization can effectively reduce the transmission resistance and over potential of the fuel cell by theoretical calculation, which is coinciding well with the simulation results.

Introduction

Proton exchange membrane (PEM) fuel cell is a kind of device that converts chemical energy directly into electrical energy by using a special proton conducting polymer electrolyte membrane that are ideally suited to the high conversion efficiency and free pollution [1–3]. Catalytic electrode, also known as catalyst layer (CL) is a crucial component for PEM fuel cell and performs several vital functions in the operation of the fuel cell system; it facilitates ions transport towards the membranes and also provides the site of the catalytic process for reacting gases.

In literature, preparations of CL material to achieve excellent ionic and electronic transport properties are conducive to prevent catalyst poisoning and improve the utilization ratio of platinum. A ceramic carbon electrode has been prepared with presence of the organic side chain, which increased the conductivity of the proton [4]. Parallel flow channel design and the layer wise structure composed of an outer and an inner CL has the least significant effect of CO poisoning for the high temperature PEM fuel cells [5,6]. Characterization methods like X-

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Nomenclature

L	geometric length (m)
H	geometric height (m)
W	geometric width (m)
I	current density (Am^{-2})
u	fluid velocity (ms^{-1})
j	transfer current density (Am^{-3})
M	molecular weight $(kg\ mol^{-1})$
F	Faraday constant $(96,487C\ mol^{-1})$
F_u	force term $(kg/(\ m^2s^2))$
w	mass fraction (%)
g	external force $(m\ s^{-2})$
x_k	mole fraction (%)
D	mass diffusivity $(\ m^2s^{-1})$
T	temperature (K)
R	universal gas constant $(8.314mol^{-1}K^{-1})$
C	molar concentration $(mol\ m^{-3})$
P	pressure (Pa)
R_s	internal resistance $(\Omega^{-1}cm^2)$
E_{eq}	equilibrium potential (V)

Greek symbols

ρ	density $(kg\ m^{-3})$
ε	porosity
μ	dynamic viscosity $(kg\ m^{-1}s^{-1})$
κ	permeability $(\ m^2)$
β_F	Forchheimer drag option $(kg^{-1}m^4)A$
σ	Conductivity $(S\ m^{-1})$
η	over potential (V)
α	electrical transfer coefficient
σ_A	specific surface area (m^{-1})

Subscripts and superscripts

c	gas channel
r	rib
gdl	gas diffusion layer
e	electrode
m	membrane
H_2	hydrogen
O_2	oxygen
H_20	water
N_2	nitrogen
a	anode
c	cathode
s	solid
∞	bulk condition
o	standard condition
f	fin
loc	location
eff	effective
ref	reference
cl	catalytic electrode
l	liquid
k	species index independently of i
i	species index

ray Tomography and Integrated Mercury Porosimetry were used to investigate the pore structure of electrode. Meanwhile, the performance of the fuel cell is optimized by the morphology analysis of platinum distribution with different electrode curing conditions [7,8].

To the best of our knowledge, the catalytic electrode designed by chemical modification or combined with advance material has better electrochemical characteristics. The use of sulfonated silica-based CL structures under ceramic carbon condition can lead to a greatly enhancement of ionic permeability [9]. A new class of coreeshell-electrocatalysts is studied by high-resolution TEM. In those conditions, the dispersion of the active electro-catalytic sites on the surface of the STps was improved [10]. However, restrictions of reactant transport are still to be addressed before liquid water can be satisfactory managed. The rGO/CB based hybrid support CL can promote to the use of high surface area of graphene and ease the diffusion of ions [11]. The inverse-opal structure of CL has good effective porosity and satisfactory water management, furthermore, the balance of hydrophobicity and hydrophilicity in electrode should also be considered [12,13].

More recently, growing interest has been focus on fractal pore structure electrode and novel fabrication process for the electrode surface structure based on inorganic mixture [14–16]. These geometries captured increasing attention mainly because of excellent surface utilization by maximizing the number of networked interfacial sites and gas accessibility [17,18]. A similar approach was followed by optimizing the macroscopic structure of the electrode surface, which enhance the local cell performance of the PEM fuel cell system due to the larger surface reaction area [19,20].

In this paper, a coupling model of three-dimensional PEM fuel cell to study the electrochemical and mass transfer mechanism is established. The fin-like or pyramidal structure is applied to the GC and the GDL to improve the mass transfer of the reactant [21–25] but it is seldom been discussed on the electrode. By analogy with the heat transfer process of fins, this study proposes a novel structure of the electrode surface and derives the mathematical equation of surface over potential by the basic Laplace equation. The influence of different fin spacing on the performance of the PEM fuel cell is analyzed by numerical simulation. The influence of both the cathode and anode under different pressure conditions on the mass transfer and electrochemical reaction characteristics of the electrode is also investigated. The optimization strategy is found by combining fin density and pressure boost. The influence of the fin structure on the electrochemical mechanism is also revealed by the mathematical model of the distribution of the fin surface.

Model definition

Geometric model

As shown in Fig. 1, the hierarchical structure on the electrode surface is significantly increasing the reaction area which is

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