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Effect of local stress concentration near the rib edge on water and electron transport phenomena in polymer electrolyte fuel cell



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Daisuke Kanda, Hirotatsu Watanabe*, Ken Okazaki

Department of Mechanical and Control Engineering, Graduate School of Science and Engineering, Tokyo Institute of Technology, 2-12-1-16-7, Ookayama, Meguro-ku, Tokyo 152-8552, Japan

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ABSTRACT

The performance of polymer electrolyte fuel cell (PEFC) depends on transport phenomena in the gas diffusion laver (GDL). To elucidate the relationship between the local stress concentration near the rib edge and current density distribution, contact stress analysis and charge transport calculations were performed. Subsequently, the effect of GDL deformation caused by the local stress concentration on water transport was investigated. As a result, contact stress analysis showed that through-plane stress in GDL was concentrated near the rib edge. However, the stress was not concentrated on the catalyst layer even when the compression ratio and curvature radius of the rib were varied over a wide range. By solving the charge conservation equation, the potential and current density distribution were obtained. The current density, although not concentrated on the catalyst layer, was concentrated in GDL near the rib edge because the GDL conductivity near the rib edge increased locally from the stress concentration. Calculation showed that to decrease the effect of local stress, rounding off the rib is more effective than decreasing the compression ratio. From scanning electron microscopy (SEM) images of the GDL after clamping, the stress concentration caused the breakup of fibers and polytetrafluoroethylene (PTFE), which caused the hydrophobicity to deteriorate. Therefore, the preferential pathways of water behavior were observed near the rib edge. It was shown that local stress concentration near the rib edge affected the water behavior and GDL characteristics although it did not affect the catalyst layer.

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1. Introduction

Global warming and fossil fuel depletion are being significantly aggravated as energy consumption and carbon dioxide emission increase [1] from industrialization, but industrialization has made our lives more comfortable, a comfort that we do not wish to give up. A power system that holds tremendous promise because of its high efficiency is the polymer electrolyte fuel cell (PEFC). However, technical problems such as performance, cost, and durability must be solved before PEFC can be used widely. The major voltage losses in PEFCs arise from the limitation in mass transport, which is influenced by the flow field geometry and properties of the porous gas diffusion layer (GDL). The GDL plays an important role in electrical conduction and water management because it promotes the diffusion of reactant gasses and emission of liquid water from catalyst layer to channel. The excess water causes flooding and prevents reactant gasses from diffusing [2]. Mass and water transport in GDL has been studied through numerical simulation [3] and visualization [2,4].

* Corresponding author. Tel./fax: +81 3 5734 2179. E-mail address: watanabe.h.ak@m.titech.ac.jp (H. Watanabe).

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A rib, which is the solid wall of a separator, is closely attached to the GDL by clamping force. Clamping is needed to seal the cell to prevent the leakage of reactant gasses. Several researchers have investigated the effect of this compression on GDL properties [5–9]. Nitta et al. [5] have reported that such GDL properties as permeability, bulk conductivity, and contact resistance are dependent on clamping force. Radhakrishnan et al. [6,7] have investigated the effect of cyclic compression on the GDL properties of surface morphology, surface roughness, pore size, void fraction, thickness, electrical resistance, contact angle, water uptake, and inplane permeability. Fester et al. [8] have shown that clamping forces decrease in-plane permeability and porosity. Freunberger et al. [9] have reported that in-plane and through-plane conductivities and contact resistance are changed by compression. Although much research on GDL compression has been conducted, most of the studies have focused on changes in the overall GDL characteristics caused by the clamping force. Little effort has been made to study the local stress concentration near the rib edge, even though it is expected to initiate cracking [10], to improve electrical conductivity, and to locally change the pathway for water removal. Therefore, local stress might be a trigger for the deterioration of the catalyst layer.

 $\sigma_{\rm max}$

 $\sigma_{\rm bulk}$

Nomenclature

ϕ	potential (V)
σ_{xx}	in-plane conductivity (S/m)
σ_{yy}	through-plane conductivity (S/m)
r _c	stress concentration ratio (-)

The purpose of this study is to investigate the effect of local stress concentration near the rib edge on the GDL and catalyst layer by using a contact stress analysis. In addition to this, charge transport calculations with considering GDL deformation are performed, and the relationship between local stress concentration and current density distribution is investigated. Furthermore, the effect of GDL deformation caused by local stress concentrations on water transport is studied.

2. Methodology

2.1. Numerical analysis

Fig. 1 shows a schematic diagram for stress analysis, which is composed of the rib, GDL, and membrane. Contact stress analysis was performed by using Abaqus version 6.8 for obtaining the stress distributions in GDL and the membrane. In the stress analysis, the origin was on the bottom-left corner of the membrane. The number of elements for the analysis was 30,000.

Both of the side edges of the GDL and membrane were fixed in the *x*-direction, and the bottom of the membrane was fixed in the *y*-direction. On the top surface and interface between the GDL and membrane, no constraint condition was applied. In the contact stress analysis, the deformation of GDL is considered by setting the compression ratio at 10%, 20%, and 30%. The compression ratio was calculated by dividing the displacement by the initial thickness of the GDL, as shown in Fig. 2 [11]. The effect of the curvature radius of the rib was investigated by using various curvature radii (R0.2, R0.1, R0.02, and vertical) on local stress concentration. The curvature radius of the rib used in this experiment was measured with a digital microscope as being R0.02.

Table 1 shows geometric and physical properties of the GDL and cell. The macro-structural approach applying a homogenized microstructure is used in this paper. Although Young's modulus is sometimes assumed to be constant for simplification [12], it is a function of strain [13,14]. However, the simplest approach (fixed value) was used in this paper because through-plane Young's modulus is barely assumed to be constant when the compressive stress is small, and it is difficult to estimate exact Young's modulus near the rib edge where local stress is concentrated, leading to the breakup of fibers of GDL as described later. In addition to this, our primary purpose is to investigate the effect of local stress concentration near the rib edge on the whole catalyst layer which the dependence of Young's modulus on strain is not likely to influence.



Fig. 1. Schematic diagram of GDL, rib, and membrane.



maximum stress on the surface of GDL (MPa)

bulk stress on the surface of GDL (MPa)

Fig. 2. Schematic diagram of compressed GDL.

Table 1

Geometric and physical properties of GDL and the cell.

Parameter	Value
Rib width Channel width Channel handle	5 mm 5 mm
Channel length	50 mm
Thickness of GDL	$200 \times 10^{-6} \text{ m}$
Thickness of membrane	$50 \times 10^{-6} \text{ m}$
Through-plane Young's modulus of GDL In-plane Young's modulus of GDL [12]	$\begin{array}{l} \textbf{6.39} \text{ MPa} \\ \textbf{1} \times \textbf{10}^{3} \text{ MPa} \end{array}$
Young's modulus of membrane [9]	50 MPa
Poison ratio of GDL [9]	0.35
Poison ratio of membrane [16]	0.35
Curvature radius of rib (measured)	R0.02

In this paper, GDL compression along vertical direction is focused. Some researchers have used a similar macro-structural approach, and the Poisson's ratio of GDL ranged from 0.25 to 0.35 [9,15]. Therefore, the Poisson's ratio was set to 0.35 in this paper.

Fig. 3 shows the calculation domain for the electron transport calculation. The domain consisted of computational and noncomputational cells used to express GDL configuration after compression had been determined by stress analysis. The computational cells indicated the GDL, and noncomputational cells indicated the rib and space made by GDL deformation.

After the stress distribution was calculated, the GDL configuration after compression was determined. By defining computational and noncomputational cells, the current density distribution was calculated. Electron transport in the GDL was governed by the charge conservation equation, which is expressed in a two-dimensional coordinate system as:

$$\frac{\partial}{\partial x} \left(\sigma_{xx} \frac{\partial \phi}{\partial x} \right) + \frac{\partial}{\partial y} \left(\sigma_{yy} \frac{\partial \phi}{\partial y} \right) = 0 \tag{1}$$



Fig. 3. Calculation domain for electron transport (200×30 cells; white cells are computational cells; gray cells are noncomputational cells).

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