研　究　速　報

Finite Element Modeling of Electrochemical-Mechanical Response of Ionic Conducting Polymer-Metal Composite Plates

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1. Introduction

Much attention has been focused on ionic conducting polymer-metal composites (abbreviated as IPMC) shown in Fig. 1 as an intelligent material of artificial muscles and MEMS. The electro-chemical-mechanical behaviors of IPMC materials have been theoretically and experimentally studied for recent years[1-5].

The purpose of the present study is to develop a prototype program of the computational tool for the design of IPMC actuators. The one-dimensional basic equations governing the electro-chemical behavior of IPMC materials are discretized by the Galerkin finite element method[6]. The calculated results are compared with the finite difference solutions in order to check the validity of the present formulation. The three-dimensional finite element analysis for the deformation response of an IPMC plate is conducted by using the calculated water distribution as an eigen-strain.

2. Electrochemical Finite Element Formulation

2.1 Forward motion

When a Nafion membrane is under an electric field by the step voltage on platinum plates, hydrated cations are subjected to the electric force to the anode side. Hydrated cations are also subjected to viscous resistance force and diffusion force in the cathode direction. Based on the balance of these forces, the total charge $Q(x,t)$ is expressed as follows[5]:

$$\eta_1 \frac{\partial Q(x,t)}{\partial t} = kT \frac{\partial^2 Q(x,t)}{\partial x^2} - \frac{\partial Q(x,t)}{\partial x} \times \left\{ \frac{e}{\varepsilon_e S_x} \left[\int_0^t i(\tau) d\tau + Q(x,t) - Q(x,0) \right] \right\} \quad \cdots\cdots\cdots\cdots (1)$$

where i is the electric current as shown in Fig. 2. The initial and boundary conditions are given as follows[4]:

$$\left\{ Q^{(e)}(x,0) \right\} = N_a e S_x c_0 x \quad \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots (2)$$

$$\left\{ Q^{(e)}(0,t) \right\} = 0$$

$$\left\{ Q^{(e)}(d,t) \right\} = N_a e S_x c_0 d \quad \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots (3)$$

Table 1 shows the material constants and calculation conditions for eqs. (1)-(3) in which $c_0 = c(x,0) = 1147$ mol/m^3.

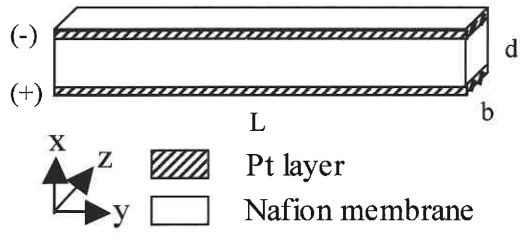

Fig. 1 IPMC plate model

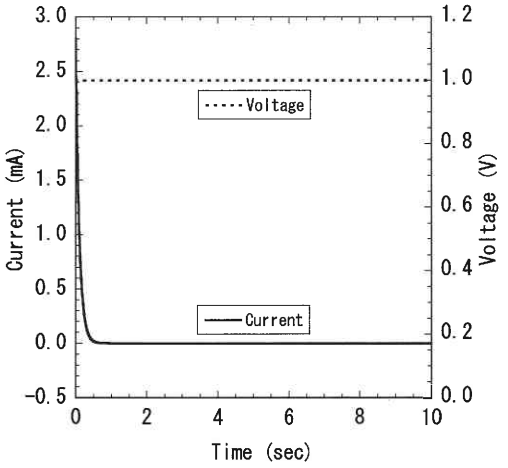

Fig. 2 Input step voltage and current profile

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The charge density is calculated from the total charge by the following equation[4].

$$Q(x,t) = N_a e S_x \int_0^x c(\xi,t)\,d\xi \quad \cdots\cdots (4)$$

Zero slopes are assumed as the boundary conditions.

The finite element formulation is conducted for eqs. (1) and (4). The total charge $Q(x,t)$ is assumed to be a linear function of the element coordinate in each element as shown in the following equation:

$$\left\{Q^{(e)}(x,t)\right\} = [N]\left\{Q^{(e)}\right\} = \left[1 - \frac{x}{h}\ \frac{x}{h}\right]\begin{Bmatrix} Q_i \\ Q_j \end{Bmatrix} \quad \cdots\cdots (5)$$

where Q_i and Q_j are the nodal total charges. h is the element length. The following equation is obtained by the finite element formulation based on Galerkin method[6]:

$$\int_0^h [N]^T \left(\eta_1 \frac{\partial Q(x,t)}{\partial t} - kT \frac{\partial^2 Q(x,t)}{\partial x^2} + \frac{\partial Q(x,t)}{\partial x} \right.$$

$$\left. \times \left\{ \frac{e}{\varepsilon_e S_x} \left[\int_0^t i(\tau)\,d\tau + Q(x,t) - Q(x,0) \right] \right\} \right) dx = 0 \quad \cdots (6)$$

Substituting eq. (5) into eq. (6) and integrating numerically by Euler method, the following form of equation[7] is obtained:

$$\begin{bmatrix} A_{11}^{(e)} & A_{12}^{(e)} \\ A_{21}^{(e)} & A_{22}^{(e)} \end{bmatrix} \left\{Q^{(e)}(x,t+\Delta t)\right\} = \begin{bmatrix} B_{11}^{(e)} & B_{12}^{(e)} \\ B_{21}^{(e)} & B_{22}^{(e)} \end{bmatrix} \left\{Q^{(e)}(x,t)\right\} \quad \cdots (7)$$

The following equation is obtained by the Galerkin finite element formulation[6] for eq. (4):

$$\int_0^h [N]^T \left(\frac{\partial Q(x,t)}{\partial x} - N_a e S_x c(x,t) \right) dx = 0 \quad \cdots\cdots (8)$$

The substitution of eq. (5) into eq. (8) leads to the following form of equation[7]:

$$\begin{bmatrix} C_{11}^{(e)} & C_{12}^{(e)} \\ C_{21}^{(e)} & C_{22}^{(e)} \end{bmatrix} \left\{c^{(e)}(x,t)\right\} = \begin{bmatrix} D_{11}^{(e)} & D_{12}^{(e)} \\ D_{21}^{(e)} & D_{22}^{(e)} \end{bmatrix} \left\{Q^{(e)}(x,t)\right\} \quad \cdots\cdots (9)$$

2.2 Backward motion

The second process is the slow diffusion of free water molecules in the anode direction. The density of water molecules $w(x,t)$ is calculated by the following equation[4]:

$$\frac{\partial w(x,t)}{\partial t} = \frac{kT}{\eta_2} \frac{\partial^2 w(x,t)}{\partial x^2} \quad \cdots\cdots (10)$$

Table 1 Material constants and calculation conditions for forward motion

Coefficient of viscosity for hydrated Na^+ moving through membrane	$\eta_1 = 1.18\times10^{-11}$ (N·s/m^2)
Boltzman constant	$k = 1.380\times10^{-23}$(N·m/K)
Absolute temperature	$T = 293$(K)
Elemental charge	$e = 1.6\times10^{-19}$(C)
Dielectric constant of hydrated Nafion membrane	$\varepsilon_e = 2.8\times10^{-3}$ (C^2/N·m^2)
Time interval	$\Delta t = 5\times10^{-4}$s
Space interval	$h = 2\mu$m
Cross section area	$S_x = 34.2\times10^{-6}$(m^2)
Avogadro number	$N_a = 6.02\times10^{23}$(/mol)

Table 2 Material constants and calculation conditions for backward motion

Concentration of bound water to the fixed SO_3^- groups	$w_1 = 4381$(mol/m^3)
Concentration of free water molecules	$w_2 = 4381$(mol/m^3)
Time of ending of first stage and beginning of second stage	$t_1 = 0.11$s
Hydration number of Na^+ ions in swollen Nafion	$n = 4.7$
Coefficient of viscosity for free water molecules	$\eta_2 = 11.6\times10^{-11}$(N·s/m^2)
Time interval	$\Delta t = 5\times10^{-3}$s

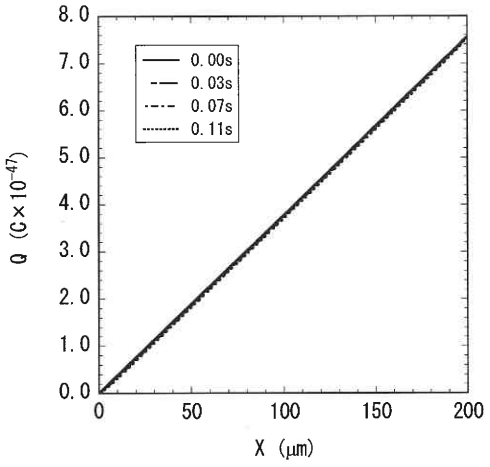

Fig. 3 Total charge distribution in membrane

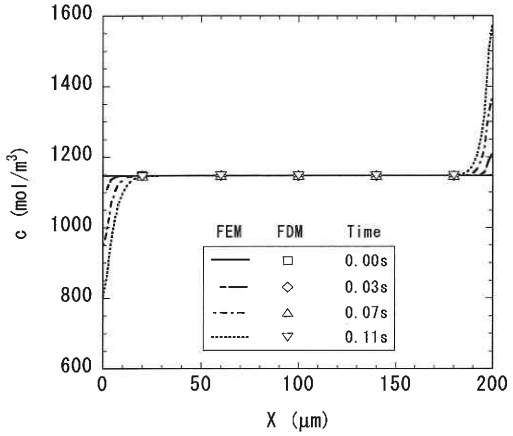

Fig. 4 Charge concentration distribution in membrane

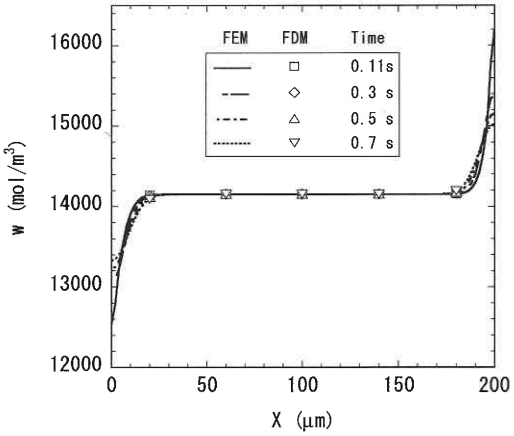

Fig. 5 Water distribution

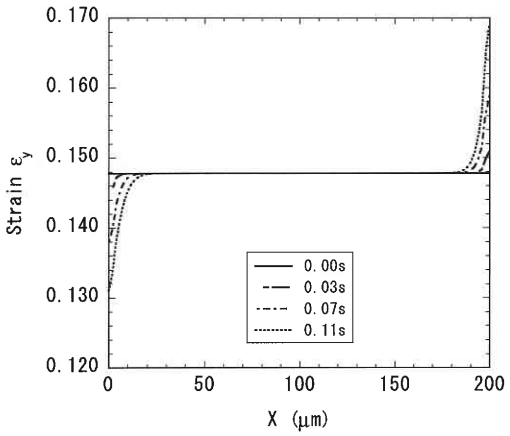

Fig. 6 Strain distribution (forward motion)

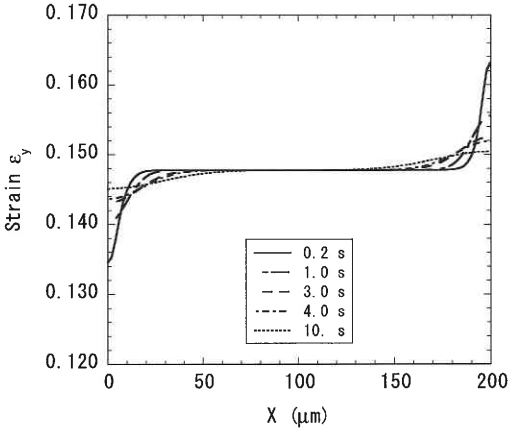

Fig. 7 Strain distribution (backward motion)

The initial and boundary conditions are given by eqs. (11) and (12), respectively[5].

$$w(x,0) = w_1 + w_2(x,0) + nc(x,t_1) \quad \cdots\cdots\cdots\cdots (11)$$

$$\frac{\partial w(0,t)}{\partial x} = 0, \frac{\partial w(d,t)}{\partial x} = 0 \quad \cdots\cdots\cdots\cdots\cdots\cdots (12)$$

Table 2 shows the material parameters and calculation conditions for the backward motion.

The finite element formulation based on Galerkin method[6] for eq. (10) leads to the following equation:

$$\int_0^h [N]^T \left(\frac{kT}{\eta_2} \frac{\partial^2 w(x,t)}{\partial x^2} - \frac{\partial w(x,t)}{\partial t} \right) dx = 0 \quad \cdots\cdots\cdots (13)$$

Assuming linear interpolation function for $w(x,t)$, the following form of equation[7] is obtained from eq. (13):

$$\begin{bmatrix} A_{11}^{(e)} & A_{12}^{(e)} \\ A_{21}^{(e)} & A_{22}^{(e)} \end{bmatrix} \left\{ w^{(e)}(x, t+\Delta t) \right\} = \begin{bmatrix} E_{11}^{(e)} & E_{12}^{(e)} \\ E_{21}^{(e)} & E_{22}^{(e)} \end{bmatrix} \left\{ w^{(e)}(x,t) \right\} \cdots (14)$$

3. Finite Element Analysis of Mechanical Response

The water mol $W_i(x,t)$ is calculated as follows[5]:

$$W_i(x,t) = S_x \int_{x_{i-1}}^{x_i} w(\xi, t) d\xi \quad \cdots\cdots\cdots\cdots\cdots\cdots (15)$$

The water content m_i in each element is calculated by multiplying the weight of water per mol (=18g/mol) with the water mol M_w as below[5].

$$m_i = W_i \cdot M_w \quad \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots (16)$$

The standard water content m_R is calculated by the following equation[5]:

$$W = m_i / m_R,\ m_R = S_x \cdot h \cdot \rho_w \quad \cdots\cdots (17)$$

where ρ_w (=1379000g/m^3) is the density of hydrated Nafion membrane. W is the water content of each element. The distribution of eigenstrain is evaluated by using the experimental relation between the strain and the water content, which is almost linear.

The three-dimensional finite element deformation analysis with eight-noded hexahedron element can be conducted by using the estimated eigenstrain $\{\varepsilon_y(x,t)\}$ as the initial strain in the IPMC plate. The incremental stiffness equation for the initial strain increment $\{\Delta\varepsilon_i\}$ is expressed as follows:

$$[k]\{\Delta u\} = \{\Delta f_i\} \quad \cdots\cdots (18)$$

where

$$\{\Delta f_i\} = \int_{V_e} \{B\}^T \{\Delta\sigma_i\} dV \quad \cdots\cdots (19)$$

$$\{\Delta\sigma_i\} = [D]\{\Delta\varepsilon_i\} \quad \cdots\cdots (20)$$

4. Numerical Example

The calculated results for the IPMC plate for the material properties of Table 3 are shown in Figs. 3–9. The results for the charge concentration distribution (Fig. 4) and the water distribution (Fig. 5) agree well with those by the finite difference modeling[5].

5. Concluding Remarks

The finite element formulation for the electrochemical-mechanical behaviors of IPMC materials has been conducted and its validity has been demonstrated by the numerical study for the IPMC plate. The multi-dimensional formulation for the electrochemical behavior and the application to other materials such as Flemion are the topics of future study.

The authors appreciate Prof. M. Taya, University of Washington, who gave advices in the course of the present study.

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Table 3 Material properties for IPMC plate

	Young's modulus (GPa)	Poisson's ratio
Nafion membrane	0.23	0.49
Platinum layer	146.8	0.39

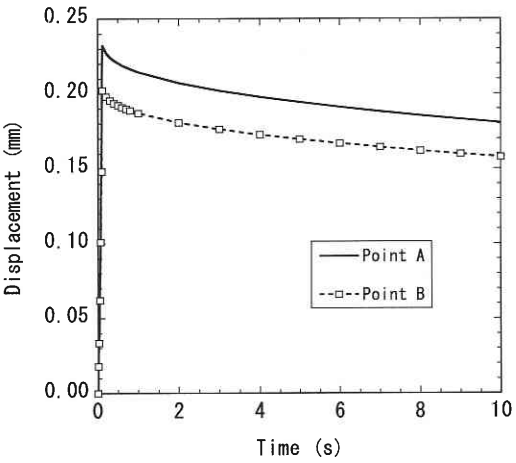

Fig. 8 Time-history of displacement for IPMC plate (L = 20 mm, d = 200 μm, b = 20 mm)

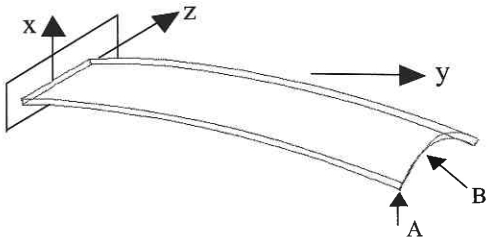

Fig. 9 Deformation of IPMC plate

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