Modeling of Hydrogel Coated Fiber Bragg Grating pH Sensor

Ian Yulianti, A. S. M. Supa'at, Sevia M. Idrus, Ojo Kurdi, and M. Ridwanto S. Anwar

***Abstract*—This paper present the modeling and simulation of the hydrogel coated FBG for pH sensor application. The hydrogel swelling was modeled by using Poisson-Nernst-Planck equation and mechanical equilibrium equation. The simulation was done by assuming that the hydrogel was coated on unetched fiber and etched fiber. The strain induced at the fiber core was analyzed using finite element method. It was found that at the region near the jacketed fiber, the strain is distributed nonuniformly. The non uniform area for etched fiber is shorter than that of unetched fiber. The Bragg wavelength shift due to strain of the etched fiber is much larger than that of the unetched fiber.**

***Index Terms*—Optical pH sensor, fiber bragg grating, hydrogel, strain.**

I. Introduction

To overcome the limitation of conventional pH sensors, optical pH sensors have been rapidly developed [1]-[6]. Most of the current optical pH sensor are intrinsic fiber optic sensor based on absorption and fluorescence methods [5] which are optical intensity modulated; therefore, fluctuations in the intensity of light source, and variations in light attenuation through the optical fiber due to changes in the degree of bending may result in measurement errors. Hydrogel coated long period fiber grating (LPFG) based pH sensor has been developed by detecting the resonance wavelength shifts due to the change of the refractive index of the hydrogel coating [7]. However, LPFGs suffer from temperature and bending cross-sensitivities [8], and the measurement accuracy is limited due to their multiple resonance peaks and broad transmission resonance. Hydrogel has also been coated to fiber Bragg grating (FBG) for measuring salinity [9]-[10]. One of the most important advantages of FBG sensors is that the measurand information is wavelength encoded, i.e., the sensed information is encoded directly into wavelength, which is an absolute parameter; therefore the output signal does not depend on the input light level and losses along the optical system. This paper presents the modeling and simulation of the pH sensitive hydrogel coated FBG for pH sensor application. Modeling and simulation was done in three steps: modeling and simulation of mechanical expansion of hydrogel coating due to pH change, analysis the induced strain in the FBG using finite element method and then calculated the λ_B shift due to strain.

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II. Fiber Bragg Grating pH Sensor Principle

Basically, the sensing process of FBG sensor is done through a detection of Bragg wavelength shift. The Bragg wavelength value of FBG is determined by the effective refractive index and the grating period as defined by

$$\lambda_B = 2n_{eff}\,\Lambda \tag{1}$$

where neff is the effective refractive index and Λ is the grating period. Since both parameters are sensitive to external perturbation, i.e. mechanical perturbation (strain, pressure) and thermal perturbation, the Bragg wavelength value will be shifted if such external perturbation is applied to the FBG. For silica fiber, the measured strain response at constant temperature is found to be

$$\frac{1}{\lambda_B}\frac{\delta\lambda_B}{\delta\varepsilon} = 0.78\times10^{-6}\,\mu\varepsilon^{-1} \tag{2}$$

pH sensing through FBG can be realized by applying thin pH sensitive hydrogel coating on the FBG as shown in Fig .1. Hydrogel are made up of a combination of a solid crosslinked polymeric chain and a neighboring aqueos solution. Large reversible mechanical expansions occur if the material is subjected to the value change of the stimuli [11-14]. In pH sensitive hydrogel coated FBG, the mechanical expansion of the hyrogel coating due to pH change stretch the FBG and thus the FBG grating period is expanded. As a result, the Bragg wavelength is shifted.

III. Simulation Method

A. Hydrogel Expansion Simulation

The multi-effect-coupling of pH Stimulus (MECpH) model [13]-[14] was used to simulate the mechanical expansion of the hydrogel under pH value change. At steady state, the one dimensional Nernst-Planck equation is defined by:

$$\frac{\partial^2 c_k}{\partial x^2} + \frac{z_k F}{RT}\frac{\partial c_k}{\partial x}\frac{\partial \psi}{\partial x} + \frac{z_k F c_k}{RT}\frac{\partial^2 \psi}{\partial x^2} = 0 \tag{3}$$

where c_k is the concentration of the kth ionic species inside the hydrogel, z_k is the valency of the kth ion, the index k describes the ionic species present in the solution. ψ is the electric potential, F is the Faraday constant (9.6487 $\times10^4$ C/mol), R is universal gas constant (8.314 J/mol K), and T is absolute temperature (K).

The electric field is defined by Poisson equation as given

by

$$\nabla^2\psi = -\frac{F}{\varepsilon\varepsilon_0}\left(\sum_{k=1}^{N} z_k c_k + z_f c_f\right) \quad (4)$$

where ε_0 is the dielectric constant of vacuum and ε is the relative dielectric constant of the solvent. The quantities z_f and c_f are the valency and concentration of the fixed charge in the hydrogel. The fixed charge concentration depends on the hydrogel volume change as defined by

$$z_f c_f = \frac{1}{H}\left(\frac{z_f c^s_{mo} K}{K + c_{H^+}}\right) \quad (5)$$

where H is the local hydration of the hydrogel and defined as the ratio of fluid volume, V_f, to solid volume,V_s, K is the dissociation constant of the acidic groups, c^s_{mo} is the total concentration of the acidic groups in the dry gel, and c_{H+} the concentration of hydrogen ions H^+ within the hydrogel.

The osmotic pressure is obtained through the following equation:

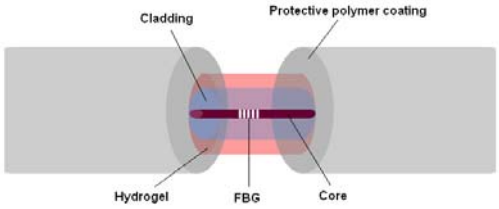


Fig. 1. Hydrgoel coated FBG pH sensor

$$P_{osmotic} = RT\sum_{k=1}^{N}\left(c_k - c_k^0\right) \quad (6)$$

where c^0_k is the concentration of the kth ion in the stress-free state in the outside solution.

The hydrogel deformation, at steady state, is defined by mechanical equilibrium equation

$$\frac{\partial\sigma}{\partial x} = \frac{\partial}{\partial x}\left\{(2\mu+\lambda)\left(\frac{\partial u}{\partial x} + \frac{1}{2}\left(\frac{\partial u}{\partial x}\right)^2\right) - P_{osmotic}\right\} = 0 \quad (7)$$

where σ is the stress tensor of the hydrogel, u is the hydrogel displacement. λ and μ are the Lame's coefficient of the solid matrix which are defined as

$$\lambda = \frac{\nu E}{(1+\nu)(1-2\nu)} \quad (8a)$$

$$\mu = \frac{E}{2(1+\nu)} \quad (8b)$$

where E and ν are modulus Young and Poisson's ratio of the hydrogel. Analytical solution to these coupled nonlinear partial differential equation is impossible, thus the model was solved numerically using the finite cloud meshless method [15].

In this work, the pH sensitive hydrogel was assumed to be 2-hydroxyethyl methacrylate (HEMA) and ethylene glycol dimethacrylate [14], [16] and the acidic groups bound to the polymer chains are carboxyl groups [12]. The simulation was done by assuming that the hydrogel coated FBG is placed in solution with ionic strength of 300 mM.

The hydrogel coating thicknesses (hydrogel thickness in dry state) was taken to be 50 μm. The hydrogel was assumed to be coated on the fiber with diameter of 125 μm (unetched) and 40 μm (etched). Mechanical expansion in the axial direction is restricted by protective polymer coating of the fiber as shown in Fig.1, thus the expansion only occur in radial direction.

B. Induced Strain in the hydrogel coated Fiber Bragg Grating

Finite element analysis of the induced strain within the FBG due to mechanical expansion of the hydrogel was carried out by employing commercial software ABAQUS 6.8. The simulations were done by assuming that the FBG is inscribed into standard telecommunication single-mode optical fiber (Corning SMF-28) with n_{eff} = 1.468. Bragg wavelength was set at 1550 nm. The fiber jacket (protective polymer coating) is removed in the region where the grating should be written and its vicinity. The unjacketed fiber was assumed to be 1 cm.

The fiber was modeled in 3D solid model and was meshed using hexahedral (C3D8R) shape. To minimize the calculation time and computer memory, the simulation was done by analyzing half of the model. The modulus Young and Poison's ratio of the fiber are 73 GPa and 0.165, respectively. Whereas, the modulus Young and Poison's ratio of the acrylic protective coating are 2.88 GPa and 0.402, respectively. The volume change of the hydrogel was converted to a mechanical perturbation as a pressure change and was used as pressure load acting on the fiber.

IV. Results

A. Hydrogel Expansion Simulation

The hydrogel was assumed to be coated along the unjacketed fiber which its length is 1 cm. As expected, hydrogel coating is swelling as the ambient pH change. The hydrogel thicknesses at low pH of unetched fiber are almost the same as that of the etched fiber as shown in Fig.3(a). For unetched fiber, at pH ≥ 7, the hydrogel thicknesses are more than 175 μm. Whereas, for etched fiber, the hydrogel thicknesses are more than 140 μm. These thickness differences occurred due to the difference of volume of hydrogel coating. However, the hydration values for all pH range are almost the same for both fibers as shown in Fig.3 (b).

The strain of the swollen hydrogel due to pH change is depicted in Fig.4 (a). For unetched fiber, the strain increased from 0.4 up to 2.5 for pH value of 4 to 7. At pH >7, as the pH increase, it is observed that the strain is almost constant at value of ~ 2.5. At high pH, it was observed that strain of hydrogel coated on unetched fiber is larger than that of hydrogel coated on etched fiber. The stress on hydrogel corresponding to strain for unetched and etched fiber is in the range of 0.5 to 6 MPa and 0.5 to 4.4 MPa, respectively.

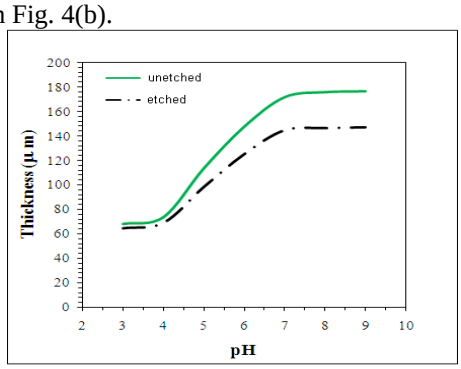
The stress occurred in the hydrogel is converted as pressure acting on the fiber, as defined by

$$P = \frac{\sigma A_h}{A_F} \quad (9)$$

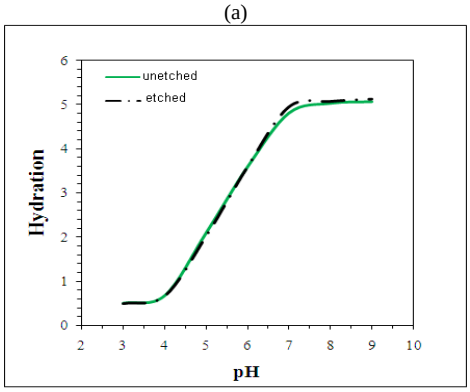
where P is the pressure acting on the fiber, A_h is the cross section area of the hydrogel coating and A_f is the cross

section area of the fiber.

As expected, the pressure induced by hydrogel volume expansion acting on the etched fiber is much larger than that acting on the unetched fiber since the cross section area of etched fiber is much smaller than that of unetched fiber, as shown in Fig. 4(b).

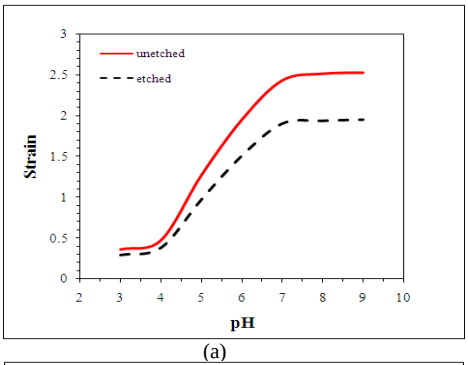


(a)

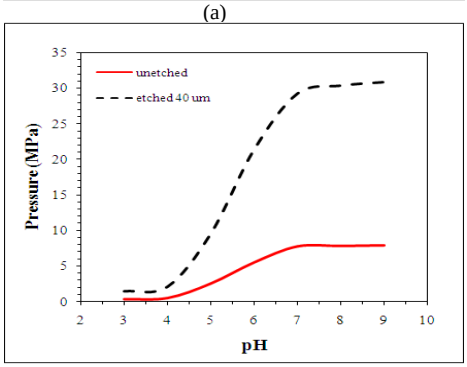


(b)

Fig. 3. Thickness (a) and hydration (b) of hydrogel coating as function of pH value of the unetched and etched fiber.



(a)



(b)

Fig. 4. Strain of the swollen hydrogel coating (a) and pressure acting on the fiber (b) as function of pH value for unetched and etched fiber.

The induced axial strain distribution along *z* direction at the center of the fiber core due to hydrogel expansion at pH of 3 for unetched and etched fiber are depicted in Fig. 5 and Fig. 6, respectively. It is shown that the strain is distributed uniformly along *z* direction. However, the distribution became non uniform at the region near the end of the unjacketed fiber. Non uniform region lengths of unetched and etched fiber are 0.14 mm and 0.04 mm. It is clear that the etched fiber provides shorter non uniform strain distribution area than the unetched fiber. This value is the same for all pH value. To ensure that the induced strain in the FBG is uniform so that the FBG spectral is not distorted, it is necessary to locate the FBG at the uniform region.

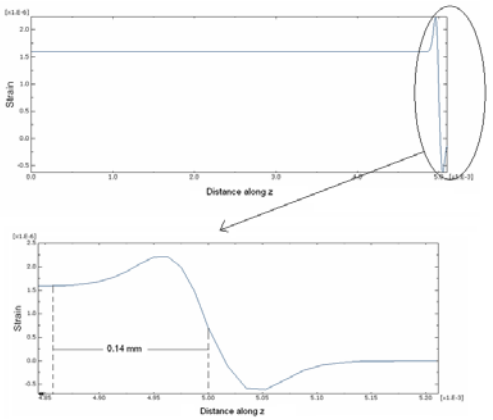


Fig. 5. Strain distribution along z direction of half model of the unetched fiber.

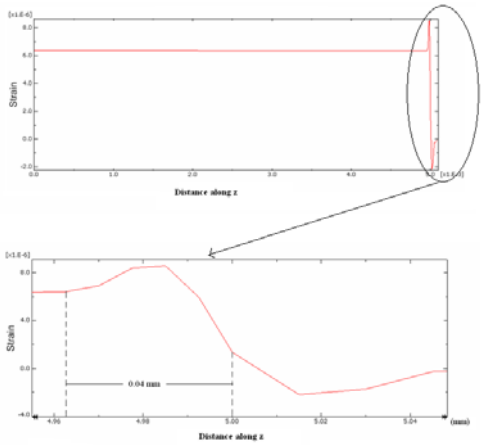
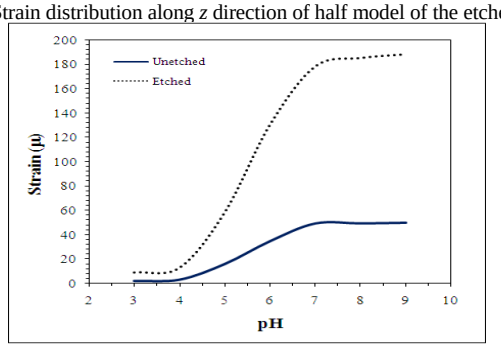
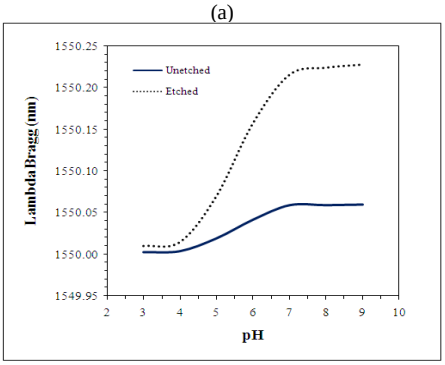


Fig. 6. Strain distribution along z direction of half model of the etched fiber



(a)



(b)

Fig. 7. Strain at the fiber core (a) and Bragg wavelength (b) as function of pH value of the unetched and etched fiber

B. Induced Strain in the Hydrogel Coated Fiber Bragg Grating

As shown in Fig. 7(a), by etching the fiber, strain at the fiber core is significantly increased for pH of above 4. Strain of more than 180 με was achieved at pH of 7. Meanwhile, for unetched fiber, the strain at pH of 7 is only 40 με. As consequence, the Bragg wavelength of the etched fiber is larger shifted than that of the unetched fiber as shown in Fig. 7(b) and thus improve the sensor sensitivity. The response is linear in the pH range of 4 to 7. The sensor sensitivity is 68.8 pm/pH unit and 18.9 pm/pH unit for etched and unetched fiber respectively.

V. Conclusion

As conclusions, modeling the hydrogel coated FBG pH sensor has been done by simulating the hydrogel swelling as response to the change of surrounding pH and its mechanical effect to the FBG. The results show that the sensor with etched fiber provides better performance in terms of strain distribution uniformity, induced strain value and sensor sensitivity.

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