# Optimization of Thermo-Optic Parameters for Temperature-Insensitive LPWG Refractometers

Dongseok Lee, Kyong Hon Kim, Seok Hyun Hwang, Min-Hee Lee, and El-Hang Lee

In this paper, we report numerically calculated results of testing a temperature-insensitive refractive sensor based on a planar-type long-period waveguide grating (LPWG). The LPWG consists of properly chosen polymer materials with an optimized thermo-optic coefficient for the core layer in a four-layer waveguide structure. The resonant wavelength shift below the spectral resolution of the conventional optical spectrum analyzer is obtained accurately over a temperature change of  $\pm 7.5^{\circ}\mathrm{C}$  even without any temperature control. The refractive index sensitivity of the proposed grating scheme is about 0.004 per resonant wavelength shift of 0.1 nm for an optimized thermo-optic coefficient.

Keywords: Bragg grating, long-period grating (LPG), planar waveguide, photonic integrated circuit, refractive index sensors.

## I. Introduction

Recently fiber-type temperature-insensitive long-period gratings (LPGs) have attracted significant interest due to their potential for application in biosensors and environmental pollution sensors [1]-[4]. The fiber-type LPGs have been investigated extensively by many research groups, and their superior characteristics with respect to coupling efficiency to transmission fiber and/or fiber devices and their low optical losses have been well recognized. However, they are not easy to integrate with other photonic devices and are not suitable for mass-production. On the other hand, planar-type long-period waveguide gratings (LPWGs) on polymer materials can be easily fabricated with an embossing technology, which is useful for low cost mass production. In addition, LPWGs are suitable for multi-functional photonic integration.

Various thermal characteristics of LPWGs can be obtained with different waveguide materials. The most popular materials used for the planar waveguides are silica (SiO<sub>2</sub>) and polymer [5]-[8]. The typical values of the refractive index n and thermo-optic coefficient dn/dT of the SiO<sub>2</sub> are 1.4463 and +1×10<sup>-5</sup>/°C at 1550 nm, respectively. However, those of the polymer materials can be optimized to be in ranges from 1.4 to 1.7 and from  $-0.5 \times 10^{-4}$  to  $-3.0 \times 10^{-4}$ /°C, respectively, by changing polymer material compositions and by illuminating ultraviolet (UV) radiation on polymers [9]-[13]. The variation of the refractive indices and thermooptic coefficients of sol-gel-derived inorganic-organic hybrid materials (hybrimers) composed of silica and organic material and of aromatic polyimides containing sulfur atoms have been demonstrated recently. Typically thermal expansion coefficient  $\alpha$  of polymer materials (approximately  $2.5 \times 10^{-4}$  /°C) is about 200 times larger than that of silica

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(approximately 1.4×10<sup>-6</sup>/°C).

Theoretical and numerical analyses of the temperature sensitivity of LPWGs have been reported in [6], [14], [15]. These studies in particular describe the temperature-dependent tuning characteristics of LPWGs with various waveguide parameters. In addition, the temperature-insensitive properties of fiber-type long-period gratings have been analyzed in [2], [3]. The numerical analysis of temperature-insensitive LPWG schemes was previously reported by us in [16], [17], though we have expanded on those ideas in the current study by performing a detailed and precise numerical analysis.

In this research we have performed a numerical analysis to design a temperature-insensitive LPWG-type refractometer especially with a planar-type waveguide by optimizing the thermo-optic parameter of the core layer in a four-layer waveguide. Numerical analysis of the effect of the material properties of the waveguides on the temperature dependency of the LPWGs will be described in the following sections and a temperature-insensitive scheme of LPWGs is proposed.

### II. Theory

The resonant wavelength for the phase matching condition between the propagating core and clad modes can be determined by

$$\lambda_0 = \left( n_{co\_eff} - n_{m, cl\_eff} \right) \Lambda , \qquad (1)$$

where  $n_{co\_eff}$  and  $n_{m, cl\_eff}$  are the effective refractive indices of the fundamental core mode and the m-th order clad mode at the resonant wavelength, and  $\Lambda$  is the period of the LPWG. The effective refractive indices can be calculated from the wave propagation functions in the core and clad layers by using the boundary conditions at the layer interfaces [18]. The effective refractive index of each layer is affected not only by the refractive indices of the core and clad layers but also by those of the substrate and upper clad layers. From the equations given in [18] we can derive combined and modified equations (2) and (3) for the effective refractive indices of the fundamental core and the m-th order clad modes, respectively.

$$\begin{split} & \sqrt{n_{co}^2 - n_{co\_eff}^2} \, \tan \left[ \sqrt{n_{co}^2 - n_{co\_eff}^2} \, k d_{co} - \tan^{-1} \left( \frac{n_{co\_eff}^2 - n_{sb}^2}{n_{co}^2 - n_{co\_eff}^2} \right) \right] \\ &= \sqrt{n_{co\_eff}^2 - n_{cl}^2} \, \coth \left[ \sqrt{n_{co\_eff}^2 - n_{cl}^2} \, k d_{cl} + \tanh^{-1} \left( \frac{n_{co\_eff}^2 - n_{cl}^2}{n_{co\_eff}^2 - n_{up}^2} \right) \right], \end{split}$$

$$\sqrt{n_{co}^{2} - n_{m,cl\_eff}^{2}} \times \tan \left[ \sqrt{n_{co}^{2} - n_{m,cl\_eff}^{2}} k d_{co} - \tan^{-1} \left( \frac{n_{m,cl\_eff}^{2} - n_{sb}^{2}}{n_{co}^{2} - n_{m,cl\_eff}^{2}} \right) - m_{1} \pi \right] 
+ \sqrt{n_{cl}^{2} - n_{m,cl\_eff}^{2}} \times \tan \left[ \sqrt{n_{cl}^{2} - n_{m,cl\_eff}^{2}} k d_{cl} - \tan^{-1} \left( \frac{n_{m,cl\_eff}^{2} - n_{up}^{2}}{n_{cl}^{2} - n_{m,cl\_eff}^{2}} \right) - m_{2} \pi \right] 
= 0,$$
(3)

where  $n_{co}$ ,  $n_{cl}$ ,  $n_{sb}$ , and  $n_{up}$  are the refractive indices of the core, clad, substrate, and upper clad waveguide materials as shown in Fig. 1. The thickness of the core and clad layers are denoted by  $d_{co}$  and  $d_{cl}$ . The wave propagation constant in a free space is denoted by k. Positive integers starting from zero are denoted by  $m_1$  and  $m_2$ . The clad mode number can be determined to be  $m = m_1 + m_2$  if both of the angle terms of the tangents in (3) are not greater than  $\pi/2$ ,  $m = m_1 + m_2 + 1$  if one of the angle terms is not greater than  $\pi/2$  and the other is greater than  $\pi/2$ , and  $m = m_1 + m_2 + 2$  if both of the angle terms are greater than  $\pi/2$  [18].

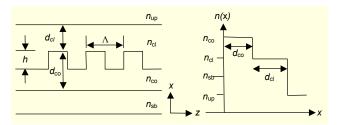


Fig. 1. Considered grating structure and refractive index profile of the LPWG.

In order to study the temperature-dependent properties of LPWGs, we take a derivative of the phase matching condition with respect to temperature as

$$\frac{d\lambda_0}{dT} = \left(\frac{dn_{co\_eff}}{dT} - \frac{dn_{m,cl\_eff}}{dT}\right)\Lambda + \left(n_{co\_eff} - n_{m,cl\_eff}\right)\frac{d\Lambda}{dT}.$$
 (4)

The resonant wavelength drift with temperature change is related to the thermo-optic coefficients of the core and clad modes and the thermal expansion of the grating period.

For a temperature change of  $\Delta T$ , the drifted resonant wavelength becomes

$$\lambda'_{0} = \lambda_{0} + \frac{d\lambda_{0}}{dT} \cdot \Delta T = \left(n'_{co\_eff} - n'_{m,cl\_eff}\right) \Lambda + \left(n_{co\_eff} - n_{m,cl\_eff}\right) \Delta \Lambda,$$
(5)

where  $n'_{co\_eff}$  and  $n'_{m, cl\_eff}$  are the effective indices of the core and clad modes after the temperature change  $\Delta T$ , and  $\Delta \Lambda$  is the

thermally expanded portion of the grating period for  $\Delta T$ . The thermal expansion effect can also change the thickness of the waveguide layers and affect the effective indices.

#### III. Numerical Analysis and Results

We have considered a four-layer waveguide structure which consists of a silica substrate, polymer core and clad layers, and the upper clad layer for materials or analytes to be tested. A silica wafer having a refractive index of 1.45 is considered as a substrate as well as a buffer due to its low cost and easy fabrication. The considered polymer materials of the core and clad layers have refractive indices of n equal to 1.53 and 1.48, respectively. The thermo-optic coefficients (dn/dT) of the SiO<sub>2</sub> substrate and the polymer clad layer are  $1.0 \times 10^{-5}$ /°C and  $-1.0 \times 10^{-4}$ /°C, respectively. The same thermal expansion coefficient  $\alpha = 2.5 \times 10^{-4}$ /°C is assumed for both the polymer core and clad layers. For the first simple calculation we have considered the upper clad to be an air space with a refractive index of 1.0. The considered thicknesses of the core and clad layers are 2.0  $\mu$ m and 6.0  $\mu$ m, respectively.

The validity of our numerical analysis was tested by comparison with the results reported in [19]. Figure 2 shows the resonant coupling wavelength of the fundamental core to clad modes of the LPWG with our waveguide structure described above as a function of the grating period. The chosen grating period is  $45.0~\mu m$  for the resonant wavelength of 1558.63~nm for the TE1 clad mode coupling when there is no temperature change. The length and corrugation depth of the LPWG are set to be 5.5~mm and 20~nm, respectively, which can be formed with a conventional imprinting technology.

The temperature-dependent resonant wavelength change of

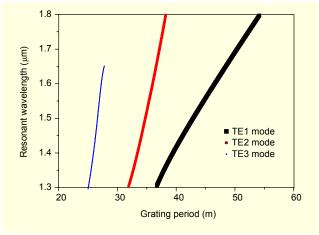


Fig. 2. Resonant coupling wavelength for the fundamental core to clad modes of the LPWG as a function of the grating period. ( $n_{core}=1.53,\,n_{clad}=1.48,\,n_{sub}=1.45,\,n_{upper}=1.0,$  thickness of core and clad = 2.0  $\mu$ m and 6.0  $\mu$ m)

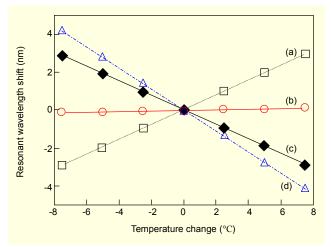


Fig. 3. Resonant wavelength shift of an LPWG due to (a) the thermal expansion ( $\alpha = 2.5 \times 10^{-4}/^{\circ}\text{C}$ ) of the grating period and the thermo-optic coefficients dn/dT of (b) -1.05×  $10^{-4}/^{\circ}\text{C}$ , (c) -1.19×10<sup>-4</sup>/°C, and (d) -1.25×10<sup>-4</sup>/°C.

LPWGs consists of the contributions from the effective index change and the thermal expansion of the grating as described in (5). The calculated result is shown in Fig. 3. The thermal expansion of the thickness of the waveguide layer affects the effective index values of the core and clad modes according to (2) and (3). Curve (a) corresponds to the effect due to the thermal expansion of the grating period only. Curves (b), (c), and (d) correspond to the thermo-optic effects due to the dn/dT values of the core layer of  $-1.05 \times 10^4$ /°C,  $-1.19 \times 10^4$ /°C, and  $-1.25 \times 10^4$ /°C, respectively.

Figure 4 shows their combined effect on the temperaturedependent resonant wavelength change. Each of the curves represents the summation of thermal expansion effect line (a) with each of the dn/dT effect lines from (b) to (d). In order to cancel out the positive wavelength shift due to the thermal expansion, a core material having a negative dn/dT value is needed. When the dn/dT of the core is  $-1.19 \times 10^{-4}$ °C which correspond to the curve (a)+(c), the total resonant wavelength change is below the spectral resolution of the conventional optical spectrum analyzer (OSA), which ranges between 0.05 nm and 0.1 nm, for the temperature change between -7.5°C and +7.5°C. The inset of Fig. 4 shows the detailed resonant wavelength variation over a range of temperatures for the curve. Further calculations to achieve a lowest level limitation of the temperature-dependent resonant wavelength change can be performed by optimizing the dn/dT value of the core material; however, our calculation indicates that a large number of digit accuracy below the decimal of the dn/dT value is required and is more difficult to obtain in the real world. In addition the resonant wavelength shift increases significantly temperature changes larger than ±7.5 °C.

Figure 5 shows the calculated resonant wavelength change

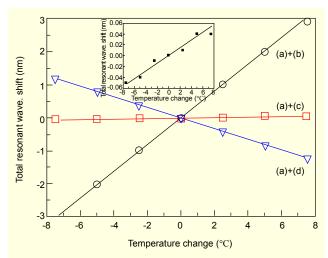


Fig. 4. Total resonant wavelength shift of an LPWG due to the combined effect of thermal expansion ( $\alpha = 2.5 \times 10^{-4}/^{\circ}\text{C}$ ) of the grating period and the thermo-optic coefficients specified in Fig. 2. The inset shows the details of the curve (a)+(c).

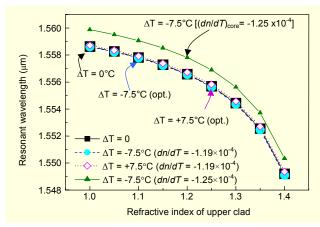


Fig. 5. Calculated resonant wavelength change vs. the refractive index of the upper clad for the optimized temperature-insensitive LPWG and un-optimized LPWG for  $\Delta T = 0$  and  $\pm 7.5^{\circ}$ C ( $dn/dT = -1.19 \times 10^{-4}/^{\circ}$ C and  $-1.25 \times 10^{-4}/^{\circ}$ C for optimized and un-optimized cases, respectively).

as a function of the refractive index of the upper clad for the optimized temperature-insensitive LPWG scheme compared to the un-optimized LPWG case. Our calculations consider the resonant wavelength corresponding to the coupling of the fundamental core mode to the TE1 clad mode. The refractive index of 1.0 indicates an air upper clad, and the corresponding resonant wavelength is 1558.63 nm with no temperature change (curve with black squares). As the upper clad index increases, the resonant wavelength shifts to a shorter wavelength. When the refractive index of the upper clad is 1.4, the resonant wavelength becomes 1549.20 nm. This mean that a refractive index change of 0.4 in the upper clad causes a resonant wavelength change of

about 10 nm. For the 0.1 nm spectral resolution of a conventional OSA, the refractive index sensitivity of the LPWG is 0.004. Further improvement of the refractive index sensitivity can be obtained by optimizing the thermo-optic coefficient up to a larger number of digit accuracy below a hundredth of  $10^{-4}$  and by using a high resolution spectrometer.

As illustrated in Fig. 5, the curve with small triangles corresponding to the un-optimized LPWG shows a significant wavelength shift even for a temperature change of 7.5°C. The wavelength shift due to temperature change is significantly large compared to the refractive index change of the upper clad. The dn/dT values used for the optimized and un-optimized LPWGs shown in Fig. 5 are  $-1.19 \times 10^4$ /°C and  $-1.25 \times 10^4$ /°C. respectively. The curves with circles and open diamonds correspond to the response curves of the optimized LPWG for  $\Delta T = -7.5$ °C and +7.5°C, respectively. Both of them overlap with the curve of  $\Delta T = 0^{\circ}$ C. The wavelength shift of the optimized LPWG is within ±0.06 nm for the temperature change of  $\Delta T = \pm 7.5$ °C. The wavelength shift is close to the resolution limit of the conventional OSA. This means that the optimized LPWG is suitable for a temperature-insensitive precision refractometer. Since the typical values of dn/dT for polymer materials are within a range between  $-1.0 \times 10^{4}$ /°C and  $-3.0 \times 10^{4}$ /°C, a polymer material with the optimized dn/dTvalue of -1.19×10<sup>-4</sup>/°C can be obtained through a composition change or UV illumination processes of polymer materials [10]-[12]. The hybrimers and aromatic polyimides containing sulfur atoms are potentially good candidate materials for such applications.

In an experimental demonstration of the proposed scheme, an optimization process may be required to achieve the specified refractive indices and the thermo-optic coefficients of the core and clad polymer materials. Particularly because of the large thermal expansion coefficient of polymer materials compared to that of the silica substrate, a significant thermal stress may appear in the polymer core near the substrate when the temperature change is large. The thermo-optic coefficient of polymer is negatively proportional to the thermal expansion coefficient, which means that the refractive index of polymer decreases with a volume expansion [11], [12]. Near the boundary of the polymer core and the silica substrate the decrease of the refractive index of the core polymer will be smaller than that of the other parts of the core polymer; therefore, the average refractive index change with temperature variation may be smaller than the calculated value. In addition, from the boundary between the core and the substrate in the upper clad direction, the refractive index of the core polymer may change gradually due to stress caused by a slight thermal expansion of the substrate at a large temperature change. This material and device stress as well as the gradual refractive

index variation may also cause a change in the beam propagation properties of the LPWG. The calculated results described in this paper give design guidelines for a temperature-insensitive refractive index sensor scheme based on a four-layer waveguide long-period grating, but some further optimization process on the polymer materials and device parameters may need to be demonstrated experimentally.

#### IV. Conclusion

We have designed a temperature-insensitive LPWG for potential application to precision refractometers with no external temperature controller by calculating the optimized dn/dT value for the core waveguide material to cancel out the thermal expansion effect. For a four-layer waveguide structure of silica substrate, polymer core and clad layers, and an upper clad layer of test material or analyte, the optimized LPWG provides a resonant wavelength shift below ±0.06 nm over a temperature change of ±7.5 °C and a refractive index sensitivity of 0.004 per resonant wavelength shift of 0.1 nm. The optimized dn/dT value for our proposed scheme turns out to be -1.19×10<sup>4</sup>/°C, which can be obtained by changing polymer material compositions and by illuminating UV radiation on polymers in the real world. The numerical calculation proposed in this paper was performed on only a few specific combinations of the substrate, core, clad, and upper clad materials, but the idea and methodology could be extended to other material and geometry configurations.

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