Simulation of a Long-Period Waveguide Grating on BCB/PMMA Polymers for Temperature Sensitivity

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Abstract—**Long-Period Gratings (LPG) has become attractive in recent years. It is relatively small in size and has the potential integration with various optoelectronic devices applied in the sensor applications. The ttemperature sensitivity of a Long-Period Waveguide Grating (LPWG) formed by Benzociclobutane BCB (core) and PolymethylmethacrylatePMMA (cladding) polymers is simulated, both polymers are used for microelectronic packaging and interconnect applications. We report the characterization and theoretical simulation of polymeric waveguide grating. Thus, a large variety of LPWG industrial devices with well-controlled characteristics can be obtained based on the phase-matching condition.**

Keywords—Simulation; Waveguide-Grating; Optical-polymers.

I. INTRODUCTION

A Long-Period Grating is capable of coupling light between the guided mode and the co-propagating cladding modes at specific wavelengths and hence results in a series of sharp rejection bands in the transmission spectrum [1]. Long-Period Fibers Gratings (LPFG) have been extensively studied and found numerous applications, such as filters, gain flatteners for erbium-doped fiber amplifiers, and sensors, etc. [2]. However, the geometry and material constraints of a fiber impose significant limitations on the functions that an LPFG can achieve, especially on the realization of active devices [3]. Moreover, optical fiber is not suitable for making compact low-cost devices and does not satisfy the demand for mass production and integration.

Therefore, to remove the constraints of the fiber and develop integrated-optical filters, Long-Period Waveguide Gratings (LPWGs) is formed in planar waveguides have been proposed. Although the light-coupling mechanisms in an LPWG and an LPFG are basically the same, LPWGs exhibit much richer optical characteristics because of the additional degrees of freedom available in the design and fabrications of optical waveguides, it is relatively small in size and has the potential integration with various optical components on the silicon substrate with optical polymers [4]. In addition, it can be used in producing useful optical devices applied in the sensor applications.

By another hand, optical signal processing is increasingly an important role in current measurement, instrumentation and communication technologies. Aspects such as the generation of signals, its modulation, measure and your address are already essential in all technological devices based on photonics, instead of electronics [5]. In this type of technology, optical fibers are widely used for driving light over long distances, but to the treatment necessary to that light, we need to have optical integrated circuits and electrooptical devices [4].

Finally, the fundamental element of the integrated optics are optical guides, which can be manufactured using a variety of techniques and materials, the optical guides integrated on glass by ion-exchange technique, and polymers through exchange photonic [6].

II. MATERIALS FOR LPWG

Optical waveguides using polymer material have been widely investigated because of simple processing steps and low production cost compared to silica-based materials. In addition, polymer materials can be molecularly engineered, allowing for fine-tuning of optical properties such as index of refraction and reduced absorption loss in spectral regions of interest, and lowered scattering losses. Most polymer materials have thermo-optic coefficients (about ten times larger than that of silica) and thus these devices can be temperature-tuned over a wider spectral range [7].

Moreover, they can be deposited directly onto any kinds of substrates; unlike other optical waveguide materials such as silica (SiO_2), lithium niobate ($LiNbO_3$), and III-V compound semiconductor materials. Such properties are important factors for the practical implementation of complex integrated optical waveguide devices. The key requirements imposed on the polymer materials are low propagation loss simple and flexible processing scheme, and good adhesion to the substrate. Propagation loss is a function of the launching wavelength and the quality of the optical waveguide. Simple and flexible processing scheme is achieved when the materials is sensitive to either ultraviolet (UV) exposure or electron-beam exposure, thus requiring no other subsequent process after development, therefore decreasing the duration of fabrication process.

Polymeric LPG have extensively demonstrated with different operating principles in various substrates. Electro-optical modulation up to 110 GHz has been reported, demonstrating that fast electronic response is possible in polymer materials as well as low operating voltage [8].

Thermo-optical devices have also been designed, simulated and fabricated, and these polymers exhibit low thermal conductivity and a large thermal index change. By another hand, the waveguides used at optical frequencies are typically a dielectric structure, e.g. BCB or PMMA, with high transmission and high index of refraction surrounded by a material with lower %T. The structure guides optical waves by total internal reflection. Integrated optics/photonics is becoming more pervasive as devices communicate with one another.

The refractive indices of the waveguide core, cladding and substrate are essential input parameters necessary to predict system behavior. Above a wavelength of 400nm, the transmission of BCB is greater than 95%. BCB is optically transparent at 632.8nm as well as at the telecommunications wavelengths of 1330 nm and 1550 nm [9-10]. BCB is therefore a suitable material for optical waveguides. A sensor/detector waveguide stripe interferometer can be formed from BCB with a reactive clad coating that changes optical properties upon interaction with the substance to be detected. Finally, the PMMA is a versatile polymeric material that is well suited for many imaging and non-imaging microelectronic applications. PMMA is most commonly used as a high resolution positive resist for direct write e-beam as well as x-ray and deep UV microlithographic processes. PMMA is also used as a protective coating for wafer thinning, as a bonding adhesive and as a sacrificial layer [11].

III. DEVELOPMENT

The LPWG presented in this work is designing and simulated using a software package for analysis and resolution by finite elements and partial derivative equations, where the electromagnetism module provided interfaces and formulations adapted to LPWG polymer substrates in different materials. Multiphysics simulation can be used to evaluate the performance of electromagnetic devices and accurately model relevant phenomena such as Joule heating, electric currents, and magnetic flux. In such a way that simulates the grating using the properties of the materials mentioned previously, multiphysics capability allows the coupling of simulations with heat transfer of structural mechanics, thermo-optical and electromagnetics, for the electromagnetic field inside the partially filled rectangular guide with isotropic or anisotropic dielectric material whether there is or not analytical solution uses the method of coupled modes.

The LPWG is produced by introduction of a periodic deformation along a waveguide, which may be in the form of modulation index of refraction or surface. The work was to simulate a dynamic LPWG using the effects thermo-optics of polymeric materials, where the grating is induced thermally, and simulation details are those of the BCB and PMMA, according to manufacturer information of the optical polymer with results from other authors [12].

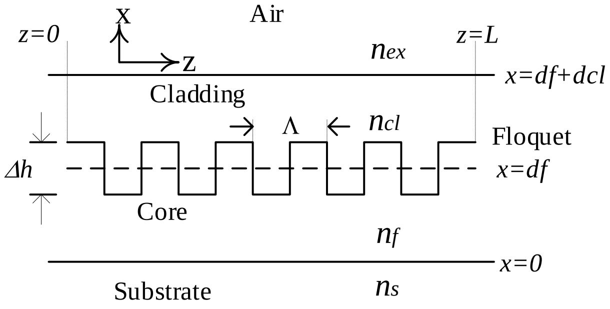

Fig. 1. Side-view of the LPWG and its refractive index profile

Fig. 1 shows the design of simulated grating, in which the corrugation is introduced into the surface of the core guide, the LPWG consists of a film (*substrate*) with an index of refractionn_s, a movie guide with $n_f$refractive index, and a movie like cover with an index of refractionn_{cl}, d_{cl} thickness and an external environment with a refractive index n_{ex} which extends infinitely, where: $n_f > n_{cl} > n_s, n_{ex}$. A schematic of polymer based corrugated LPWG along with its refractive index profile is shown in Fig. 2. The proposed LPWG structure consists of Si substrate, thick layer of PMMA having refractive index of 1535 with thermo-optic coefficient of -1.28x10^{-4}/°C [13] is used as under-cladding as well as over-cladding layers, whereas the BCB polymer having relatively higher index of 1561 with thermo-optic coefficient of -1.55x10^{-4} /°C is considered as the guiding layer[13].

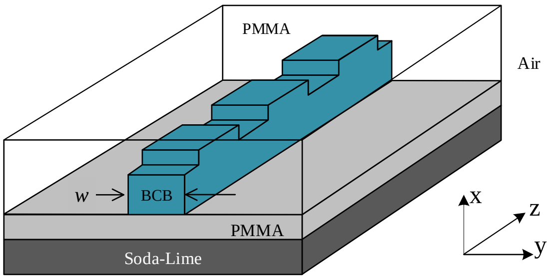

Fig. 2. PMMA/BCB polymer based LPWG structure

The resonant wavelenght of the LPWG can be determined by the use of phase-matching condition between forward propagating core and higher order cladding modes, which can be represented as:

$$\lambda_{0m} = \left(N^0{}_{eff} - N^m{}_{eff}\right)\Lambda(1)$$

Where $N^0{}_{eff}$ and $N^m{}_{eff}$ are the effective modal indices of fundamental core mode and higher order cladding modes respectively and Λ is a period of grating. The effective refractive indices can be calculated by using boundary condition at the interface of layers. In order to study the temperature-sensitivity of grating, we take a derivative of the phase matching condition with respect to temperature as:

$$\frac{d\lambda_0}{dT} = \Lambda \frac{d\left(N^0{}_{eff} - N^m{}_{eff}\right)}{dT} + \left(N^0{}_{eff} - N^m{}_{eff}\right)\frac{d\Lambda}{dT} \quad (2)$$

IV. MODELLING AND SIMULATION

The directional LPWG sensor using In-Plane Hybrid-Mode Waves was modelled and simulated to determine the electro-magnetic (EM) field distribution of the multilayer stack. In the same simulation environment, we have carried out thermal and optical investigations, without approximations on the refractive index distribution and consequently on the effective indices of the structures. Typically, the two analysis are developed in two different simulation environments, so requiring some methods to export the refractive index distribution. The systems based on planar optical waveguide with input grating sensor are of interest as they offer multiple tuning parameters for the LPWG design and their high sensitivity. In the present paper, an algorithm based on the Finite-ElementsMethod (FEM) is proposed for finding the chip response and optimizing the temperature sensitivity. The modelling and simulation were carried out in ComsolMultiphysics™[14] software using the radio-frequency (RF) moduleas described in the following:

V. THERMO-OPTICAL ANALISYS

The finite element method (FEM) has been used to solve both thermal and wave propagation problems (at the wavelength of 1550nm) in optical waveguides. The thermal problem is solved and the obtained temperature distribution is used to evaluate the refractive index change, caused by the thermo-optic effect, in the heated regions. This distribution of refractive index is then usedto solve the optical problem. The analysis of waveguides is carried out in the *x-y* plane, perpendicular to the lightpropagation direction *z*. The mathematical equation for heat transfer by conduction is the heat equation:

$$\rho C \frac{\partial T}{\partial t} + \nabla \cdot (-k\nabla T) = Q \qquad (3)$$

Where T is the temperature [K], *Q* is a heat source or heat sink [W/m^3], ρ is the density [kg/m^3], *C* is the heat capacity [J/kg·K] and *k* is the thermal conductivity [W/m·K] of the medium. These three thermo-physic properties determine the thermal diffusivity α [m^2/s], which gives information on how rapidly a temperature variation at the medium surface propagates through the medium itself. If the thermal conductivity is isotropic, the equation (3) becomes:

$$\rho C_p \frac{\partial T}{\partial t} - k\nabla^2 T = Q \qquad (4)$$

The partial differential equation that describes the light propagation is the wave equation:

$$\nabla^2 E_t + \nabla\left(\frac{\nabla n^2(x,y) \times E_t}{n^2(x,y)}\right) + \left(\frac{2\pi}{\lambda}\right)^2 n^2(x,y)E_t = \left(\frac{2\pi}{\lambda}\right)^2 n_{eff}\,E_t \, (5)$$

This derived from Maxwell's equations, where E_t is the transverse electric field, λ is the wavelength, n(*x*,*y*) is the refractive index distribution and $n_{eff}$is the effective index (eigenvalue of the wave equation). We have considered the absence of generation terms and a scalar conductivity forboth static and dynamic analysis. Table1 collects the thermo-physical values used in the simulations for the materials involved in the waveguide. In this work, constant values for the conductivity, density and heat capacity of the air are used. However, since air conductivity and density are almost linear in the temperature range 30-100°C.

Table 1. Thermal-physic constants to polymers

Material	k [W/m·K]	ρ [kg/m^3]	C [J/kg·K]	Source
PMMA (@23°C)	0.22	1188	1450	[14]
BCB (@25°C)	0.29	2190	1400	[14]
Air (@ 30°C)	0.026	1.167	1005	[14]

VI. GEOMETRY

A 10 element step-phase grating geometry was modelled in order to represent a symmetric waveguide of the multilayer stack. Illumination from the bottom boundary of the stack was describe as a port-boundary condition specifying the **H** field as light source (λ_0=1,550 nm) with in-plane polarization. The Wave Optics Module provides dedicated tools for electromagnetic wave propagation in linear optical media for accurate component simulation and optical design optimization. With this module, we can model high-frequency electro-magnetic wave simulations in either frequency or time-domain in optical structures. It also adds to your modeling of optical media by supporting inhomogeneous and fully anisotropic materials, and optical media with gains or losses. The periodic nature of the nature of the problem was described through the combination of Floquetboundary conditions in concert with the Port boundary condition, the Floquet boundary condition being critical to Finite Element Method (FEM) modelling as it indicates the main distinction between leaky waves along periodic structures and multilayer structures, through a single propagation factor, *kp* [14].

VII. BOUNDARY CONDITIONS

A planar dielectric step waveguide demonstrates the principles behind any kind of dielectric waveguide such as a ridge LPWG, and has a known analytic solution. This model solves for the effective index of a dielectric step waveguide as well as for the fields, and compares to analytic results.

Table 2 describes the applied boundary conditions to material refractive indices (RI) for the multilayer structure.

Table 2. Optical Properties-Multilayer Material

Material	Layer	RI (*n*)	Source
PMMA	Cladding	1.535	[13]
BCB	Core	1.561	[13]
Soda-Lime	Substrate	1.349	[13]
Air	Air	1	NA

Some additional Comsol and FEM modeling techniques were required namely:

1. The concept and application of assembly versus composite geometry;
2. Application of identity pairs at the boundaries of assemblies to establish source and destinations boundaries for an excitation source;
3. Application of the Floquet Boundary Conditions (FBC) as previously outlined;
4. Setting the port conditions for the identity pairs outlined in 2

The model geometry (Fig. 1) was extended to include additional layers (Air *n*=1) below the Soda-Lime substrate to serve as the source and destination for the excitation *p* polarized source. The left and right external boundaries were set up with Floquet conditions and the upper and lower external boundaries together with the identity pair boundary were set as Perfect Magnetic Conductors (PMC)[15], the internal boundaries all remained as continuity.

VIII. SIMULATION RESULTS

The way finite element analysis obtains the temperatures, stresses, flows, or other desired unknown parameters in the finite element model are by minimizing an energy functional. An energy functional consists of all the energies associated with the particular finite element model. Based on the law of conservation of energy, the finite element energy functional must equal zero.

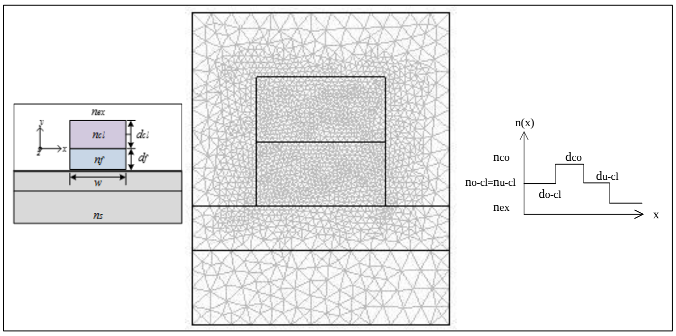

Fig. 3 FEM analysis in the longitudinal section.

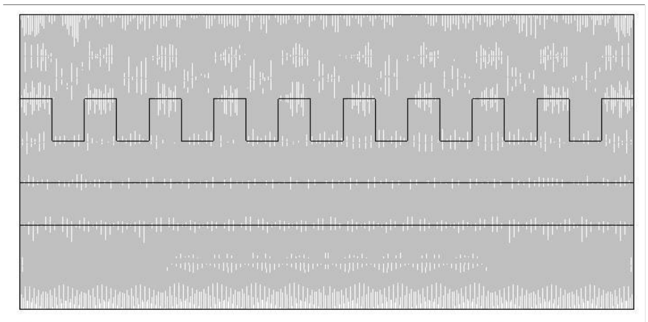

Fig. 4. Final model geometry and boundary conditions with FEM mesh.

The resulting plots (Figs. 3 and 4) show the mesh and final model geometry and boundary conditions, mesh generation is the practice of generating a polygonal or polyhedral mesh that approximates a geometric domain. The temperature gradient is a physical quantity that describes in which direction and at what rate the temperature changes the most rapidly around to the cladding, core, substrate and air (Fig 5).

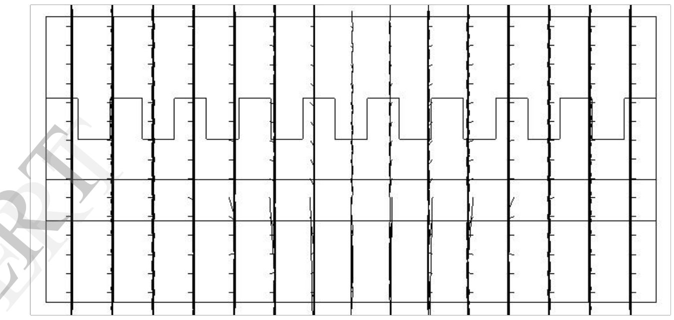

Fig. 5. The temperature gradient vectors.

The refractive index arises from the molecular polarizability a according to the Lorentz–Lorenz formula.Differentiating Eq. 2 with respect to temperature gives the temperaturedependence of refractive index or thermo-optic coefficient (Fig 6). Decreasing density with temperature (positivethermal expansion coefficient, the usual case) decreasesrefractive index, whereas a positive change in polarizabilitywith temperature (the usual case) increasesrefractive index [16].

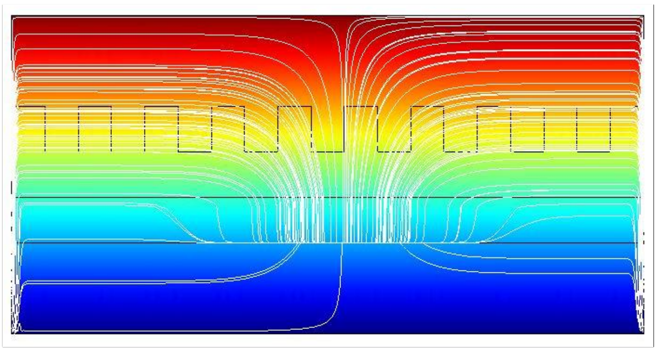

Fig.6. Thermo-optical effect in polymeric sections and thermal flux lines.

IX. RESULTS AND DISCUSSIONS

The phase matching graph are plotted for tree TE modes (Fig. 7) governed by Eq. 1. Attention has been focused to achieve resonance wavelength for the LPWG in the infrared spectra.

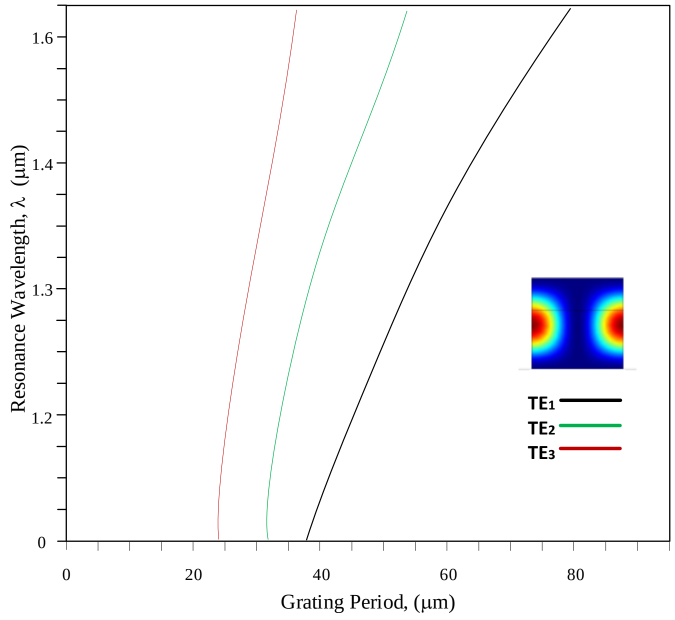

Fig. 7:Phase matching plot for LPWG withdco=4.0□m, du-cl=do-cl=6.8□m.

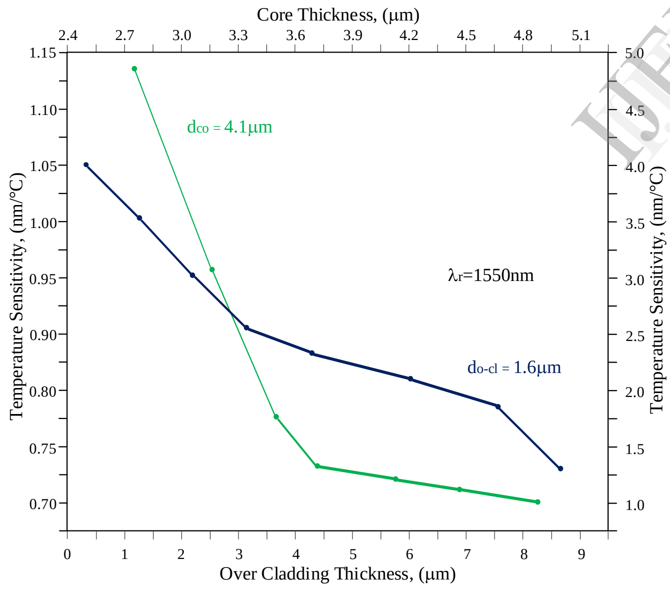

Fig. 8. Variation of temperature sensitivity of LPWG (having fixed under-cladding thickness of 6.8□m with core and over-cladding thickness for a resonance wavelength of 1550nm.

Temperature sensitivity of LPWG is shown in Fig. 8. The effect of varying core and cladding thickness is described for itsresonance wavelength in infrared region (1550 nm) where the sensitivity value decreases with theincrease of core and over-cladding thickness. Effect of varying core thickness is found to be dominating in this region. A similar type of result is observed in also earlier reports [4,9,11,17]. This describes that a range of temperature sensitivity of LPWG is achievable by varying core and over-cladding thickness. However, LPWG has somelimitation in terms of selecting core and cladding thickness, as this plays an important role in scattering/ radiation losses and number of propagating modes. Therefore, the LPWG parameters can be chosen as per the requirement for any specific application.

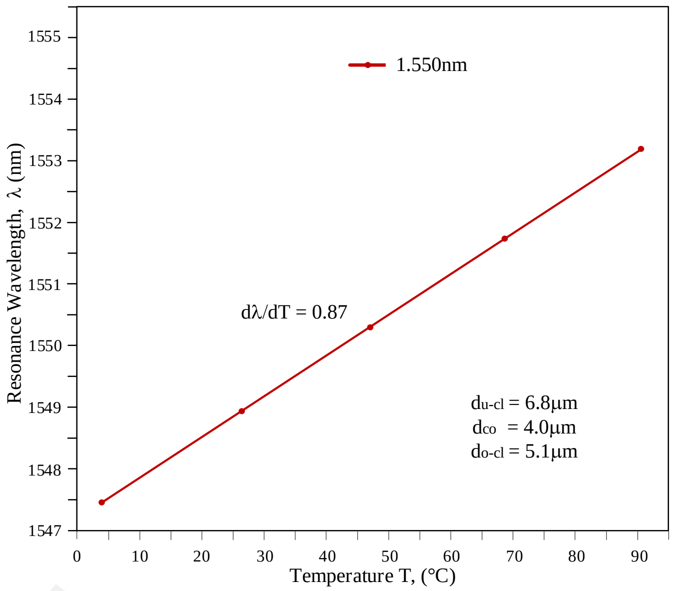

Fig. 9. Variation of Resonance wavelength with temperature for resonance wavelength in infrared region (1550nm).

In a typical case, the LPWG has been optimized for core thickness of 4.0mm and over-cladding thickness of 5.1mm with grating period of 70µm. The temperature sensitivity values are found to be 0.87nm/°C for LPWG resonance wavelengths of 1550nm. The Fig. 9 describe the resonance wavelength shift for the LPWG with temperature at this wavelength region.

X. CONCLUSIONS

A theoretical investigation and simulation of the thermo-optic effect in a LPWG has been carried out, by means of the finite element method. Finite Element Analysis is a numerical method, which provides solutions to problems that would otherwise be difficult to obtain. The central key of this analysis is the calculation and use of the effective thermo-optic coefficient that is a property of the whole waveguide structure, taking into account all geometrical and material parameters, and the multiphysics integration of both optical and thermal investigations. This integration is fundamental to remove the approximation on the refractive index distribution.

Temperature sensitivity of PMMA/BCB polymers based LPWG is analyzed theoretically. Grating period is chosen in order to get resonance wavelength, in infrared region. Effect of core, cladding and over-cladding thickness on temperature sensitivity is observed in resonating wavelength.

Temperature sensitivity for an optimized LPWG structure is found to be 0.87nm/°C for resonant wavelength of 1550nm.

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