

Study of a low-cost trimodal polymer waveguide for interferometric optical biosensors

Jhonattan C. Ramirez,¹ Laura M. Lechuga,^{1,2} Lucas H. Gabrielli,¹
and Hugo E. Hernandez-Figueroa^{1,*}

¹*School of Electrical and Computer Engineering (FEEC), University of Campinas (UNICAMP), 13083-970 Campinas, SP, Brazil*

²*Nanobiosensors and Bioanalytical Group, Institut Català de Nanociència i Nanotecnologia (ICN2), CSIC and CIBER-BBN, 08193 Bellaterra (Barcelona), Spain*

**hugo@decom.fee.unicamp.br*

Abstract: A novel evanescent wave biosensor based on modal interaction between the fundamental mode and the second order mode is proposed and numerically demonstrated. By taking advantage of their symmetries, it is possible to design a device where only the fundamental and the second order modes can propagate, without excitation of the first order mode. With this selection of modes it is possible to achieve a high sensitivity behavior in the biosensor configuration, due to the strong interaction between the evanescent field and the outer surface as compared to previous evanescent wave-based biosensor designs.

© 2015 Optical Society of America

OCIS codes: (130.6010) Sensors; (130.0130) Integrated optics; (230.7370) Waveguides; (130.5460) Polymer waveguides.

References and links

1. M. C. Estevez, M. Alvarez, and L. M. Lechuga, "Integrated optical devices for lab-on-a-chip biosensing applications," *Laser Photonics Rev.* **6**(4), 463–487 (2012).
2. F. Prieto, B. Sepulveda, A. Calle, A. Llobera, C. Domínguez, A. Abad, A. Montoya, and L. M. Lechuga, "An integrated optical interferometric nanodevice based on silicon technology for biosensor applications," *J. Opt. A: Pure Appl. Opt.* **14**(8), 907–912 (2003).
3. K. E. Zinoviev, A. González-guerrero, C. Domínguez, and L. M. Lechuga, "Integrated bimodal waveguide interferometric biosensor for label-free analysis," *J. Lightwave Technol.* **29**(13), 1926–1930 (2011).
4. D. Duval, A. González-Guerrero, S. Dante, J. Osmond, R. Monge, L. J. Fernández, K. E. Zinoviev, C. Domínguez, and L. M. Lechuga, "Nanophotonic lab-on-a-chip platforms including novel bimodal interferometers, microfluidics and grating couplers," *Lab Chip* **12**(11), 1987–1994 (2012).
5. R. Bruck and R. Hainberger, "Sensitivity and design of grating-assisted bimodal interferometers for integrated optical biosensing," *Opt. Express* **22**(26), 32344–32352 (2014).
6. M. Hiltunen, J. Hiltunen, P. Stenberg, J. Petäjä, E. Heinonen, P. Vahimaa, and P. Karioja, "Polymeric slot waveguide at visible wavelength," *Opt. Lett.* **37**(21), 4449–4451 (2012).
7. M. Wang, J. Hiltunen, C. Liedert, S. Pearce, M. Charlton, L. Hakalahti, P. Karioja, and R. Myllylä, "Highly sensitive biosensor based on UV-imprinted layered polymeric-inorganic composite waveguides," *Opt. Express* **20**(18), 20309–20317 (2012).
8. M. Mrozowski, *Guided Electromagnetic Waves: Properties and Analysis* (Research Studies, 1997).
9. J. D. Joannopoulos, S. G. Johnson, J. N. Winn, and R. D. Meade, *Photonic Crystals: Molding the Flow of Light* (Princeton, 2008).
10. W. P. Huang and J. Mu, "Complex coupled-mode theory for optical waveguides," *Opt. Express* **17**(21), 19134–19152 (2009).
11. J. Leuthold, C. Koos, and W. Freude, "Nonlinear silicon photonics," *Nat. Photonics* **4**(8), 535–544 (2010).

1. Introduction

Nowadays most clinical, chemical and biological diagnostics are performed in laboratories with complex equipment that produce accurate results. They require long processing periods and dedicated, highly trained staff, resulting in high costs and delayed results. This situation can be improved using integrated optical sensors, which can be incorporated in portable point-of-care platforms. Most of these integrated optical sensors make use of the evanescent wave working principle. Different evanescent wave integrated sensors have been developed to date, such as interferometers, ring resonators, grating couplers, photonic crystal and silicon wire based sensors. Among all of them, interferometric devices have shown the highest sensitivity: around 1×10^{-7} or 1×10^{-8} RIU, and have become one of the preferred options for achieving truly point-of-care tools with label-free and fast detection [1–3].

In 2011 a new type of interferometric biosensor based on the modal interaction between the fundamental mode and the first order mode of the light—the so called bimodal waveguide interferometer (BiMW) [3–5]—was proposed. This new type of interferometric biosensor, fabricated in silicon-related technologies and operating at the visible range, showed bulk sensitivities around 1×10^{-7} RIU ensuring a compact device of high sensitivity, which was very beneficial for the sake of integration in lab-on-chip platforms [4]. Using the concept of the BiMW sensor as starting point, in this work we propose and numerically demonstrate a new and highly sensitive trimodal interferometric waveguide biosensor to be implemented in polymer technology. The choice of polymer material addresses the need of having a cheap mass-production process to manufacture the devices in resource-constrained settings, due to the simpler fabrication process (etchless fabrication) and larger tolerances for the waveguide dimensions [6, 7].

The advantages of the proposed trimodal device for sensing applications are two-fold: first, the second order mode shows a greater depth of evanescent tail than the first one, resulting in higher sensitivity; second, because we employ a channel waveguide instead of a rib one, the single mode to multimode transition will occur in width instead of thickness, increasing the region of interaction between the evanescent field of the waveguide and the sensing area.

2. Theoretical calculation

We have considered an interferometric device based on the interaction between the fundamental and first or second order TE modes of a channel waveguide. Our structure is divided in three sections, the central one is the interferometric section, which supports either two or three TE modes, while both extremities are single-mode and constitute the input and output waveguides of the device, respectively. All sections have the same core thickness, such that the multi-mode characteristic at the center is due to a larger lateral dimension of the waveguide.

This geometry, illustrated in Fig. 1, leads to simpler fabrication processes in comparison to previous proposals. Having the high order modes distributed laterally also allows greater interaction between the waveguide and the substances to be analyzed at the sensing surface area. From Fig. 1 we can observe two important design regions in the device: the transition from single mode to multimode waveguide operation and its opposite, which are the entrance and exit coupling regions and are analyzed in the next section.

It is very important to remark that, in principle, the TM polarization should be more sensitive for both the bimodal and the trimodal waveguide, since its evanescent tail extends longer outside of the waveguide core (due to the boundary conditions for the electric field in the normal direction), but other factors contribute as well to the final sensitivity, such as the cut-off

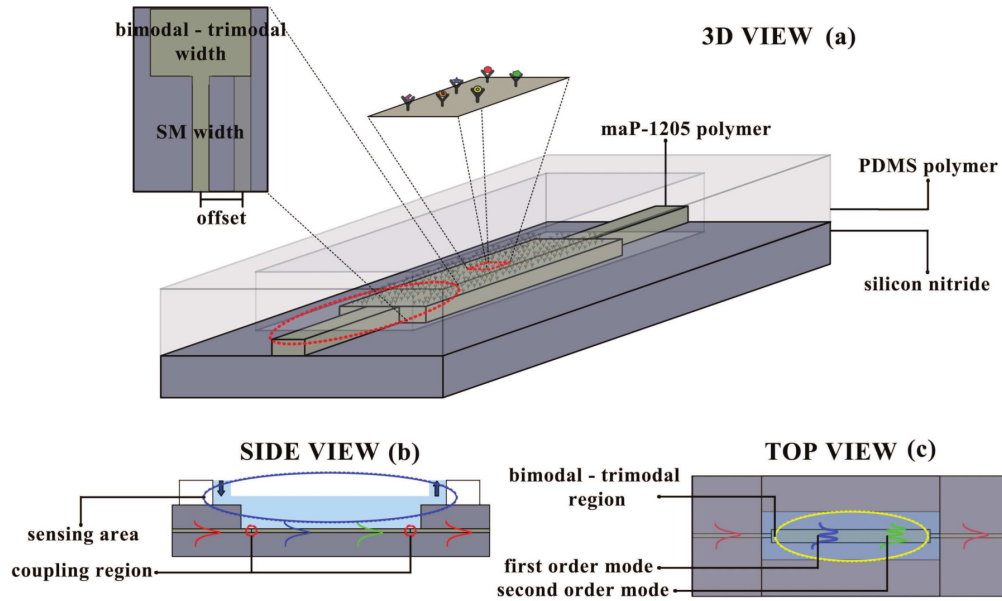


Fig. 1. Multimode interferometric biosensor scheme. (a) Three-dimensional view of the multimode interferometer and its sensing area. (b) Side view of the waveguide coupling region. (c) Top view showing the region where high-order modes are excited and interact with the bioactive region.

frequencies, the waveguide dimensions, and the coupling efficiency. The interplay between all of those parameters must be taken into account during design. The waveguide dimensions are directly related to the cut-off frequencies and they are limited by fabrication conditions. In our case, the reduced dimensions required for the single mode access waveguides led to a higher sensitivity for the TE mode.

2.1. Mode orthogonality

The coupling coefficient determines the percentage of light coupled from the fundamental mode in the single mode waveguide to each high-order mode propagating in the multimode waveguide. At the output of our interferometric device we can observe the same effect, but in this case the coupling coefficient is the percentage contribution of each mode of the multimode waveguide to the formation of a single mode at the output.

We analyze the excitation of the multimode waveguide using conventional field overlap integrals. Because both single-mode waveguides (input and output) have the same shapes and offsets with respect to the multimode waveguide, the analysis performed on one junction is valid for the other one as well.

We start recollecting the unconjugated orthogonality relation between guided modes m and n with propagation constants β_m and β_n respectively [8–10]:

$$(\beta_m^2 - \beta_n^2) \iint_S \vec{e}_n \times \vec{h}_m \cdot d\hat{s} = 0 \quad (1)$$

where S is the waveguide cross-section.

For the input waveguide, we calculate and optimize the coupling between the single input mode ($\vec{E}, \vec{H}$) and the modes from the multimode waveguide that we want to interfere ($\vec{e}_n, \vec{h}_n$):

$$\vec{E} = \sum_{n=0}^N c_n \vec{e}_n + \text{radiation modes} \quad (2)$$

Using the orthogonality relation Eq. (1), the butt-coupling coefficients c_n can be calculated by:

$$c_n = \frac{\iint_S \vec{E} \times \vec{h}_n \cdot d\hat{s}}{\iint_S \vec{e}_n \times \vec{h}_n \cdot d\hat{s}} \quad (3)$$

We calculate the excitation of the output waveguide resulting from the mode interference in the sensing region considering the different propagation constants of each mode and the total length L of the interferometer:

$$\sum_{n=0}^N c_n \vec{e}_n e^{-j\beta_n L} = d\vec{E} + \text{radiation modes} \quad (4)$$

$$d = \sum_{n=0}^N c_n e^{-j\beta_n L} \frac{\iint_S \vec{e}_n \times \vec{H} \cdot d\hat{s}}{\iint_S \vec{E} \times \vec{H} \cdot d\hat{s}} \quad (5)$$

If the modes are properly normalized, $|d|^2$ is the power in the output waveguide.

2.2. Bulk sensitivity

The bulk (or homogeneous) sensitivity relates to the effective mode variation between the interfered modes with respect to a bulk refractive index change at the sensing area of the device (the outer cladding of our structure). The intrinsic bulk sensitivity can be calculated by:

$$\eta_{\text{bulk}} = \frac{\partial(\Delta n_{\text{eff}})}{\partial n_{\text{clad}}} \quad (6)$$

$$\Delta n_{\text{eff}} = n_{\text{eff},i} - n_{\text{eff},0} \quad (7)$$

where n_{clad} is the cover refractive index and Δn_{eff} is the difference between the refractive indexes of the high order mode in question and the fundamental. The index i represents the high-order mode that we want to interfere; in our case it takes the values 1 (for a bimodal waveguide) or 2 (for a trimodal waveguide).

The sensitivity of the device due to the variation of the effective index difference directly affects the phase difference between the two modes at the end of the interferometric region, which determines the power coupled to the single mode waveguide at the output:

$$\Delta\phi = \frac{2\pi\Delta n_{\text{eff}}L}{\lambda} \quad (8)$$

$$S_{\text{bulk}} = \frac{\partial(\Delta\phi)}{\partial n_{\text{clad}}} = \frac{2\pi L}{\lambda} \eta_{\text{bulk}} \quad (9)$$

where λ is the vacuum wavelength at the operating frequency, and S_{bulk} is the bulk sensitivity of our device.

2.3. Surface sensitivity

When a bimolecular interaction takes place on top of the sensing area, the mode properties are affected by a refractive index variation at their evanescent tail due to a biorecognition event. In

order to use the interferometric device as a biosensor, it is necessary to previously functionalize the sensor surface with affinity bioreceptors that will capture the specific analyte [1]. In that manner, the surface sensitivity is defined with respect to the thickness of a bioreceptor layer. Owing to the evanescent profile of the guided modes in the sensing area of the device, this sensitivity should reach a maximum value asymptotically as the biolayer thickness increases.

The intrinsic surface sensitivity is defined as:

$$\eta_{\text{surf}} = \frac{\partial(\Delta n_{\text{eff}})}{\partial b} \quad (10)$$

where b is the thickness of the biolayer.

Following Eq. (8), the surface sensitivity is defined as:

$$S_{\text{surf}} = \frac{\partial(\Delta\phi)}{\partial b} = \frac{2\pi L}{\lambda} \eta_{\text{surf}} \quad (11)$$

For high sensitivity, it is necessary to have a high penetration depth δ_i , which is inversely proportional to the evanescent tail decay α_i , defined as:

$$\alpha_i = \frac{1}{\delta_i} = \frac{2\pi}{\lambda} \sqrt{n_{\text{eff},i}^2 - n_{\text{clad}}^2} \quad (12)$$

A large penetration depth means that increases the evanescent field penetrates more deeply into the cladding. To ensure a high sensitivity it is necessary to minimize the penetration depth of the fundamental mode while maximizing the penetration of the high order mode. This way the high order mode feels the variation in the sensing area more strongly than the fundamental, thereby creating the interferometric response.

3. Numerical results

Based on modal analysis it is well known that the higher the modal order, the larger the penetration depth of the evanescent wave in channel waveguides. To verify it numerically, we compare the behaviour of the trimodal interferometer with a bimodal device with the same structural characteristics (materials and overall length of the device), and with the highly sensitive BiMW interferometer based on silicon technology [3]. We studied the bulk and surface sensitivities for the three structures and the coupling efficiency between the single-mode and the higher order modes.

The coupling efficiency will determine the fringe visibility at the output signal of the interferometric device, i.e., the more balanced the excitation of the interfering modes, the higher the power swing due to their interference at the output. Therefore, the dimensions of each waveguide and their coupling coefficients will directly determine the sensitivity of the device and its performance as a biosensor.

For the calculations, we have used a channel waveguide operating at 633 nm composed of an ma-P 1205 photoresist (micro resist tech) core over a SiO₂ substrate. The refractive indexes of core and substrate at the operating wavelength are, respectively, 1.644 and 1.457 [11]. The cladding over the sensing area is considered water (refractive index of 1.33). It is important to keep the device input and output covered to avoid impurities and extra noise affecting the interferometric signal. A PDMS cladding with refractive index 1.42 has been chosen in order to prevent these undesired phenomena and guarantee a high index contrast.

The dimensions of the waveguides were chosen taking into account fabrication conditions. The thickness and width of the waveguide core are at least 100 nm and 400 nm, respectively, limited by the material viscosity and the lithography resolution. We varied the thickness of the guiding layer between 400 nm and 1.0 μm and for each thickness; we calculated the modal

curves and the mode coupling varying the width of the waveguide core. We display in Fig. 2(a) the modal curves for the PDMS-covered region (single mode operation), and in Fig. 2(b) the modal curves on the multimode sensing area, covered with water. Knowing that our fabrication error is close to 20 nm, we are guaranteed to operate with the desired number of modes in each region, as shown by Fig. 2(c). The closest to the cut-off width of the high order mode, the more sensitive the device should become, due to the longer evanescent tail.

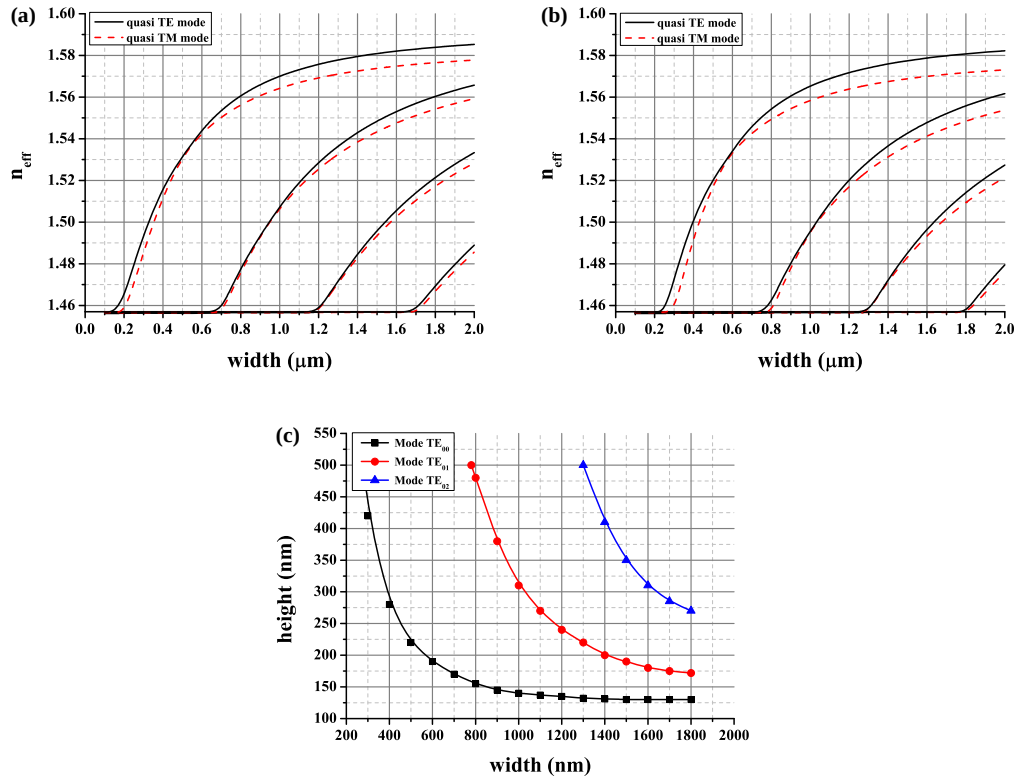


Fig. 2. Modal curves for a waveguide of 500 nm thickness with cladding of (a) PDMS polymer, (b) water. (c) Cut-off relation between width and height in the polymer waveguide at the sensing area.

The width will also affect the coupling coefficients between the single mode and multimode regions, which are directly proportional to the interferometric fringe visibility and impact in the final sensitivity when we take into account the photodetector and its noise floor. In Fig. 3 we show the coupling coefficients and sensitivity of the bimodal and trimodal devices, respectively.

At this stage we chose the dimensions that give the highest sensitivity, since both cases show coupling coefficients above 10 %, which seems to be acceptable in terms of detectable signal [3].

It must be pointed out that in the case of the bimodal device we have an extra design parameter: the offset between single mode and multimode regions. This offset can be used to adjust the coupling coefficients as close as possible to 50% (for maximal fringe visibility). In the case of the trimodal device, the waveguides must be aligned (zero offset) so that the first order mode is not excited (because of modal symmetry). Thus the only parameter we can freely use to equalize the coupling is the width of the single-mode region. According to our analysis, the optimal dimensions for the bimodal and trimodal devices are summarized in table 1.

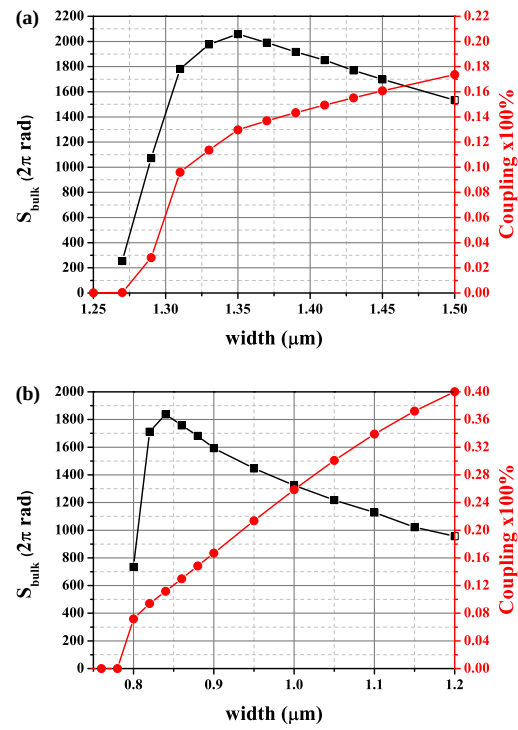


Fig. 3. Variation of the coupling coefficient and sensitivity as function of the multimode waveguide width. (a) Trimodal case with single-mode waveguide width 610 nm. (b) Bi-modal case with single-mode waveguide width 610 nm.

Table 1. Selected dimensions for each proposed device.

Dimensions (nm)	Polymer BiMW	Polymer TriMW	Si ₃ N ₄ BiMW	Si ₃ N ₄ TriMW
Core thickness	500	500	150	150
Single-mode width	610	610	400	400
Multimode width	820	1350	680	1000
Offset	110	0	140	0

We have studied both the bulk and the surface sensitivities of the device, comparing it with the one presented in [3], considering a 15 mm sensing length for all cases. Results are shown in Fig. 4. We can clearly observe that for both analyses the trimodal device outperforms the bimodal one. This can be expected due to the longer evanescent tail of the higher order modes and their stronger interaction with the analyte. For the calculation of the surface sensitivity the biolayer was modelled with a refractive index of 1.45 (standard value for a protein monolayer). It is important to note the difference between the curves in Fig. 4(b): particularly around 10 nm thickness the trimodal polymer device has almost twice the sensitivity of the bimodal polymer design. As expected, both curves reach a similar peak and decay once most of the energy of the evanescent tail is inside the biolayer. The numerical studies were performed in Comsol Multiphysics.

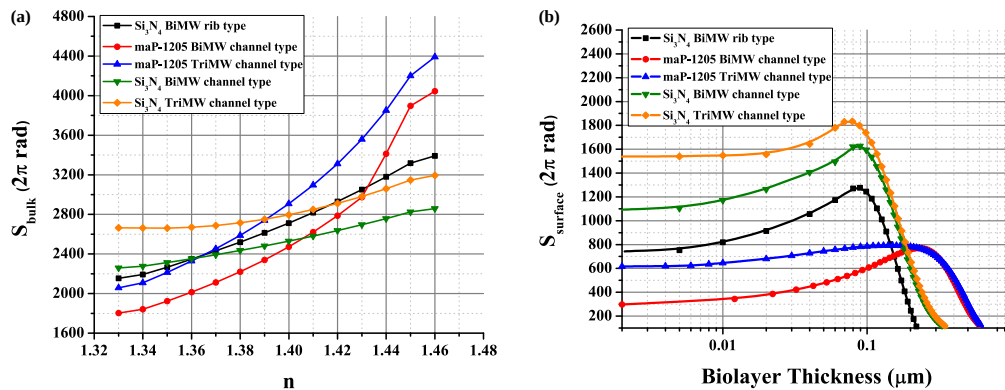


Fig. 4. Comparison between the proposed and current state-of-the-art devices for the (a) bulk and (b) surface sensitivities.

Analyzing Fig. 4(a) when the refractive index in the cover is 1.33, we can observe that the bimodal and trimodal polymer channel waveguides have, respectively, 18% and 7% less sensitivity than the Si_3N_4 bimodal sensor presented in [3], i.e., the rib type waveguide. Nonetheless, with a Si_3N_4 channel waveguide we obtain 4% and 25% more sensitivity for the bimodal and trimodal cases, respectively. In terms of bulk sensitivity the contrast remains lower than for a Si_3N_4 structure, but the advantage of using a higher order mode leads to comparable or better results depending on the refractive index of the bulk matrix. We can observe that by increasing the cover refractive index, the sensitivity increases. This is due to the fact that when the index contrast of the core to the cladding is lower, a higher fraction of the mode energy propagates in the cladding. This effect is more visible for polymer waveguides, as presented by Fig. 4(a), since they have a lower index contrast by design.

When evaluating the performance of our biosensor with a 10 nm biolayer as in Fig. 4(b), the difference between the bimodal and the trimodal waveguide sensitivities becomes remarkable. We obtained surface sensitivities for the TriMW with polymer and Si_3N_4 cores respectively 54% and 74% greater than for BiMW.

Although the Si_3N_4 waveguide is, as expected, more sensitive, an important issue comes up: the nanometric device dimensions make it less attractive as a commercial product. Since they can only be fabricated with state-of-the-art lithography, they turn out to be economically unfeasible. Nevertheless, the use of a lower refractive index material allows us to find a compromise between the fabrication costs and a good sensitivity biosensor design.

Finally, we show the interferometric plot of the device output calculated using Eq. (5) in Fig. 5. We show the coupling coefficients and their variation with the offset in position between

each section of the device in Fig. 5(a). If, for example, we consider a misalignment of 10 nm, it results in a variation of at most 0.21% in the coupling coefficient of the trimodal waveguide and 10% for the bimodal case. These variations lead, in turn, to changes in the interferometric fringes of the devices and, ultimately to a possible loss of sensitivity. A stronger dependence with the offset error is observed for the BiMW, because the bimodal offset is on a slope, whereas the TriMW offset is on stable region of zero offset.

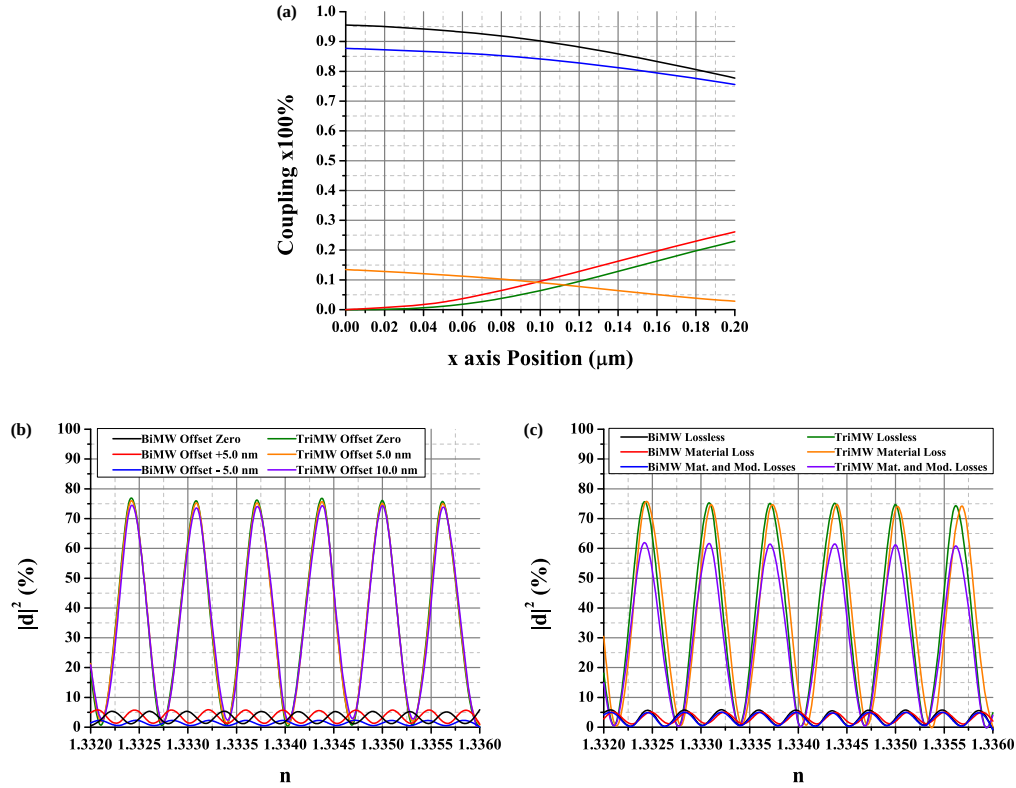


Fig. 5. Effects of misalignment and losses in the biosensors. (a) Effects of offset error in the coupling coefficients. (b) Trimodal transfer function $|d|^2$ for TE polarization under offset error. (c) Effects of losses in the transfer function for TE polarization.

In Fig. 5(b) we demonstrate that the effects of misalignment in the transmission function are minimal. This plot shows the interferometric fringes of the bimodal and trimodal designs when the cladding index varies slightly and under the effect of the offset error. We can see a 3% loss in fringe visibility, which means that the proposed device presents good tolerance to fabrication imperfections.

The material proposed for this work has an extinction coefficient below 2×10^{-2} [12]. On this basis and in order to test the effect of losses on our device, in Fig. 5(c) we illustrate a transfer function showing three different scenarios: the first one lossless, the second with only the influence of the material losses and the third one considering both material and an estimation of scattering of losses. Scattering losses were estimated at 1 dB/cm for the fundamental mode, and, knowing that higher order modes usually present higher losses, 1.25 dB/cm and 1.74 dB/cm for the first and second order modes, respectively (i.e., 20% and 67% higher than the fundamental). We can see that material losses are minimal and do not affect any of the devices. Scattering losses have a more significant impact, it decreases the fringe visibility for the TriMW in about

20%. Nevertheless, these levels are still far beyond the results for the BiMW and should not represent a limitation for the practical realization of the biosensor.

According to [3, 4], the limit of Detection (LOD) of a device is related to the visibility, noise floor, and sensitivity. Using the interferometric output signal in Fig. 5 and assuming an RMS noise of 0.04 [3], we predict that the LOD of our polymer device in bulk will be around 7.34×10^{-7} RIU. This sensitivity is very similar to that obtained in [3–5].

These results clearly demonstrate that the use of a higher order mode in the design of a polymer interferometric device leads to an overall sensitivity improvement, as should be expected from the waveguide dispersion curves. Nevertheless, a compromise exists between a cheaper device fabricated with polymer material of lower index versus the more sensitive device fabricated in Si₃N₄.

4. Conclusion

We have proposed and numerically demonstrated that a trimodal waveguide polymer interferometric sensor has the potential to show higher sensitivity than a bimodal waveguide with similar characteristics. This is because the penetration depth of the evanescent tail of the second order mode is fundamentally greater than that of the first when compared to the fundamental mode, thereby allowing greater interaction between the light traveling inside the waveguide and any physical, chemical, or biological phenomena that may be present on the surface of the structure.

The precise coupling between the single-mode and the multimode waveguides is of great importance, because it will define the visibility of the interferometer in terms of optical power at the output. The wide multimode waveguide enables easy implementation of a trimodal biosensor with suppression of the first order mode due to their different symmetries.

Polymeric waveguides have been proposed to reduce fabrication costs however, due to the low refractive index of the polymeric material it has not been possible to obtain a sensitivity biosensor comparable to the ones obtained by silicon photonic technology.

Therefore, our proposal has two combined special features to increase the sensitivity of a modal biosensor interferometer: first, a novel modal interferometer, with larger penetration depth by high order mode evanescent tail and second, a high modal interaction by coupling mode theory optimization. This aspect is a key factor in enabling that lab-on-chip technologies can be available and mass produced in developing regions of the world.

Acknowledgements

The Authors would like to thank the Brazilian C&T Institute FOTONICOM (CNPq project no. 574017/2008-9 and FAPESP project no. 2008/57857-2), the Brazilian Program Science without Frontiers for International Cooperation - MEC/MCTI/CAPES/CNPq/FAPs, project no. 313690/2013-8, for their financial support and resources for our research.