Semiconductor lasers as integrated optical biosensors: sensitivity optimisation

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Abstract. Semiconductor lasers contain both a light source and waveguide, rendering them suitable for adaptation to evanescent field biosensing. One-dimensional simulations using the beam propagation method have been carried out for planar semiconductor waveguide structures, with a view to maximising sensitivity of the effective index to changes in the refractive index and thickness of a film on the waveguide surface. Various structural parameters are investigated and it is found that thinning the upper cladding layer maximises the sensitivity. Implications for laser operation are considered, and an optimised structure is proposed. Surface layer index and thickness resolutions of 0.2 and 2nm are predicted.

1. Introduction
Optical biosensors offer highly sensitive detection of trace amounts of analyte, with applications in a range of fields from medical diagnostics to security detection. However, well-established evanescent field sensing techniques such as surface plasmon resonance [1] and dual-polarisation interferometry [2] are limited by sensitivity, cost and convenience due to size constraints. Other sensors such as grating couplers [3] are also limited by noise when the measured signal is an amplitude or phase difference, and by the difficulty of coupling light into the waveguide from an external source. Semiconductor laser chips contain both a light source and a waveguide, so could potentially be used as integrated optical sensing chips. In addition, a distributed feedback (DFB) laser contains a Bragg grating embedded in the waveguide, allowing laser amplification only at or near the Bragg wavelength, which is strongly dependent on the effective index of the lasing mode. This in turn is highly sensitive to changes in the refractive index of the medium within the mode volume. Therefore, if the lasing mode can be made to extend beyond the surface of the laser waveguide, any changes in refractive index at the surface, brought about by for example physisorption of biomolecules, should be detectable by a change in the lasing wavelength. The critical factor in determining sensitivity of an evanescent field sensor is the optical power of the evanescent field at the sensing interface. We have investigated various 1-D waveguide structures achievable through surface modifications to commercially available devices. Mode-solving by the Beam Propagation Method (BPM) [4] determines the sensitivity of the modal effective index of various structures to changes in the index and thickness of a surface layer. Thinning the upper p-cladding layer dramatically increases the sensitivity due to increased overlap of the optical field with the sample. However, a limit to how thin this upper layer can be made is imposed by the need to maintain optical confinement in the active region of the laser and minimizing losses. Based on our findings, structures optimised for sensitivity whilst maintaining laser action will be proposed.
2. Waveguide design and simulations

Figure 1 shows a band gap diagram for a basic InP/InGaAsP multiple quantum well (MQW) laser with a separate confinement heterostructure (SCH) [5], where $\lambda_{gw}$ and $\lambda_{qw}$ are the band gap wavelengths of the SCH layer and the quantum wells respectively. For this simulation, three layer planar waveguides were designed based on Figure 1, with InP substrate and cladding layers of index 3.17 and an InGaAsP waveguide layer with a variable index between 3.2 and 3.45 [6]. Typical uses of an evanescent field optical biosensor are for bio-affinity assays, where a biological molecule that selectively binds to the substance of interest is immobilized on the sensor surface, and for monitoring thin layer formation of protein molecules. In both cases, changes in the index and thickness of the biolayer occur. To evaluate the sensitivity of a particular structure to such changes, a thin test layer was added to the waveguide surface, and the effective index calculated as a function of test layer index ($\mu$) and thickness ($t$) for the ranges $0<t<10\text{nm}$ and $1<\mu<2$, which are typical for a protein monolayer [7]. Calculations of the optical mode and effective index were carried out using BeamPROP™, a commercial mode-solver employing the beam propagation method [4]. The sensitivity for a particular waveguide structure was defined as $S_\mu=\partial N/\partial \mu$ or $S_t=\partial N/\partial t$, where $N$ is the mode effective index of the fundamental TE mode at a wavelength of 1.55 $\mu$m.

Three methods of maximising the overlap of the evanescent field with the test layer were investigated: (i) by decreasing the index step between the InP layers and the InGaAsP waveguide layer; (ii) by thinning the upper cladding layer and (iii) by adding one or two high index layers above the guiding layer. A generalised transverse index profile showing the variable parameters is shown in figure 2, along with cross sections of three types waveguide investigated.

3. Results and discussion

$N$ increases linearly with $t$ up to a certain thickness and then flattens out; the gradient of the $N$ vs $\mu$ curve gradually increases with $\mu$ (figure 3). This can be understood by noting that the evanescent field in the test layer is proportional to $\exp(-k_z z)$ where $z$ is the transverse direction (perpendicular to the direction of propagation) and $k_z$ is the transverse wavevector [8]. The sensitivity is proportional to the integrated optical power in the test layer:

$$S = \int_{z_1}^{z_2} \exp(-2k_z z) dz = -\frac{1}{2k_z} \exp(-2k_z z + t) \exp(z)$$

(1)

Raising $\mu$ therefore results in an exponential increase in sensitivity, since $k_z$ decreases as $\mu$ increases [8]. With $\mu$ constant, raising $t$ increases the transverse distance covered by the test layer, thereby including more optical power. $E$ decays approximately linearly over small distances, but rapidly drops to zero at greater distances, giving rise to the shape of the $N$ vs $t$ curve in figure 3. Hereafter, $S_\mu$ and $S_t$.
are estimated as the gradients of the tangents to the curves of \( N \nu \mu \) at \( t=5\)nm and \( N \nu t \) at \( \mu=1.45 \) respectively.

**Figure 2:** A: Waveguide transverse index profile illustrating variable parameters \( \Delta n \) (index step), \( l \) (cladding layer thickness), \( l_1 \) (distance of high index layer from waveguide layer – note these are only present in five and seven layer waveguides), \( \mu \) and \( t \). B: Waveguide cross sections for (i) three layer waveguide with variable \( l \) and \( \Delta n \); (ii) five layer waveguide with variable \( l_1 \); (iii) seven layer waveguide.

3.1. Effect of structural parameters

Mode profiles for the waveguide structures with various parameters can be seen in figures 4, 5 and 6. Qualitatively we can measure the effects on sensitivity by examining the area bounded by the curves and the test layer boundaries, as shown in the plots on the right hand side of the figures. Decreasing the index step and the cladding layer thickness both dramatically improve sensitivity. In the former case, reducing \( \Delta n \) from 0.28 to 0.03 results in a 24-fold increase in both \( S_\mu \) and \( S_t \), due to reduced confinement of the mode in the waveguide. In the latter case the improvement from \( l=1\mu m \) to \( l=0\mu m \) is of the order \( 10^3 \) for both \( S_\mu \) and \( S_t \), due to the exponential decay of the field with transverse distance, although this is mitigated slightly by greater modal confinement with decreasing \( l \). The effect of high index layers in the cladding region is to extend or “stretch” the evanescent field, once again increasing sensitivity. As can be seen from figure 6, the optimum position for a single layer is mid-way between the waveguide and test layers, and the sensitivity shows a 10-fold improvement on a three-layer waveguide with \( l=1\mu m \). Adding a second high index layer (mode profiles not shown) further multiplies this sensitivity by a factor of 3.

3.2. Practical Laser Performance

The strongest sensing effect is obtained by thinning the upper cladding layer. However, thinning this layer indefinitely is not feasible since a p-doped layer is required to inject carriers into the device and for waveguiding. In addition, the threshold gain \( \alpha_{th} \) at which gain due to stimulated emission exceeds losses in a Fabry-Perot laser is given by [9]
Here, $L$ is the length of the laser cavity, $R$ is the reflectivity of the laser facets, $\alpha_{\text{ac}}$ and $\alpha_{\text{ex}}$ are the loss coefficients for the active region and surrounding regions respectively and $\Gamma$ is the confinement factor, defined as the fraction of total optical power confined in the active region. According to equation 2, decreasing the optical confinement to improve sensitivity will also lead to an increase in threshold gain. Figure 7 shows a plot of $\Gamma$ and its inverse computed for the central 20nm width of a three layer waveguide structure with $\Delta n=0.23$. $\Gamma$ increases as $l$ is reduced for $l>1\mu m$, due to the high index step between the waveguide and the air forcing the mode into the waveguide layer. Eventually however, $\Gamma$ decreases as the mode is pushed into the substrate, as can be seen for $l<1\mu m$. The minimum at around $l=1.5\mu m$ suggests an optimum cladding layer thickness at this value.

3.3. Sensitivity

Based on the above results, a device with $\Delta n=0.23$ and $l=0.15\mu m$ offers high sensitivity while still operating as a laser, and modification of an existing laser device is practicable. For this structure $S_t\sim 10^{-2}\mu m^{-1}$, approximately 2 orders of magnitude greater than $S_{\mu}\sim 10^{-4}$. Changes in effective index can be translated to changes in wavelength for a DFB laser by [10]

$$ \frac{\Delta \lambda}{\lambda} = \frac{\Delta N}{N} \tag{3} $$

Assuming a minimum measurable $\Delta \lambda$ of 0.01nm with an optical spectrum analyser and taking $N=3.28$, we have a detection limit on $\Delta N$ of $2\times10^{-5}$. Using the values for $S_t$ and $S_{\mu}$ quoted above, minimum detectable changes in test layer index and thickness are $\Delta \mu_{\text{min}}=0.2$ and $\Delta t_{\text{min}}=2nm$. The size of a protein molecule is generally of the order 2-10nm, so this value for $\Delta t_{\text{min}}$ is promising. Although predicted sensitivity is still roughly two orders of magnitude less sensitive than SPR and the integrated optical sensors described by Lukosz [3], sensitivity may be improved by using two lasers simultaneously, with one device isolated from the analyte as a reference.
Figure 4: Left: mode profiles for three layer waveguide with index step $\Delta n$ as parameter. Right: mode profiles in test layer (magnified view).

Figure 5: Left: mode profiles for three layer waveguide with cladding layer thickness $l$ as parameter. Right: magnified view showing positions of test layer for various $l$.

Figure 6: Left: mode profiles for five layer waveguide showing high index layer at a distance $l_1$ from the waveguide layer. $l_1$ is parameter. Right: magnified view of test layer.
The beat frequency between the two signals can be measured with an electrical spectrum analyser, allowing for detection of much smaller wavelength shifts, for example a beat frequency of 100MHz corresponds to a wavelength difference of 0.8pm, giving a detection limit $\Delta N=2\times10^{-6}$. Twinned lasers could also help to compensate for wavelength noise induced by environmental temperature variations, since both devices should be equally affected.

4. Conclusion

If a semiconductor laser is to be used as a biosensing device, it is necessary to modify the upper layers of the laser waveguide to allow the optical mode to overlap with material on the surface. Of the methods investigated, thinning the upper p-type cladding layer yields the greatest improvement in sensitivity to changes in both the index and the thickness of a test layer. An optimized structure with $l=0.15\mu m$ and corresponding layer index and thickness resolutions of 0.2 and 2nm are predicted. There is also potential for improvement by using twinned lasers, and this type of sensor would have the advantage of being compact, portable and cost effective, and easily adapted from existing technology.

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