Heteroepitaxial bonding for hybrid integration of nanostructured optical devices

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Abstract

The field of photonic is nowadays developing very fast, and new advances on bonding technics rise the interest of doing hybrid devices with III-V materials bonded on IV materials. Fabrication of buried photonic crystals is now possible and offers new opportunities in tuning devices. In this report, I will study a new approach to reduce simulation computation time of such devices, using an old theory applied to a new goal: the Effective Medium Theory. I will show that this method improves computation time for mode analysis, in a laser cavity for example. I will also compare the results of simulation to actual waveguides modal behaviour.

Note to the reader

This report was made in collaboration with the CNRS under a confidentiality clause. Some parts of this public report were thus eluded to respect that clause. For more information on the complete report, please contact Anne Talneau: anne.talneau@lpn.cnrs.fr

Confidential parts are noted with a [CONFIDENTIAL] at the beginning of the section’s name.
1 Context & Objectives

1.1 Context

The field of photonics is very active with numerous research being done on the subject. One of the hot topics deals with integrated circuits consisting of III-V semiconductors on Silicon. The interest of this is quite simple: III-V materials such as InP have great properties as for active photonic devices such as lasers or amplifiers operating at 1.55µm. But III-V semiconductors are rare, and thus expensive. Their technology is not as mature as that of Silicon. Silicon on the contrary is well-known due to its large scale use in microelectronics, it is cheap being the most abundant element on Earth’s crust and has very good properties for light guiding, but it is also known to have poor emission or active properties on account of its indirect bandgap. Therefore comes the idea to integrate III-V materials on Silicon, to have the light amplification part on top of silicon and the electronic and guiding parts on silicon. These devices are therefore called hybrid ones.

<table>
<thead>
<tr>
<th>Material</th>
<th>Lattice Constant</th>
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<tbody>
<tr>
<td>Si</td>
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</tr>
<tr>
<td>InP</td>
<td>5.86 Å</td>
</tr>
<tr>
<td>GaAs</td>
<td>5.65 Å</td>
</tr>
</tbody>
</table>

Table 1: Lattice constant of different crystalline materials

But a problem arises for the actual fabrication of such devices. The III-V materials and Silicon have different lattice constants and that difference is too large to enable epitaxial growth, so the two materials need to be bonded by another way. Several groups include a bonding layer made of dielectric having a poor thermal conductivity, thus probably leading to some thermal roll-off visible on the output power current curve of operating lasers. (see figure 1 for the specific example of the Bowers’ group in Santa Barbara).

1.2 The COHEDIO project

The COHEDIO project (Heteroepitaxial bonding for hybrid integration of nanostructured optical devices), which was the frame for my internship, is a national project funded by the ANR (Agence Nationale de la Recherche, national agency for research).

- The LPN (Laboratory of Photonics and Nanostructures), main shareholder in the project, which I am part of
- IOGS (Institute of Optics Graduate School)
- IEF (Institute of Fundamental Electronics)
- P’ Institute, Poitiers university
- III-V lab by Alcatel Thales Lucent Leti
The objective of this project is to open a new avenue for the design and fabrication of hybrid integrated photonic devices developing new interfaces such as heteroepitaxial interfaces. This bonding technique has the capability to associate two materials that cannot be grown epitaxially, and achieves this feature without an intermediate dielectric layer: it reconstructs the atomic bonds at the interface and preserve the crystalline properties of each material, as well as any patterning previously defined on one of the surfaces, without burying the pattern in an intermediate layer material, as occurs in prior art. The project studies this bonding technique, promising for the development of a new generation of devices, and demonstrates its relevance on several carefully selected integrated devices as test vehicles. The project studies the bonding on silicon of two classes of materials that are fundamental for the operation and fabrication of photonic integrated circuits (PICs): III-V semiconductors of InP type for the obtaining of essential emission/amplification functions, and magneto-optical garnets for the equally critical function of optical isolation. These materials will be bonded

Figure 1: (a) Device fabricated by the group of Bowers with thin oxide bonding. (b) Optical output power of that device in function of injection current. The optical power shrinks rapidly for larger intensities. The yield is low for high temperatures. Figures reproduced from [1]
on silicon, taking advantage of the optimised high performance of guide technology available on Si, and of the capability to nanostructure them. The bonded surfaces will be of limited area, on the order of cm², enough for the realization of a single device ("die"). We will study telecom key-devices such as DFB laser diodes and semiconductor optical amplifiers (SOA), both electrically pumped, as well as optical isolators. For lasers and SOA, the silicon nanopatterning, performed simultaneously with the guide patterning, will broaden the parametric design space in order to mitigate the limiting heat transfer value of present designs. Beyond individual devices, this technique will contribute to boost the performances of more complex integrated circuits, such as the commutation matrices based on SOA integrated on SOI guides. This project, fundamental in character, shall make new hybrid integration architectures available for photonic devices, thanks to the preservation of the integrated nanopatterns upon heteroepitaxial bonding. This integration of nanostructures in the central part of architectures adds functions such as confinement/periodicity to the palette, and it also has a large potential to stabilise frail or brittle interfaces. It will have the potential to lengthen their lifetime and to make them immune to thermal cycling or to stress occurring during e.g., contact definition or packaging steps.

The project got started in 2011 and has since then given many interesting results, including heteroepitaxial bonding [2] and design[3] (see figure 2). This is the method that will be used to elaborate the samples studied during this internship. A PHD student I am working with is currently developing a method to bond InP to Silicon with a thin layer (2 – 4nm thick) of Silicon oxide. State of the art techniques used by the III-V lab feature for example more than 10nm thick bonding layer.

![Figure 2: SEM picture of an interface bonded with heteroepitaxial bonding. The transition zone is only a few atoms thick and no dislocation can be seen out of the grain boundary.](image)
1.3 Objectives of the internship

My role in the project is first to develop a tool to simulate the guiding properties of the different designs proposed to optimise the geometry of the device and secondly to confront that simulation to actual waveguides.

The idea of the COHEDIO project concerning the design of laser cavity is to replace the air lateral cladding by a nanostructure material made of air holes in a silicon matrix (see figure 3). This will enable to tune efficiently the confinement factor of the modes inside the guides and should improve heat dissipation from InP toward the substrate. The main difficulty to simulate that geometry is that we have a truly 3D waveguide, a 3D simulation is thus necessary. I will use the effective medium theory to describe the nanostructured material by a homogeneous material, which improves computation time a lot. This theory must be implemented and compared to simulation with actual geometry, and then compared to actual devices guides elaborated at the LPN by my supervisor.

Figure 3: Layout of the proposed device for the COHEDIO project. Scale is not respected.
2 Effective Medium theory for a nanostructured material

We want to study a waveguide with a structured material acting as the cladding of the guide. That geometry can be simulated with a mesh close to its exact shape, but it requires a great amount of computation. One way to reduce the computation time is to consider the structured material as a continuous material with the adequate properties. That approximation is called the Effective Medium Theory (EMT) and can be used in many fields. In our case, the EMT approximation is valid if the wavelength is large compared to the characteristic length of the structured material, which summarizes as \( \alpha = \frac{\text{period}}{\lambda} \ll 1 \) [8] for a periodic structure. This method has been used for diffraction calculation [9] or photonic band structure calculation [10] [11]. Here we will apply it to mode analysis of waveguides with nanostructured lateral cladding.

2.1 Effective Medium Theory in 1 Dimension

This part summarizes the EMT approach for a 1D structured medium, for example a periodic array of silicon slabs separated by air. The incoming wave has a wavelength of \( \lambda \). As said earlier, the array must satisfy the condition \( \alpha = \frac{\text{period}}{\lambda} \ll 1 \). In this configuration, one must take into account the direction of the electric field compared to the slabs [8]. From now on, we call \( \epsilon_\perp \) and \( \epsilon_\parallel \) the relative dielectric constant of the effective medium when the field is perpendicular and parallel to the interface respectively.

That approach is summarised on figure 4. The associated equations for the effective medium are as follows[8]:

\[
\frac{1}{\epsilon_\perp^{(0)}} = \frac{1}{\epsilon_2} + \frac{1-f}{\epsilon_1} \tag{1}
\]

\[
\epsilon_\parallel^{(0)} = f \epsilon_2 + (1-f) \epsilon_1 \tag{2}
\]
for better precision, one can take a correction from [12] and use a second order approximation in \( \alpha \)

\[
\epsilon^{(2)}_{\parallel} = \epsilon^{(0)}_{\parallel} \cdot [1 + \frac{2}{3} \cdot \alpha^2 \cdot \epsilon^2_{0} \cdot (1 - f)^2 \cdot (\epsilon_2 - \epsilon_1)^2] \\
\epsilon^{(2)}_{\perp} = \epsilon^{(0)}_{\perp} \cdot [1 + \frac{2}{3} \cdot \alpha^2 \cdot \epsilon^2_{0} \cdot (1 - f)^2 \cdot (\epsilon_2 - \epsilon_1)^2 \cdot \epsilon^{(0)}_{\parallel} \cdot \epsilon^{(0)}_{\perp}] 
\]

with \( \alpha = \Lambda / \lambda \), \( \Lambda \) being the period of the structuration and \( \lambda \) the wavelength.

The calculus gives different results depending on the direction of the electric field: the medium acts as a uniaxial anisotropic dielectric where \( n_\perp = \sqrt{\epsilon_\perp} \) is the extraordinary index and \( n_\parallel = \sqrt{\epsilon_\parallel} \) is the ordinary index. The two indices with second order correction are represented figure 5 for \( \alpha = 0.1 \) and different values of the fill factor.

![Figure 5](image)

Figure 5: Values of the parallel and perpendicular indexes for slabs of air in silicon with second order correction, \( \alpha = 0.1 \)

With this figure, we can see that the extraordinary index \( (n_\perp) \) is always lower than the ordinary index \( (n_\parallel) \). That is \( \Delta n = n_{ex} - n_{ord} < 0 \), our material is thus called negative uniaxial.

### 2.2 Effective Medium Theory in 2 Dimensions

We now consider a proper 2D photonic crystal as considered in figure 6. The main variables are the following:

- the size of the lattice compared to the wavelength through the parameter \( \alpha = \frac{\Lambda}{\lambda} \)

- The linear filling factor of the grating \( f_i = \frac{d_i}{\Lambda_i} \), \( i = \{ x, z \} \). In this study, we always take the case of symmetric holes, \( f_x = f_z \) but some calculations are given for generic fill factors\(^1\).

\(^1\)In the world of EMT, scientists use mainly square holes with linear fill factor as described here. In the photonic crystal world, scientists use surface fill factors with either round or square holes, see section 2.3.
We want to describe that 2D grating by an effective homogeneous medium and see how far that approximation can be pushed. We have to take into consideration the direction of polarisation: the results will not be the same depending on whether the polarisation of the electric field is in the direction of invariance (along the x-axis) or in the plane of the grating (in the plane defined by axis y and z). The case of the electric field in the direction of invariance was studied before[9] and give the following result:

\[
\epsilon_y = (1 - f_x f_z) \epsilon_1 + f_x f_z \epsilon_2
\]

(5)

Figure 6: Diagram of a photonic crystal with relevant entities

When the field is not aligned along the direction of invariance, there is no exact formula to get the effective index[12]. We have to make the averaging in the two directions: we can make the first average considering the field parallel to the holes and then perpendicular or the reverse (figure 7). In detail that gives for \(\epsilon_{\parallel \perp}\) and \(\epsilon_{\perp \parallel}\):

\[
1/\epsilon_{\| \perp} = (1 - f)/\epsilon_1 + f/\epsilon_{\parallel}
\]

(6)

\[
\epsilon_{\perp \parallel} = (1 - f)\epsilon_1 + f\epsilon_{\perp}
\]

(7)

with \(\epsilon_{\parallel}\) and \(\epsilon_{\perp}\) being the same as in equations 1 and 2. The formulas are valid in the case of a square lattice. The two ways of calculating the effective medium give two different results, one value always lower than the other. We call them lower and upper bound, following ref. [9], associated respectively to \(\epsilon_{\| \perp}\) and \(\epsilon_{\perp \parallel}\):

\[
\epsilon_{\| \perp} \rightarrow n_{\text{upper}}
\]

\[
\epsilon_{\perp \parallel} \rightarrow n_{\text{lower}}
\]

These formulas were implemented through a MATLAB routine to give the results plotted figure 8. The actual effective index is located somewhere between the upper and the lower bound. In the zone of interest, that makes a relative uncertainty on the index value of about 10%. The fabrication of an actual device enables precision in the pattern up to a certain point that would give
uncertainty on the effective index of a few percents. We therefore see that the 10% uncertainty is too large to be used without further treatment.

First we can try to determine if the result is better when taking a higher order EMT, using equations 3 and 4. Where $\epsilon^{(0)}_\perp$ and $\epsilon^{(0)}_\parallel$ are the permittivities at zeroth order from equations 1 and 2 respectively. The results are shown figure 9. The upper and lower bounds at second order in $\alpha$ are shifted up compared to zeroth order, but the relative uncertainty for the real index is not changed and is still around 10%. Again we must find another way.

The article from R. Bräuer and O. Bryngdahl [12] gives a method to approximate the actual effective index. They discovered that the following formula gave results very close to those calculated with a full analysis of a 2D photonic crystal with Bloch waves.

$$\epsilon_{eff}^{1/2} = \left[\epsilon^{1/2}_\perp + 2.\epsilon^{1/2}_\parallel + 2.\epsilon^{1/2}_\perp\parallel\right]/5$$  \hspace{1cm} (8)

Figure 7: effective medium by averaging perpendicular then parallel (a) and parallel then perpendicular (b)

Figure 8: Effective medium theory index for upper and lower bounds. Fill factor is linear fill factor (see section 2.3).
The results are shown figure 10. The exact calculation was adapted from a MATLAB script provided by Henri Benisty from IOGS (Institute of optics graduate school, [3] is a recent article written by them related to EMT) that originally calculated the band structure of a photonic crystal, thus at any \( \alpha \). The effective index was extracted from the dispersion relation and then plotted for each value on the graph. As a result, we can see that the approximation in the zone of interest provided by Brüer and Bryngdahl is very close to the effective index with 2D photonic crystal calculation, and is even better when taking into account the second order rectification. For large values of the fill factor, the real effective index drops. In that case, we are getting close to the photonic band-gap, which the EMT cannot describe properly as such. Studies were made to show that EMT can be applied with corrections to fit even close to the band-gap [13], but that goes out of our study.

As for the EMT with 1D structuration, we find that the right EMT representation for the structured medium is an anisotropic uniaxial medium, with extraordinary index along the axis of invariance of the hole array. To summarize, we have (following the notation of figure 6):

\[
\epsilon_x = \epsilon_z = \left[ \epsilon_1^{1/2} + 2.\epsilon_{\perp}^{1/2} + 2.\epsilon_{\parallel}^{1/2} \right]/5
\]

\[
\epsilon_y = (1 - f_x.f_z).\epsilon_1 + f_x.f_z.\epsilon_2
\]

The spacing between the two indexes is shown figure 11

Since a script for calculating the exact effective index is available, the rest of the study will be made with values taken from that script and not from the Bräuer-Bryngdahl approximation. The validity of that approximation was nevertheless demonstrated in case the exact calculation is not available.

![Figure 9: Effective medium theory index: zeroth order vs second order for \( \alpha = 0.2 \). Fill factor is linear fill factor (see section 2.3).](image-url)
2.3 Note on the use of linear fill factor and surface fill factor

There are two norms for the fill factor in the scientific community, one for people dealing with effective medium and one for people dealing with photonic crystals. The one used in all this part is based on linear fill factor, which is defined as

\[ f_{\text{lin}} = \frac{\text{size of air slabs/holes}}{\text{period of structuration}} \]

and is applicable only to square holes, whereas the surface fill factor is defined as

\[ f_{\text{surf}} = \frac{\text{surface occupied by air}}{\text{surface of a cell of periodic structure}} \]

In the case of 1D structuration (ex: slabs), the two definitions are equivalent. In the case of a 2D structuration (ex: square holes), the definitions are not equivalent and we have the relation:

\[ f_{\text{surf}} = f_{\text{lin}}^2 \]

In the special case of air holes, the right value is the surface fill factor. But

Figure 10: EMT upper and lower bounds with and without corrections to second order in \( \alpha = 0.1 \) plotted with the Bräuer approximation with and without correction and the exact effective index. Fill factor is linear (see section 2.3).

Figure 11: Anisotropy of effective medium composed of air holes in silicon
one can transfer to linear fill factor by considering a square lattice with same surface fill factor and take its linear fill factor. That gives $f_{surf} = f_{lin}^2 = \frac{\pi}{4} \frac{d^2}{\text{period}^2}$, where $d$ is the diameter of the round holes. From now on, all fill factors will be surface fill factors.
3 [CONFIDENTIAL] Application of the Effective Medium Theory to eigen mode calculation supported by optical waveguides

The previous section described the effective medium theory. All those results are well known and were published in earlier reviews [12][16]. They were performed with an incoming plane wave that impinges onto the structured medium. In this part we will demonstrate that the EMT is still relevant and can be applied to the case where the structured medium is used for the lateral cladding of a waveguide. The core of the guide is made of bulk silicon and the lateral cladding is made of a structured medium of air holes/trench made in silicon. The following parts will demonstrate the validity of the EMT approximation for a nanostructured waveguide and the limitations of this theory. First in a simple to simulate case where the cladding is made of trenches of air in silicon and the second case with a lattice of holes in silicon.

CONFIDENTIAL

The following sections of the report were considered confidential and property of the CNRS. They are thus not printed in the public report. See Anne Talneau for the complete report anne.talneau@lpn.cnrs.fr
4 Measurement of fabricated PhC-Si waveguides

The COMSOL models from the previous section need to be confronted to reality. In that optic, my supervisor created waveguides in the clean room of the laboratory, both with and without a 400nm thick InP layer bonded on top. The InP mesa is here simpler than the full-laser stack implemented for previous simulations. The COMSOL models are thus adapted to fit the real guides as close as possible. In this section, I will describe the setup used first for field cartography and then for spectral analysis of the guide.

In this section, I will use guides, either covered with InP on top or not. They are taken from two different arrays with guides, each of them is partly covered with InP, partly uncovered (see figure 12). The main geometry features are:

- Width of the ridge: 0.6, 0.8, 1.0, 1.2 & 1.4 µm
- Hole diameter: 50nm or 60nm
- the holes have different depth depending on their diameters: 50nm → 200nm and 60nm → 250nm
- Silicon thickness: 550nm
- When InP is bonded on top, it has a thickness of 400nm. It is a simple layer of InP and not the complex stack used for simulation in section 3.

![Figure 12: Microscope photograph of arrays of waveguides, uncovered on left and covered on right. Magnifying: 20X.](image)

The layers thickness is SEM controlled, but the geometry of the holes would be better described by a cone than by a cylinder (see figure 13), which concurs in a 10-15% uncertainty on air filling factor and can disturb the electric field distribution.

4.1 Field cartography

A first experiment can be made with the setup figure 14. The goal is to obtain a field cartography on the output cleaved facet. The camera used is an InGaAs camera with a high sensitivity in the 1.5µm wavelength rang. Many filters were set between the first lens and the camera, so that the field picture
Figure 13: Scanning Electron Microscope picture of the cleaved face of one of the measured guide. This one is covered with InP.

uses all the extend of the camera sensibility range. The input fiber is a microlensed (west of 2µm) polarization maintaining fiber with polarization tuned along the horizontal axis. Therefore only TE modes are investigated. No direct quantitative information can be extracted from light intensity with this method, but a method for roughly detecting the presence of a second order mode can nevertheless be performed.

Figure 14: Camera setup used for taking photographs of field distribution.

Some comparison on field distribution between reality and simulation is given on figure 15, for bonded and unbonded guides. The shapes are different from that calculated by simulations. This is due to the diffraction limit of our photography: an objective with numerical aperture of 1 can see details of minimum size equal to $\lambda/2 = 0.75\mu m$. The width of the mode is of that order, and the numerical aperture is most certainly far below 1 (the exact value was not measured), therefore the maximum resolution of the setup is too low to be able to really compare them to the modes obtained with simulation. But taking this setup was a very valuable tool to align the input fiber with the center of the
guide in the end-fire setup described section 4.2.

Figure 15: Field distribution of real guides on left versus the same geometry simulated with comsol on right, for (a) covered guide, $w_{\text{ridge}} = 0.6\mu\text{m}$ and $d_{\text{holes}} = 50\text{nm}$, (b) covered guide $w_{\text{ridge}} = 1.4\mu\text{m}$ and $d_{\text{holes}} = 50\text{nm}$ and (c) uncovered guide $w_{\text{ridge}} = 1.4\mu\text{m}$ and $d_{\text{holes}} = 50\text{nm}$

All the previous photographs were taken with the input fiber aligned with the center of the guide. If I put the fiber slightly off the center of the ridge ($1.3\mu\text{m}$ aside for $w = 1.4\mu\text{m}$ and $0.6\mu\text{m}$ aside for $w = 0.6\mu\text{m}$), then I sometimes get the shape of the mode that changes to look very much alike the second order mode (see figure 16). That phenomenon only occurs when a higher order mode is detected in the Fourier spectrum (see section 4.2), but it is not always visible enough to be detected. So I interpret this as the input fiber exciting preferentially the $TE^1$ mode. This mode is asymmetric and is thus favoured when putting the fiber off-axis. If the fiber is put between the center and most favourable position for $TE^1$, then I can picture a combination of the two modes. The fundamental is the most important, but some field corresponding to the $nth$ order mode is "leaking" out of the main mode. And that effect can be used to have a quantitative detection of the presence of a second mode. I use a program made previously that can integrate the field given by a picture over a localized area. So I do two integrations: the first on a small window very close to the main spot and the second, much larger, that is used for normalization purposes. I repeat that operation for many wavelength. I do this with the fiber centered, shifted left and shifted right (see figure 16). The fiber is shifted so that its center is facing the structurated lateral cladding. With a west of $2\mu\text{m}$,
some light still comes into the guide, but on the side of it. The values I calculate and compare are the following:

$$\rho_i = \frac{\int_{\text{close window}} \text{intensity on camera}}{\int_{\text{wide window}} \text{intensity on camera}}, \quad i = \{\text{centered, left, right}\} \quad (9)$$

Figure 16: Field cartography when fiber is (a) centered (b) shifted on side so that both modes are excited (c) shifted more on side so that only $TE^1$ mode is excited

These analysis have been made only on uncovered guide. The results for $w = 0.6\mu m$ and $w = 1.4\mu m$ are show figure 17. Some of the points calculated are wrong because the alignment of the main spot changes with wavelength. This results in the main spot moving across the camera field during acquisition: for some wavelength, the main spot is out of the close window.

Figure 16: Field cartography when fiber is (a) centered (b) shifted on side so that both modes are excited (c) shifted more on side so that only $TE^1$ mode is excited

The results shows a visible difference between what was calculated with the $w = 1.4\mu m$ and the $w = 0.6\mu m$. For the narrower waveguide, the main spot is very constant versus wavelength: there is almost no change in field distribution when the fiber is centered than when it is shifted left or right. There is only one mode present. The larger waveguide on the contrary shows more chaotic results. That is partially due to the fact that the position of the main spot on camera is very sensitive to wavelength, so sometimes the main spot goes out of the small window. Nonetheless the difference in field distribution is much larger in this case than in the narrow ridge, here we have at least two modes present. This method is not very accurate but enables to have a quick estimation of the presence or not of higher mode in the guide. Alignment and sampling is quick compared to the end-fire setup (about 30 min, compared to 1h30, and analysis of results is easier).

4.2 Measuring with the end-fire setup

4.2.1 setup & analysis method

From previous section we get rough information on mode shape, but now we need quantitative information. To do that, we use an end-fire setup (see figure 18). The entrance and exit fibers are aligned with the center of the guide. The
Figure 17: \( \rho \) calculated versus wavelength in nm for (a) \( w = 0.6 \mu m \) and (b) \( w = 1.4 \mu m \). The red ellipse indicates points where the close window was not centered on the main spot.

wavelength sent by the input fiber can be tuned, and a power meter measures the power coupled to the fiber. We thus get the spectrum of our guide. The guide in itself has cleaved facets at both end. It will therefore act as a Fabry-Perot cavity. The light will reflect on the end face and go both way, thus creating interferences. These will make fringes in the acquired spectrum. And these fringes can be used to get information via a Fourier transform, such as the number of modes that can propagate and their group index. The script used to analyze raw data was created by a previous student in internship. I actualized and adapted the code for my own use. The script features an interesting functionality: the Fourier transform by window. The script takes the convolution of the spectrum by a Gaussian function and then takes the Fourier transform. With that, we get the Fourier transform on a small window of wavelength (see figure 19). From that we can get information such as dispersion relation of the modes.

The length of the guide array is \( L_{\text{physical}} \). From the optical length at resonance (i.e at optical length of a cavity eigenmode), \( L_{\text{optical}} = n_g L_{\text{physical}} \) where \( n_g \) is the group index of the mode. If the signal is good, a secondary peak can be seen that correspond to light going twice through the cavity. Therefore the relation for \( n_g \) becomes \( L_{\text{optical}} = 2n_g L_{\text{physical}} \)

From the comsol simulations, we can only get the phase index. The group index is linked to the phase index by the relation:
Figure 18: Camera setup used for taking photographs of field distribution.

Figure 19: (a) Spectrum of a waveguide (One measured during the previous internship) in blue, and the same guide convoluted with a Gaussian window (in red). (b) The corresponding Fourier transform. This figure was adapted from the internship report of Mikael Saada, made at the LPN in 2002.

\[ n_g = n_\phi - \frac{d n_\phi}{d \lambda_0} \]  

(10)  

From measurement we only have \( n_g \). COMSOL simulations can provide the phase index and its variation with wavelength. From that I deduce the simulated group index and can compare it to that of the real guide.

4.2.2 [CONFIDENTIAL] measurement of waveguides

The following sections of the report were considered confidential and property of the CNRS. They are thus not printed in the public report. See Anne Talneau for the complete report anne.talneau@pn.cnrs.fr
5 Conclusion & further work

This internship enabled me to prove the validity of the EMT theory when it is applied to modal analysis with a nanostructured medium, be it with air trenches or air holes. The gain in computation time for these simulation was very high and the loss in precision acceptable. The EMT simulation were able to simulate fine results such as mode hybridization, even though some work could be done to further improve the exact localization of the anti-crossing with EMT theory. I also demonstrated the measurement of covered waveguides with an end-fire setup and showed some differences between covered and uncovered guides, thus demonstrating the usefulness of these hybrid devices. Further work will be to use the results and tools developed during that internship in order to design an actual cavity and, in the end, have a proper device and compare its efficiency to the ones obtained before. Another step to do is to complete the work already done on thermal dissipation by IOGS [3].
Appendix

A The simulations with COMSOL and MATLAB

A.1 basic models

The models are originally made with the COMSOL interface. They can sometimes call matlab functions directly from the model or be exported to a .m file for scripting with MATLAB.

The 2D models (the exact geometry with 1D structuration for example, see figure ??) are built so that the size of the whole box does not change with variation of parameters such as the ridge width. The size of the mesh is taken so that every zone of the model has at least 2 elements across each dimension. A slab of 10nm width will for example have mesh elements of maximum size 5nm.

The remaining elements of geometry not stated for in section ?? or ?? (i.e all excluding the 3D model) are featured table 2

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<th>Index</th>
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<tr>
<td>Quantum Wells</td>
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<td>SCH</td>
<td>0.25</td>
</tr>
<tr>
<td>InP top</td>
<td>1</td>
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</tbody>
</table>

Table 2: Geometry features not staged in the core of the report

A.2 Parametric study of a comsol model with matlab

In this section, my interest will be to explain how I could produce results such as seen figure ??, The COMSOL interface is quite efficient to solve some categories of problems, including simple parametric studies for example. But the manipulation of data produced directly by COMSOL is somehow inconvenient. There comes MATLAB, which is a very efficient software to manipulate data. The idea is to write a MATLAB script that will communicate with the COMSOL server. MATLAB will ask COMSOL to perform some calculations and then get the results back, which can then be manipulated. We can therefore make loops in MATLAB to make the simulations for all the parameters that are required. The flowchart of that script is proposed figure 20. Data is plotted and saved in a .txt file that can be reinterpreted later, for further manipulation without the need to relaunch the whole calculation.

This method seems quite efficient, but it has nonetheless some limitations, the COMSOL model is created from the graphical interface and then exported in .m that can be read by MATLAB. The COMSOL programs turn around the notion of domain, which are different from the simple definition of geometrical shapes. For example two circles drawn with same center but with different radius will define 3 zones : First outside the outer circle, second between outer...
Figure 20: Flow chart of the script using 2D models. Can be applied to exact model with slabs of air, EMT model for 1D structuration and EMT model with 2D structuration.

and inner circle and third inside inner circle. These zones are numerated in ascending order from first met to last met. Scanning is made from bottom left to top right. All properties like material are assigned to a domain and not to a geometry. COMSOL standalone is capable of redefining materials and others to the right geometrical zone if ever the numeration changes following a change in geometry. But when the model is exported in matlab, the assignment of material is made to a numerated number. For example air is assigned to domain 1 & 2. If I now change the geometry and send it to COMSOL, it will do the numeration anew and the domain that correspond to air might be numerated 3 & 5 instead of 1 & 2. So, to be scriptable, the model must be built so that the domain numeration will not change with variation of parameters. An alternative would be to use selection boxes, but that would mean create one selection box for each domain, but that solution comes impossible to apply with my models that can have up to 100 domains. This is the reason why I put SiO$_2$ on sides of the structured medium figure 22. It is designed to always go a bit under the InP mesa, so that the slabs of air would not be either below InP or below air, depending on the ridge width. The material is chosen to be SiO$_2$ so that the mode will not confine itself in the small cavity so-formed. The geometry with effective medium did not require that, but was created to fit as close as possible to the reference geometry.

A.3 mode analysis for a 3D model

Doing a mode analysis for a 3D model was quite challenging since COMSOL does not provide a module for mode analysis in 3D. Only frequency analysis of the cavity is available: COMSOL calculates the eigenfrequencies of the cavity and corresponding field distribution. The trick is to use periodic conditions
with phase matching (Floquet periodicity). The phase at entrance is shifted from the phase at exit by a factor \(2\pi n_{eff} \frac{\text{thickness}}{\text{wavelength}}\). \(n_{eff}\) is the effective index of the mode we search, at frequency \(\nu = \frac{c}{\lambda} = 1.934 \times 10^{14}\ \text{Hz}\). If the index is set right then the cavity has an eigenmode with eigenfrequency equal to the searched frequency. Since I had already developed a model with EMT, I chose to use the results from that model, extract the effective index of the modes found that way and inject it as guess index in the 3D model. The error in eigenfrequency is related to the error of the effective index. We thus get a customized method to check the validity of EMT in 2D structured media for guiding mode. I had nevertheless one big technical problem with that script. In the .m models, geometries, materials, etc. are identified by a name, for example 'geom1'. The problem is that when exporting the model, COMSOL exports it with 'geom1' for for 2D and 3D model. Thus if I load the two models at the same time, conflicts appear and the script crashes. The names cannot be changed directly on COMSOL and must be changed manually at every occurrence, which is not practical at all. Two solutions: integrate both models in one directly inside COMSOL. But a bug from COMSOL prevented me from doing that. I think that bug was corrected in the later version (4.3.a), but that version was extremely slow on my computer due to a bad graphic chipset, so I chose the second option instead, which is to load and clear the models every time needed, so that only one model is loaded at a time. That manipulation slows the script, but the loading time is short compared to calculation time. A flowchart of the script I used is shown on figure 21.

As for the implementation of the model, the two faces used for periodic conditions must have the same mesh. That can have some consequences when some parts of a domain are squeezed thin, for example between the front face and the holes. Because of this, COMSOL sometimes throws an error when building the mesh; it cannot place a mesh element with all the constraints given, such as maximum size and standard growth of mesh size to adapt zone with different characteristic sizes. The condition that every layer must have at least 2 elements on every length can also cause problems since the number of points to calculate can grow extremely large and saturate memory. The case \(f=0.1\) for example saturates memory. Mesh size is the main reason why I could not reproduce the same geometry as for the 2D models, inducing strong border effects for low confined modes.

I also tried to use PML on the sides to avoid border effects, but I might have set them wrong because I still had border effects, the InP mesa would still act as a confining cavity. And more, many modes would be found confined inside the PML. So I decided to abandon them for the moment.

### A.4 automatic mode identification

When COMSOL runs a calculation with the mode analysis module, it computed the eigenmodes of the model that are close to a reference effective index. It will search the eigenmodes close to that value in effective index. It is then the role of the user to identify the modes and get out the wrong ones. As a matter of fact, COMSOL can find modes that are not possible in reality, which shows seemingly random field distribution. When running hundreds of simulations, it becomes interesting to automate this process, and therefore find a good way to discriminate the modes we are interested in. The fundamental modes \(TE^0\) and
Figure 21: Flow chart of the script using the 3D model helped with the 2D.

$TM^0$ are mainly located inside the ridge. So I decided identify the fundamental modes on that characteristic: they have the highest field confinement inside the ridge, with direction of electric field mainly directed along predilection axis. In equations:

$$mode \; TE^0 \; identified \rightarrow \max \frac{\int_{\text{ridge}} E_x^2}{\int_{\text{all}} E^2}$$ (11)

$$mode \; TM^0 \; identified \rightarrow \max \frac{\int_{\text{ridge}} E_y^2}{\int_{\text{all}} E^2}$$ (12)

That system works well for the 2D models, either exact or EMT, since no border effects disturb the field distribution. With the 3D model, for small ridge values, detection with those equations can be wrong as discussed in ?? . The fundamental mode also has a high field in the top part in the InP mesa. The idea is to use that zone in addition to the ridge to improve mode detection. The
field is now integrated over the ridge but also a column above the ridge (cf figure ??), including first layer of InP, quantum wells and SCH. Detection is still not perfect that way but the right mode is thus sometimes identified, when it was almost never before.
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