Investigation of plasmonic structures and spontaneous emission in semiconductor lattices

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Abstract

In this thesis, the author begins by introducing some fundamental concepts of LASERs, in order to contextualise the theoretical work conducted throughout the project. This thesis investigates the reflectance, transmission and density of modes of a variety of semiconductor lattices. This study depends on the transfer matrix method (TMM), which is commonly used in theoretical photonics modelling. Later in the thesis, the TMM is adapted for increased versatility, and is used to calculate the rate of spontaneous emission within several different semiconductor lattices. Finally, this thesis introduces the concept of a SPASER (with some discussion of various approaches), and the results of a series of plasmonic simulations are shown and discussed.
Declaration

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Chapter 1

Introduction

1.1 Objectives

The core objectives of this thesis are to provide a comprehensive introduction to the theoretical methods that can be used to investigate several types of LASERs. The transfer matrix method for photonic crystal structures is discussed, and the calculation of spontaneous emission enhancement within a photonic structure will also be investigated. Later in the thesis, some of the methods that can be used to investigate plasmonic activity are discussed.

1.2 Introduction to LASERs

1.2.1 LASER definition

The word LASER is an acronym for ”Light amplification and stimulated emission of radiation”. Light amplification refers to the multiplying of photons as they pass through the active part of the LASER. ”Stimulated emission of radiation” refers to the fact that emission of photons in the active region of the laser is no longer random spontaneous emission. The photons interact with excited electrons in the active material, causing the electrons to lose energy and drop to a lower energy level. This causes the release of a new photon with energy and phase corresponding to the incident photon [1].
1.2 Introduction to LASERs

1.2.2 History of LASERs

Einstein first theorised the possibility of stimulated emission in 1917, in the paper "Zur Quantentheorie der Strahlung" (The Quantum Theory of Radiation) [2]. It was not until many years later however, that the first operational LASERs were demonstrated. The first key experimental step took place in the 1950s. Charles Townes and others produced an operational MASER (Microwave analogue of a LASER) [3], which was the first experimental proof of stimulated emission of radiation. Next, in 1960 Theodore Maiman created the first true LASER. This LASER used ruby as the active medium and operated at a wavelength of 693 nanometres [4]. Looking at figure 1.1, the basic structure of the LASER can be understood. The coiled bulb is a quartz flash tube which generates a population inversion in the ruby, and the ruby crystal inside is highly mirrored on both ends to allow photon oscillation (and therefore stimulated emission of photons).

![Simplified schematic of the basic ruby LASER from 1960. The inner core is a ruby crystal with mirrored ends, wrapped around the outside of this core is a quartz flash tube (image from [5])](image)

In 1962, the first LASER diode (a forward biased GaAs P-N junction) was demonstrated [6]. It was identified to be a LASER as it had a threshold current beyond which the emission intensity is greatly increased and the spectral peak narrowed significantly [6]. There was another leap forward in LASER technology in
1.2. Introduction to LASERs

1974, as the quantum well LASER was developed. This was demonstrated experimentally the following year [7], and was particularly exciting as the wavelength of QW LASERs could be controlled by the thickness of the quantum wells in the active region. Prior to this, the wavelength of a LASER was entirely dependent on the properties of the materials used to fabricate the LASER. In the early 1990s, several alternative LASER designs such as VCSELs [8] (A laser device in which emission occurs perpendicular to the top surface) and quantum dot LASERs [8] were developed and demonstrated. But the final huge step forward occurred in 1994, with the invention of the quantum cascade LASER (QCL). This was significant as these are the first LASER devices that do not depend on conduction-valence band electron transitions [9], instead relying on transitions occurring entirely within the conduction band. QCLs are also capable of reaching wavelengths that are typically difficult to attain with previous LASER designs, which gives them great potential for future applications.

1.2.3 Applications

When many people hear the word LASER, perhaps the first thing that comes to mind is a simple LASER pointer (or perhaps a futuristic weapon in a sci-fi film). In fact, LASERs are currently used for a great deal of essential applications. High power LASERs can be used to cut metal with extreme precision for industrial purposes [10]. LASERs are also used in the fabrication process of microscopic electrical devices, as they are required to break down photoresist layers so they can be removed by etching. LASERs can be used in medicine, achieving analgesic effects through a process called LLLT (low level LASER therapy) [11], and more famously for LASER eye surgery. They also have extensive applications in the electronics and communications industry, a well-known example being computer CD drives [12] and data transmission [13]. There are a myriad of applications for LASERs in modern society, and with LASER technology still undergoing development, they will only become more ubiquitous as time goes on.
1.2. Introduction to LASERs

1.2.4 Recent work

As was mentioned in section 1.2.2, the advent of the quantum cascade LASER has increased hopes of developing a device capable of easily producing THz radiation. This would allow a great deal of applications to become a reality, such as illicit substance detection [14], as well as applications in astrophysics [15] and communications [16]. Recently, there have been multiple routes to advance LASER technology, such as incorporating a graphene layer into a grated QCL waveguide. If a bias is applied to the graphene layer, then the lasing mode frequency can be changed. This offers the potential for electronically tunable LASERS, which could be used for many applications [17]. There are also several groups working on improving the temperature range at which QCLs can be operated (as currently many QCLs require extremely low temperatures). This would be a useful development as it would increase the ease of use and allow QCLs to be used for more commercial applications.

1.2.5 Future prospects

The future of LASERs is very bright indeed, as there are many new and exciting ways in which LASERs are being applied, often with potential to revolutionise entire fields of science. Carbon nanotube SPASERs, a new development in the field of photonics and plasmonics, have great potential as it may be possible to use them to create ultrafast nanocircuits [18]. In recent years there have been a number of medical advances using LASERs (specifically in dermatology) [19], and future applications will involve using wavelengths outside the visible and infra-red range [19]. Other possible future applications of radiation in the THz region (perhaps using a THz QCL as the source) include improved security [20], medical scanning [21], data transmission [22] and many others.
1.3 Principles of Lasers

1.3.1 Stimulated and spontaneous emission

Spontaneous emission is the emission of a photon (with random phase and direction), caused by an electron moving from a high-energy orbital to a lower energy orbital. The energy of the emitted photon is equal to the energy difference of the orbitals, and the frequency is correlated to the energy difference by a constant $h$ (i.e. $E = hν$, where $h$ is Planck’s constant) [1].

![Energy state diagram for spontaneous and stimulated emission.](image)

Stimulated emission is somewhat different. Although the radiation is still emitted by the transition of an electron from a higher to a lower energy state (as in spontaneous emission), stimulated emission is induced by a collision between a photon and the excited electron. This differs from spontaneous emission because spontaneous emission occurs randomly, whereas stimulated emission is triggered. After the
collision, the incident photon also continues to propagate, meaning the number of photons involved in the interaction has doubled. The photon that was released by the electron in this interaction is a "stimulated" photon, and has identical properties (phase, polarisation and wavelength) to the incident photon [23]. It is important to note however, that not every incident photon leads to a stimulated photon.

1.3.2 Population inversion

A "population inversion" refers to the state of a system having more electrons in an excited state than in a lower energy state. It is called an "inversion" because it is the inverse of the usual state, in which the majority of electrons are in the lower energy levels. This state can be achieved by using an external LASER to "pump" electrons from the lower energy state to the higher energy state. A population inversion is desirable because if the population of electrons is greater in the higher energy state than the lower energy state, then the material can act as a "photon amplifier" and lasing can occur [23]. If the population of electrons is greater in the lower energy state however, then the material will act as a photon absorber.

![Figure 1.3: (a) Electrons are in the ground state (green) (b) Electrons have been "pumped" to a higher energy state (red) by an external energy source [1]](image)

1.3.3 Optical and electrical pumping

Optical pumping is the process of using a second LASER to produce the population inversion. Initially light is input from an external source into the active region of the LASER which excites the electrons into a higher energy state, meaning they can take part in stimulated emission. For a simple two-level system, this method of pumping would not work in the steady-state, as the absorption and stimulated emission will compensate one another and cause electronic transparency of the material [23].
increasing the number of energy levels used in the pumping process to three or four, it is possible to achieve a population inversion. In a three-level system for example, if there is pumping from ground level to level three, and then a rapid transition from level three to level two, it is then possible to achieve a population inversion between level two and the ground state [23].

In diode LASERs, pumping can be electrical rather than optical, meaning the pump takes the form of an input current. Electrical pumping can also be used to pump quantum cascade lasers, in which the gain in the LASER is caused by an increase in the number of electrons.

1.3.4 Gain and Loss

In an active material, energy can be stored as potential energy via the existence of high energy state electrons and holes. Gain (synonymous with amplification) is the process by which some of the energy stored in the active material is transferred to an electromagnetic wave. This energy transfer takes place by recombination of an electron and a hole, which releases a photon.

A positive value of gain corresponds to amplification of the propagating wave. If the value of gain is negative however, then the power of the wave will decrease as it passes through the active material (referred to as loss/absorption). Without a population inversion, the absorption rate will be higher than the gain as there will be more electrons in the lower state becoming excited, than electrons in the excited state being stimulated. As a result of this we would not expect lasing without a population inversion. The lasing threshold is the level of electron excitation that results in a net gain equal to zero, meaning that the gain is exactly balanced with the losses in the active material.

1.3.5 Bragg gratings

Bragg gratings are an important component of some types of LASERs, although they can also be implemented in materials without gain to create a passive optical filter. We will now discuss the basic principles of the Bragg grating.
A Bragg grating is a periodic structure that can be used to selectively allow certain frequencies of radiation to pass through. An example of this phenomenon is the colourful pattern that occurs on the back of a CD ROM when viewed under white light, this is caused by Bragg diffraction [12].

We now consider a structure comprised of alternating layers of different refractive index (as shown in figure 1.5). In such a structure, the coefficient of reflection is given by

$$r_n = \left( \frac{b_0}{a_0} \right)_{b_N=0}$$

(1.3.1)

This is the ratio of the reflected amplitude $b_0$ to the incident amplitude $a_0$ [24], assuming that there is no incident light at the far end of the structure.

It is possible to use a matrix method to solve for the reflectance, however this will not be shown until later in the thesis.

The main feature of a Bragg reflector is a high reflectance over a certain frequency band (centred around a frequency known as the Bragg frequency), which is determined by the thickness of the alternating strata. A classic example is the "quarter wave stack" in which the thickness of each layer is one quarter of the Bragg wavelength of the radiation in that material (ie: $d = \frac{\lambda}{4n_m}$, where $\lambda$ is the vacuum wavelength of the Bragg wavelength and $n_m$ is the refractive index of material $m$).
If we think of each 2 layered section as a "unit", then it can be seen that the optical path length for a round trip from one unit cell is a full Bragg wavelength. This means that at the Bragg wavelength, the backward propagating reflected waves will interfere constructively with each other, which will cause high reflectance.

Gain is not a necessary feature of a Bragg reflector, and it is possible to have an optical filter that does not change the energy of the light, this is called a "passive" filter [23]. If there is gain in the filter however, then it is called an "active" filter. Both of these models will be discussed in more detail later in the report.

1.3.6 Grating coupling constant $\kappa$

We can also introduce the "grating coupling constant" $\kappa$ at this point. This is a measure of the reflection per unit length in a grating. This can be easily calculated for a Bragg grating reflecting at the Bragg frequency. This is done by considering a single "unit" of one high refractive index and one low refractive index section (of length $d_m = \frac{\lambda}{4n_m}$). In such a structure the reflectance for this unit is [12]:

$$\rho = \frac{n_1 - n_2}{n_1 + n_2} \quad (1.3.2)$$
Which can be extrapolated to find the reflectance per unit length, which is:

\[ \kappa = \frac{4}{\lambda_m} \rho = \frac{4}{\lambda_m} \frac{n_1 - n_2}{n_1 + n_2} \]  
(1.3.3)

If we multiply this by the length of the grating then we retrieve \( \kappa L \), which is a useful parameter to determine the performance of the grating [12]. A typical values for \( \kappa L \) is approximately 2.

### 1.3.7 Density of modes (DOM)

The density of modes is defined to be the number of modes per unit frequency \((dk/d\omega)\), and it is a useful measure of whether a LASER is lasing. When the DOM is high it indicates a lasing mode, and where the DOM is low it indicates a non-lasing mode or suppressed region. The DOM can also be used to predict threshold gain and the frequency of the lasing modes in a photonic structure and so it is an incredibly powerful tool. The DOM can be found analytically [25], however the derivation of the DOM is dependent on the transfer matrix method (which has not yet been discussed). We will quote the result here however.

Using the transfer matrix method, it is possible to find a single matrix that defines the output radiation in relation to the input. In this matrix \( M \), the transmission coefficient is defined to be \( t = 1/M_{11} \), and the transmission coefficient has real and imaginary components \((t = x + iy)\). After some differentiation and algebraic manipulation, it can be found that the DOM \((dk/d\omega)\) is [26] [25]:

\[ \rho(\omega) = \frac{dk}{d\omega} = \frac{1}{d} \frac{y'x - x'y}{x^2 + y^2} \]  
(1.3.4)

where \( \rho \) is the DOM, \( d \) is the total length of the photonic structure and the dash refers to a derivative with respect to \( \omega \) (which can be calculated numerically).

### 1.4 Types of Lasers

#### 1.4.1 Fabry-Perot

Fabry-Perot (FP) LASERs are an important type of LASER, and of the original diode LASERs all were FP LASERs [12]. FP LASERs are useful to consider as the
phase and gain conditions necessary for lasing are relatively simple to understand compared to many modern LASERs. We will now follow and discuss the derivation for the oscillation conditions of a FP LASER from [12].

If we begin by considering a simple plane wave oscillating back and forth in the FP cavity. Then to establish an ansatz for the equation of the plane wave, we must consider the angular frequency, propagation constant and also the gain and loss occurring as the wave propagates.

The wave will have propagation constant $\beta = \frac{2\pi}{\lambda_m}$ and will have angular frequency of $\omega = 2\pi f$. If we also consider that the wave will have scattering losses and gain per unit length, we can also include a term $(g_m - a_m)$ to account for the overall gain/loss per unit length. We can form the ansatz for the forward propagating (left-right) wave. This will be:

$$E_{\text{forward}}(z) = E_0 e^{(g_m - a_m)z} e^{-i\beta z} e^{i\omega t} \quad (1.4.5)$$

for a FP cavity of length $L$ (also assuming that reflection causes no phase shift in the wave). Note at this point that the gain and absorption terms have been expressed separately as $g_m$ and $a_m$ respectively. This is not necessary and they could be expressed as a combined term (negative for a lossy material and positive for an active material). The equation of the wave travelling ”backwards” (right-left) after reflection, will be given by:

$$E_{\text{backward}}(z) = [E_0 \rho_{\text{right}} e^{(g_m - a_m)L} e^{-i\beta L}] e^{(g_m - a_m)(L-z)} e^{-i\beta(L-z)} \quad (1.4.6)$$

This wave then travels backwards towards the left facet (starting point) and will once again be reflected, joining the forwards travelling wave we have considered previously. For the system to be oscillating stably, we require that the phase after the round trip is equal to the initial phase, we require that the amplitude is equal also.

The equation describing the forward propagating wave reflected from the left facet is given by:

$$E_{\text{forward}}(z) = [E_0 e^{(g_m - a_m)(2L)} e^{-i\beta(2L)}] (\rho_{\text{right}} \rho_{\text{left}}) e^{(g_m - a_m)z} e^{-i\beta z} e^{i\omega t} \quad (1.4.7)$$
1.4. Types of Lasers

For this to fit the amplitude and phase conditions for stable oscillation, we require
that this has the same phase and amplitude as the initial wave. This allows us to
derive an amplitude and a phase condition.

The amplitude condition is given as:

\[ E_0 e^{(g_m - a_m)(2L)} e^{-i\beta(2L)} (\rho_{\text{right}}\rho_{\text{left}}) = E_0 \tag{1.4.8} \]

\[ (\rho_{\text{right}}\rho_{\text{left}}) e^{(g_m - a_m)(2L)} = 1 \tag{1.4.9} \]

With the phase condition being given by:

\[ e^{-i\beta(2L)} = 1 \tag{1.4.10} \]

\[ \beta L = N\pi \tag{1.4.11} \]

Where \( N \) is an integer \([12]\).

![Relative power spectrum](image)

Figure 1.6: FP LASER spectrum (image from [12]) operating around the central
wavelength of 1.55\(\mu m\). Power is highest at the central wavelength, and reduces
further from this wavelength. We can use such plots to find the gain profile of an
FP laser.

This is a very oversimplified model, as both the absorption and the gain coef-
ficients are (in reality) dependent on the frequency of the radiation. Which means
this model is not completely accurate, however for the purposes of demonstration it will be sufficient.

In a FP LASER, the initial excitation is caused by spontaneous emission, which occurs over a range of frequency values. The gain spectrum of a FP LASER also covers a range of values, and is highest in the centre and decays away from the peak. We find that in a FP cavity there can be several amplified modes, but it is the central modes that have greatest amplitude. This is shown in figure 1.6.

The standard FP LASER can also be adapted to have other features such as: high power, narrow spectrum or high modulation capability [12]. However these adaptations will not be discussed here.

1.4.2 Distributed Bragg reflector LASER

The next two LASERs (distributed Bragg reflector LASER and distributed feedback LASER) both use a Bragg grating as a key component. The distributed Bragg reflector (DBR) LASER shares some similarities with a FP LASER, however the DBR uses a Bragg grating in addition to the FP cavity. The benefit of including a Bragg grating is that it is a relatively low cost method to achieve single frequency emission.

In a DBR LASER, there is a central cavity (similar to a FP cavity) but on either side (outside the facet) there is a Bragg reflector etched into the device (shown in figure 1.7).

![Figure 1.7: Diagram of a Bragg reflector LASER (image from [12]). There is a Bragg grating on either side of the gain section, which produces frequency dependent mirroring.](image)
The purpose of etching the Bragg grating is so that rather than simply reflecting light of any frequency back into the gain region (as in a FP cavity), the Bragg grating will reflect multiple small reflections back into the cavity [12]. These reflections only interfere constructively at certain wavelengths (specifically those close to the Bragg wavelength). This results in a method for inducing single frequency lasing, rather than multi-mode lasing (as in a FP device).

1.4.3 Distributed feedback LASER

The distributed feedback (DFB) LASER, is similar to the distributed Bragg reflector LASER. However, while the gain and grating regions are two separate entities in a DBR LASER, they are not separated in a DFB LASER. In a DFB LASER the grating is contained within the LASER cavity.

Figure 1.8: Diagram of a wave propagating through a DFB LASER (image from [12]). It can be seen that the grating and the gain section are part of the same structure in this laser.

This means that within the cavity both the forward and backward propagating waves are growing in power due to the material gain and the constructive reflection (shown in figure 1.8). A DFB LASER can operate at two possible frequencies, neither of which is the Bragg frequency. This is because the phase condition in this LASER cannot be met by a wave at the Bragg frequency [12].
1.4. Types of Lasers

Defects can be introduced into the periodic structure in order to achieve single frequency lasing with a DFB LASER. If a defect is introduced with length \( d = \frac{\lambda}{4} \) at the centre of the LASER, then single frequency lasing will occur. The reason for this is that by inserting a defect of this length into the centre of the LASER, an analogue of a DBR LASER is formed. There is a cavity in the centre (formed of the defect section), and then frequency-sensitive, highly reflective mirrors on either side of the cavity (formed by the DFB grating).

1.4.4 Quantum cascade LASER

The quantum cascade LASER (QCL) has a very different operating principle than any of the LASERs discussed thus far. Rather than using the photons produced when an excited electron drops from the conduction band to the valence band, the QCL instead uses the photons produced when an electron drops from one energy level in the conduction band to a lower level in the conduction band. The QCL requires very exact fabrication methods [27], and so is more difficult to fabricate than many other types of LASER.

![Diagram of the energy band structure in a QCL](image.png)

Figure 1.9: Diagram of the energy band structure in a QCL (image from [9]). The electron transitions are intra-band, and it can be seen that one electron can undergo many transitions (thus producing multiple photons).
The inter sub-band transitions are implemented by using a series of quantum wells and also by applying a bias to the material. The purpose of the quantum wells is to induce sharp changes in the energy potential, thus causing quantised energy states [9]. The bias is used to cause sloping of the energy potential along the laser (shown in figure 1.9). Electrons are then passed through the structure, tunnelling through the potential barriers and dropping to a lower energy level, thus releasing an electron. As there is a bias causing sloping of the potential, this cycle can be repeated, meaning that each electron can contribute more than one photon, which is a significant difference to the other LASERs we have discussed (in which each excited electron contributes only one photon).

Looking at figure 1.9, the incoming electron starts at energy level 3, and then tunnels through the potential barrier to energy state 2 (releasing a photon). The electron then tunnels from energy state 2 to energy state 1 and then is passed through to the next unit cell so the cycle can be repeated.

Figure 1.10: Schematic of a QCL (image from [17]). There is a gold waveguide on top of the QCL structure to provide confinement. Some QCLs will also have a metal layer underneath for further confinement, but heavily doped semiconductor can also be used.

One of the key advantages of a QCL over a standard LASER configuration is that frequencies of radiation that can be difficult to attain with a standard LASER can be achieved with a QCL, as the emission frequency of the QCL is largely determined by the QW thickness [28]. Another advantage is that multiple photons can be produced per electron, and so photonic output can be high [28]. Some QCLs (such as mid-
IR) can be operated at room temperature and continuous wave [29], however room temperature lasing remains elusive for the THz region. Finally, QCLs have a higher modulation speed than other semiconductor lasers. This is due to the fact that the electron transitions in a QCL are intraband transitions which occur significantly faster than interband transitions (which occur in other semiconductor lasers).

Figure 1.11: Schematic of single (a) and double (b) metal waveguide, showing confinement of EM radiation (image from [30]). There is distinctly less confinement when a double metal waveguide is not used.

The physical design of a QCL is shown in figures 1.10 and 1.11. The core components are the active region, the waveguide, and the grating (if there is one). The gold waveguide is most visible as it is on the top of the structure, and acts to confine the radiation to the active region below. Beneath the waveguide is the active region (where the QWs are located). The substrate layer below is a heavily doped semiconductor region which also acts to confine the EM radiation (though not as strongly as the gold layer on top). A common adaptation of this QCL design is a double metal QCL (gold on the top and bottom of the active region), the advantage of this is that the EM radiation is even more highly confined than in the single metal design [30].

By using focused ion beam milling, it is possible to cut a grating into the gold waveguide layer. This grating can be periodic or aperiodic, and the resulting reflectance can be calculated using a transfer matrix method. This standard design has been modified in some previous work by incorporating a graphene layer on top of the grating [17]. A bias can then be applied to the graphene, resulting in some
"undoing" of the grating effects. The final result of this is effectively a tuneable QCL, as the lasing characteristics can be changed by the gating of the graphene.
Chapter 2

Theoretical investigation of LASERs

2.1 Transfer matrix method (TMM)

The transfer matrix method is a useful tool for investigating layered photonic structures. Scientific software such as MATLAB can be used to quickly solve the matrix multiplications for greater convenience.

Essentially the method involves alternately multiplying together a sequence of matrices, which correspond to either scattering at the material boundaries or propagation through a layer of material [24]. A full explanation of the method will now be discussed.

If the electric field in a material with refractive index \( n_1 \), between \( x = 0 \) and \( x = L \) (such as figure 2.1) is considered. It can be considered to be composed of a forward propagating and a backward propagating wave. The equation of the field in this material will be given by:

\[
E(x) = E_1 e^{ik_{1x}x} + E'_1 e^{-ik_{1x}x}, \quad 0 < x < L
\]  

(2.1.1)

where \( E_1 \) and \( E'_1 \) are the initial amplitudes of the forward and backward wave respectively, and \( k_{1x} \) is the wavenumber. Mathematically, this is equivalent to the derivation that was covered in the earlier chapter (regarding FP lasers). However, now the term \( E'_1 \) has absorbed the constant exponential term \( e^{ik_{1}L} \) (for algebraic
2.1. Transfer matrix method (TMM)

Figure 2.1: Electric field in material with refractive index $n_1$, it can be seen that there is field propagation in both directions, this can be described by complex exponential terms.

simplicity). Collectively $\phi = k_{1z}x$ is the phase of the field ($k_{1z} = 2\pi n_1/\lambda_0$).

Propagation through a layer of dielectric material can be modelled using a phase matrix to relate the field at each end of the dielectric layer. The fields at the left and right of the dielectric layer are related by the equation:

$$\begin{pmatrix} E^+_{\text{left}} \\ E^-_{\text{left}} \end{pmatrix} = P_1 \begin{pmatrix} E^+_{\text{right}} \\ E^-_{\text{right}} \end{pmatrix}$$

(2.1.2)

with $P_1$ defined by [31]:

$$P_1 = \begin{pmatrix} e^{ik_{1z}L} & 0 \\ 0 & e^{-ik_{1z}L} \end{pmatrix}$$

(2.1.3)

which represents the phase that the field will accumulate as it passes through the dielectric layer.

In addition to the changing phase, it is also necessary to consider the effect of interfaces between materials of different refractive indices in order to formulate the transfer matrix.

Fresnel coefficients are used to create the scattering matrix at the boundary between the two materials. These coefficients are:
2.1. Transfer matrix method (TMM)

The scattering matrix at the interface of layer \( m-1 \) and \( m \) is given by [31]:

\[
S_{m-1,m} = \frac{1}{t_{m-1,m}} \begin{pmatrix} 1 & r_{m-1,m} \\ r_{m-1,m} & 1 \end{pmatrix} 
\]  \hspace{1cm} (2.1.6)

Scattering matrices and phase matrices can be concatenated in order to find the transfer matrix of a more complex structure (such as a Bragg reflector). For example, the field at the left and right of a unit cell is related by:

\[
\begin{pmatrix} E_{+LHS} \\ E_{-LHS} \end{pmatrix} = P_1 S_{12} P_2 S_{21} \begin{pmatrix} E_{+RHS} \\ E_{-RHS} \end{pmatrix} 
\]  \hspace{1cm} (2.1.7)

This method can be extended to any arbitrary lattice structure, simply by concatenating further matrices. So for a Bragg reflector with \( n \) unit cells, the transfer matrix would simply be:

\[
\begin{pmatrix} E_{0+}^n \\ E_{0-}^n \end{pmatrix} = (P_1 S_{12} P_2 S_{21})^n \begin{pmatrix} E_{n+1}^+ \\ E_{n+1}^- \end{pmatrix} = M^n \begin{pmatrix} E_{n+1}^+ \\ E_{n+1}^- \end{pmatrix} 
\]  \hspace{1cm} (2.1.8)

Figure 2.2: Electric field at the interface between a material with refractive index \( n_1 \) and a material with refractive index \( n_2 \).

\[
r_{m-1,m} = \frac{n_m - n_{m-1}}{n_m + n_{m-1}} \]  \hspace{1cm} (2.1.4)

\[
t_{m-1,m} = \frac{2n_{m-1}}{n_m + n_{m-1}} \]  \hspace{1cm} (2.1.5)
where $M$ represents the transfer matrix for a single unit cell. Finally, the total transfer matrix can be used to calculate the transmission and reflection coefficients. This can be done by considering the total transfer matrix $M_{Total}$, this is shown below.

\[
M_{Total} = M^N = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} = \begin{pmatrix} \frac{1}{t_{tot}} & -\frac{r_{tot}}{t_{tot}} \\ \frac{r_{tot}}{t_{tot}} & \frac{1}{t_{tot}} \end{pmatrix}
\]

(2.1.9)

The transmission coefficient is given by

\[
t_{tot} = \frac{1}{M_{11}}
\]

(2.1.10)

and the reflection coefficient is given by

\[
r_{tot} = \frac{M_{21}}{M_{11}}
\]

(2.1.11)

The power reflection and transmission are found by calculating the amplitude squared of these coefficients. The final result is [31]:

\[
T = |t_{tot}|^2 = \frac{1}{|M_{11}|^2}
\]

(2.1.12)

and the reflection coefficient is given by

\[
R = |r_{tot}|^2 = \frac{|M_{21}|^2}{|M_{11}|^2}
\]

(2.1.13)

Gain can also be included in the TMM, by including it as a part of the phase in the propagation matrix. For a standard gainless material, the phase from passing through a material with thickness $d$ is $\phi = k_{1d}d = 2\pi dn_m/\lambda$. If gain is to be included in the model, then a complex component $\phi_i$ is introduced to the phase $\phi$. The complex term will be:

\[
\phi_i = \frac{igd}{2}
\]

(2.1.14)

where $g$ is the power gain coefficient. When this is multiplied into the propagation matrix $P$, it will become:

\[
P = \begin{pmatrix} e^{i\phi} & 0 \\ 0 & e^{-i\phi} \end{pmatrix} = \begin{pmatrix} e^{i(2\pi d/d_n)}e^{(-gd/2)} & 0 \\ 0 & e^{-i(2\pi d/d_n)}e^{(gd/2)} \end{pmatrix}
\]

(2.1.15)
2.1. Transfer matrix method (TMM)

This matches intuition, as now in the propagation matrix there is an exponential term with a real exponent. This means that there will be exponential growth or decay, which is what would be expected in a system with gain. It can also be seen that if \( g = 0 \), then the propagation matrix for the standard gainless optical filter is retrieved.

The TMM can also be used to calculate the density of modes. A full derivation of this is covered in the literature [25], however the key points will be covered here also. As mentioned previously, the definition of the density of modes is:

\[
\rho (\omega) = \frac{dk}{d\omega} \tag{2.1.16}
\]

The transfer matrix method can be used to extract the density of modes [25]. The derivation is started by considering the transmission coefficient \( t \). This coefficient is complex and can be expressed in either cartesian or polar coordinates:

\[ t = x + iy = \sqrt{T} e^{i\phi} \tag{2.1.17} \]

It was stated earlier in the thesis that \( \phi = kd \), and it can be seen from equation 2.1.17, that \( \tan(\phi) = y/x \). This can then be differentiated and simplified to:

\[
\frac{d}{d\omega} (\tan (kd)) = \frac{d}{d\omega} \left( \frac{y}{x} \right) \tag{2.1.18}
\]

\[
\sec^2 kd \frac{dk}{d\omega} = \frac{1}{d} \frac{y'x - x'y}{x^2} \tag{2.1.19}
\]

\[
\left( \tan^2 kd + 1 \right) \frac{dk}{d\omega} = \frac{1}{d} \frac{y'x - x'y}{x^2} \tag{2.1.20}
\]

\[
\left( \frac{y^2}{x^2} + 1 \right) \frac{dk}{d\omega} = \frac{1}{d} \frac{y'x - x'y}{x^2} \tag{2.1.21}
\]

\[
\frac{dk}{d\omega} = \frac{1}{d} \frac{y'x - x'y}{x^2 + y^2} = \rho (\omega) \tag{2.1.22}
\]

This can be calculated numerically from the transfer matrix.
2.2 TMM for a periodic lattice

Now a TMM approach to investigating a periodic lattice will be considered. This is one of the simpler models, however it is useful to discuss before considering an aperiodic lattice structure.

![Figure 2.3: Schematic of a Bragg reflector. This has alternating layers of refractive index \( n_1 \) and \( n_2 \). Each layer has a width of \( d_m = \lambda_0 / 4n_m \).](image)

One of the benefits to studying a periodic structure is that due to the repetitive nature of the structure, the matrices involved in the calculation will repeat also. This can significantly improve the simulation performance as there are several ways to increase efficiency of matrix algebra if the matrices are repeating.

2.2.1 Without gain or loss

A gainless and lossless model is the simplest possible model, so this will be discussed first with simulation results. This model is a distributed feedback structure with each layer having a thickness of \( d_m = \lambda / 4n_m \). The layers have no gain or loss, and so the value of \( \phi \) in the propagation matrix is purely real. The Bragg wavelength used in the simulation is 700nm (roughly 430GHz). The layers are assumed to have refractive indices of 3.6 and 3 (approximately GaAs and AlAs respectively). A range of frequencies are considered to show how this affects the reflectance of the structure.

The first stage is to consider the sections of material that the radiation passes through so the ”unit cell” can be determined. When the transfer matrix of the unit
cell is identified, it can be exponentiated to find the transfer matrix of the complete structure.

\[
E_{Left} = S_{21} P_2 S_{12} P_1 E_{Right} = M E_{Right} \quad (2.2.23)
\]

In order to find the transfer matrix for the entire structure, the unit cell transfer matrix is concatenated \( N \) times (where \( N \) is the number of unit cells in the total structure).

\[
E_{Left} = M^N E_{Right} = (S_{21} P_2 S_{12} P_1)^N E_{Right} \quad (2.2.24)
\]

and \( M \) is the transfer matrix of a single unit cell. The simulation was completed using MATLAB and \( N = 30 \) unit cells to make the complete structure. The reflectance, transmission and DOM results from the simulation will now be discussed.

It can be seen from figure 2.5 that there is high reflectance at the Bragg frequency. This is to be expected due to the nature of a Bragg reflector (discussed in section 1.4.2). This region of high reflection is called a reflection band, and in this example has a bandwidth of roughly \( 0.04 \lambda_{Bragg} \). In this region, very little radiation penetra-
2.2. TMM for a periodic lattice

Figure 2.5: Reflectance at frequencies near to the Bragg frequency (2.897 THz), \( n_1 = 3.6, n_2 = 3.73 \) and \( N = 30 \)

Figure 2.6: Transmission at frequencies near to the Bragg frequency (2.897 THz), \( n_1 = 3.6, n_2 = 3.73 \) and \( N = 30 \)

Successive smaller reflectance peaks can also be seen as the frequency difference from the Bragg frequency increases.

The graph of transmission has a trough at the Bragg frequency, which shows
that a low proportion of the incident radiation is transmitted through the structure. This is expected as the reflectance is high at the Bragg frequency. Small troughs in transmission can be seen as the frequency difference from the Bragg frequency increases. In a gainless and lossless system such as this, it can be shown that $R + T = 1$ due to conservation of energy. This is a useful check that the MATLAB code is running without errors.

### 2.2.2 With loss

The simulation can be repeated with the introduction of absorption in the material, which results in energy loss as the radiation passes through. The method is essentially the same as before except now there will be a complex component to $\phi$ in the propagation matrix. The absorption axis in figure 2.7 is found by using a constant absorption per unit length and multiplying by the total length of the structure.

![Figure 2.7: (a) Reflectance and (b) transmission at frequencies near to the Bragg frequency (2.897 THz), as a function of both frequency and absorption (negative gain)](image)

From the graph of reflectance, it can be seen that as absorption is increased the reflectance decreases, although the overall shape of the curve remains similar. It can also be seen that as the absorption is increased, the side bands of reflection vanish. This is likely because they are smaller in amplitude than the central band even at zero absorption, and so with absorption they are negligible in amplitude.

Looking at the transmission graph, a similar trend can be seen. As the absorption is increased, the transmission amplitude decreases. This is intuitively reasonable as
if some of the radiation is being absorbed then the transmitted proportion should be reduced.

![Reflectance+Transmission of periodic structure (log10)](image)

Figure 2.8: Reflectance+Transmission is non-constant, as total energy of the wave has changed due to absorption

By plotting a graph of the sum of transmission and reflectance (figure 2.8), the change in total energy can be seen as a function of frequency and absorption. In the gainless/lossless model this would have a constant value of unity.

### 2.2.3 With gain

The model including gain will now be investigated, the differences between this and the model with absorption can now be studied.

Firstly looking at the reflectance graph, the general trend is that as the gain increases, the reflectance increases also. As well as this, there are specific values of frequency and gain where there are significant spikes of reflectance. These are most likely points where lasing will occur, though it is important to verify this by looking at the DOM also.

In previous discussions high reflectance has indicated a lack of wave propagation. In a system with gain however, if we see a point with high reflectance, the transmission must also be checked to see if that is correspondingly high also. If both reflectance and transmission are approaching a singularity then this can indicate lasing.
2.2. TMM for a periodic lattice

Figure 2.9: (a) Reflectance (verified against reflectance plot in [32]) and (b) transmission at frequencies near to the Bragg frequency (2.897 THz), as a function of both frequency and absorption (negative gain)

Next looking at the graph of transmission, the most striking feature is the region of very low transmission through the centre of the frequency band. This is due to the Bragg reflector structure causing reflectance within the central frequency band. In the frequency region outside the low transmission band, it can be seen that there are singularities at points corresponding to singularities in the reflectance. This is increasingly good evidence for lasing, however it is still important to check the DOM at these points also.

From the DOM graph, it can be seen that the singularities agree with the singularities in the reflectance and transmission graphs (and therefore confirm lasing). It may also be noticed however, that for higher levels of gain, the DOM becomes negative. This is a limitation of the transfer matrix method, as it is not physically possible to have a negative density of modes. This issue is often circumvented in the literature simply by labelling these regions < 1. Here the result has been left as a < 0 quantity, but it is important to note that for these higher levels of gain the results are non-physical.
2.3 TMM of an aperiodic lattice

An aperiodic lattice is simply a lattice in which the layers do not have a simple repeating pattern like the structure discussed previously.

Aperiodic lattices can be modelled using the same transfer matrix methods as the periodic lattice, however a shorthand technique for labelling the order of the layers must be developed so that the structure can be described to the computer and the transfer matrix can be formed.

Figure 2.11: Example of the ADFB (aperiodic distributed feedback) vector input into MATLAB

\[
ADFB = [1 \hspace{0.5cm} -1 \hspace{0.5cm} -1 \hspace{0.5cm} -1 \hspace{0.5cm} 1 \hspace{0.5cm} 1 \hspace{0.5cm} -1 \hspace{0.5cm} 1]
\]
2.3.1 Defect modes in a single defect lattice

The effect of including a single $\lambda/(4n_m)$ defect in the centre of a DFB structure will now be discussed. The transfer matrix of this structure can be found relatively easily given the results of section 2.2.

It has been stated earlier that the transfer matrix of a full periodic lattice with $N$ unit cells is:

$$E_{Left} = M^N E_{Right} = (S_{21} P_2 S_{12} P_1)^N E_{Right} \quad (2.3.25)$$

If the single defect structure is broken into sections, the transfer matrix will become apparent. First the periodic structure up to the defect is considered (Section 1 in figure 2.12). This will have $N/2$ unit cells in it, and so the transfer matrix of this section will be:

$$E_{RightDefect} = (S_{21} P_2 S_{12} P_1)^{N/2} E_{Right} \quad (2.3.26)$$

Then the defect matrix is considered, and so for the current matrix:

$$E_{LeftDefect} = P_1 (S_{21} P_2 S_{12} P_1)^{N/2} E_{Right} \quad (2.3.27)$$

Finally the periodic structure after the defect is included, which is the same as the transfer matrix of the first periodic section. So the total transfer matrix will be:

$$E_{Left} = (S_{21} P_2 S_{1,2} P_1)^{N/2} P_1 (S_{21} P_2 S_{1,2} P_1)^{N/2} E_{Right} \quad (2.3.28)$$
From this, the methods used previously can be applied to investigate reflectance, transmission and density of modes.

Figure 2.13: (a) Reflectance and (b) transmission near the Bragg frequency (2.897 THz) for a gainless single defect structure, $n_1 = 3.6$, $n_2 = 3.73$ and $N = 50$.

In figure 2.13, there is now a sharp drop in reflectance in the centre of the high reflectance band at the Bragg frequency, and also there is a sharp peak in the centre of the low transmission region. This is because of similar physics to that discussed in section 1.4.2. These peaks are expected as the structure is effectively a FP structure enclosed in frequency selective mirrors.

The sum of the reflectance and transmission is equal to one, as is the case in the periodic gainless system. This is because the structure is not absorbing or supplying energy to the radiation as it propagates through, so the total power reflected and transmitted is equal to the total initial power.

The result of introducing gain into a single defect structure can be seen from figure 2.14. It can be seen that there is a singularity at the Bragg frequency for a relatively low gain. There are also further singularities at higher gain values with frequency above and below the Bragg frequency. This is a similar DOM plot to that of the periodic structure. However, lasing is now possible at the Bragg frequency also.
2.3. TMM of an aperiodic lattice

2.3.2 Modes in a fully aperiodic lattice

So far, the standard periodic lattice and the single defect lattice have been discussed. Next, the fully aperiodic lattice will be investigated. This is a lattice in which there is no pattern to the order of the layers.

In this model, each layer again has thickness $\lambda/(4n_m)$, however the ordering of the layers is now randomised. The ordering of the layers is represented in MATLAB as a vector of 1s and $-1$s, with 1 corresponding to the high refractive index material and $-1$ corresponding to the low refractive index material.

The transfer matrix is then calculated in the same way as previously, by repeatedly concatenating the relevant matrices. The reflectance and transmission can then be found from the resultant transfer matrix, and the DOM can be calculated as before.

Looking at the reflectance and the transmission surfaces, it can be seen that there are singularities at corresponding points, which is a sign of lasing. The singularities are still symmetric around the Bragg frequency as they were in the models studied previously (periodic and single defect).

Next looking at the DOM of the aperiodic structure, the singularities again
2.3. TMM of an aperiodic lattice

Figure 2.15: (a) Reflectance and (b) transmission of an aperiodic DFB LASER around the Bragg frequency (2.897 THz). Lattice can be described by: 
\[ M^6 D M^9 D M^8 D M^2 M^2 D M^9 D M^8 D M^8 D M^{17} \]  
(M represents a unit cell and D represent a layer of high refractive index)

Figure 2.16: DOM of an aperiodic DFB structure around the Bragg frequency (2.897 THz) with gain, this is the same lattice described in figure 2.15

appear at corresponding points to the reflectance and transmission, thus indicating lasing. The aperiodic lattice is a very versatile lattice as it can be used to generate lasing at a given frequency. This is done by using a Fourier transform technique and reverse engineering the required lattice from the desired spectrum [32] [33].
2.3.3 Other work done involving aperiodic lattice and graphene

There has been significant previous research in our group involving aperiodic lattices [17] [34]. The research involved placing a layer of graphene over the top of the grating cut into the gold waveguide layer of a QCL. It is then possible to electronically dope the graphene in order to change the Fermi level. The result of doping is that the behaviour of the grating is altered, if this can be completely controlled then the outcome could be a fully tunable LASER.

2.4 Spontaneous emission modelling

Though the spontaneous emission in LASERs is random, there are factors that can cause enhancement or suppression of the spontaneous emission rate. The Purcell effect will be discussed first, which quantifies the enhancement of spontaneous emission rate [35]. Fermi’s golden rule will also be discussed. This rule relates the DOM of an EM wave to the probability of an excited electron decaying to a lower energy level [36].

2.4.1 Purcell effect

The Purcell effect is the phenomena by which the spontaneous emission rate of an atom is enhanced by the environment it is in. The spontaneous emission can be enhanced by the atom being at the edge of a photonic band gap, or it can be suppressed by being inside the band gap [26].

The "Purcell factor", which is a measure of the enhancement of the spontaneous emission, can be quantified using the equation [37]:

\[ F_P = \frac{3Q}{4\pi^2V} \left( \frac{\lambda}{n_{eff}} \right)^3 \]  

(2.4.29)

where \( F_P \) is the Purcell factor, \( Q \) is the cavity quality factor, \( V \) is the mode volume and \( n_{eff} \) is the effective refractive index [37].
2.4.2 Fermi’s golden rule

Fermi’s golden rule is given by [26] and [38] as:

\[ \Gamma_{if} = \frac{2\pi}{\hbar} \rho(\omega) \langle f|\mu.E|i \rangle \]  \hspace{1cm} (2.4.30)

where \( \Gamma \) is the probability of transitioning from the initial to the final state, \( \rho(\omega) \) is the density of modes, \( \langle f| \) and \( |i \rangle \) from \( \langle f|\mu.E|i \rangle \) refer to the final and initial wavefunctions of the electron. \( \mu \) refers to the dipole moment, and \( E \) is the electric field.

The spontaneous emission rate is dependent on the density of modes. So for a structure with high DOM at a certain frequency, an enhancement in spontaneous emission at that frequency would be expected.

It is possible to produce an analytical equation for the power enhancement of spontaneous emission using the density of modes in a 1D structure for some simple structures. This is done in a paper by Tocci et al [36], however a more general numerical method will be discussed here.

For this method, it is required to find the amplitude of the electric field at all points along the structure. This can be done by adapting the transfer matrix method [39] to consider the electric field at all points in the structure (rather than only at interfaces). For this method, it is necessary to calculate the forward and backward wave components using the TMM, and then interpolate the field between the interfaces using the equation [39]:

\[ E_i(z) = \Omega_i^+ \exp(i[k_i(z - z_{i-1})]) + \Omega_i^- \exp(-i[k_i(z - z_{i-1})]) \]  \hspace{1cm} (2.4.31)

in which \( \Omega_i^{+-} \) is the coefficient of the forward and backward electric field respectively, \( z_{i-1} \) is the position of the \( (i - 1) \)th material interface and \( k_i = n_i\omega/c \).

This will be combined with the DOM in order to find the enhancement of spontaneous emission (to within a scaling constant) as shown below [36]:

\[ P_\omega(z) = C \rho_\omega |E_\omega|^2 \]  \hspace{1cm} (2.4.32)
2.4.3 Methodology for modelling spontaneous emission

Initially, the method to calculate the electric field within the Bragg reflector will be discussed in detail. While this work can be completed analytically (following the method described in [40]), later work (single defect and aperiodic lattices) cannot be solved as simply. As a result of this, the method discussed here is computational and can be applied to any arbitrary lattice.

The first step in the calculation is to calculate the transfer matrix of the field passing through the lattice. This is done using the same method as described in section 2.1.

In this instance, it is not only the total transfer matrix of the structure that is important. The transfer matrix of the structure leading up to each interface is required in order to calculate the electric field throughout the structure. This is because in order to describe the electric field within the strata, it is essential to know the forward and reverse wave components at the interfaces.

The incident wave can be shown as a vector, with forward and backward components:

The method used to calculate the coefficients of the electric field at each interface is a version of the TMM [39]. We first define matrices to describe the reflection and transmission at the interfaces:

\[
D_j = \begin{pmatrix}
1 & 1 \\
n_j & -n_j
\end{pmatrix}
\] (2.4.33)

in which \(j = 1, 2\) represents the high/low refractive index section of the periodic structure. We also must define propagation matrices:

\[
P_i = \begin{pmatrix}
\exp(ik_j d_j) & 0 \\
0 & \exp(-ik_j d_j)
\end{pmatrix}
\] (2.4.34)

in which \(k_j = n_j \omega/c\), and \(d_j\) is the thickness of the \(j\)th layer in the structure.

Now that these matrices have been defined, it is simple to formulate the transfer matrix at each interface of the structure. An \(N\) period periodic structure can be calculated to be:

\[
T = D_0^{-1}(D_2 P_2 D_2^{-1} D_1 P_1 D_1^{-1})^N D_0
\] (2.4.35)
From this matrix, it is possible to calculate the coefficient of reflectance \( r(\omega) = 1/T_{1,1} \), this is then used to define the coefficients of the incident field.

\[
E_0 = \begin{pmatrix} \Omega_0^+ \\ \Omega_0^- \end{pmatrix} = \begin{pmatrix} 1 \\ r(\omega) \end{pmatrix}
\] (2.4.36)

In order to calculate the coefficients of the field at each interface, it is necessary to calculate the transfer matrices leading up to the interface.

\[
E_1 = D_2^{-1} P_1 D_1 E_0
\] (2.4.37)

This is done iteratively, using the formula:

\[
E_j = \begin{pmatrix} \Omega_j^+ \\ \Omega_j^- \end{pmatrix} = D_{j+1}^{-1} P_j D_j E_{j-1}
\] (2.4.38)

When the field coefficients at each interface are calculated, the field can be interpolated between the interfaces to find a description of the electric field at all points in the structure. This can be done using the formula:

\[
E_i(z) = \Omega_j^+ \exp(ik_i(z - z_{i-1})) + \Omega_j^- \exp(-ik_i(z - z_{i-1}))
\] (2.4.39)

Where \( i \) indicates the layer number, \( z \) is the position along the structure, and \( z_{i-1} \) is the \( z \)-coordinate of the preceding interface. Finally, the intensity of the electric field can be calculated by:

\[
I_i(z) = n_i^2 |E_i(z)|^2
\] (2.4.40)

In addition to being useful for calculating the intensity of the electric field throughout the structure, this method can be used to calculate the spontaneous emission rate of a dipole positioned within the layered structure. This is done simply by multiplying the magnitude of the electric field by the density of modes, as shown [40]:

\[
P(\omega, z) = C \rho(\omega) |E_i(z)|^2
\] (2.4.41)

### 2.4.4 Modelling spontaneous emission in a periodic lattice

The results of this calculation for a periodic structure will now be demonstrated and compared to a verified source [39] to validate the method used.
Figure 2.17: Electric field magnitude in periodic lattice from (a) calculations conducted by the author and (b) calculations from [39] (N = 50, n_1 = 1.6170, n_2 = 2.9546, λ = 848nm)

As can be seen from figure 2.17, the code has been verified to be correct and it can be seen that in the centre of the lattice, the intensity is significantly increased (by a factor of approximately 30) when compared to the field than at the outer edges. This increase is due to constructive interference of the field in this region of the lattice.

The spontaneous emission is proportional to the intensity in this case, as the calculation has been conducted at a single frequency. At all points in the lattice the DOM is identical and so this will simply scale the result of figure 2.17 (which is subject to a scaling constant already).

The effect of the DOM on the spontaneous emission can be observed by extending the previous work and considering a range of frequencies. As the method has been verified by comparison to published work, a quarter wave stack (QWS) will be considered next. A classic feature of the QWS is that the DOM is low at frequencies near the Bragg frequency and high at the band edge, this leads to an increase in spontaneous emission at the band edge. The results of the spontaneous emission calculation are displayed in figure 2.18.

It can be seen in figure 2.18 that the simulation does indeed produce the expected
2.4. Spontaneous emission modelling

2.4.5 Modelling spontaneous emission in a single defect lattice

The calculation is now repeated for the single defect lattice and the results are displayed in figure 2.19. It can be seen that the profile of the electric field intensity is markedly different than in the periodic lattice. In this structure the electric field intensity is notably higher before the defect, this could be explained by high
2.4. Spontaneous emission modelling

reflectance (caused by the defect) resulting in a half-length periodic lattice to the left of the defect. This explains why the profile of the electric field before the defect is very similar to that of field within the periodic lattice (shown in figure 2.17). This is further supported by the low field intensity to the right of the defect, as a large proportion of the field is reflected backwards rather than passing through the defect. It can also be seen that in this structure, the maximum intensity is significantly lower than it was in the periodic lattice, showing that overall the defect has inhibited constructive interference.

![Electric field intensity - Single-defect lattice](image)

Figure 2.19: Electric field magnitude in a single defect lattice with the defect located centrally \((N = 50, n_1 = 1.6170, n_2 = 2.9546, \lambda = 848\text{nm})\)

2.4.6 Modelling spontaneous emission in an aperiodic lattice

As can be seen from figure 2.20, the field intensity at the left hand side (beginning) of the lattice is significantly higher than in the centre, as it has dropped to a lower intensity after encountering a defect in the structure. This is consistent with what has been seen with the previous simulations (figure 2.19 and figure 2.17 a)
As discussed previously (in section 2.4.4), the DOM has no effect when a single frequency is considered, this is because the DOM is constant throughout the structure. When multiple frequencies are considered however, the DOM will have a significant effect on the spontaneous emission. This is shown in figure 2.21, as it can be seen that the spontaneous emission is strongly inhibited except for very narrow frequency bands (in which the SE is notable).

![Electric field intensity - Aperiodic lattice 1](image)

Figure 2.20: Electric field magnitude in aperiodic lattice 1, lattice structure shown by red line (refractive indices are scaled, \(n_1 = 1.6170, n_2 = 2.9546, \lambda = 848\)nm). Lattice can be described by: \(M^{14}D^2M^2D^2MD^5MD^2M^2D^2M^4D^3MD^2MD^2M^{14}\) (\(M\) represents a unit cell and \(D\) represent a layer of high refractive index)

From figure 2.21, it can be seen that in addition to frequency, the spontaneous emission is affected by position in the lattice (as it was with the periodic lattice). In the high frequency band, the spontaneous emission rate is enhanced throughout the whole lattice (albeit by a varied amount). Whereas in the lower frequency band, the spontaneous emission rate decreases in the far side of the lattice. It is notable however that the enhanced frequency bands are far narrower in this lattice than any of the previously considered lattices.
2.5 Chapter summary

This chapter begins with a discussion of the transfer matrix method, and how it can be used to model the physics in a layered dielectric structure. Following this several lattices are investigated, and the results will be discussed here.

The first lattice that was investigated was a Bragg reflector structure. This was chosen because the transfer matrix has already been used to investigate this structure in the literature, and so by repeating this investigation and comparing the result to results from the literature [32], I was able to verify that the simulation was running as it should be. This also demonstrated how plotting the reflectance and transmission plots can be used to find lasing conditions. Finally, this first model demonstrated a key limitation of the transfer matrix method. Which is that under certain conditions of gain and frequency, the transfer matrix can produce sub-zero results for the density of modes, which is unphysical and should be disregarded.

Following the investigation of the Bragg reflector, a single defect lattice was investigated, and was again compared to previous work from the literature for validation. The key difference between the periodic lattice and the single defect lattice

Figure 2.21: Spontaneous emission in aperiodic lattice 1 ($n_1 = 1.6170$, $n_2 = 2.9546$, $\lambda_b = 848\text{nm}$). This is the same lattice as described in figure 2.20.
was that lasing at the Bragg frequency is permitted in a single defect lattice (as demonstrated by the reflectance, transmission and density of modes plots). After this the TMM was used to investigate a fully aperiodic lattice. This yielded the interesting result that the lasing modes were again symmetric around the Bragg frequency (not necessarily an intuitive result).

The key results of this chapter come with the investigation of spontaneous emission enhancement. This uses results from [39] and [40], and combines these methods in order to calculate the spontaneous emission rate enhancement of a dipole emitter at any point in an arbitrary lattice. This is done by using the standard TMM in order to calculate the density of modes, and also using an adapted TMM to calculate the electric field at all points in the lattice by interpolating between the interfaces of the dielectric layers. This investigation produced intuitively reasonable results for the Bragg reflector, showing a suppression of spontaneous emission around the Bragg frequency, and enhancement at the band edges. The results for the aperiodic lattice are a much narrower frequency band with spontaneous emission enhancement, with suppression at all other frequencies. There is also an asymmetric distribution of enhancement along the length of the cavity, which may be expected for an aperiodic lattice.
Chapter 3

Plasmons

3.1 Introduction to plasmons

"Plasmons" are collective oscillations of the electron plasma of a material induced by incident radiation [41] at the boundary between certain materials. Plasmons allow electromagnetic energy to be localised to length scales shorter than the wavelength of the incident radiation. As a result of the tight confinement, the intensity can be very high compared to free-space radiation.

Although the effects of plasmons were first noticed in 1899, the physics was not understood for many more years. There was some development in the 1950s, but plasmonics in its modern form only became a field of interest in the late 1990s, after the publication of a seminal paper [42]. In this paper it was realised that at certain frequencies of light, the emission through an array of sub-wavelength holes was greatly enhanced, and this was correctly attributed to plasmonic activity.

3.1.1 Current and potential applications

Due to the fact that plasmons can be confined to small length scales [43], plasmonic technology lends itself to applications in which downsizing of components is desirable. An example of such an application is nanolithography [44]. As plasmons are not limited by the Abbe diffraction limit [44], this technology is very promising in this field. As well as this, the physics of plasmons is more clearly understood than the photon transport methods in similar near-field optical energy devices [45].
Due to the extreme sensitivity of plasmons to the topology of material interfaces, and also due to their high intensity, plasmons can be very useful for sensing. Plasmonic technology can enable the detection of a single molecule bound to a metal particle [46].

It is also hoped that in the future plasmonics may be able to significantly improve computing technologies by improving integration of photonic devices [44] [47].

### 3.2 SPASER (Surface plasmon amplification and stimulated emission of radiation)

The concept of SPASERs was introduced in 2003. In the SPASER, the fundamental component is surface plasmon polaritons (SPPs). SPPs are propagating plasmons and have useful properties such as tight confinement [43]. The SPASER is the surface plasmon version of a LASER. In a SPASER, surface plasmons act analogously to photons in a LASER [48], as they are amplified by an active medium. This is possible because the SPs share many necessary relevant features with photons. There are several possible approaches to making the SPASER a viable and useful tool, and some SPASER concepts will be discussed now.

#### 3.2.1 Plasmonic LASER antenna

This is a surface plasmon device that is heavily based on the usual LASER diode structure, except at the end facet there are gold nanorods [41]. The result of this is that the field in the region of these nanorods is greatly enhanced (by a factor of approximately 800). The spot size of this SPASER was observed to be on the order of tens of nanometers, which means it could be used in several applications (such as near field optical microscopy).

This SPASER can also be altered to have a "bow-tie" shaped gold structure on the end facet, the result of this is a further increase in the field intensity.
3.2. SPASER (Surface plasmon amplification and stimulated emission of radiation)

3.2.2 Metal-dielectric nanoshell SPASER

A promising type of SPASER is the metal-dielectric nanoshell SPASER [48]. This consists of a dielectric nanoparticle core, with a metal shell surrounding it, and an outer coating of several monolayers of quantum dots.

In this type of SPASER, when an incident photon is absorbed, it causes an
3.2. SPASER (Surface plasmon amplification and stimulated emission of radiation)

electron-hole (E-H) pair to form in the QD layer, which then drops to an excitonic state [45]. When the exciton recombines, the energy is transferred to the metal nanostructure to form resonant surface plasmons (SPs).

A complementary SPASER design is to have a metal nanoparticle surrounded by the dielectric. This is discussed in a paper by Noginov et al [49], but will not be discussed further here.

3.2.3 V-shaped SPASER

![Diagram of V-shaped SPASER](image)

Figure 3.3: Local field amplitude within the V-shaped structure (diagram from [46])

Another category of SPASER is a V-shaped metallic nanostructure on a dielectric [46]. The gain in this system seems to be best when provided by semiconductor quantum dots for several reasons, such as the potential for frequency tunability due to quantum confinement in the QDs [46].

In the far zone, the spasing will be seen as having very narrow spectrum and high spectral intensity, which are desirable features for a SPASER.

3.2.4 Carbon nanotube SPASER

Another potential SPASER device is one made up of carbon nanotubes (CNTs) and a graphene nanoflake. This has great potential for applications such as flexible electronics to make “smart-clothing” [50]. This type of SPASER is investigated
3.3. Plasmons from first principles

theoretically in a paper by Rupasinghe et al [18], in which the system has a pump LASER causing excitons to form in the CNT, these excitons then interact with the SPs in the graphene flake to provide gain.

Figure 3.4: Schematic of a CNT SPASER, excitons in the CNT excite plasmons in the graphene nanoflake (diagram from [18])

This SPASER design has great potential as several theoretical studies have shown that graphene has superior plasmonic properties when compared to noble metals, such as improved tunability, and better field confinement [18].

3.3 Plasmons from first principles

A preliminary investigation into simple plasmonic models is very useful to assist with developing overall understanding of how plasmons may behave in different situations. This becomes useful for identifying potential errors in more advanced simulations.

In this section, a first principles approach is taken to investigate the behaviour of plasmons in some simple situations (such as those described in "Introduction to Graphene plasmonics" [47]).
### 3.3.1 Single boundary

The simplest model to consider is a 2D model consisting of an infinitely long interface between a metal and a dielectric (Shown in figure 3.5).

![Figure 3.5: Schematic of a single interface between dielectric and metal](image)

In this model, surface plasmon polaritons (SPPs) can propagate along the interface. The field will penetrate further into the dielectric than the metal as the skin depth of metal is very low (approximately 25nm) [48]. First, the transverse-magnetic (TM) modes are considered, these are modes with no magnetic field in the direction of propagation. The TM modes can be written as:

\[
E_j (r, t) = (E_{j,x} \hat{x} + E_{j,z} \hat{z}) e^{-\kappa_j |z|} e^{i(qx - \omega t)}
\]

\[
B_j (r, t) = (B_{j,y} \hat{y}) e^{-\kappa_j |z|} e^{i(qx - \omega t)}
\]

The equations make intuitive sense as there is a term that causes exponential decay as the distance to the interface increases and a term that captures the oscillation in both the x direction and in time. The subscript \( j \) represents the material (material 1 is the dielectric and material 2 is the metal).

The next step is to use Maxwell’s equations to investigate the situation mathematically. \( E_j (r, t) \) and \( B_j (r, t) \) are substituted into the Maxwell equations:
\[ \nabla \times \mathbf{E}_j = -\frac{\partial \mathbf{B}_j}{\partial t} \]  
(3.3.3)

\[ \nabla \times \mathbf{B}_j = \frac{\varepsilon_j}{c^2} \frac{\partial \mathbf{E}_j}{\partial t} \]  
(3.3.4)

It can then be found that:

\[ B_{j,y} = \frac{-\omega \varepsilon_j}{c^2 q} E_{j,z} \]  
(3.3.5)

\[ B_{j,y} = -i \text{sgn}(z) \frac{\kappa_j}{q} E_{j,x} \]  
(3.3.6)

\[ E_{j,x} = -i \text{sgn}(z) \frac{\kappa_j}{q} E_{j,z} \]  
(3.3.7)

\[ \kappa_j = \sqrt{q^2 - \frac{\varepsilon_j \omega^2}{c^2}} \]  
(3.3.8)

Due to boundary conditions on the Maxwell equations at boundaries (continuity of tangential components of electric and magnetic fields) [47]:

\[ E_{1,x} = E_{2,x} \]  
(3.3.9)

\[ B_{1,y} = B_{2,y} \]  
(3.3.10)

This means that the magnetic field can be eliminated, so:

\[ E_{1,x} = E_{2,x} \]  
(3.3.11)

\[ \frac{\varepsilon_1}{\kappa_1} E_{1,x} = -\frac{\varepsilon_2}{\kappa_2} E_{2,x} \]  
(3.3.12)

Which can be solved by:

\[ \frac{\varepsilon_1}{\kappa_1(q, \omega)} + \frac{\varepsilon_2}{\kappa_2(q, \omega)} = 0 \]  
(3.3.13)

This is the dispersion relation, and the value of \( q \) for the SPPs can be determined from this. For this to be satisfied, the signs of the permittivity \( \varepsilon_j \) in each material must be different to one another, an example of this is a metal and an insulator [47].

For this example, the dispersion relation can be solved analytically for \( q_{SPP} \) to find that:

\[ q_{SPP} = \frac{\omega}{c} \sqrt{\frac{\varepsilon_1 \varepsilon_2(\omega)}{\varepsilon_1 + \varepsilon_2(\omega)}} \]  
(3.3.14)
3.3. Plasmons from first principles

The Drude model can be used to model the permittivity of the metal $\epsilon_2$. If there is no loss then the permittivity can be described by:

$$\epsilon_2(\omega) = 1 - \frac{\omega_p^2}{\omega^2}$$  \hspace{1cm} (3.3.15)

Where $\omega_p$ is the plasmon frequency. The results of a simulation of this form can be seen in figure 3.6.

Figure 3.6: (a) E-field at the interface between a metal and a dielectric (b) Profile view of the E-field (Parameters: $\omega_C = 10$THz, $\omega_P = 2$THz, $\epsilon_1 = 3.9$, $\epsilon_2 = -24$)

A wavelike pattern can be seen in the x-direction (along the interface) and an exponential decay can be seen in the z-direction (perpendicular to the interface). From figure 3.6 the penetration depth into the metal layer is seen to be lower as the decay is faster, but close to the interface the electric field is stronger in the metal region. Also by inspection of figure 3.6 we can see that the plasmon has a wavelength along the x-direction of approximately 70$\mu$m. The penetration depth can also be found by considering the length scale it takes for the intensity to reduce by a factor of $e$, however this is not done here.

3.3.2 Double boundary

A slightly more complex example is a model in which there is a layer of one material sandwiched between two layers of a different material.
3.3. Plasmons from first principles

The derivation of the underlying physics is very similar to the single boundary, only in this case there are more boundary conditions to satisfy. The D-M-D model will be considered first. Considering again the TM wave described by:

\[ E_j(r, t) = (E_{j,x} \hat{x} + E_{j,z} \hat{z}) e^{-\kappa_j |z|} e^{i(qx - \omega t)} \]  \hfill (3.3.16)

\[ B_j(r, t) = (B_{j,y} \hat{y}) e^{-\kappa_j |z|} e^{i(qx - \omega t)} \]  \hfill (3.3.17)

Maxwell’s equations are again used and then boundary conditions are applied to find that for \( z < 0 \) \((j = 1)\) and \( z > d \) \((j = 3)\):

\[ B_{j,y} = -\frac{\omega \epsilon_j}{c^2 q} E_{j,z} \]  \hfill (3.3.18)

\[ B_{j,y} = -i \text{sgn}(z) \frac{\omega \epsilon_j}{c^2 \kappa_j} E_{j,x} \]  \hfill (3.3.19)

\[ E_{j,x} = -i \text{sgn}(z) \frac{\kappa_j}{q} E_{j,z} \]  \hfill (3.3.20)

\[ \kappa_j = \sqrt{q^2 - \frac{\epsilon_j \omega^2}{c^2}} \]  \hfill (3.3.21)

In the middle region \( 0 < z < d \) \((j = 2)\), the field is somewhat more complicated. As it is a superposition of two decaying fields, it can be described as:

\[ E_j(r, t) = \left[ \left( E^{(+)\, 2}_{j,z} \hat{x} + E^{(+)\, 2}_{j,z} \hat{z} \right) e^{\kappa_{2z} z} + \left( E^{(-)\, 2}_{j,z} \hat{x} + E^{(-)\, 2}_{j,z} \hat{z} \right) e^{-\kappa_{2z} z} \right] e^{i(qx - \omega t)} \]  \hfill (3.3.22)

\[ E_j(r, t) = \left[ \left( B^{(+)\, 2}_{j,y} \hat{y} + B^{(-)\, 2}_{j,y} \hat{y} \right) e^{\kappa_{2z} z} \right] e^{i(qx - \omega t)} \]  \hfill (3.3.23)

Figure 3.7: (a) D-M-D double interface structure (b) M-D-M double interface structure
These must satisfy the relations:

\[ B_{2, y}^{(+)} \left( \begin{array}{c} + \\ + \end{array} \right)_{2, y} = -\frac{i\omega\epsilon_2}{c^2} E_{2, x}^{(+)} \]  
(3.3.24)

\[ B_{2, y}^{(+)} = -\frac{i\omega\epsilon_2}{c^2} E_{2, x}^{(+)} \]  
(3.3.25)

\[ B_{2, y}^{(-)} = -\frac{\omega\epsilon_2}{c^2} E_{2, z}^{(-)} \]  
(3.3.26)

\[ B_{2, y}^{(-)} = -\frac{i\omega\epsilon_2}{c^2} E_{2, x}^{(-)} \]  
(3.3.27)

\[ \kappa_2 = \sqrt{q^2 - \frac{\epsilon_2\omega^2}{c^2}} \]  
(3.3.28)

There are now two sets of boundary condition as there are two interfaces. The BCs at \( z = 0 \) are:

\[ E_{1, x} = E_{2, x}^{(+)} + E_{2, x}^{(-)} \]  
(3.3.29)

\[ B_{1, y} = B_{2, y}^{(+)} + B_{2, y}^{(-)} \]  
(3.3.30)

and the BCs at \( z = d \) are:

\[ E_{2, x}^{(+)} e^{\kappa_2 d} + E_{2, x}^{(-)} e^{-\kappa_2 d} = E_{3, x} e^{-\kappa_3 d} \]  
(3.3.31)

\[ B_{2, y}^{(+)} e^{\kappa_2 d} + B_{2, y}^{(-)} e^{-\kappa_2 d} = B_{3, y} e^{-\kappa_3 d} \]  
(3.3.32)

These equations are solved for the dispersion relation:

\[ (1 + \frac{\epsilon_2\kappa_1}{\epsilon_1\kappa_2})(1 + \frac{\epsilon_2\kappa_3}{\epsilon_3\kappa_2}) = (1 - \frac{\epsilon_2\kappa_1}{\epsilon_1\kappa_2})(1 - \frac{\epsilon_2\kappa_3}{\epsilon_3\kappa_2}) e^{-2\kappa_2 d} \]  
(3.3.33)

Next, some simulation results will be discussed.

From figure 3.8, it can be seen that there is some interference between the plasmons at each metal-dielectric interface. This is shown by the fact that the overlap of the E-field in figure 3.8, and also by the fact that the field does not fully decay in figure 3.8. The decay is sharp in the central (metal) region, however because of the small size of the structure the field does not fully decay. If the metal layer were thinner, it would be possible that the E-field would be enhanced within the metal structure due to the fact that the field is a sum of the fields decaying from each side.

Comparatively, for the MDM structure the decay is weak within the central region (dielectric) and strongest in the outer regions (metal). From figure 3.9, it can
3.3. Plasmons from first principles

Figure 3.8: (a) E-Field in a D-M-D layered structure (b) Profile of E-Field in D-M-D structure (Parameters: $\omega_C = 10$THz, $\omega_P = 2$THz, $\epsilon_1 = \epsilon_2 = 3.9$, $\epsilon_2 = -24$)

Figure 3.9: (a) E-Field in a M-D-M layered structure (b) Profile of E-Field in M-D-M structure (similar structure to many QCLs) (Parameters: $\omega_C = 10$THz, $\omega_P = 2$THz, $\epsilon_1 = \epsilon_1 = -24$, $\epsilon_2 = 3.9$)

be seen that the electric field decays rapidly on either side of the dielectric region, and the field is largely confined within the dielectric. This is conceptually similar to the design of a double metal QCL waveguide. In which the active region is trapped between two metal layers, which act to confine the E-field to the active region.

3.3.3 Single boundary with graphene

Another interesting model to consider is a single interface between two materials, with a layer of graphene sandwiched between the layers. Due to the presence of the
3.3. Plasmons from first principles

graphene, the system now allows for surface plasmons even at the interface between two dielectric or two metal layers, whereas before the presence of a dielectric-metal interface was required.

Figure 3.10: Schematic of a single graphene interface between two different materials. The presence of graphene removes the restriction that these materials must be metal and dielectric (image from [47]).

For this model, the conductivity for graphene must be considered. This is because the boundary conditions of the Maxwell equations involve conductivity. This was assumed to be zero in the previous models but in this model the graphene conductivity is non-zero.

The conductivity of graphene is comprised of two components: intraband (transitions within either conduction or valence band where momentum is not conserved), and also interband (where transitions are from valence to conduction band, and momentum is conserved). In the THz region, at room temperature and with usual doping conditions the conductivity of the graphene is dominated by the intraband conductivity. So the conductivity is modelled as [47]:

$$\sigma_g(\omega) \approx \frac{\sigma_0}{\pi} \frac{4E_F}{\hbar\gamma - i\hbar\omega}$$  \hspace{1cm} (3.3.34)

Where $$\sigma_0 = \pi e^2/2h$$.

The method of investigation is similar to before, except now the boundary conditions will be [47]:

$$E_{1,x}(x, z) |_{z=0} = E_{2,x}(x, z) |_{z=0}$$ \hspace{1cm} (3.3.35)

$$B_{1,y}(x, z) |_{z=0} - B_{2,y}(x, z) |_{z=0} = \mu_0 \sigma_{xx} E_{2,x}(x, z) |_{z=0}$$ \hspace{1cm} (3.3.36)
Note that in the situation of a metal-dielectric, the right hand side of the boundary condition will be zero. Also, the graphene conductivity is considered to be \( \sigma(\omega) = \sigma_{xx} = \sigma_{yy} \) (which is the case if the graphene is unstrained). This ultimately leaves us with the dispersion relation:

\[
\frac{\epsilon_1}{\kappa_1(q, \omega)} + \frac{\epsilon_2}{\kappa_2(q, \omega)} + \frac{i\sigma(\omega)}{\omega \epsilon_0} = 0 \tag{3.3.37}
\]

Due to the fact that \( \sigma(\omega) \) depends on frequency and \( \kappa_j \) depends on frequency and \( q \), this is an implicit equation with no analytical solution. As a result this must be solved numerically.

Figure 3.11: E-Field at a single graphene interface between air and silicon dioxide \( (\epsilon_{\text{air}} = 1, \epsilon_{\text{SiO}_2} = 3.9, \omega_c = 2\pi \text{THz}, q_c = 0.051 \mu m^{-1}) \) (Same parameters used as in [47])

The plasmonic activity at a single graphene interface between two dielectrics (air and \( \text{SiO}_2 \)) can now be considered. The electric field is shown as a function of \( x \) and \( z \) allowing the spatial distribution of the plasmons to be seen. A noteworthy point is that the plasmons are significantly less confined in this case, as there is no metal to cause rapid decay of the field. It is also important to realise that this graph is flipped relative to the earlier schematic diagram (figure 3.10), and so in this plot the upper layer is \( \text{SiO}_2 \) and the lower layer is air.

It can also be seen that the penetration into the \( \text{SiO}_2 \) layer is greater than the penetration into the air. This is because \( \kappa_2 < \kappa_1 \), meaning that the exponential
3.3. Plasmons from first principles

decay of the field is weaker in material 2 (SiO$_2$).

3.3.4 Spherical particle

The methods that have been previously discussed can be extrapolated to modelling the surface of a small metal nanoparticle in a dielectric medium. This is done by making the assumption that the plasmons are resonant at certain wavelengths [51]. It is assumed that the resonance is formed by a standing wave of two oppositely propagating SPP waves, meaning the plasmon wavelength (of an $m$th order plasmon) will be $\lambda_m = 2\pi r / m$. The wavevector can then be found from $k_m = 2\pi / \lambda_m = m / r$.

![E-Field on the surface of a gold nanoparticle (m = 3, $\epsilon_{air} = 1$, $\epsilon_{Gold} = -8.4953$ at $\omega_c$ [52], $\omega_c = 510$THz, $q_c = 1.809\mu m^{-1}$)](image)

Figure 3.12: E-Field on the surface of a gold nanoparticle ($m = 3$, $\epsilon_{air} = 1$, $\epsilon_{Gold} = -8.4953$ at $\omega_c$ [52], $\omega_c = 510$THz, $q_c = 1.809\mu m^{-1}$)

By combining this approach with the approach we have discussed previously (solving the dispersion relation from Maxwell’s equations), we can achieve a plasmon model for a nanoparticle. In this model the wavevector was found by using the same technique as was used for the single interface planar model that was discussed in section 3.3.1, which was to use the dispersion relation to find $q_{SPP}$ as a function of $\omega_c$, $\epsilon_1$ and $\epsilon_2 (\omega)$. The particle radius (at resonant values) was then calculated in order to complete the model. This model can be considered to be the simple planar model that was initially discussed but rolled into a circular shape. This imposes the requirement that the circumference of the particle be a length that allows resonance
of the wave [51], but overall is very similar.

It can be seen from the model that the E-field has taken a wavelike form with alternating sections of high and low intensity. The model in figure 3.12 has order 3 ($m = 3$), meaning there are that the total circumference of the particle is equivalent to two full wavelengths.

### 3.4 Chapter summary

After a brief introduction to SPASERs, this chapter began by considering a single interface between a metal and a dielectric, and used Maxwell’s equations to derive the properties of surface plasmons appearing at this interface (following work done in [47]). This led to the expected oscillatory behaviour along the interface and the exponential decay as distance from the interface increased.

Following the investigation of a single interface model, double interface models (Both DMD and MDM) were then studied. The MDM model is of particular interest in this thesis, as this most resembles a QCL (with the metal layer above and below the active region). This model demonstrates the optical confinement caused by the metal layers, and it can be seen that the field decays very quickly in the metal layer. This model could be improved by considering a thin metal layer, followed by air (rather than a thick metal layer), as this would be a closer analogue to a QCL. This model is relatively simplistic, and a more complex model could be generated using a physics simulation software such as COMSOL. However, in this thesis a first-principles investigation serves to demonstrate some of the key features of plasmons.

The next model considered was a single interface between two dielectrics with a single layer of graphene at the interface. This is also of interest when considering a QCL, as it is possible to modify the waveguide of a QCL by the addition of a graphene layer. The key result of this model is that the existence of graphene at the interface removes the constraint that materials must have permittivity of different signs, and also that there is a lack of confinement caused by the removal of the metal layer. This model could be furthered by including a grating structure in the metal layer, and then layering the graphene over the grating. However, as this would
hugely increase the complexity of the model, it would be necessary to investigate this using simulation software such as COMSOL.

Finally, the model was extended to investigate a metal nanoparticle, as these are a component in several SPASER designs. This model assumed that due to the extremely short penetration depth of electric field into metals, there would be no interference of fields from opposite sides of the particle. This model incorporated both the work done in [47] And [51]. To further this investigation, it would be useful to verify the results using a simulation software such as COMSOL, or to use Mie theory to investigate the effect of the metal nanoparticle on the field.

In summary, first principles models such as those mentioned throughout section 3.3 can be very useful for improving understanding and developing an intuition for plasmon behaviour. However for more complicated systems, it is usually preferable to use a modelling software such as COMSOL which can take into account many variables that it would be incredibly difficult and time consuming to consider manually.
Chapter 4

Conclusion

I will now summarise some of the key points of the work undertaken within this thesis, and I will endeavor to contextualize some of this work into the wider fields of photonics and plasmonics. I will then consider possible future developments and extensions of the work completed within this thesis.

4.1 Summary

The core goals of this thesis are to build upon previous theoretical work by adapting established methods (such as the TMM and first-principles plasmonic models) so that they can be extended beyond their previous usage.

In section 2.1, the typical formulation of the TMM is described and some results are displayed in order to demonstrate the validity of the methodology used in this thesis. This is done by replicating earlier work produced within our research group [32]. With this formulation of the TMM it is possible to calculate useful quantities such as the reflectance, transmission and the density of modes for an arbitrary crystal lattice. However, this formulation of the TMM is limited, as it can only be used to investigate behavior at the interfaces between layers of a photonic crystal, and cannot be used to study the field within the layers themselves.

Later in the thesis, in section 2.4.3, the TMM is adapted using techniques described in [39] in order to extend the capabilities of the TMM. The alteration of the method enables the study of the field within the layers of the photonic crystal, as
opposed to being limited to the study of the field at the interfaces.

The two formulations of the TMM are then combined in order to calculate the rate of spontaneous emission within an arbitrary crystal lattice. This is a highly useful capability as spontaneous emission is a core component of many laser and SPASER systems, and therefore fine control of this may offer interesting capabilities in the future of these systems.

In addition to this, in section 3.3, a series of first-principles plasmonic models are considered and investigated. This begins with a single metal-dielectric interface, and is then extended to more complex models. The final model considered is a spherical metal nanoparticle, this was selected as it is a component of some SPASER models. This simulation was created by adapting the models discussed earlier in the chapter, with influence from [51].

The overarching theme of the thesis is the study of new and novel nanodevices, specifically SPASERs. However due to the nature of new technology, and the wide range of different approaches to achieving SPASER properties, it is difficult to say which of the SPASER concepts (if any) will become dominant over time. As a result of this, much of the work done in this thesis is fundamental research, rather than being directly applied to any given type of SPASER concept.

## 4.2 Future work

An obvious next step would be to verify the results produced in section 3.3.4 by replicating them using another theoretical method. One approach to this would be to use Mie theory, which is commonly used to investigate the effect of nanoparticles on electromagnetic radiation. After verification, the model could also be extended to investigate the effect of a graphene layer surrounding a dielectric nanoparticle, which is similar to some plasmonic models in which a thin metal layer surrounds a dielectric nanoparticle.

Other possible avenues to extend the plasmonic research would be to replace the first-principles calculations by using a commercial software such as COMSOL to increase the complexity of the models considered. If this were to be done then
more elaborate models such as graphene plasmonic waveguides could be considered, and the behavior of the system with electrical doping at each pixel of the waveguide could be studied further.

Finally, further research may make it possible to bring together the (currently separate) studies of spontaneous emission and plasmonics detailed in this thesis. If a system is considered in which there is a plasmonic waveguide (either metallic or graphene) placed upon a layered semiconductor laser, then by calculating the rate of spontaneous emission in the laser, and using this as the input field for a plasmonic system, the resulting behavior could then be investigated. As this system is conceptually similar to a graphene-altered QCL (due to the plasmonic waveguide), it may provide some insight into the behavior in the graphene QCL system (which is not yet thoroughly understood). As this calculation would be complex, it would be advisable to use commercial software such as COMSOL (which is not discussed significantly within this thesis) rather than the first-principles calculations used here.
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