A FULL-VECTORIAL THEORY OF THIRD-ORDER NONLINEAR OPTICAL EFFECTS IN ALUMINUM GALLIUM ARSENIDE WAVEGUIDES

by

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Abstract

A Full-Vectorial Theory of Third-Order Nonlinear Optical Effects in Aluminum Gallium Arsenide Waveguides

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A full-vectorial theory of third-order nonlinear effects is used to derive expressions for the nonlinear coefficients (NLCs) of waveguide modes in high-confinement Aluminum Gallium Arsenide (AlGaAs) waveguides. The dependence of the NLCs on the crosssection and orientation of AlGaAs-on-insulator (AlGaAsOI) waveguides is investigated via simulation.

The results of the full-vectorial theory are compared to those of various scalar theories used in previous studies of AlGaAs waveguides. It is found that the scalar theories tend to underestimate the NLCs for high-confinement AlGaAsOI waveguides. Two of the three investigated scalar theories do not accurately predict the waveguide geometries that optimize the NLCs.

Examples of applications of the full-vectorial theory to wavelength conversion are demonstrated for AlGaAsOI and plasmonic slot waveguides.

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Chapter 1

Introduction

With the rise of digital technology in modern times, faster, denser data transmission has become necessary. Optical communication and signal processing has the potential to provide higher bandwidth and lower power consumption than conventional electronic methods. Optical signals over fibre are already commonly used for long distance communication and are increasingly used over shorter distances, for example in intra-data center interconnects [1, 2]. Converting between optical and electrical signals for signal processing is undesirable due to high energy consumption and large component size, so it is preferable to perform as much signal processing as possible in the optical domain.

This can be achieved using integrated optical circuits (IOC), which perform signal transmission and processing on a monolithic chip using optical waves channelled through waveguides [3, 4]. IOCs have a lower cost, smaller footprint, higher stability and provide increased optical intensities and longer interaction lengths compared to bulk optics. However, integrated devices that can perform the necessary functions for optical signal processing, including signal generation, modulation, multiplexing, and wavelength conversion, are still under development.

1.1 Integrated Optics

Integrated optical chips can consist of many different materials, including glass or semiconductors. A waveguide is defined by a variation in the refractive index n of the chip material. If a high index material (the "core") is surrounded by a lower index material (the "substrate" below and the "cladding" above the core) it is possible for light to be trapped inside and propagate through the high index core. In general the index can vary in three dimensions, however this thesis will mainly be concerned with waveguides that are invariant in the z (longitudinal) direction, with n varying in the x and y (transverse) directions. In such waveguides, the electric field **E** oscillating at a given frequency ω_0 can be written in terms of a sum of waveguide modes, where a single mode is given by:

$$\mathbf{E}(\mathbf{r},t) = \mathbf{e}(x,y)exp(-i\omega_0 t + i\beta_0 z)$$
(1.1)

where **e** is the mode profile, $\mathbf{r} = (x, y, z)$ is the position, t is time and β_0 is the propagation constant. In this thesis, boldface variables are vectors, while subscripted variables, such as e_x , denote the components of the vector. The concept of waveguide modes will be explored further in Chpt. 2.

Integrated optical waveguides are generally vary small, with dimensions on the order of a few microns down to hundred of nanometers. They are usually fabricated using a process called lithography, which involves the sequential layering and etching of different materials. The limits of lithography impose many constraints on the fabrication of optical circuits and must be considered during the design of waveguide devices.

1.2 Nonlinear Optics

Nonlinear optical processes can potentially perform many of the functions required for optical signal processing [5, 6], including signal regeneration [7], wavelength conversion for wavelength division multiplexing (WDM) [8], frequency comb generation [9], and entangled photon generation [10]. The interaction of an electric field \mathbf{E} with matter is mediated by the polarization \mathbf{P} of the medium. In nonlinear materials the polarization can be expressed as a Taylor expansion:

$$\mathbf{P} = \chi^{(1)} |\mathbf{E} + \chi^{(2)}| \mathbf{E}^2 + \chi^{(3)} |\mathbf{E}^3 + \dots$$
(1.2)

where $\chi^{(i)}$ is the *i*th order susceptibility [11], which is an (i + 1)th order tensor, and the vertical bar | denotes tensor multiplication. Typically the nonlinear terms are much weaker than the linear term and can be ignored. However, for high powers in waveguides with a small cross-section they can become significant. Second order effects are nonexistent in materials that possess inversion symmetry, such as silicon and silica. Third order effects are present in all materials though the strength of these effects depends on the material. Effects of the fourth and higher orders are generally ignored in integrated devices.

Third order nonlinear processes, which involve the third order susceptibility $\chi^{(3)}$ and depend on the third power of **E**, involve the interaction of four optical waves with the nonlinear medium [11]. Common third-order effects include self-phase modulation (SPM)

and cross-phase modulation (XPM), which modify the refractive index of the medium in an intensity dependent manner. Another third-order effect is degenerate four-wave mixing (DFWM), which involves the absorption of two "pump" photons with frequency ω_p and the emission of "signal" and "idler" photons with frequencies ω_s and ω_i in a parametric process obeying conservation of energy $(2\omega_p = \omega_s + \omega_i)$.

There have been many demonstrations of third-order nonlinear devices in various material systems, including AlGaAs [12, 13, 14], silicon-on-insulator (SOI) [15], and silica fibres [16].

1.3 High-Confinement Waveguides

Much of modern integrated optics research has focused on the SOI platform due to its low cost, CMOS compatibility, and the prevalence of silicon fabrication infrastructure from the integrated electronics industry. However, silicon has some limitations, in particular an indirect bandgap which makes it a poor material for the creation of light sources or detectors. These limitations are often surmounted by hybrid integration of III-V semiconductors to perform the required active functions, however this introduces additional fabrication steps. For nonlinear applications silicon is also limited by two-photon absorption (TPA), a nonlinear process that induces loss that scales with intensity, limiting the possible power in the waveguide. Due to these drawbacks, research in alternative material systems for integrated optical circuits continues.

A common material for integrated nonlinear devices is Aluminum Gallium Arsenide (AlGaAs) [17]. AlGaAs has a high second- and third-order nonlinearity, transparency in the telecoms wavelength range, and a direct bandgap which is tunable via variation of the Aluminum fraction, allowing the reduction of TPA [18]. These qualities make it ideal for nonlinear devices. Second order nonlinear effects in AlGaAs can be used to perform many of the same functions as third order effects, however due to the phase-matching requirements complicated structures are required [19], increasing the complexity, and therefore the cost, of fabrication.

Traditionally, AlGaAs waveguides have been fabricated as ridge waveguides (for example [20]), or deep-etched nanowire waveguides (for example [21]). The index change in the vertical direction in these waveguides is created by varying the Al concentration, with a higher concentration having lower n. However this variation in n is not very high, resulting in weak optical confinement in the vertical direction. With a small index contrast between the core and the substrate/cladding, the spatial mode profile will not be well confined in the core and will extend a greater distance into the lower index material. In deep-etched nanowire waveguides the horizontal confinement is provided by etching through the core layer, creating strong confinement in the horizontal direction. However, there is still low confinement in the vertical direction, and the deep (several micron) etch also makes it difficult to create some of the structures found in systems with a shallower etch, for example SOI circuits.

Recently, there has been an increase in interest in high-confinement AlGaAs waveguides, for example suspended AlGaAs [22] and AlGaAs-on-insulator (AlGaAsOI) [23, 24, 25], which alleviate some of the drawbacks of the ridge and nanowire waveguide geometries. High confinement waveguides have a small waveguide core cross-section with subwavelength dimensions, as well as a large refractive index contrast between the waveguide core and the cladding/substrate in all transverse directions. The high confinement of these systems means a smaller mode effective area, resulting in higher optical intensities and therefore stronger nonlinear effects. They also have the added benefits of a smaller device footprint, lower bend losses, and increased dispersion control.

A common approach for modelling nonlinear effects in low-confinement waveguides is described in [26], which was developed for silica fibres. In low-confinement waveguides the electric field profile of the modes is primarily in a single, transverse component, mainly resides in the core, and the group velocity is roughly equal to the group velocity in the bulk core material. As the confinement of the waveguide is increased these assumptions are not longer accurate, and therefore a more detailed theory that takes into account these facts is required for high-confinement waveguides.

1.4 Content of this Thesis

The goal of this thesis is to apply a full-vectorial approach to derive expressions for, and calculate the values of, the NLCs for high-confinement AlGaAs waveguides. The full-vectorial approach will take into account the interactions of the various components of the electric field in the waveguide modes, the unique qualities of the AlGaAs third-order susceptibility tensor, and the orientation of the waveguide with respect to the AlGaAs crystal.

Full-vectorial models of waveguide nonlinearities have been developed, primarily for SOI [27, 28, 29, 30, 31, 32] and silica waveguides [33]. However the third-order susceptibility tensor for AlGaAs is different than that of silica and SOI [34], so a new analysis is needed for AlGaAs waveguides. Studies of the anisotropy of the AlGaAs third-order susceptibility tensor have been performed in the past [18, 35], however they have focused on plane waves in bulk media or low-confinement waveguides, not in high-confinement waveguides where multiple electric field components are involved. The results of these analyses will be combined with the full-vectorial theory developed for SOI waveguides to derive expressions for the NLCs suitable for high-confinement AlGaAs waveguides. The characteristics of this model will be investigated via simulations of AlGaAs waveguides of various geometries.

The orientation of the AlGaAs waveguide in the plane perpendicular to the growth direction of [001] will be kept as a variable in the derivation of the expressions for the NLC. The anisotropy of the nonlinearity of bulk materials like silicon [36] and AlGaAs [18] has been studied in the past, however the full-vectorial approach of this thesis will show that the anisotropy of the NLCs is different than that of the bulk material and depends on the mode profiles involved.

As the focus of the thesis is on the NLCs, the dispersion, scattering losses, two-photon absorption, free carrier effects, and Raman scattering will not be investigated. Models that include these effects have been developed for SOI (see, for example, [27, 28]), which could be adapted for AlGaAs waveguides. The results for the NLCs presented here could then be used in this more complete model.

For simplicity, in this thesis the analysis will mainly be focused on a specific type of AlGaAsOI waveguide, that of a rectangular Al_{0.18}Ga_{0.82}As core with width w, height h, completely surrounded by SiO₂ (see Fig. 1.1). At a wavelength of $\lambda = 1550$ nm Al_{0.18}Ga_{0.82}As has a refractive index of n = 3.28 [37] and SiO₂ has an index of n = 1.44 [38].

The band-gap of AlGaAs increases with increasing Al fraction, reducing the effects of two-photon absorption. However, this also reduces both the refractive index n and the Kerr index n_2 , which is undesirable for nonlinear devices. 0.18 is the lowest Al fraction where TPA is negligible at typical optical powers so it is chosen for the core material.

In Chpt. 1 the motivation for this thesis as well as basic concepts in integrated nonlinear optics and high confinement-waveguides has been introduced. Chpt. 2 will further introduce the concept of waveguide modes and develop the theoretical framework that will be used to model third-order nonlinear effects in high-confinement AlGaAs waveguides. Expressions for the nonlinear coefficient for the single-mode case will be derived and its dependence on waveguide geometry and mode type will be investigated in Chpt. 3. A similar analysis will be performed in Chpt. 4 for the cross-phase modulation and four wave mixing nonlinear coefficients involved in two-mode propagation in AlGaAsOI waveguides. In Chpt. 5 the results of our model will be compared to those produced by other approaches that have been used to model AlGaAs waveguides in the past, for both AlGaAsOI and AlGaAs nanowire waveguides. In Chpt. 6 the full-vectorial model



Figure 1.1: Cross section of an AlGaAsOI waveguide with z as the direction of propagation.

will be used to predict the performance of wavelength conversion devices. In Chpt. 7 the results of this thesis will be summarized and potential directions of future research will be proposed.

Chapter 2

Theory

In this chapter I will develop the theory of the propagation of electromagnetic fields inside a high-confinement AlGaAs waveguide. First I will introduce the basics of electromagnetic propagation in optical waveguides in terms of waveguide modes, ignoring nonlinear effects. Then I will introduce third-order nonlinear effects as a perturbation to the linear theory, deriving coupled differential equations describing the change of mode amplitudes as the modes propagate down the waveguide. I will conclude by discussing the properties of the AlGaAs third-order susceptibility tensor.

2.1 Waveguide Modes

2.1.1 Derivation

The propagation of electromagnetic fields is determined by a set of coupled differential equations called Maxwell's equations. Integrated optics is primarily concerned with materials with no free charges, free current or magnetization. In this case, Maxwell's curl equations take the form:

$$\nabla \times \mathbf{E} = -\mu_0 \frac{\partial \mathbf{H}}{\partial t} \tag{2.1}$$

$$\nabla \times \mathbf{H} = \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} + \frac{\partial \mathbf{P}}{\partial t}$$
(2.2)

(2.3)

where **E** is the electric field, **H** is the magnetic field, **P** is the polarization of the medium, ε_0 is the permittivity of free space, and μ_0 is the permeability of free space. Assume the electric field oscillates at a single frequency ω_0 . The complex electric field therefore takes the form

$$\mathbf{E}(\mathbf{r},t) = \tilde{\mathbf{E}}(\mathbf{r})exp(-i\omega_0 t) \tag{2.4}$$

where $\mathbf{r} = (x, y, z)$ is the position vector. If the polarization is assumed to be linear, it is given by $\mathbf{P}(\mathbf{r}, t) = \tilde{\mathbf{P}}(\mathbf{r})exp(-i\omega_0 t) = \varepsilon_0\chi^{(1)}(\omega_0)\tilde{\mathbf{E}}(\mathbf{r})exp(-i\omega_0 t)$, where $\chi^{(1)}$ is the linear susceptibility of the medium. If these expressions for the electric field and the polarization are inserted into Maxwell's curl equations, we obtain:

$$\nabla \times \tilde{\mathbf{E}} = i\mu_0 \omega_0 \tilde{\mathbf{H}} \tag{2.5}$$

$$\nabla \times \tilde{\mathbf{H}} = -i\omega_0 \varepsilon_0 n^2(\mathbf{r}, \omega_0) \tilde{\mathbf{E}}$$
(2.6)

Where $n = \sqrt{1 + \chi^{(1)}}$ is the refractive index of the medium. A waveguide oriented in the z direction is defined by n, which will only depend on x, y, and ω_0 . In this case, different (bounded) solutions to this equation take the form $\tilde{\mathbf{E}}^{(m)} = \mathbf{e}^{(m)}(x, y, \omega_0)e^{i\beta_0^{(m)}z}$, and are referred to as waveguide modes [39]. Here $\beta_0^{(m)}$ is the propagation constant, $\mathbf{e}^{(m)}$ is the mode profile, and m is a mode index. Note that there can be multiple modes for a given ω_0 . The different waveguide modes can be found by numerically solving Eqs. (2.5) and (2.6). No exact solutions to these equations for a rectangular waveguide exist, however there are approximate analytic solutions that can be found, for example, using Marcatili's method [3].

Throughout this thesis, Lumerical MODE Solutions finite element method software is used to simulate the waveguides and determine their mode profiles, propagation constants and other characteristics. Instead of frequency, the vacuum wavelength $\lambda = 2\pi c/\omega_0$ is often used, particularly in the optical and infrared ranges. The analyses in this thesis will be focused on wavelengths near $\lambda = 1550$ nm, which is commonly used for telecoms applications. Unless otherwise specified, the simulations in this thesis will be performed at that wavelength.

2.1.2 Mode Characteristics

Modes in rectangular waveguides have several common characteristics that are relevant to the work in this thesis. In general, the dominant component of the mode profile **e** will be either the x component, e_x , in which case it is referred to as a (quasi-) transverse electric (TE) mode, or the e_y component, in which case it is referred to as a (quasi-) transverse magnetic (TM) mode. This is sometimes referred to as the "polarization" of the mode. For waveguides confined in two dimensions the modes are not truly TE or TM modes, as all of the electric field components will be non-zero (though some components will be small). However, for simplicity they well be referred to as such in this thesis.

As mentioned previously, for low-confinement waveguides the dominant transverse component (e_x for TE modes and e_y for TM modes) will be the only significant component of the mode profile. For high-confinement waveguides with a small core the magnitude of the longitudinal (e_z) component will increase in magnitude. This can be demonstrated quantitatively using the longitudinal fraction f_z of a waveguide mode [40], defined as

$$f_z = \frac{\iint |e_z|^2 dA}{\iint |e_x|^2 + |e_y|^2 + |e_z|^2 dA}$$
(2.7)

where dA denotes integration over the x - y plane, and the integration symbol without subscripts \iint denotes integration over the entire plane. This is equal to 1 - T, where T is the transversality of the mode [33]. Using Lumerical MODE simulation software to evaluate the profile of the fundamental transverse electric (TE) mode of the AlGaAsOI waveguide at a wavelength of $\lambda = 1550$ nm, the longitudinal fraction f_z for AlGaAsOI waveguides with various widths was calculated. The waveguide height used was h = 400nm. The results are shown in Fig 2.1.



Figure 2.1: The values of f_z for AlGaAsOI waveguides with various widths. The mode was the fundamental TE mode evaluated at a wavelength of 1550 nm. The height of the waveguide was h = 400 nm.

Fig 2.1 shows that f_z increases with decreasing waveguide width, demonstrating the increased magnitude of the e_z component of the mode profile. It can also be seen that, when the waveguide width is small enough, the mode profile begins to extend further out of the waveguide core, and f_z begins to reduce.

Another important concept is that of mode order. Depending on the size and refractive index profile of the waveguide, there can be several, a single, or no bounded modes at a given frequency. In general, a larger waveguide has more possible modes. Inside the waveguide core the dominant component of the electric field will follow a roughly sinusoidal distribution in both the x and y directions. The number of zeroes in these distributions denotes the "order" of the mode. There is one TE (TM) mode with no zeroes in the e_x (e_y) profile, which is referred to as the "fundamental" TE (TM), or TE₀₀ (TM₀₀), mode. In general, if there are n zeros in the x direction and m zeros in the y direction in the profile of the dominant electric field component, the mode will be referred to in this thesis as the TE_{nm} or TM_{nm} mode. The normalized mode profiles of the TE₀₀, TM₀₀, TE₁₀ and TM₁₀ modes for an AlGaAsOI waveguide with w = 800 nm, h = 600 nm and $\lambda = 1550$ nm are shown in Fig. 2.2. The waveguide modes can be normalized in such a way that the transverse components are purely real and the longitudinal component is purely imaginary [39].



Figure 2.2: Normalized mode profiles of an AlGaAsOI waveguide with w = 800 nm, h = 600 nm, at a wavelength of $\lambda = 1550$ nm. Lines denote the edges of the waveguide core. Top row: TE₀₀ mode. Second row: TM₀₀ mode. Third row: TE₁₀ mode. Fourth row: TM₁₀ mode.

Another important property of a waveguide mode is the effective index, which influences the mode's linear and nonlinear coupling with other modes. It is defined as $n_{eff} = \beta_0 c/\omega_0$, where c is the speed of light in vacuum. In general, for a rectangular waveguide $n_{cladding} < n_{eff} < n_{core}$ for all bound modes. Higher order modes tend to have a lower effective index than lower order modes with the same polarization. The calculated n_{eff} of the fundamental TE $(n_{eff,TE})$ and TM $(n_{eff,TM})$ modes of an AlGaAsOI waveguide as a function of w with $\lambda = 1550$ nm and h = 500 nm are shown in Fig. 2.3.



Figure 2.3: Effective indices of the fundamental TE and TM modes of an AlGaAsOI waveguide with h = 500 nm, $\lambda = 1500$ nm, and various widths.

From this figure it can be seen that w > h implies $n_{eff,TE} > n_{eff,TM}$, when w = h, then $n_{eff,TE} = n_{eff,TM}$, and w < h, implies $n_{eff,TE} < n_{eff,TM}$ for AlGaAsOI waveguides. It is also clear that w has a stronger effect on $n_{eff,TE}$ than on $n_{eff,TM}$, though the effect on $n_{eff,TM}$ is non-zero, particularly at low w. The inverse is true for h. It is also generally true for most modes that as the dimensions of the waveguide decrease, the n_{eff} will decrease.

With a basic understanding of waveguide modes and their properties, the theory of third-order nonlinear effects in high-confinement waveguides can now be developed.

2.2 Nonlinear Coupled Mode Theory

The equations required to describe how different waveguide modes interact through the third-order nonlinearity will now be derived. A formalism that takes into account the fullvectorial nature of the waveguide mode and can be generalized to any number of modes at different frequencies is required. There are several examples of theoretical frameworks for vectorial nonlinear pulse propagation designed for different situations, primarily for SOI [28, 29] and silica [33] waveguides. Some examples make simplifying assumptions, such as focusing on pulses centered at a single frequency [31, 33], quasi-continuous wave (quasi-CW) pulses that ignore dispersion effects [32], or single spatial modes [30]. As far as I am aware, a full-vectorial approach has not been applied to AlGaAs waveguides in the literature.

In general, in these treatments the electric field is written as a superposition of waveguides modes whose complex amplitudes are coupled through the various nonlinear effects, changing their magnitudes and phases as they propagate down the waveguide. For simplicity, the focus of this thesis will be on quasi-CW modes at wavelengths near $\lambda = 1550$ nm in AlGaAs waveguides. Under the quasi-CW approximation, the electric field in the time domain can be written:

$$\mathbf{E}(\mathbf{r},t) = \frac{1}{2} \sum_{n} \frac{A_n(z)}{\sqrt{N_n}} \mathbf{e}^{(n)}(x,y,\omega_0^{(n)}) exp(i\beta_0^{(n)}z - i\omega_0^{(n)}t) + c.c.$$
(2.8)

where c.c. denotes the complex conjugate, and N_n is a normalization constant:

$$N_n = \frac{1}{4} \iint (\mathbf{e}^{(n)} \times \mathbf{h}^{*(n)} + \mathbf{e}^{*(n)} \times \mathbf{h}^{(n)}) \cdot \mathbf{z} dA$$
(2.9)

such that $|A_n|^2$ is the optical power in the *n*th mode. The magnetic field **H** is similarly defined:

$$\mathbf{H}(\mathbf{r},t) = \frac{1}{2} \sum_{n} \frac{A_n(z)}{\sqrt{N_n}} \mathbf{h}^{(n)}(x,y,\omega_0^{(n)}) exp(i\beta_0^{(n)}z - i\omega_0^{(n)}t) + c.c.$$
(2.10)

Here $\mathbf{h}^{(n)}$ is the magnetic field mode profile of the *n*th mode.

2.2.1 Propagation Equation

To determine how the mode amplitudes vary along the waveguide due to nonlinear effects, the starting point of this derivation will be the propagation equation from [32]:

$$\frac{\partial A_n}{\partial z} = \frac{i\omega_n}{4\sqrt{N_n}} \iint \mathbf{e}^{*(n)}(\mathbf{r}) \cdot \mathbf{P}^{NL}(\mathbf{r},\omega_n) exp(-i\beta_0^{(n)}z) dA$$
(2.11)

where the integration is over the entire x - y plane, the * denotes complex conjugation, and $\mathbf{P}^{NL}(\mathbf{r}, \omega_n)$ is the nonlinear polarization at a frequency ω_n , given by:

$$\mathbf{P}^{NL}(\mathbf{r},t) = \frac{1}{2} \sum_{n} [\mathbf{P}^{NL}(\mathbf{r},\omega_n) exp(-i\omega_n t) + \mathbf{P}^{NL^*}(\mathbf{r},-\omega_n) exp(i\omega_n t)]$$
(2.12)

This equation (or equations very similar to this) can be derived directly from Maxwell's equations [31, 41] or using the reciprocity theorem [28, 29, 33].

Due to the quasi-CW approximation the dispersion effects or the shock term seen in other treatments are not included. In Al_{0.18}Ga_{0.82}As TPA is negligible at $\lambda = 1550$ nm so nonlinear absorption and free carrier effects can be neglected as well.

If the model is to be used for shorter pulses, dispersion effects would need to be included. The distance at which dispersion becomes significant is given by the dispersion length $L_D = T_0^2/|\beta_2|$, where T_0 is pulse duration and β_2 is the group velocity dispersion parameter [26]. Typical $|\beta_2|$ values for the fundamental TE mode AlGaAsOI waveguides with w = 0.5 - 1 microns are on the order of 1 ps²/m, so for a waveguide with length L = 0.01 m, dispersion becomes significant at a pulse duration of around $T_0 = \sqrt{L|\beta_2|} =$ 0.1 ps. For a derivation of a full-vectorial model that includes dispersion effects, see [29].

Eq. (2.11) determines how the amplitudes of the modes change as they propagate down the waveguide in the z direction. To explicitly determine the right hand side an expression for the nonlinear polarization P^{NL} in terms of the mode amplitudes A_n is required.

2.2.2 Nonlinear Polarization

For simplicity, the electric field is rewritten as:

$$\mathbf{E}(\mathbf{r},t) = \frac{1}{2} \sum_{n} \frac{A_n(z)}{\sqrt{N_n}} \mathbf{e}^{(n)}(x,y) exp(-i\omega_0^{(n)}t + i\beta_0^{(n)}z) + c.c.$$
(2.13)

$$=\frac{1}{2}\sum_{n}\tilde{\mathbf{E}}^{(n)}(\mathbf{r})exp(-i\omega_{0}^{(n)}t)$$
(2.14)

where the complex conjugate term of term n is indexed as the corresponding negative integer, -n. This means $\omega_0^{(-n)} = -\omega_0^{(n)}$ and $\tilde{\mathbf{E}}^{(-n)} = \tilde{\mathbf{E}}^{*(n)}$. Note that this sum could include modes with the same frequency but different spatial distributions as well as modes with similar mode profiles but distinct frequencies.

It will be assumed that the nonlinear polarization is due to electronic transitions and therefore is instantaneous. In general, for electric fields consisting of a sum of monochromatic waves the components of the third-order nonlinear polarization at frequency $\omega_0^{(n)}$

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are given by [42]:

$$\mathbf{P}^{NL}(\mathbf{r},\omega_{0}^{(n)}) = \varepsilon_{0} \sum_{(pqr)} K\chi^{(3)}(-\omega_{0}^{(n)};\omega_{0}^{(p)},\omega_{0}^{(q)},\omega_{0}^{(r)}) |\tilde{\mathbf{E}}^{(p)}(\mathbf{r})\tilde{\mathbf{E}}^{(q)}(\mathbf{r})\tilde{\mathbf{E}}^{(r)}(\mathbf{r})$$
(2.15)

where (pqr) indicates a sum over distinct combinations of modes where $\omega_0^{(p)} + \omega_0^{(q)} + \omega_0^{(r)} = \omega_0^{(n)}$, and the vertical bar | denotes tensor multiplication. K is a degeneracy factor that accounts for the different permutations of the frequencies, as well as the various 1/2 factors from the definitions of the polarization and electric field. Note a subtle difference between the treatment here and that of [42]: in that textbook the summations are over distinct frequencies, while in this derivation the summations are over modes that may or may not have the same frequency. The spatial dependence of the polarization and the electric fields is also included here. Inserting Eq. (2.14) into Eq. (2.15) gives an expression for the μ component of \mathbf{P}^{NL} :

$$P_{\mu}^{NL}(\mathbf{r},\omega_{0}^{(n)}) = \varepsilon_{0} \sum_{(pqr)} K \frac{A_{p}A_{q}A_{r}}{\sqrt{N_{p}N_{q}N_{r}}} exp(i(\beta_{0}^{(p)} + \beta_{0}^{(q)} + \beta_{0}^{(r)})) \\ \times \sum_{\alpha\beta\gamma} \chi_{\mu\alpha\beta\gamma}(\omega_{0}^{(n)};\omega_{0}^{(p)},\omega_{0}^{(q)},\omega_{0}^{(r)})e_{\alpha}^{(p)}e_{\beta}^{(q)}e_{\gamma}^{(r)}$$
(2.16)

where $\chi_{\mu\alpha\beta\gamma}$ are the elements of the fourth-rank tensor $\chi^{(3)}$. The integrand in Eq. (2.11) can therefore be written as:

$$\mathbf{e}^{*(n)} \cdot \mathbf{P}^{NL}(\mathbf{r}, \omega_{0}^{(n)}) exp(-i\beta_{0}^{(n)}z) = \varepsilon_{0} \sum_{(pqr)} K \frac{A_{p}A_{q}A_{r}}{\sqrt{N_{p}N_{q}N_{r}}} \\ \times \sum_{\mu\alpha\beta\gamma} \chi_{\mu\alpha\beta\gamma}(\omega_{0}^{(n)}; \omega_{0}^{(p)}, \omega_{0}^{(q)}, \omega_{0}^{(r)}) e_{\mu}^{*(n)} e_{\alpha}^{(p)} e_{\beta}^{(q)} e_{\gamma}^{(r)} \\ \times exp(i(-\beta_{0}^{(n)} + \beta_{0}^{(p)} + \beta_{0}^{(q)} + \beta_{0}^{(r)})z)$$
(2.17)

The terms where $\omega_0^{(p)}, \omega_0^{(q)}$ and $\omega_0^{(r)}$ are all positive result in third harmonic generation. However, due to the phase mismatch (see Chpt. 3), these terms will in general be insignificant and can therefore be neglected. Only terms including one negative frequency and two positive frequencies will have a small phase mismatch. Taking the negative frequency to be $\omega_0^{(p)}$, the integrand can be written:

$$\mathbf{e}^{*(n)} \cdot \mathbf{P}^{NL}(\mathbf{r}, \omega_{0}^{(n)}) exp(-i\beta_{0}^{(n)}z) = \varepsilon_{0} \sum_{(pqr)} K \frac{A_{p}^{*}A_{q}A_{r}}{\sqrt{N_{p}N_{q}N_{r}}} \\ \times \sum_{\mu\alpha\beta\gamma} \chi_{\mu\alpha\beta\gamma}(\omega_{0}^{(n)}; \omega_{0}^{(p)}, \omega_{0}^{(q)}, \omega_{0}^{(r)}) e_{\mu}^{*(n)} e_{\alpha}^{*(p)} e_{\beta}^{(q)} e_{\gamma}^{(r)} \quad (2.18) \\ \times exp(i(-\beta_{0}^{(n)} - \beta_{0}^{(p)} + \beta_{0}^{(q)} + \beta_{0}^{(r)})z)$$

now with the sum over only positive mode indices in (pqr). Note that, due to the fact that the first frequency $\omega_0^{(p)}$ is taken to be negative, this expression includes the complex conjugates of A_p and $e_{\alpha}^{(p)}$. Inserting this into Eq. (2.11) gives:

$$\frac{\partial A_n}{\partial z} = i \sum_{(pqr)} \gamma_{npqr} A_p^* A_q A_r exp(i\Delta\beta_{npqr}z)$$
(2.19)

where

$$\gamma_{npqr} = \frac{K\omega_n \varepsilon_0}{4\sqrt{N_n N_p N_q N_r}} \sum_{\mu\alpha\beta\gamma} \iint \chi_{\mu\alpha\beta\gamma}(\omega_0^{(n)}; \omega_0^{(p)}, \omega_0^{(q)}, \omega_0^{(r)}) e_{\mu}^{*(n)} e_{\alpha}^{*(p)} e_{\beta}^{(q)} e_{\gamma}^{(r)} dA \qquad (2.20)$$

are referred to as the nonlinear coefficients (NLCs) and $\Delta\beta_{npqr} = -\beta_0^{(n)} - \beta_0^{(p)} + \beta_0^{(q)} + \beta_0^{(r)}$ is the phase mismatch.

The NLCs are important parameters that denote the strength of the different nonlinear interactions between the modes. Accurately determining their value is crucial for predicting the performance of nonlinear devices. Investigating their dependence on waveguide geometry will be the focus of much of this thesis. For an in-depth study of various third-order nonlinear effects and the roles played by the NLCs, see [26].

2.2.3 Nonlinear Susceptibility

To evaluate the NLCs an expression for the third-order nonlinear susceptibility $\chi_{\mu\alpha\beta\gamma}$ is required. As previously mentioned, TPA is negligible at $\lambda = 1550$ nm in AlGaAs if the Al fraction is greater than 0.18. Therefore, $\chi_{\mu\alpha\beta\gamma}$ will be taken to be purely real.

AlGaAs has cubic symmetry so there are four independent elements of $\chi_{\mu\alpha\beta\gamma}$: χ_{xxxx} , χ_{xxyy} , χ_{xyxy} , and χ_{xyyx} [18]. The tensor can therefore be written as [33]:

$$\chi_{\mu\alpha\beta\gamma} = \chi_{xxyy}\delta_{\mu\alpha}\delta_{\beta\gamma} + \chi_{xyxy}\delta_{\mu\beta}\delta_{\alpha\gamma} + \chi_{xyyx}\delta_{\mu\gamma}\delta_{\alpha\beta} + (\chi_{xxxx} - \chi_{xxyy} - \chi_{xyyy} - \chi_{xyyx})\delta_{\mu\alpha\beta\gamma}$$
(2.21)

where δ_{ij} is the Kronecker delta.

With this frequency ordering, $\chi_{xyxy} = \chi_{xyyx}$ by permutation symmetry, assuming that $\omega_0^{(q)} \approx \omega_0^{(r)}$ [35]. This equation can then be written in terms of anisotropy parameters used for relating the tensor elements in AlGaAs [35]:

$$\sigma = \frac{\chi_{xxxx} - \chi_{xxyy} - 2\chi_{xyxy}}{\chi_{xxxx}} \tag{2.22}$$

$$\delta = \frac{\chi_{xxxx} + \chi_{xxyy} - 2\chi_{xyxy}}{2\chi_{xxxx}} \tag{2.23}$$

The parameter σ is a measure of the anisotropy of the material and δ is referred to as the induced birefringence, which denotes the difference in SPM strength between linearly and circularly polarized light [18]. In general, σ is negative, implying the nonlinearity is weakest when the electric field is oriented along a crystal axis. In this work we will take the values of $\sigma = -0.54$ and $\delta = 0.18$ for Al_{0.18}Ga_{0.82}As, which were obtained via SPM and XPM experiments [20]. However, there are several different values obtained for these parameters in AlGaAs from experiment and theory [18]. For example, theoretical predictions based on low-temperature band structure data for light at the half-band gap energy of GaAs give $\sigma = -0.82$ and $\delta = 0.08$ [34], suggesting more experimental and theoretical work is needed to determine these parameters to a higher accuracy.

It is common to write the susceptibility element χ_{xxxx} in terms of the Kerr index n_2 using $\chi_{xxxx} = \frac{4}{3}\varepsilon_0 cn^2 n_2$, where n_2 is evaluated along the [001] axis of the crystal lattice. Strictly speaking n_2 will depend on all of the frequencies involved. However, there is not sufficiently detailed experimental evidence to include this dispersion in our model. We will assume it is constant, and take n_2 to be $n_2 = 1.43 \times 10^{-17} \text{ m}^2/\text{W}$ [18] at wavelengths close to $\lambda = 1550 \text{ nm}$. Note that n_2 is found for both the TE and TM modes of a [001] grown wafer in [18]. The n_2 for the TM mode must be used, as this is the value for fields oriented along the [001] axis.

Writing the tensor in terms of the parameters n_2, σ and δ gives:

$$\chi_{\mu\alpha\beta\gamma} = \frac{4}{3} \varepsilon_0 cn^2 n_2 \left(\left(\delta - \frac{\sigma}{2} \right) \delta_{\mu\alpha} \delta_{\beta\gamma} + \frac{1}{2} \left(1 - \delta - \frac{\sigma}{2} \right) \left(\delta_{\mu\beta} \delta_{\alpha\gamma} + \delta_{\mu\gamma} \delta_{\alpha\beta} \right) + \sigma \delta_{\mu\alpha\beta\gamma} \right)$$
(2.24)

However, this tensor is expressed in the coordinate system of the cubic crystal lattice of AlGaAs. The susceptibility tensor will change depending on the orientation of the waveguide coordinate system and the coordinate system of the lattice. The tensor elements in the waveguide coordinate system are written as [27]:

$$\chi_{\mu\alpha\beta\gamma} = \frac{4}{3} \varepsilon_0 c n^2 n_2 \left(\left(\delta - \frac{\sigma}{2} \right) \delta_{\mu\alpha} \delta_{\beta\gamma} + \frac{1}{2} \left(1 - \delta - \frac{\sigma}{2} \right) \left(\delta_{\mu\beta} \delta_{\alpha\gamma} + \delta_{\mu\gamma} \delta_{\alpha\beta} \right) + \sigma \sum_q R_{q\mu} R_{q\alpha} R_{q\beta} R_{q\gamma} \right)$$
(2.25)

where R is the rotation matrix that converts vectors in the waveguide coordinate system to that of the crystal, and q = 1, 2, 3.

AlGaAs wafers are often grown in the [001] direction. Waveguides created on such wafers can be oriented in any direction in the plane formed by the [100] and [010] directions. The rotation matrix for the crystal growth direction [001] is:

$$R_{[001]}(\theta) = \begin{bmatrix} \cos(\theta) & 0 & \sin(\theta) \\ \sin(\theta) & 0 & -\cos(\theta) \\ 0 & 1 & 0 \end{bmatrix}$$
(2.26)

where the angle θ is the angle between the propagation axis (z) of the waveguide and the $[0\overline{1}0]$ crystal axis (see Fig. 2.4).



Figure 2.4: Orientation of the waveguide coordinate system (dashed lines) and crystal axis coordinate system (solid lines).

With this rotation matrix, along with Eq. (2.19) and Eq. (2.25), expressions for the

propagation of the mode amplitudes $A_n(z)$ in Eq. (2.8) can now be derived if the modes involved are specified.

2.3 Conclusion

In this chapter, the basic concepts of waveguide modes were introduced and a fullvectorial theory of quasi-CW mode propagation in waveguides consisting of a material with cubic symmetry was described. Treating the third-order nonlinearity as a perturbation coupling the linear modes of the waveguide, propagation equations for an arbitrary number of modes with different spatial distributions and frequencies were derived. The third-order susceptibility tensor of AlGaAs was discussed for an arbitrary waveguide orientation in a wafer with a [001] growth direction.

Chapter 3

Single-Mode Nonlinear Coefficient

In this chapter the full-vectorial theory developed in the previous chapter will be used to derive explicit expressions for the NLCs involved in single-mode propagation. The numerical value of this single-mode NLC will be obtained via simulation for the fundamental TE and TM modes of AlGaAsOI waveguides to investigate its dependence on waveguide height h, width w and orientation θ .

3.1 Single-Mode NLC Expressions

Dropping the mode index subscripts/superscripts for simplicity, the electric field for a single mode is given by:

$$\mathbf{E}(\mathbf{r},t) = \frac{1}{2} \frac{A(z)}{\sqrt{N}} \mathbf{e}(x,y) exp(-i\omega_0 t + i\beta_0 z) + c.c.$$
(3.1)

With only one mode propagating in the waveguide, there is only one term on the right hand side (r.h.s.) of Eq. (2.19):

$$\frac{\partial A}{\partial z} = i\gamma |A|^2 A \tag{3.2}$$

where

$$\gamma = \frac{3\omega_0\varepsilon_0}{16N^2} \sum_{\mu\alpha\beta\gamma} \iint \chi_{\mu\alpha\beta\gamma}(\omega_0; -\omega_0, \omega_0, \omega_0) e^*_{\mu} e^*_{\alpha} e_{\beta} e_{\gamma} dA$$
(3.3)

where K = 3/4 [42] has been used. This differential equation has the solution:

$$A(z) = A(0)exp(i\gamma|A(0)|^{2}z)$$
(3.4)

This indicates that the nonlinearity will impart a power-dependent phase shift on the mode, referred to as self-phase modulation (SPM). The NLC γ will be referred to as the single-mode NLC. Note that, as will be discussed in a Chpt. 6, this NLC will also be used in the case of several modes with the same spatial profile but different carrier frequencies to determine the strength of SPM, cross-phase modulation (XPM) and four wave mixing (FWM).

If dispersion and group velocity terms are included, and a change of variables is used to convert the coordinate system to the pulse frame, this equation becomes the well-known nonlinear Schrödinger equation (NLSE):

$$\frac{\partial A}{\partial z} = -\frac{i\beta_2}{2}\frac{\partial^2 A}{\partial T^2} + i\gamma |A|^2 A \tag{3.5}$$

where T is the time coordinate in the pulse coordinate system and β_2 is the group velocity dispersion (GVD).

NLCs in general can be calculated directly using Eq. (2.20), though in some cases an explicit expression in terms of the mode profile components can be derived to help gain a deeper understanding of what influences the strength of nonlinear effects inside the waveguide. For the single mode case, a relatively simple expression for γ can be derived for AlGaAs waveguides fabricated in a wafer grown in the [001] direction. Inserting Eq. (2.25), along with Eq. (2.26), into Eq. (3.3), gives:

$$\gamma = \frac{\varepsilon_0 \omega_0}{4\mu_0 c N^2} \iint n^2 n_2 \left(\left(\delta - \frac{\sigma}{2} \right) |\mathbf{e} \cdot \mathbf{e}|^2 + \left(1 - \delta - \frac{\sigma}{2} \right) |\mathbf{e}|^4 + \sigma B(\theta) \right) dA \tag{3.6}$$

where $|\mathbf{e} \cdot \mathbf{e}|^2 = (\mathbf{e} \cdot \mathbf{e})(\mathbf{e}^* \cdot \mathbf{e}^*)$ and $|\mathbf{e}|^4 = (\mathbf{e} \cdot \mathbf{e}^*)(\mathbf{e} \cdot \mathbf{e}^*)$. $B(\theta)$ is the angle-dependent term given by:

$$B(\theta) = \sum_{\mu\alpha\beta\gamma} \sum_{q} R_{q\mu} R_{q\alpha} R_{q\beta} R_{q\gamma} e_{\mu}^{*} e_{\alpha}^{*} e_{\beta} e_{\gamma}$$

$$= \frac{1}{4} (\cos(4\theta) + 3) (|e_{x}|^{4} + |e_{z}|^{4}) + \frac{1}{2} (1 - \cos(4\theta)) |e_{x}|^{2} |e_{z}|^{2} + |e_{y}|^{4}$$
(3.7)

where the fact that the modes of a non-absorbing waveguide can be written in such a way that the transverse components are entirely real and the longitudinal component is entirely imaginary has been used [39]. Note that only the θ -dependent B term will be different for the various wafer growth directions, but the other terms will remain the same. This can be algebraically simplified to:

$$\gamma = \frac{\varepsilon_0 \omega_0}{4\mu_0 c N^2} \iint n^2 n_2 \left((|\mathbf{e}|^4 - \sigma \left(\frac{\sin^2(2\theta)}{2} (|e_x|^2 - |e_z|^2)^2 + 2|e_x|^2 |e_y|^2 \right) - 4\delta(|e_x|^2 + |e_y|^2) |e_z|^2 \right) dA$$
(3.8)

The normalization constant can also be approximated as [43]:

$$N = \frac{1}{4} \iint (\mathbf{e} \times \mathbf{h}^* + \mathbf{e}^* \times \mathbf{h}) \cdot \hat{\mathbf{z}} dA \approx \frac{v_g \varepsilon_0}{2} \iint n^2 |\mathbf{e}|^2 dA$$
(3.9)

where v_g is the group velocity of the mode, the integral is over the entire x - y plane, and we have assumed $\lambda(dn^2/d\lambda) \ll 2n^2$. To verify this approximation, the ratio between the right and left sides of the above equation was calculated for the fundamental TE mode of an AlGaAsOI waveguide for various w up to a micron. The ratio for this range of w was approximately 0.96-0.97. The expressions for the NLCs that use this approximation (including the two-mode XPM and FWM NLCs, derived in Chpt. 4) will tend to overestimate the true value of the NLC. For higher accuracy, expressions that do not make this approximation, such as Eqs. (3.6) or (3.3) can be used instead. The approximation could also be reversed by multiplying the calculated NLC with the appropriate factor from Eq. (3.9). Throughout this thesis, unless otherwise specified I will use Eq. (2.20) to calculate the NLCs without making the approximation in Eq. (3.9).

Inserting this into the expression for γ gives:

$$\gamma = k_0 n_g^2 \left(\frac{\iint n^2 n_2 |\mathbf{e}|^4 dA}{(\iint n^2 |\mathbf{e}|^2 dA)^2} - \sigma \frac{\iint n^2 n_2 ((\frac{\sin^2(2\theta)}{2} (|e_x|^2 - |e_z|^2)^2 + 2|e_x|^2 |e_y|^2) dA}{(\iint n^2 |\mathbf{e}|^2 dA)^2} - \delta \frac{\iint 4n^2 n_2 (|e_x|^2 + |e_y|^2) |e_z|^2 dA}{(\iint n^2 |\mathbf{e}|^2 dA)^2} \right)$$
(3.10)

where $k_0 = \omega_0/c$ is the vacuum wavenumber and $n_g = c/v_g$ is the group index. Eq. (3.10) can be further simplified into a more intuitive expression if some assumptions are made. Assuming the waveguide consists of a single nonlinear core with index $n = n_{core}$ and Kerr index n_2 surrounded by a cladding with negligible Kerr index, and the waveguide mode is quasi-TE or quasi-TM such that $\iint_{NL} |e_x|^2 |e_y|^2 dA \approx 0$ (here NL indicate integration over the nonlinear core), γ can be written as:

$$\gamma = \eta_{NL} \left(\frac{n_g}{n_{core}}\right)^2 \frac{k_0 \overline{n_2}}{A_{eff}} \tag{3.11}$$

where η_{NL} is the mode overlap with the nonlinear core:

$$\eta_{NL} = \frac{\iint_{NL} (n^2 |\mathbf{e}|^2)^2 dA}{\iint_{\infty} (n^2 |\mathbf{e}|^2)^2 dA}$$
(3.12)

 A_{eff} is the effective area, which is defined here as:

$$A_{eff} = \frac{(\iint_{\infty} n^2 |\mathbf{e}|^2 dA)^2}{\iint_{\infty} (n^2 |\mathbf{e}|^2)^2 dA}$$
(3.13)

and $\overline{n_2}$ is the effective Kerr index of the mode:

$$\overline{n_2} = n_2 \left(1 - \overline{\sigma} \frac{\sin^2(2\theta)}{2} - 4\overline{\delta} \right) \tag{3.14}$$

where $\overline{\sigma}$ is the effective anisotropy of the waveguide mode:

$$\overline{\sigma} = \sigma \frac{\iint_{NL} (|e_x|^2 - |e_z|^2)^2 dA}{\iint_{NL} |\mathbf{e}|^4 dA}$$
(3.15)

and similarly $\overline{\delta}$ is an effective δ :

$$\overline{\delta} = \delta \frac{\iint_{NL} (|e_x|^2 + |e_y|^2) |e_z|^2 dA}{\iint_{NL} |\mathbf{e}|^4 dA}$$
(3.16)

Subscripts have been added to the integrals to make clear whether the integral is over the nonlinear core (indicated by NL) or the entire x - y plane (indicated by ∞). Writing γ in this way clarifies what influences its value: the size of the mode profile and therefore the intensity for a given power (A_{eff}) , how much of the mode profile overlaps with the nonlinear section of the waveguide (η_{NL}) , and the group velocity enhancement (n_g/n_{core}) . The effective Kerr index $\overline{n_2}$ is modified by the orientation of the waveguide θ and the relative strengths of the different electric field components.

Similar expressions to Eq. (3.11) have been found using a full-vectorial approach before, for example in [31, 32, 33, 43]. In particular, the dependence on n_g , A_{eff} and η_{NL} are well known, though various definitions of A_{eff} are used in the literature. However, to the best of my knowledge, the expressions for \bar{n}_2 , $\bar{\sigma}$, and $\bar{\delta}$ have not been found before.

3.2 Geometric Dependence

The dependence of the single-mode NLC γ on AlGaAsOI waveguide geometry will now be investigated. The value of γ for the TE₀₀ (TM₀₀) mode, which will be referred to as γ_{TE} (γ_{TM}) was calculated using Eq. (3.11) for an AlGaAsOI waveguide with various values of height h and width w at $\lambda = 1550$ nm and $\theta = \pi/4$. The results are shown in Fig. 3.1. In general, reducing the size of the waveguide core will increase γ by reducing A_{eff} and



Figure 3.1: Calculated values for a) γ_{TE} and b) γ_{TM} for an AlGaAsOI waveguide at $\lambda = 1550$ nm and $\theta = \pi/4$.

increasing n_g . However when the core becomes too small and the mode profile begins to expand into the cladding, η_{NL} and n_g will begin to decrease, reducing γ . This behaviour can be seen in more detail in Fig. 3.2, where the calculated A_{eff} , η_{NL} and n_g/n_{core} are shown for the fundamental TE and TM modes. From Fig. 3.2 a) and b) it can be seen that A_{eff} generally decreases as h or w are reduced, with a stronger dependence on the dimension perpendicular to the polarization of the mode (h for the TE mode and w for the TM mode). This pattern is reversed if the waveguide core becomes too small, at which point the mode profile begins to spread out into the cladding, increasing A_{eff} . This occurs at dimensions of around λ/n_{core} .

This effect can also be seen in Fig. 3.2 c) and d), where η_{NL} is plotted for the TE₀₀ and TM₀₀ modes, respectively. η_{NL} is roughly equal to unity until the dimension parallel to the polarization decreases below approximately 400 nm, at which point η_{NL} begins to decrease. This is especially evident for η_{NL} of the TM₀₀ mode for the waveguide with h = 250 nm, which is much lower than η_{NL} for the waveguides with h = 500 nm or h = 750 nm.

Similar to η_{NL} , The group index n_g for the TE (TM) mode is largely independent of



Figure 3.2: A_{eff} (top row), η_{NL} (middle row), and n_g/n_{core} (bottom row) for the TE₀₀ (left column) and TM₀₀ (right column) modes of an AlGaAsOI waveguide at $\lambda = 1550$ nm. The legend in a) applies to all plots.

h(w) (see Fig. 3.2 e), f)), but increases as the direction parallel to the polarization of the mode is decreased. This changes when the waveguide dimensions are reduced below around 400 nm, when the mode profile begins to spread out of the core and n_g starts to decrease.

The unique aspects of the AlGaAs tensor are contained in \overline{n}_2 . Calculated values for \overline{n}_2/n_2 , $\overline{\sigma}/\sigma$ and $\overline{\delta}/\delta$ for the TE₀₀ and TM₀₀ modes at $\lambda = 1550$ nm for AlGaAsOI waveguides with $\theta = \pi/4$ are shown in Fig. 3.3. In this figure it can be seen that \overline{n}_2/n_2 , $\overline{\sigma}/\sigma$ and $\overline{\delta}/\delta$ for the TE₀₀ mode depend strongly on w but only weakly on h, while the opposite is true for the TM₀₀ mode.

From Fig. 3.3 c) it can be seen that $\overline{\sigma}/\sigma$ for the TE₀₀ mode is approximately equal to unity for waveguides with a *w* larger than a micron, but begins to decrease as *w* is reduced. For the TM₀₀ mode, on the other hand, $\overline{\sigma}/\sigma$ is negligible for waveguides with



Figure 3.3: Calculated $\overline{n_2}/n_2$ (top row), $\overline{\sigma}/\sigma$ (middle row), and $\overline{\delta}/\delta$ (bottom row) for the TE₀₀ (left column) and TM₀₀ (right column) modes of an AlGaAsOI waveguide at $\lambda = 1550$ nm. The legend in a) applies to all plots.

h > 500 nm, but reaches a value of approximately 0.26 when h is reduced to 250 nm.

This is due to the fact that $\overline{\sigma}$ is proportional to the integral of $(|e_x|^2 - |e_z|^2)^2$. In general, the magnitude of the e_z component increases when decreasing the waveguide dimension perpendicular to the dominant electric field component of the mode. This can be demonstrated using a modified expression for f_z . Note that in Eqs. (3.15) and (3.16), the integrals are only over the nonlinear core. The equation for f_z is modified to include integrals over the core, giving f_z^{core} :

$$f_z^{core} = \frac{\iint_{NL} |e_z|^2 dA}{\iint_{NL} |\mathbf{e}|^2 dA} \tag{3.17}$$

The calculated values of f_z^{core} for the fundamental modes of an AlGaAsOI waveguide with $\lambda = 1550$ nm are shown in Fig. 3.4.



Figure 3.4: Simulated values of f_z^{core} for AlGaAsOI waveguides of various cross-sections. a) TE₀₀ mode. b) TM₀₀ mode.

This shows how the magnitude of e_z in the waveguide core is mostly dependent on the dimension of the waveguide parallel with the mode polarization.

TE modes have a strong e_x component which means an increase in $|e_z|^2$ leads to an overall decrease in the integral of $(|e_x|^2 - |e_z|^2)^2$. For a TM mode the e_x component is negligible and therefore $(|e_x|^2 - |e_z|^2)^2 \approx |e_z|^4$. This means that reducing h, and therefore increasing $|e_z|^2$, will lead to an overall increase in $\overline{\sigma}$ for the TM₀₀ mode.

As can be seen in Fig. 3.3 d) and e) the opposite is true for $\overline{\delta}/\delta$ which is proportional to the integral of $(|e_x|^2 + |e_y|^2)|e_z|^2$. This means increasing $|e_z|$ will increase $\overline{\delta}$ for both fundamental modes.

From Fig. 3.3 a) these effects on $\overline{\sigma}, \overline{\delta}$ combine to decrease $\overline{n_2}$ with reduced w for the TE₀₀ mode. Changing h has little effect. For the TM₀₀ mode, decreasing h will decrease $\overline{n_2}$, while changing w has little effect. The overall change in $\overline{n_2}$ is around 10%. By comparing Figs. 3.1, 3.2, and 3.3 it can be seen that, for a given θ , the value of γ is largely dependent on A_{eff}, η_{NL} and n_g rather than $\overline{n_2}$.

Note that, though the focus of this thesis is on AlGaAs, the expressions for γ derived here are valid for any material with cubic symmetry. They can be used, for example, for silica waveguides by setting $\delta = 1/3$ and $\sigma = 0$, in which case they can be reduced to expressions derived in [33]. We can see from Eq. (3.10) in this case there will no angular dependence for γ , as expected for an isotropic material. The anisotropy of silicon waveguides is usually expressed using the factor $\rho = 1 - \sigma = 1.27$ [31] at a wavelength of 1550 nm. If Kleinmann symmetry is applicable, $\delta = 1/3 + \sigma/6$ [44]. With these values, these expressions for γ can be used for SOI waveguides as well. However, for silicon waveguides various other effects, such as TPA and free carrier effects, should be included in the propagation equation [31].

3.3 Angular Dependence

How γ_{TE} and γ_{TM} depend on waveguide orientation θ will now be examined. From Eq. (3.11), the angular dependence of γ on θ is entirely determined by a term proportional to $\sin^2(2\theta)$. This means that γ will increase as θ increases from 0 to $\pi/4$, then decrease again as θ goes from $\pi/4$ to $\pi/2$. This can be seen in Fig. 3.5, where simulated γ_{TE} and γ_{TM} values for high confinement (h = 300 nm, w = 350 nm) and low confinement (h = 1500 nm, w = 1750 nm) AlGaAsOI waveguides at $\lambda = 1550 \text{ nm}$ are shown as a function of θ . The NLCs were calculated using Eq. (3.3), and are normalized to their value when $\theta = 0$. Physically this is because the e_x and e_z components are directed off the crystal



Figure 3.5: The normalized nonlinear coefficients for the fundamental TE and TM modes of a high confinement (h = 300 nm, w = 350 nm) and a low confinement (h = 1500 nm, w = 1750 nm) AlGaAsOI waveguide.

axes when $\theta = \pi/4$, which increases γ due to the anisotropy of the AlGaAs $\chi^{(3)}$ tensor.

We can see from Fig. 3.5 that the variation with θ is high for γ_{TE} and negligible for γ_{TM} in a low-confinement waveguide. As discussed above, this is due to the fact that $|e_z| \approx 0$ in a low confinement waveguide, so $\overline{\sigma} \approx \sigma$ for the TE₀₀ mode and $\overline{\sigma} \approx 0$ for the TM₀₀ mode. As the confinement of the waveguide is increased, $|e_z|$ increases as well, leading to a decrease in $\overline{\sigma}$ for the TE₀₀ mode and an increase in $\overline{\sigma}$ for the TM₀₀ mode. This leads to a lower change in γ_{TE} and a larger change in γ_{TM} as θ is increased from 0 to $\pi/4$, as seen in Fig. 3.5.
The magnitude of the angular dependence of γ can be quantified by defining the normalized maximum change in γ with θ as $\Delta \gamma$:

$$\Delta \gamma = \frac{\gamma(\theta = \pi/4) - \gamma(\theta = 0)}{\gamma(\theta = 0)} = -\frac{\overline{\sigma}}{2(1 - 4\overline{\delta})}$$
(3.18)

The magnitude of this variation could be important for quasi-phase matching broadband FWM processes, as suggested in [45]. From these expressions it can be seen that, for low-confinement waveguides where $|e_z| \approx 0$, $\Delta \gamma_{TE} \approx -\sigma/2$ and $\Delta \gamma_{TM} \approx 0$.

The quantity $\Delta\gamma$, calculated using Eq. (3.3), is plotted for the fundamental TE and TM modes at $\lambda = 1550$ nm for various waveguide cross-sections in Fig 3.6. From this figure it can be seen that, due to its dependence on $\overline{\sigma}$ and $\overline{\delta}$, $\Delta\gamma$ depends strongly on the dimension parallel to the dominant component of the electric field in the mode, and only depends weakly on the perpendicular direction. For large w, $\Delta\gamma$ for the fundamental TE mode approaches around 0.25, then as w decreases $\Delta\gamma$ decreases as well, approaching 0.125. For the fundamental TM mode, $\Delta\gamma$ is negligible for large h, but approaches 0.09 as h is reduced.



Figure 3.6: Simulated values of $\Delta \gamma$ for AlGaAsOI waveguides of various cross-sections. a) Fundamental TE mode. b) Fundamental TM mode.

3.4 Low Confinement Approximation

In the low-confinement limit, either $\mathbf{e} \approx e_x \hat{\mathbf{x}}$ (for a TE mode) or $\mathbf{e} \approx e_y \hat{\mathbf{y}}$ (for a TM mode). This is also known as a "scalar" approximation. Under this limit the mode profile is almost entirely contained inside the waveguide core. When these approximations

are applied to Eqs. (3.12)-(3.16), along with the additional assumption that material dispersion is negligible, the following low confinement approximations are obtained:

$$\eta_{NL} \to 1 \tag{3.19}$$

$$A_{eff} \rightarrow \frac{\left(\int \int |e_t|^2 dA\right)^2}{\int \int |e_t|^4 dA} \tag{3.20}$$

$$n_g \to n_{core}$$
 (3.21)

$$\overline{\sigma} \to \sigma(TE), 0(TM)$$
 (3.22)

$$\overline{\delta} \to 0$$
 (3.23)

$$\overline{n}_2 \to n_2 \left(1 - \sigma \frac{\sin^2(2\theta)}{2} \right) (TE), n_2(TM)$$
(3.24)

where e_t is the dominant transverse electric field component (e_x for a TE mode and e_y for a TM mode). From these results the low-confinement expressions for the NLC of the fundamental modes, γ_{TE}^{LC} and γ_{TM}^{LC} , are found:

$$\gamma_{TE}^{LC} = k_0 n_2 \left(1 - \sigma \frac{\sin^2(2\theta)}{2} \right) \frac{\iint |e_x|^4 dA}{(\iint |e_x|^2 dA)^2}$$
(3.25)

$$\gamma_{TM}^{LC} = k_0 n_2 \frac{\iint |e_y|^4 dA}{(\iint |e_y|^2 dA)^2}$$
(3.26)

These expressions can be compared to those found using the scalar approximation in [26]. The expression for γ_{LC}^{TM} is identical. The expression for γ_{LC}^{TE} has an extra factor of $(1 - \sigma \sin^2(2\theta)/2)$ to account for the anisotropy of the AlGaAs tensor. In Fig. 3.5, it can be seen that for the low confinement waveguide γ_{TE} varies by around 26%, as would be expected according to Eq. (3.25).

3.5 Conclusion

In this chapter explicit expressions for the single-mode NLC in terms of the mode profile components were derived. Its dependence on waveguide cross-section geometry and orientation for the fundamental TE and TM modes have been investigated via simulation. It was found that increasing the confinement of AlGaAsOI waveguides will decrease the effective anisotropy $\overline{\sigma}$ of TE modes but increase $\overline{\sigma}$ of TM modes. Low-confinement, scalar approximations to the NLCs were also found.

The results presented in this chapter show that care must be taken to properly opti-

mize the waveguide cross-section geometry for nonlinear devices. There are many factors that play a role in determining the values of the NLCs, including A_{eff} , η_P , n_g , and θ , which must be considered when designing an AlGaAsOI waveguide for nonlinear applications. In general, it was found that the NLCs increase with decreasing waveguide cross-section until the mode profiles begin to spread into the cladding, decreasing the nonlinearity.

Chapter 4

Two-Mode Nonlinear Coefficients

In this chapter, the case of two modes with different spatial mode profiles at the same frequency ω_0 propagating in a high-confinement AlGaAsOI waveguide will be considered. This scenario has applications in, for example, correlated photon generation [46] or intermodal FWM applications [47]. The interactions between the two modes will lead to two new nonlinear coefficients corresponding to cross-phase modulation (XPM) and four wave mixing (FWM). These NLCs will have a different dependence on the waveguide geometry and tensor elements than the single-mode NLC γ .

4.1 Two-Mode NLC Expressions

The first scenario that will be examined is that of the fundamental TE (index of 1) and TM (index of 2) modes. This is the same situation that was studied using full-vectorial models in SOI waveguides in [31] and fibre waveguides in [33].

Consider Eq. (2.19), with n, p, q, r as 1 or 2, where 1 corresponds to the TE₀₀ mode and 2 corresponds to the TM₀₀ mode. Because the modes have the same frequency the conservation of energy condition $-\omega_0^{(p)} + \omega_0^{(q)} + \omega_0^{(r)} = \omega_0^{(n)}$ is automatically satisfied for all mode combinations. There are in total eight terms in the (pqr) sum of Eq. (2.19) for two modes with the same frequency. If we assume that the waveguide geometry has reflection symmetry in the x and y directions, as is the case with the AlGaAsOI waveguide, the fundamental mode profiles will have certain symmetries (see Fig. 2.2). The dominant components (e_x for the TE₀₀ and e_y for the TM₀₀ mode) are even functions of x and y. The e_z profile for the TE₀₀ mode is an odd function of x and an even function of y, and vice versa for the TM₀₀ mode) are odd functions of both x and y but they are negligible, even for high-confinement waveguides. This means that the low-confinement orthogonality relation

$$\iint \mathbf{e}^{(i)} \cdot \mathbf{e}^{*(j)} dA \propto \delta_{ij} \tag{4.1}$$

still holds for the fundamental TE and TM modes in a waveguide with this symmetry. Due to this fact, the NLCs that contain odd numbers of either of the modes, such as γ_{1112} or γ_{1222} , will be approximately zero. These terms can therefore be neglected [31]. For waveguides that lack this symmetry, such as fibres, these terms must be considered, as they were in [33].

With this in mind, from Eq. (2.19) the following propagation equations are obtained:

$$\frac{\partial A_1}{\partial z} = i\gamma_{1111}|A_1|^2 A_1 + i2\gamma_{1212}|A_2|^2 A_1 + i\gamma_{1122}A_2^2 A_1^* e^{-i2\Delta\beta z}$$
(4.2)

$$\frac{\partial A_2}{\partial z} = i\gamma_{2222}|A_2|^2A_2 + i2\gamma_{2121}|A_1|^2A_2 + i\gamma_{2211}A_1^2A_2^*e^{i2\Delta\beta z}$$
(4.3)

where $\Delta\beta = \beta^{(1)}(\omega_0) - \beta^{(2)}(\omega_0)$ is the phase mismatch. The factor of two in the second term on the r.h.s. has been included to allow for better comparison to the case of multiple modes with the same spatial profile. Note that if the modes had different frequencies, the last term on the r.h.s. would not exist, but the others would be the same.

From Eq. (2.20) and the expression for $\chi_{\mu\alpha\beta\gamma}$ it can be seen that, if the modes have the same frequency, $\gamma_{1212} = \gamma_{2121}$ and $\gamma_{1122} = \gamma^*_{2211}$. Simulations show that in general $Im(\gamma_{1122}) << Re(\gamma_{1122})$ so it will be assumed that $\gamma_{1122} = \gamma_{2211}$.

Similar propagation equations to this have been previously derived [48], with the dispersion terms included. The main difference between our model and the previously studied cases is in different definitions of the NLCs. For low-confinement isotropic waveguides such as silica fibres, it is often assumed $\gamma_{1111} = \gamma_{2222} = 3\gamma_{1212} = 3\gamma_{1122}$ [26] or $\gamma_{1111}/\gamma_{1212} = \gamma_{2222}/\gamma_{2121}$ [48], however as shown below this is not the case for AlGaAsOI waveguides.

The first term on the r.h.s of Eqs. (4.2) and (4.3) is the self phase modulation (SPM) term which will induce a phase shift dependent on the power of the mode. This induces a power-dependent phase shift in the temporal domain. The second term represents cross-phase modulation (XPM), which is similar to SPM but depends on the power of a different mode. The last term on the r.h.s. is the four wave mixing (FWM) term, which represents a transfer of energy between the pulses. Which direction the energy is transferred depends on the phase of this term. If the phase mismatch $\Delta\beta$ is large the phase will change rapidly, causing the direction of power transfer to change quickly as well. This prevents a significant transfer of power from one mode to the other. If the process is "phase-matched" ($\Delta\beta \approx 0$) then the power transfer from one mode to the other can accumulate over a large distance, resulting in a large total power transfer.

The strength of these different terms is determined by the different NLCs involved. The NLCs γ_{iiii} , where i = 1, 2, correspond to SPM. From Eq. (2.20):

$$\gamma_{iiii} = \frac{3\omega_0\varepsilon_0}{16N_i^2} \sum_{\mu\alpha\beta\gamma} \iint \chi^{(3)}_{\mu\alpha\beta\gamma} e^{*(i)}_{\mu} e^{*(i)}_{\alpha} e^{(i)}_{\beta} e^{(i)}_{\gamma} dA \tag{4.4}$$

This is the same expression as γ from the previous section, evaluated for mode *i*. This means that $\gamma_{1111} = \gamma_{TE}$ and $\gamma_{2222} = \gamma_{TM}$. Results from the previous chapter, including the different ways of writing this factor, therefore also apply here.

The XPM NLC is γ_{1212} , given by:

$$\gamma_{1212} = \frac{3\omega\varepsilon_0}{16N_1N_2} \sum_{\mu\alpha\beta\gamma} \iint \chi^{(3)}_{\mu\alpha\beta\gamma} e^{*(1)}_{\mu} e^{*(2)}_{\alpha} e^{(1)}_{\beta} e^{(2)}_{\gamma} dA \tag{4.5}$$

Inserting Eq. (2.25) into this expression gives:

$$\gamma_{1212} = \frac{\varepsilon_0 \omega_0}{4\mu_0 c N_1 N_2} \iint n^2 n_2 \left(\left(\delta - \frac{\sigma}{2} \right) |\mathbf{e}^{(1)} \cdot \mathbf{e}^{(2)}|^2 + (1/2) \left(1 - \delta - \frac{\sigma}{2} \right) (|\mathbf{e}^{(1)}|^2 |\mathbf{e}^{(2)}|^2 + |\mathbf{e}^{(1)} \cdot \mathbf{e}^{*(2)}|^2) + \sigma B_{1212}(\theta) \right) dA$$

$$(4.6)$$

where $|\mathbf{e}^{(1)} \cdot \mathbf{e}^{(2)}|^2 = (\mathbf{e}^{*(1)} \cdot \mathbf{e}^{*(2)})(\mathbf{e}^{(1)} \cdot \mathbf{e}^{(2)})$ and $|\mathbf{e}^{(1)} \cdot \mathbf{e}^{*(2)}|^2 = (\mathbf{e}^{*(1)} \cdot \mathbf{e}^{(2)})(\mathbf{e}^{(1)} \cdot \mathbf{e}^{*(2)})$. Note that the integral is over the square of the dot products of the two modes, so these terms will not integrate to zero, despite Eq. (4.1). The angle-dependent term B_{1212} is given by:

$$B_{1212}(\theta) = \frac{1}{4} (\cos(4\theta) + 3) (|e_x^{(1)}|^2 |e_x^{(2)}|^2 + |e_z^{(1)}|^2 |e_z^{(2)}|^2) + |e_y^{(1)}|^2 |e_y^{(2)}|^2 + \frac{1}{4} (1 - \cos(4\theta)) (|e_x^{(1)}|^2 |e_z^{(2)}|^2 + |e_x^{(2)}|^2 |e_z^{(1)}|^2)$$

$$(4.7)$$

If the two modes under consideration are low confinement TE and TM modes the terms involving dot products between the mode profiles will be approximately zero. For high confinement waveguides the overlap between the e_z components will become significant and these terms must be considered.

The $(1/2)(1 - \delta - \frac{\sigma}{2})|\mathbf{e}^{(1)}|^2|\mathbf{e}^{(2)}|^2$ term is the only term that does not depend on an overlap between the mode profile components of the two modes. In a low-confinement waveguide, if the modes have different polarizations this will be the only significant term. In terms of the susceptibility tensor elements, it is proportional to $(1/2)(1 - \delta - \frac{\sigma}{2}) =$

 χ_{xyxy}/χ_{xxxx} . For an isotropic material $\chi_{xyxy}/\chi_{xxxx} = 1/3$, and the expression $2\gamma_{1212} = 2\gamma_{1111}/3$ from [26] is recovered (recall the extra factor of 2 in front of γ_{1212} in Eqs. (4.2) and (4.3)).

 $B_{1212}(\theta)$ will only be significant if there is overlap between the modes or if the e_z components of the mode profiles are significant. This means there will be no angular variation in γ_{1212} for the fundamental TE and TM modes in a low confinement waveguide, but the magnitude of the angular variation will increase as the e_z components of the modes increase.

The last term in Eqs. (4.2) and (4.3) represents four wave mixing (FWM). The FWM NLC γ_{1122} is given by:

$$\gamma_{1122} = \frac{3\omega\varepsilon_0}{16N_1N_2} \sum_{\mu\alpha\beta\gamma} \iint \chi^{(3)}_{\mu\alpha\beta\gamma} e^{*(1)}_{\mu} e^{*(1)}_{\alpha} e^{(2)}_{\beta} e^{(2)}_{\gamma} dA \tag{4.8}$$

Inserting Eq. (2.25) gives:

$$\gamma_{1122} = \frac{\varepsilon_0 \omega_0}{4\mu_0 c N_1 N_2} \iint n^2 n_2 \left(\left(\delta - \frac{\sigma}{2} \right) (\mathbf{e}^{*(1)} \cdot \mathbf{e}^{*(1)}) (\mathbf{e}^{(2)} \cdot \mathbf{e}^{(2)}) + \left(1 - \delta - \frac{\sigma}{2} \right) (\mathbf{e}^{*(1)} \cdot \mathbf{e}^{(2)})^2 + \sigma B_{1122}(\theta) \right) dA$$
(4.9)

where

$$B_{1122}(\theta) = \frac{1}{4} (\cos(4\theta) + 3) (|e_x^{(1)}|^2 |e_x^{(2)}|^2 + |e_z^{(1)}|^2 |e_z^{(2)}|^2) + |e_y^{(1)}|^2 |e_y^{(2)}|^2 - \frac{1}{4} (1 - \cos(4\theta)) (|e_x^{(1)}|^2 |e_z^{(2)}|^2 + |e_x^{(2)}|^2 |e_z^{(1)}|^2 - 4e_x^{(1)} e_z^{(1)} e_x^{(2)} e_z^{(2)})$$

$$(4.10)$$

where the symmetry properties of the mode profile has been used to eliminate some terms in $B_{1122}(\theta)$. Here, and in the rest of this thesis, I have written the imaginary component of $e_z^{(i)}$, $Im(e_z^{(i)})$, as simply $e_z^{(i)}$ due to the fact that the longitudinal component of the mode profile is purely imaginary. The e_z components always appear in a product with other e_z components, so their complex nature can be accounted for by including a negative sign in front of the term they appear in. For example, the last term in B_{1122} was rewritten as follows:

$$4e_x^{(1)}e_z^{(1)}e_x^{(2)}e_z^{(2)} = 4e_x^{(1)}(iIm(e_z^{(1)}))e_x^{(2)}(iIm(e_z^{(2)}))$$

= $-e_x^{(1)}(Im(e_z^{(1)}))e_x^{(2)}(Im(e_z^{(2)}))$
 $\rightarrow -4e_x^{(1)}e_z^{(1)}e_x^{(2)}e_z^{(2)}$ (4.11)

It can be seen that the first term in the integrand of Eq. (4.9) is the only term that does

not depend on overlap between the modes. In a low-confinement waveguide, this will be the only significant term if the modes have different polarizations. In terms of the tensor elements, this term is proportional to $(\delta - \sigma/2) = \chi_{xxyy}/\chi_{xxxx}$. For an isotropic material, $\chi_{xxyy}/\chi_{xxxx} = 1/3$, and the relation $\gamma_{1122} = \gamma_{1111}/3$ from [26] is recovered. Similar to B_{1212} , $B_{1122}(\theta)$ will only be significant if there is overlap between the mode profiles or the e_z component is large in magnitude.

Similar to the single-mode NLC γ , γ_{1212} and γ_{1122} can be refactored into more intuitive forms. Using Eq. (3.9) the normalization factors N_1 and N_2 can be rewritten in terms of the group indices of mode 1 and mode 2, n_{g1} and n_{g2} , respectively. Then, assuming the waveguide consists of a single nonlinear core with core index n_{core} and neglecting a term involving the integral of $2e_x^{(1)}e_y^{(2)}e_y^{(1)}e_x^{(2)}$, γ_{1212} can be written as:

$$\gamma_{1212} = \eta_{NL}^{(12)} \frac{n_{g1} n_{g2}}{n_{core}^2} \frac{k_0 \overline{n}_2^{(XPM)}}{A_{eff}^{(12)}}$$
(4.12)

where the nonlinear overlap of the two modes with the core is:

$$\eta_{NL}^{(12)} = \frac{\iint_{NL} (n^2 |\mathbf{e}^{(1)}|^2) (n^2 |\mathbf{e}^{(2)}|^2) dA}{\iint_{\infty} (n^2 |\mathbf{e}^{(1)}|^2) (n^2 |\mathbf{e}^{(2)}|^2) dA}$$
(4.13)

the combined effective area of the two modes is:

$$A_{eff}^{(12)} = \frac{(\iint n^2 |\mathbf{e}^{(1)}|^2 dA) (\iint n^2 |\mathbf{e}^{(2)}|^2 dA)}{\iint (n^2 |\mathbf{e}^{(1)}|^2) (n^2 |\mathbf{e}^{(2)}|^2) dA}$$
(4.14)

the effective Kerr index of the XPM process is:

$$\overline{n}_{2}^{(XPM)} = n_{2} \left(1 - 4\overline{\delta}_{12} - \overline{\sigma}_{1212} \frac{\sin^{2}(2\theta)}{2} - F_{1212} \right)$$
(4.15)

where the effective δ of the two modes is:

$$\overline{\delta}_{12} = \delta \frac{\iint_{NL} (e_x^{(1)} e_x^{(2)} + e_y^{(1)} e_y^{(2)}) e_z^{(1)} e_z^{(2)} dA}{\iint_{NL} |\mathbf{e}^{(1)}|^2 |\mathbf{e}^{(2)}|^2 dA}$$
(4.16)

where again $e_z^{(i)}$ are the imaginary parts of the z component of $\mathbf{e}^{(i)}$, i.e. $e_z^{(i)} = Im(\mathbf{e}^{(i)} \cdot \hat{z})$. The effective anisotropy of XPM between the two modes is:

$$\overline{\sigma}_{1212} = \sigma \frac{\iint_{NL} (|e_x^{(1)}|^2 - |e_z^{(1)}|^2) (|e_x^{(2)}|^2 - |e_z^{(2)}|^2) dA}{\iint_{NL} |\mathbf{e}^{(1)}|^2 |\mathbf{e}^{(2)}|^2 dA}$$
(4.17)

A new factor F_{1212} is introduced here due to the mismatch in the mode's spatial profiles:

$$F_{1212} = \frac{1}{2} \left(1 + \delta + \frac{\sigma}{2} \right) \\ \times \frac{\int \int_{NL} (e_x^{(1)} e_z^{(2)} - e_z^{(1)} e_x^{(2)})^2 + (e_y^{(1)} e_z^{(2)} - e_z^{(1)} e_y^{(2)})^2 + (e_x^{(1)} e_y^{(2)} - e_y^{(1)} e_x^{(2)})^2 dA}{\int \int_{NL} |\mathbf{e}^{(1)}|^2 |\mathbf{e}^{(2)}|^2 dA}$$

$$= \frac{1}{2} \left(1 + \delta + \frac{\sigma}{2} \right) \frac{\int \int_{NL} |\mathbf{e}^{(1)} \times \mathbf{e}^{(2)}|^2 dA}{\int \int_{NL} |\mathbf{e}^{(1)}|^2 |\mathbf{e}^{(2)}|^2 dA}$$
(4.18)

Using the same approximations, a similar procedure can be performed to obtain the following expression for γ_{1122} :

$$\gamma_{1122} = \eta_{NL}^{(12)} \frac{n_{g1} n_{g2}}{n_{core}^2} \frac{k_0 \overline{n}_2^{(FWM)}}{A_{eff}^{(12)}} \tag{4.19}$$

where the effective Kerr index of the FWM process is:

$$\overline{n}_{2}^{(FWM)} = n_{2} \left(1 - 4\overline{\delta}_{12} - \overline{\sigma}_{1122} \frac{\sin^{2}(2\theta)}{2} - F_{1122} \right)$$
(4.20)

where $\overline{\delta}_{12}$ is the same as above, $\overline{\sigma}_{1122}$ is given by:

$$\overline{\sigma}_{1122} = \sigma \frac{\iint_{NL} (|e_x^{(1)}|^2 - |e_z^{(1)}|^2) (|e_x^{(2)}|^2 - |e_z^{(2)}|^2) + 2(e_x^{(1)}e_z^{(2)} - e_z^{(1)}e_x^{(2)})^2 dA}{\iint_{NL} |\mathbf{e}^{(1)}|^2 |\mathbf{e}^{(2)}|^2 dA}$$
(4.21)

and F_{1122} is given by:

$$F_{1122} = \frac{1}{\iint_{NL} |\mathbf{e}^{(1)}|^2 |\mathbf{e}^{(2)}|^2 dA} \\ \times \iint_{NL} \left(1 + \delta - \frac{\sigma}{2} \right) \left((e_x^{(1)} e_z^{(2)} - e_z^{(1)} e_x^{(2)})^2 + (e_y^{(1)} e_z^{(2)} - e_z^{(1)} e_y^{(2)})^2 \right) \\ + \left(1 - \delta + \frac{\sigma}{2} \right) (e_x^{(1)} e_y^{(2)} - e_y^{(1)} e_x^{(2)})^2 dA$$

$$(4.22)$$

Note that if equal mode profiles are assumed for the two modes, i.e. $\mathbf{e}^{(1)} = \mathbf{e}^{(2)}$, then each factor is equal to the corresponding factor for the single-mode case, except for F_{1212} and F_{1122} which equal zero.

Similar to the single-mode NLC case, the dependence of the NLCs on $A_{eff}^{(12)}$, $\eta_{NL}^{(12)}$ and the group indices are well-known. The novelty of the NLC expressions found here lies in the expressions for the effective Kerr indices $\bar{n}_2^{(XPM)}$ and $\bar{n}_2^{(FWM)}$ and the various factors they contain, which, to the best of my knowledge, have not previously been written in this way.

4.2 Geometric Dependence

The values of γ_{1212} and γ_{1122} for the TE₀₀ and TM₀₀ modes for various waveguide geometries will now be investigated. Simulations of AlGaAsOI waveguides were performed using Lumerical MODE Solutions software to determine the mode profiles $\mathbf{e}^{(j)}(x, y)$. The results were used to calculate the NLCs $\gamma_{1212}, \gamma_{1122}$ using Eqs. (4.12) and (4.19) for various waveguide cross-sections with a crystal growth direction of [001], a waveguide orientation of $\theta = \pi/4$ and a wavelength of $\lambda = 1550$ nm. The results are plotted below in Fig. 4.1. The SPM NLCs γ_{1111} and γ_{2222} for the same waveguide geometries were already examined in the previous chapter and are not included here.



Figure 4.1: The calculated values of the a) γ_{1212} and b) γ_{1122} for the fundamental TE and TM modes of an AlGaAsOI waveguide for various geometries calculated using Eqs. (4.12) and (4.19). The parameters used in the simulation were $\lambda = 1550$ nm and $\theta = \pi/4$.

The qualitative behaviour of γ_{1212} and γ_{1122} is similar to that of γ_{TE} and γ_{TM} from the previous section. They increase with decreasing width until reaching a maximum, at which point they begin to decrease as the mode profiles begin to spread into the cladding. With h = 250 nm there is a decrease in γ_{1122} when compared to a waveguide with h = 500nm, and γ_{1212} is roughly the same as with h = 500 nm for w > 400 nm.

By comparing Figs. 3.1 and 4.1 it can be seen that the SPM coefficients are higher than the XPM and FWM coefficients. This is due to the lack of significant overlap between the fundamental TE and TM modes. The SPM coefficients only involve a single mode, so all of the terms in the integrals in Eq. (3.10) are significant. γ_{1212} is roughly twice the magnitude of γ_{1122} , but they reach maximums at different waveguide dimensions. The calculated $A_{eff}^{(12)}$, $\eta_{NL}^{(12)}$, $\sqrt{n_{g1}n_{g2}}/n_{core}$ and $\overline{\delta}_{12}$, which are common to both γ_{1212} and γ_{1122} , for an AlGaAsOI waveguide with $\lambda = 1550$ nm and $\theta = \pi/4$ are shown in Fig. 4.2.



Figure 4.2: The calculated values of a) $A_{eff}^{(12)}$, b) $\eta_{NL}^{(12)}$, c) $\sqrt{n_{g1}n_{g2}}/n_{core}$ and d) $\overline{\delta}_{12}$ for the fundamental TE and TM modes of an AlGaAsOI waveguide with various waveguide geometries. The parameters used in the simulation were $\lambda = 1550$ nm and $\theta = \pi/4$. The legend in a) is used for all plots.

As they involve both the TE₀₀ and TM₀₀ modes, $A_{eff}^{(12)}$ and $\eta_{NL}^{(12)}$ depend on both waveguide width w and height h. From Figs. 4.2 a) and b), as the core size decreases, $A_{eff}^{(12)}$ decreases and $\eta_{NL}^{(12)}$ is roughly unity until dimensions are reduced below around 500 nm and the mode profile begins to spread into the cladding, at which point $A_{eff}^{(12)}$ begins to increase and $\eta_{NL}^{(12)}$ drops. The product of the group indices of the two modes $\sqrt{n_{g1}n_{g2}}/n_{core}$ in Fig. 4.2 c) is a combination of the individual group velocities whose properties were discussed in the previous chapter. The $\overline{\delta}_{12}$ term, shown in Fig. 4.2 d), is negligible due to the weak $e_y^{(1)}$ and $e_x^{(2)}$ mode profile components. The calculated values for $\overline{n}_2^{(XPM)}/n_2$, $\overline{n}_2^{(FWM)}/n_2$, $\overline{\sigma}_{1212}/\sigma$, $\overline{\sigma}_{1122}/\sigma$, F_{1212} , and F_{1122} for the TE₀₀ and TM₀₀ modes of AlGaAsOI waveguides at $\lambda = 1550$ nm and $\theta = \pi/4$ are shown in Fig. 4.3.



Figure 4.3: The calculated values of a) $\overline{n}_2^{(XPM)}$, b) $\overline{n}_2^{(FWM)}$, c) $\overline{\sigma}_{1212}/\sigma$, d) $\overline{\sigma}_{1122}/\sigma$, e) F_{1212} , and f) F_{1122} for the fundamental TE and TM modes of an AlGaAsOI waveguide for various waveguide geometries. The parameters used in the simulation were $\lambda = 1550$ nm and $\theta = \pi/4$. The legend in b) is used for all plots.

From Figs. 4.3 a) and b), it can be seen that the effective Kerr indices $\overline{n}_2^{(XPM)}/n_2$ and $\overline{n}_2^{(FWM)}/n_2$ display more complicated behaviour than the single-mode \overline{n}_2 . In the XPM case, the effective Kerr index is approximately 0.525, except for large widths and low height. This is due in part to the complicated behaviour of $\overline{\sigma}_{1212}$ shown in Fig. 4.3 c). Unlike the other effective anisotropies, $\overline{\sigma}_{1212}$ is negative. This is because $\overline{\sigma}_{1122}$ is proportional to the integral of $(|e_x^{(1)}|^2 - |e_z^{(1)}|^2)(|e_x^{(2)}|^2 - |e_z^{(2)}|^2)$. If mode 2 is a TM mode then $e_x^{(2)} \approx 0$, and therefore the integral of $(|e_x^{(1)}|^2 - |e_z^{(2)}|^2 - |e_z^{(2)}|^2)$ is negative. As long as $(|e_x^{(1)}|^2 - |e_z^{(1)}|^2)$ is positive, as it is if mode 1 is the TE₀₀ mode, then $\overline{\sigma}_{1122}$ will be negative. Due to this fact, in order to maximize XPM effects θ should be zero.

In terms of magnitude, with a large h both $e_x^{(2)}$ and $e_z^{(2)}$ are low, and therefore so is $\overline{\sigma}_{1122}$. Reducing h to 250 nm increases the magnitude of $e_z^{(2)}$ and $\overline{\sigma}_{1122}$ increases. As w is reduced, $\overline{\sigma}_{1122}$ approaches zero due to the fact that $|e_z^{(1)}|$ is increasing, which decreases $(|e_x^{(1)}|^2 - |e_z^{(1)}|^2)$.

The F_{1212} factor, shown in Fig. 4.3 e), has a value of around 0.35-0.45, and decreases with a reduction in waveguide width or height.

The effective anisotropy for the FWM NLC $\overline{\sigma}_{1122}$, shown in Fig. 4.3 d), is mostly independent of w. It increases with decreasing h, reaching values of around 0.25σ with h = 250 nm. It is positive due to the extra term involving the integral of $(e_x^{(1)}e_z^{(2)} - e_z^{(1)}e_x^{(2)})^2$ compared to the XPM effective anisotropy (see Eq. (4.21)).

The F_{1122} factor, shown in Fig. 4.3 f), is higher than F_{1212} , with a value of around 0.6-0.85. With a waveguide height of h = 500 nm or h = 750 nm F_{1122} increases with a decreasing width w. For a waveguide with h = 250 nm, however, F_{1122} has a value of around 0.8-0.85, and decreases with decreasing w. The combined behaviour of $\overline{\sigma}_{1122}$ and F_{1122} lead to the values of $n_2^{(FWM)}$ seen in Fig. 4.3 b).

From Figs. 3.2, 3.34.2, and 4.3 it can be seen that $A_{eff}^{(12)}$, $\eta_{NL}^{(12)}$ and $\sqrt{n_{g1}n_{g2}}/n_{core}$ do not significantly differ from the corresponding single-mode factors A_{eff} , η_{NL} , n_{g1}^2/n_{core}^2 and n_{g2}^2/n_{core}^2 for the fundamental TE and TM modes of the AlGaAsOI waveguide. The decrease in the magnitude of γ_{1212} and γ_{1122} when compared to the single-mode NLC γ is largely due to the decrease in their respective effective Kerr indices, and in particular to the F_{1212} and F_{1122} terms.

4.3 Angular Dependence

The dependence of the XPM and FWM NLCs on θ will now be examined. γ_{1212} and γ_{1122} for the fundamental TE and TM modes at $\lambda = 1550$ nm of high-confinement (h = 300 nm, w = 350 nm) and low-confinement (h = 1500 nm, w = 1750 nm) waveguides are shown in Fig. 4.4 as a function of θ . The NLCs are normalized to their value where $\theta = 0$. For the rest of this thesis, Eq. (2.20) was used to calculate the full-vectorial NLCs, instead of the approximate formulas such as Eqs. (3.11), (4.12), and (4.19).

It can be seen from this figure that γ_{1212} and γ_{1122} display little angular variation for the low-confinement waveguides due to the low effective anisotropies $\overline{\sigma}_{1212}$ and $\overline{\sigma}_{1122}$ in low-confinement waveguides. For high confinement waveguides, γ_{1212} decreases slightly and γ_{1122} increases significantly by a factor of around 1.35 when θ varies from 0 to $\pi/4$.

Similarly to the single-mode case, I define $\Delta \gamma_{1212} = \frac{\gamma_{1212}(\theta = \pi/4) - \gamma_{1212}(\theta = 0)}{\gamma_{1212}(\theta = 0)}$ and $\Delta \gamma_{1122} = \frac{\gamma_{1212}(\theta = \pi/4) - \gamma_{1212}(\theta = 0)}{\gamma_{1212}(\theta = 0)}$



Figure 4.4: The values of the various nonlinear coefficients for high and low confinement AlGaAsOI waveguides as a function of waveguide orientation.

$$\frac{\gamma_{1122}(\theta=\pi/4) - \gamma_{1122}(\theta=0)}{\gamma_{1122}(\theta=0)}. \text{ From Eq. (4.6):}$$

$$\Delta\gamma_{1212} = -\frac{\overline{\sigma}_{1212}}{2(1-\overline{\delta}_{12}-F_{1212})} \approx -\frac{\overline{\sigma}_{1212}}{2(1-F_{1212})} \tag{4.23}$$

where $\overline{\delta}_{12}$ was neglected due to its low value, and likewise

$$\Delta \gamma_{1212} \approx -\frac{\overline{\sigma}_{1122}}{2(1 - F_{1122})} \tag{4.24}$$

This behaviour can be investigated in detail by plotting the calculated values of $\Delta \gamma_{1212}$ and $\Delta \gamma_{1122}$ for the fundamental modes of an AlGaAsOI waveguide at $\lambda = 1550$ nm, found using Eqs. (4.5) and (4.8) (see Fig. 4.5).

When compared to Fig. 3.6, it can be seen that they display different behaviour than the SPM NLCs. The variation in XPM, $\Delta \gamma_{1212}$, generally follows the same pattern as $\overline{\sigma}_{1212}/\sigma$, as F_{1212} does not significantly vary with these waveguide geometries.

It can also be seen that $\Delta \gamma_{1122}$ increases as h decreases, and reaches up significant values up to 0.65 when h = 250 nm. With h = 250 nm, $\Delta \gamma_{1122}$ decreases with smaller w, but displays the opposite behaviour for h = 500 nm or h = 750 nm, increasing slightly as w decreases. As $\overline{\sigma}_{1122}$ does not vary significantly with w (see Fig. 4.3 d)), this is due to the behaviour of F_{1122} with respect to w (see Fig. 4.3 f)). From these figures and Eq. (4.24) it can also be seen that the high value of $\Delta \gamma_{1122}$ is not due to a high value of $\overline{\sigma}_{1122}$, which only reaches values up to around 0.3σ , but due to the high values of F_{1122} for waveguides with a low h.



Figure 4.5: Simulated values of a) $\Delta \gamma_{1212}$ and b) $\Delta \gamma_{1122}$ for the fundamental TE and TM modes of an AlGaAsOI waveguide of various cross sections evaluated at $\lambda = 1550$ nm.

4.4 Low Confinement Approximation

As in the previous section, the fundamental TE (TM) mode can be approximated as consisting entirely of the e_x (e_y) component for low confinement waveguides. If it is also assumed that the mode profile is negligible outside the waveguide core and material dispersion is ignored, the following expressions for the various factors involved in the nonlinear coefficients can be obtained:

$$\eta_{NL}^{(12)} \to 1$$
 (4.25)

$$A_{eff}^{(12)} \to \frac{(\iint |e_x^{(1)}|^2 dA)(\iint |e_y^{(2)}|^2 dA)}{\iint |e_x^{(1)}|^2 |e_y^{(2)}|^2 dA}$$
(4.26)

$$n_{g1}n_{g2} \to n_{core}^2 \tag{4.27}$$

$$\overline{\delta}_{12} \to 0 \tag{4.28}$$

$$\overline{\sigma}_{1212} \to 0 \tag{4.29}$$

$$\overline{\sigma}_{1122} \to 0 \tag{4.30}$$

$$F_{1212} \to \frac{1}{2} \left(1 + \delta + \frac{\sigma}{2} \right) \tag{4.31}$$

$$F_{1122} \to \left(1 - \delta + \frac{\delta}{2}\right) \tag{4.32}$$

$$\overline{n}_{2}^{(XPM)} \to \frac{n_{2}}{2} \left(1 - \delta - \frac{o}{2} \right) \tag{4.33}$$

$$\overline{n}_2^{(FWM)} \to n_2 \left(\delta - \frac{\delta}{2}\right) \tag{4.34}$$

These expressions lead to low confinement approximations for the XPM and FWM NLCs:

$$\gamma_{1212}^{LC} = \frac{1}{2} \left(1 - \delta - \frac{\sigma}{2} \right) \left(\frac{\omega_0 n_2}{c} \right) \frac{\int \int |e_x^{(1)}|^2 |e_y^{(2)}|^2 dx dy}{\left(\int \int |e_x^{(1)}|^2 dx dy \right) \left(\int \int |e_y^{(2)}|^2 dx dy \right)}$$
(4.35)

$$\gamma_{1122}^{LC} = \left(\delta - \frac{\sigma}{2}\right) \left(\frac{\omega_0 n_2}{c}\right) \frac{\iint |e_x^{(1)}|^2 |e_y^{(2)}|^2 dx dy}{(\iint |e_x^{(1)}|^2 dx dy) (\iint |e_y^{(2)}|^2 dx dy)}$$
(4.36)

From these equations it can be seen that there will be no angular dependence for γ_{1212} and γ_{1122} for the fundamental TE and TM modes in a low confinement waveguide, as seen in Fig. 4.4.

In an isotropic material $\delta = 1/3$ and $\sigma = 0$, which gives $(1/2)(1 - \delta - \sigma/2) = 1/3$ and $\delta - \sigma/2 = 1/3$. If a symmetric waveguide is assumed such that $|e_x^{(1)}| = |e_y^{(2)}|$ throughout the waveguide, then $\gamma_{1111}^{LC} = \gamma_{2222}^{LC} = 3\gamma_{1212}^{LC} = 3\gamma_{1122}^{LC}$, where $\gamma_{1111}^{LC} = \gamma_{TE}^{LC}$ and $\gamma_{2222}^{LC} = \gamma_{TM}^{LC}$. This matches results for isotropic, scalar models for silica fibres [26].

Plotted in Fig. 4.6 are the ratios between the full expressions $(\gamma_{1111}, \gamma_{2222}, \gamma_{1212}, \gamma_{1122})$ calculated using Eq. (2.20) and the low-confinement approximations $(\gamma_{1111}^{LC}, \gamma_{2222}^{LC}, \gamma_{1212}^{LC}, \gamma_{1122}^{LC})$ for the nonlinear coefficients for the fundamental modes of an AlGaAsOI waveguide with varying height and width, $\lambda = 1550$ nm, and $\theta = \pi/4$. The ratio of the height to the width is fixed as 4:5 to demonstrate the effect of reducing both dimensions of the waveguide. It can be seen that for large waveguide areas there is good agreement between



Figure 4.6: The ratios of the full and low confinement nonlinear coefficients for the TE₀₀ and TM₀₀ modes of an AlGaAsOI waveguide with $\lambda = 1550$ nm and $\theta = \pi/4$. The ratio of height to width is fixed at 4:5.

the low-confinement approximations and the full expressions for the NLCs. However, as the waveguide area decreases the low-confinement approximations underestimate γ_{ijkl} , in agreement with work in silica and silicon [49]. This is especially true for the XPM NLC ratio, $\gamma_{1212}/\gamma_{1212}^{LC}$, which reaches a maximum value of around 3.25. The ratios of the other NLCs have maximum values of around 2. The low-confinement approximation for γ_{1212} is also accurate until a smaller waveguide area than the others.

4.5 Higher Order Modes

The full-vectorial model is not limited to the fundamental modes of the waveguide. In fact, the higher order modes of the waveguide can have very strong longitudinal components (see Fig. 2.2), so a full-vectorial model is essential to accurately model third-order nonlinear interactions involving these modes.

As an example of applying this theory to higher order modes, the case of the TE₀₀ and TE₁₀ modes (see Figure 2.2) at the same frequency, which will be labelled with the indices 1 and 2, respectively, will be analyzed. This mode combination has been used for intermodal FWM [47] and entangled photon generation [50]. The full-vectorial model can be readily extended to situations involving modes at different frequencies, though the impact of this on $\chi^{(3)}$ must be considered.

From Fig. 2.2 it can be seen that the TE_{10} mode has different symmetry properties than the TE_{00} and TM_{00} modes. It has a very strong e_z component that is even in both the x and y directions and the e_x profile is odd in the x direction and even in the y direction. Due to these symmetries the NLCs that integrated to zero for the previous case of the fundamental modes, for example γ_{1112} and γ_{1222} , will also be negligible in this case.

All four of the NLCs from this and the previous chapter will be examined at the same time. Note that no assumptions were made about the mode profiles when deriving Eqs. (3.10), (4.6) and (4.9) (other than a symmetry assumption used to eliminate a term in $B_{1122}(\theta)$, which still applies to this case), so they still apply to this mode combination. The simplified expressions in Eqs. (4.12) and (4.19) also still apply to this mode combination. However, the low confinement approximations defined in the last section no longer apply. Even in a low-confinement waveguide, the e_z component of the TE₁₀ mode is still significant, so the scalar mode approximation is not accurate.

Plotted in Fig. 4.7 are all four NLCs discussed so far, calculated using Eq. (2.20) for the TE₀₀ and TE₁₀ modes for an AlGaAsOI waveguide grown on a [001] wafer with $\theta = \pi/4$ and $\lambda = 1550$ nm. Note the larger values of w used in this plot compared to the plots in the previous sections due to the fact that the TE₁₀ mode is not supported in AlGaAsOI waveguides with w below around 650 nm. It can be seen that γ_{2222} is slightly

lower that γ_{1111} , despite both modes having the same TE polarization. γ_{1212} is slightly more than half of γ_{1111} , similar to the case of the two fundamental modes. Also, γ_{1122} tends to reach a maximum at a larger w than the others, while γ_{1111} does not appear to reach a maximum for these ranges of h and w. These facts could be relevant for optimizing the geometry of waveguides used for intermodal FWM, for example.



Figure 4.7: The values of the various nonlinear coefficients for an AlGaAsOI waveguide for various values of h and w. The parameters used in the simulations were $\theta = \pi/4$, and $\lambda = 1550$ nm.

The variation of the NLCs with θ , normalized to their values when $\theta = 0$, as a function of θ with a fixed cross section of h = 300 nm and w = 700 nm is shown in Fig. 4.8. It can be seen that γ_{2222} has a lower maximum than γ_{1111} due to the stronger e_z component of the TE10 mode profile. For the same reason, the variation in the XPM NLC γ_{1212} is small and negative. The FWM NLC γ_{1122} has a very large variation of up to around 2.25 times its value at $\theta = 0$. This can be understood from Eqs. (4.9) and (4.10). Due to the fact that the TE₀₀ mode has a large e_x component and the TE₁₀ mode has both a large e_x and e_z component, $B_{1122}(\theta)$ reaches very high values compared to the rest of the terms in Eq. (4.9) when $\theta = \pi/4$. In Fig. 4.9 $\Delta\gamma$ is plotted for the four NLCs as a function of



Figure 4.8: The values of the nonlinear coefficients for an AlGaAsOI waveguide as a function of θ . The parameters used in the simulations were h = 300 nm, w = 700 nm and $\lambda = 1550$ nm.

waveguide width w. It can be seen that the angular variation is around 0.26 for γ_{1111} for all widths due to the negligible e_z component for the TE₀₀ mode at these values of w. $\Delta\gamma_{2222}$ is slightly less than $\Delta\gamma_{1111}$ due to the stronger e_z component of the TE₁₀ mode. $\Delta\gamma_{1212}$ starts at slightly less than $\Delta\gamma_{2222}$ when w = 1200 nm, and approaches zero as w decreases. $\Delta\gamma_{1212}$, which reaches a very large value of up to approximately 3 when w = 650 nm, as seen in Fig. 4.8.

4.6 Conclusion

In this chapter, explicit expressions for the two-mode NLCs corresponding to XPM and FWM were derived. Their dependence on waveguide geometry and orientation were investigated via simulation and compared to the single-mode NLC γ for the fundamental TE and TM modes. The case of the TE₀₀ and TE₁₀ modes was examined as well.



Figure 4.9: The values of $\Delta \gamma$ for various nonlinear coefficients for the TE_{00} and TE_{10} modes of an AlGaAsOI waveguide with varying waveguide width w. The parameters used in the simulations were h = 300 nm, and $\lambda = 1550$ nm.

Chapter 5

Comparison To Existing Theories

In this chapter the results obtained using the full-vectorial model will be compared via simulations to other models that have previously been used to describe third-order nonlinear effects in AlGaAs. Most of the focus of this chapter will be on the single-mode NLC discussed in Chpt. 3. The different expressions for the single-mode NLC that have been used for AlGaAs waveguides will be reviewed. The numerical results of those expressions will be compared to those obtained by the full-vectorial theory for AlGaAsOI and AlGaAs nanowire waveguides.

5.1 Existing Theories

Basic introductions to nonlinear optics such as [11, 42] tend to make a plane wave assumption that make them unsuitable for evaluating effects of high confinement waveguide geometry or mode size. Much of the early research on the anisotropy of the AlGaAs thirdorder susceptibility tensor involved low-confinement ridge waveguides, where the plane wave approximation is appropriate [18, 20, 35, 44]. Though the nonlinear interactions between different electric field components and different optical frequencies were investigated, the focus of these studies was generally on individual electric field components of arbitrary polarization, not on the interaction of different waveguide modes involving multiple electric field components. The results of these studies on the AlGaAs third-order susceptibility tensor $\chi^{(3)}$ and the nonlinear parameters σ, δ and n_2 , however, are used in our model.

There are many published theories regarding third-order nonlinear optical effects in waveguides, some of which are described below. Typically they share many characteristics: a coupled mode formalism is used, involving SPM, XPM and FWM terms, as in our theory, though other effects like TPA, free carrier absorption (FCA) and dispersion (FCD), and nonparametric effects like Raman scattering are often included, in particular for silicon waveguides. They mostly differ in which effects they include and how the NLCs are evaluated. Different assumptions on the mode profiles and susceptibilities are used to derive many different expressions for the NLCs.

For silica fibres, a common resource is [26], where a scalar approximation along with an isotropic third-order susceptibility assumption is applied to fibre waveguide modes. A more recent study on fibre waveguides is [33], where a full-vectorial theory of two orthogonally polarized pulses in high-confinement fibre waveguides is investigated. The expressions derived in this thesis for the various NLCs reduce to those in that work if an isotropic material is assumed, i.e. $\sigma = 0$ and $\delta = 1/3$. Interestingly, in [33] it was found that two propagating modes can affect the dispersion of the other if they are phase-matched.

Much of the integrated nonlinear optics literature has focused on SOI waveguides due to the popularity of that material system. For an in-depth introduction to thirdorder nonlinear effects in SOI waveguides, see [29, 28]. There have been extensive studies for fibre and SOI waveguides using various definitions of NLCs and effective areas, for example [32, 43, 51, 52, 53].

Perhaps most relevant to the work in this thesis is [31], where the nonlinear interaction between the fundamental TE and TM modes at the same wavelength in an SOI waveguide were investigated using a full-vectorial model. The basic theory is very similar to that demonstrated in this thesis, however (in addition to the difference in material parameters such as n, n_2, σ , etc. between AlGaAs and silicon) is the fact that Kleinmann symmetry cannot be assumed for AlGaAs due to the proximity to the half band gap at $\lambda = 1550$ nm, leading to an additional material parameter δ . If Kleinmann symmetry applies, as it does in silicon, σ and δ are related. Also, only a single waveguide orientation was considered in that work, and explicit expressions for the various NLCs in terms of the mode profile components were not derived as they are in this thesis.

To the best of my knowledge, full-vectorial theories such as these have not been applied to AlGaAs waveguides. Recent experimental research on third order effects in AlGaAs waveguides tends to borrow models developed for low confinement silica fibre or SOI waveguides and does not properly account for the anisotropy of the AlGaAs third-order susceptibility tensor.

A common general expression for the single-mode NLC is:

$$\gamma = \frac{k_0 n_2}{A_{eff}} \tag{5.1}$$

where A_{eff} is the effective area of the mode.

The exact definition of the effective area varies. The approach in [26] is often applied to AlGaAs waveguides, where A_{eff} is given by:

$$A_{eff}^{II} = \frac{(\iint |e(x,y)|^2 dA)^2}{\iint |e(x,y)|^4 dA}$$
(5.2)

where e(x, y) is the scalar electric field mode profile and the \iint symbol with no subscript indicates integration over the entire x - y plane, resulting in the NLC:

$$\gamma^{II} = \frac{k_0 n_2}{A_{eff}^{II}} = k_0 n_2 \frac{\iint |e(x, y)|^4 dA}{(\iint |e(x, y)|^2 dA)^2}$$
(5.3)

This equation was derived for low-confinement silica fibres, where it was assumed the mode profile was scalar and transverse $(\mathbf{e}(x, y) = e(x, y)\hat{x})$ and the material nonlinearity was isotropic.

It has been shown for fibres that this model tends to underestimate the magnitude of the NLC for high-confinement waveguides [33, 49]. As previously discussed, this assumption is only valid for waveguide with large core dimensions and small index contrasts between the core and cladding. However this expression is still commonly used for Al-GaAs waveguides where this scalar assumption is not valid, in particular for AlGaAs nanowires [12, 13, 21, 54, 55, 56]. Though it is occasionally not specified, I will assume that the scalar $|e(x, y)|^2$ was replaced by the vectorial $|\mathbf{e}(x, y)|^2 = |e_x|^2 + |e_y|^2 + |e_z|^2$ in these publications to account for the strong e_z component of high-confinement waveguide modes. In some studies the region of integration is modified to only include the waveguide, or is not specified.

Note that Eq. (5.3) is similar to the low-confinement approximations derived from our full expressions, Eqs. (3.25) and (3.26). However, Eqs. (3.25) and (3.26) were derived from the full-vectorial expression Eq. (3.10) by neglecting the non-dominant transverse component (e_y for the TE mode and e_x for the TM mode) and the e_z component. Eq. (5.3) includes them by replacing $|e_x|^2$ (in γ_{TE}^{LC}) or $|e_y|^2$ (in γ_{TM}^{LC}) by $|\mathbf{e}|^2$.

Another example of an effective area is used in [57], originally from [52]:

$$A_{eff}^{III} = \frac{a_{NL} \iint S_z dA}{\iint_{NL} S_z dA}$$
(5.4)

where $S_z = (\mathbf{e} \times \mathbf{h}^*) \cdot z$ is the z component of the Poynting vector, a_{NL} is the cross-section area of the nonlinear waveguide core, and NL denotes integration over the nonlinear region. This expression was designed to relate the total power to the average intensity in the nonlinear region. The NLC in this case is:

$$\gamma^{III} = \frac{k_0 n_2}{A_{eff}^{III}} = k_0 n_2 \frac{\iint_{NL} S_z dA}{a_{NL} \iint S_z dA}$$
(5.5)

Another expression for the single mode NLC, suggested in [51] for high contrast waveguides, is

$$\gamma^{IV} = k_0 \frac{\iint n_2(x, y) S_z^2 dA}{(\iint S_z dA)^2}$$
(5.6)

where n_2 is included in the integrand of the numerator to account for the inhomogeneity of the waveguide.

In some publications, the general formula of Eq. (5.1) is used, but the exact expression used for A_{eff} is not specified or is unclear [23, 24]. Though γ^{III} and γ^{IV} do not necessarily assume the mode profile is scalar, I will still refer to them as "scalar" models as they do not take into account the full vectorial nature of the waveguide mode and the AlGaAs nonlinear susceptibility tensor.

As they were mainly developed for isotropic materials, these models does not consider the orientation of the waveguide coordinate frame with that of the crystal lattice. For low-confinement waveguides where the mode may be considered scalar, for example rib AlGaAs waveguides [58], the waveguide orientation can be roughly accounted for by considering a different effective n_2 . As shown in Chpt. 3, this method is not effective for high-confinement modes with multiple electric field components where a full-vectorial approach is required to calculate the effective Kerr index.

A common reference for n_2 is [18], where n_2 was found for TE and TM modes in a low-confinement strip-loaded waveguide on a [001] grown wafer. The TE mode is oriented in the [110] direction and the TM mode is oriented along the [001] axis. Different n_2 values were found for these modes, which correspond to the effective n_2 values $n_2[110] = 1.5 \times 10^{-17} \text{ W}^{-1}\text{m}^{-1}$ and $n_2[001] = 1.43 \times 10^{-17} \text{ W}^{-1}\text{m}^{-1}$, which can be used for scalar modes with electric fields with those orientations. However, for high-confinement waveguides using a different n_2 value will still not fully account for anisotropy of the AlGaAs susceptibility tensor and the differences between the electric field components of the modes. As shown in the Chpt. 3, the magnitude of the variation in γ with changing θ depends on the relative magnitudes of the components of the mode profile. Simply varying n_2 does not account for this phenomenon.

Note that this change in n_2 between the $n_2[001]$ and $n_2[110]$ from [18] is only around 5%, while our model predicts a variation in γ of around 26% for a scalar TE mode as the orientation of the θ changes from 0 (parallel to a crystal axis) to $\pi/4$ (halfway between

two crystal axes). These discrepancies suggest further experimental work is needed to determine the values of n_2 , σ and δ to higher accuracy. These effects are irrelevant for $\theta = 0$ when all electric field components are directed along crystal axes, so the comparison presented here between the different expressions for γ will be restricted to the case where $\theta = 0$ and use $n_2[001]$ for all NLCs.

Most studies on third-order nonlinear effects in AlGaAs waveguides involve modes with the same spatial distribution, so only the single mode NLC (equivalent to γ_{iiii}) is required. An exception is [13], where an expression similar to the XPM NLC from [26] is used:

$$\gamma_{1212}^{II} = \frac{k_0 n_2}{3} \frac{\iint |e^{(1)}(x,y)|^2 |e^{(2)}(x,y)|^2 dA}{(\iint |e^{(1)}(x,y)|^2 dA)^2 (\iint |e^{(2)}(x,y)|^2 dA)^2}$$
(5.7)

where $e^{(i)}(x, y)$ is the *i*th scalar mode profile. In [26] Eq. 5.7 is multiplied by two. This factor of two in our case is not included in our XPM NLC as it is included in Eqs. (4.2) and (4.2). The factor of 1/3 is not included in [13], instead the value of n_2 is modified based on the polarization of the modes involved.

This expression is similar to the low-confinement XPM NLC derived in Chpt. 4, Eq. (4.35), though this expression uses the magnitude of the total electric field rather than just the dominant component. However, the factor of $(1/2)(1 - \delta - \sigma/2)$ factor from Eq. (4.35) is replaced by 1/3, which is the value obtained for this factor for an isotropic material where $\sigma = 0$ and $\delta = 1/3$.

For comparison, I will replace replace the factor of 1/3 with $(1/2)(1 - \delta - \sigma/2)$ to account for the AlGaAs $\chi^{(3)}$ tensor's anisotropy. As I did for γ^{II} , I replace the scalar mode profile magnitude $|e(x, y)|^2$ used in [26] with the vectorial mode profile magnitude $|\mathbf{e}(x, y)|^2$ to attempt to account for the strong e_z component in high-confinement waveguides.

Though I have not seen it used in the literature, I propose a modified form of γ^{IV} for XPM will also be compared to our full-vectorial model, given by:

$$\gamma_{1212}^{IV} = \frac{1}{2} \left(1 - \delta - \frac{\sigma}{2} \right) k_0 \frac{\iint n_2(x, y) S_z^{(1)} S_z^{(2)} dA}{(\iint S_z^{(1)} dA) (\iint S_z^{(2)} dA)}$$
(5.8)

A scalar expression for the two-mode FWM NLC γ_{1122} is also given in [26]. However, I will not compare it to our model here.

5.2 AlGaAsOI Waveguides

The different expressions for the NLCs will now be compared via simulation with the full-vectorial model for AlGaAsOI waveguides. As $\theta = 0$, the value of n_2 will be taken as $n_2[001]$ for all NLCs.



Figure 5.1: The values of the various published nonlinear coefficients for an AlGaAsOI waveguide with varying waveguide width w. The parameters used in the simulations were h = 300 nm, $\theta = 0$ and $\lambda = 1550$ nm. a) TE₀₀ mode. b) TM₀₀ mode.

Fig. 5.1 shows the calculated values of the various published single-mode NLCs for the fundamental TE and TM modes of an AlGaAsOI waveguide at $\lambda = 1550$ nm and a waveguide orientation of $\theta = 0$. Here γ is the single mode NLC from the full-vectorial model of this thesis, calculated directly from (3.3). From Fig. 5.1 a), there are significant quantitative differences between γ^{II-IV} and γ for the TE₀₀ mode. The full-vectorial NLC γ is significantly higher than the other expressions, though it follows the same general pattern. This is in agreement with results for full-vectorial models in fibre [33]. The difference in results is most apparent for smaller w of around 300-400 nm due to the increased vectorial nature of the modes when the waveguide core is smaller. For larger w the fundamental TE mode is closer to a scalar mode, so the approximate NLCs are more accurate.

Qualitatively it can be seen that all of the NLCs increase with decreasing w until reaching a maximum at which point they begin to decrease due to the mode profile leaking into the cladding. However, the maximum is reached at different values of w for different expressions. The expression γ^{IV} follows the qualitative behaviour of γ the best, with a similar optimum waveguide width of around w = 375 nm for the TE₀₀ mode. The values obtained from γ^{II} significantly differ than the other NLCs for w < 600 nm. γ^{II} reaches a maximum value at approximately w = 600 nm for the TE₀₀ mode, a much larger width than the others, then decreases while the other NLCs significantly increase.

It can also be seen that, for very small widths, γ and γ^{IV} , which are larger than the others for higher widths, begin to decrease much more quickly than γ^{II} and γ^{III} . This is because the mode is leaking out of the nonlinear core into the cladding. The expressions for γ and γ^{IV} take this into account by including n_2 inside the integrand of the numerators of those expressions, while this is not accurately accounted for in γ^{II} . The last NLC, γ^{III} includes only an integration over the nonlinear core in the denominator, however the effects of the changing mode shape are reduced due to the constant a_{NL} factor in its denominator. This result suggests that for optimizing the geometry of an AlGaAsOI waveguide, the full-vectorial theory is required, but γ^{IV} can provide a close approximation.

Similar differences can be seen for the TM_{00} mode as well in Fig. 5.1 b). The main difference is again that the full-vectorial γ is much larger than the other expressions. It can also be seen that, for $w > 600 \text{ nm } \gamma^{IV}$ is a good approximation for γ for the TM_{00} mode, performing even better here compared to the TE_{00} mode.

The same analysis was performed for the TE_{10} and TM_{10} modes. The results are shown in Fig. 5.2.



Figure 5.2: The simulated values of the various published NLCs for an AlGaAsOI waveguide with varying waveguide width w. The parameters used in the simulations were $h = 300 \text{ nm}, \theta = 0 \text{ and } \lambda = 1550 \text{ nm}.$ a) TE₁₀ mode. b) TM₁₀ mode.

Similar to the fundamental modes, it can be seen that the scalar NLC expressions underestimate γ for the higher order TE₁₀ and TM₁₀ modes. This would be expected, considering the strong e_z components of their mode profiles. Again γ^{IV} is closest to γ , particularly for the TM₁₀ mode at w > 1.2 microns. However, it fails to properly find the optimum value for maximizing γ for the TM₁₀ mode. The other scalar NLCs γ^{II} and γ^{III} severely underestimate γ and should not be used for these modes.

The values of γ_{1212} , γ_{1212}^{II} and γ_{1212}^{IV} calculated by simulation for the fundamental modes of an AlGaAsOI waveguide are shown in Fig. 5.3. The results are similar to the case of



Figure 5.3: The simulated values of the various XPM NLCs for the fundamental modes of an AlGaAsOI waveguide with varying waveguide width w. The parameters used in the simulations were h = 300 nm, $\theta = 0$ and $\lambda = 1550$ nm.

the single-mode NLC γ . The scalar expressions γ_{1212}^{II} and γ_{1212}^{IV} underestimate the value of γ_{1212} from the full-vectorial model. γ_{1212}^{IV} is a better approximation than γ_{1212}^{II} and reaches a maximum at a similar value of w as γ_{1212} .

Altogether, theses results suggest that there are significant quantitative differences between the predictions of the full-vectorial model and the various other approximations used in previous AlGaAs waveguide studies. Though it tends to underestimate the NLC, γ^{IV} is the closest approximation to γ for the TE₀₀, TM₀₀, TE₁₀, and TM₁₀ modes. This is the same result obtained for silica and silicon fibres in [33]. Results obtained from γ^{II} are farthest from γ and should not be used for high-confinement AlGaAs waveguides. A similar result is obtained for the case of the XPM NLC.

5.3 Nanowire Waveguides

The above section shows how the various published expressions for the single-mode NLC γ and the XPM NLC γ_{1212} produce significantly different results for AlGaAsOI waveguides. Here a similar comparison for the fundamental modes of an AlGaAs nanowire will be performed to determine the accuracy of the scalar models for this type of waveguide. A cross-section of a typical AlGaAs nanowire is shown in Fig. 5.4.



Figure 5.4: Diagram of the cross-section of the upper section of a typical AlGaAs nanowire waveguide.

The core of the AlGaAs nanowire that will be considered here consists of Al_{0.18}Ga_{0.82}As, with height h_{core} and width w. Above the core is the cladding layer with height $h_{cladding}$ and below is the substrate, both consisting of Al_{0.75}Ga_{0.25}As. Increasing the Al fraction reduces the refractive index, so to maximize the confinement in the vertical direction the Al fraction of the cladding and substrate should be as high as possible. A higher Al fraction than 0.75 risks being oxidized when exposed to air, so this is the fraction chosen for the substrate and cladding layers. To the left and right of the core is air. Throughout this section, the height of the core h_{core} and cladding $h_{cladding}$ will be taken to be 500 nm.

There is lower vertical confinement compared to the AlGaAsOI waveguide due to the smaller index difference of around 0.28 between the two different AlGaAs compositions. The core typically has air on either side which provides higher horizontal confinement than that of an AlGaAsOI waveguide with a large index difference of around 2.3. The waveguide is etched to a depth of 2-3 microns into the substrate layer to prevent leakage losses into the pure GaAs wafer below the substrate layer. In the simulations used in this section the computational domain did not extend the full etched distance into the substrate, essentially assuming the etch was of infinite depth.

The mode profiles for the fundamental TE and TM modes at $\lambda = 1550$ nm in a typical AlGaAs nanowire waveguide are shown in Fig. 5.5. It can be seen that the mode profiles

extend into the cladding and substrate layers due to the small index difference with the core. It is conceivable that this lower confinement may cause the difference between the full-vectorial theory and the scalar models to decrease for some or all of the modes. Note that even though the nanowire waveguide is not strictly symmetric in the y direction, as long as the cladding above the core is at least a few hundred nanometers thick the mode profile is roughly symmetric. The assumptions regarding the symmetries of the mode profiles used in the derivation of the NLCs in Chpts. 3 and 4 therefore still hold.



Figure 5.5: Diagram of the normalized mode profiles of the fundamental TE and TM modes of an AlGaAs nanowire waveguide. Parameters used in this simulation were $h_{core} = h_{cladding} = 500$ nm, w = 500 nm and $\lambda = 1550$ nm. Lines indicate outline of waveguide layers. First row: fundamental TE mode. Second row: fundamental TM mode.

As can be seen in Fig. 5.5 the longitudinal component of the TE_{00} mode is significant, while it has a much lower magnitude in the TM_{00} mode. To quantify this, the longitudinal mode fraction f_z was calculated for the fundamental TE and TM modes at 1550 nm for various values of w. The results are shown in Fig. 5.6.

It is clear that the TE mode has a very strong longitudinal component, even stronger than in the AlGaAsOI waveguide. This is because of the high index contrast between the AlGaAs and the air on either side of the waveguide. The TM mode, on the other



Figure 5.6: The longitudinal mode fraction f_z of the fundamental TE and TM modes of an AlGaAs nanowire waveguide as a function of waveguide width. The parameters used in the simulation were $h_{core} = h_{cladding} = 500$ nm and $\lambda = 1550$ nm. a) TE₀₀ mode. b) TM₀₀ mode.

hand, has a much weaker e_z component due to the low vertical confinement, and could be fairly accurately approximated as a scalar mode.

The calculated values of the various NLCs for AlGaAs nanowire waveguides are shown in Fig. 5.7. The values used were $h_{core} = h_{cladding} = 500$ nm, $\theta = 0$, and $\lambda = 1550$ nm. Care must be taken when modelling AlGaAs nanowires due to the change in n_2 with varying Al fraction. The $n_2[001]$ value for Al_{0.75}Ga_{0.25}As is approximately 9% that of Al_{0.18}Ga_{0.82}As [59, 60]. Due to this low value, and the low intensity of the mode in the substrate/cladding, it will be assumed only the core is nonlinear and $n_2 = 0$ elsewhere.

It is evident from Fig. 5.7 that the scalar approximations are much closer to the full-vectorial model for the nanowire than in the AlGaAsOI case, particularly for the fundamental TM mode. This is due to the fact that the TM mode has a low f_z which makes the scalar mode approximation more accurate. It is also interesting to note that γ^{III} very closely matches γ for the TM mode, even for very narrow waveguides, while γ^{II} and γ^{IV} also stay very close to each other for all values of w.

The same is not true for the TE case, where both γ^{III} and γ^{IV} have similar values, slightly less than γ , while γ^{II} again diverges from the others and underestimates the NLC when w < 600 nm. However, typical AlGaAs nanowire waveguides used in nonlinear applications have widths in the range of 600 nm due to the fact that this geometry places the zero dispersion wavelength at 1550 nm for the TE₀₀ mode (see Fig. 5.8).

From Fig. 5.7 a) it can be seen that for $w \approx 600$ nm the scalar NLCs are good approximations for γ for both the fundamental TE and TM modes, particularly γ^{IV}



Figure 5.7: The values of the various published nonlinear coefficients for an AlGaAs nanowire waveguide with varying waveguide width w. The parameters used in the simulations were $h_{core} = h_{cladding} = 500$ nm, $\theta = 0$ and $\lambda = 1550$ nm. a) Fundamental TE mode. b) Fundamental TM mode.

for the TE mode. However, recall that this is assuming $\theta = 0$. For other waveguide orientations the scalar approximations may not be as accurate.

5.4 Conclusion

In this chapter, the different theories used to model third-order nonlinear effects in Al-GaAs waveguides were compared with the full-vectorial theory. In particular, different expressions for the single-mode NLC used in the literature for AlGaAs waveguides were simulated along with the full-vectorial model. It was found that other scalar expressions for the single-mode NLC underestimate the full-vectorial γ for high-confinement AlGaA-sOI waveguides. Similar results were obtained for the XPM NLC γ_{1212} and its scalar approximations.

For the AlGaAs nanowire waveguide, the scalar approximations are more accurate for the fundamental TM mode due to the low confinement in the vertical direction. However, the γ^{II} and γ^{III} scalar NLCs are still inaccurate for the fundamental TE mode when w < 600 nm.

In almost all cases, γ^{IV} provided the best approximation for the full-vectorial model, with the exception being for the TM₀₀ mode of the AlGaAs nanowire, where γ^{III} performed slightly better. It should be noted that these simulations were performed with $\theta = 0$, and that the scalar models do not take into account the complicated influence of the orientation of the waveguide with respect to the crystal lattice on γ .



Figure 5.8: The values of β_2 for an AlGaAs nanowire waveguide with varying waveguide width w. The parameters used in the simulations were $h_{core} = h_{cladding} = 500$ nm, $\theta = 0$ and $\lambda = 1550$ nm. a) Fundamental TE mode. b) Fundamental TM mode.

Chapter 6

Applications

In this chapter I will demonstrate the application of the full-vectorial model to situations of practical interest and predict their performance. In particular, I will examine wavelength conversion efficiency when the signal, idler and pump are in the same spatial mode (which will be referred to as degenerate four wave mixing (DFWM)), for both AlGaAsOI and plasmonic slot waveguides (PSW) with an AlGaAs core.

6.1 Degenerate Four Wave Mixing

DFWM involves three modes called the pump, signal and idler with frequencies ω_1, ω_2 and ω_3 respectively, all in the same spatial mode. The frequencies must satisfy the energy conservation condition $2\omega_1 = \omega_2 + \omega_3$. It will be assumed that the frequencies are close enough together such that they have identical mode profiles and the dispersion of the $\chi^{(3)}$ tensor can be neglected. By considering Eq. (2.20) it can be seen that the SPM, XPM and FWM NLCs will be almost identical in this case. The only difference between the NLCs will be due to the degeneracy factor K, and the different ω values in the prefactor.

With this in mind, the propagation equations can be found from Eq. (2.11):

$$\frac{dA_1}{dz} = i\gamma(|A_1|^2 + 2|A_2|^2 + 2|A_3|^2)A_1 + 2i\gamma A_1^*A_2A_3exp(i\Delta\beta z)$$
(6.1)

$$\frac{dA_2}{dz} = i\gamma(|A_2|^2 + 2|A_1|^2 + 2|A_3|^2)A_2 + i\gamma A_3^* A_1^2 exp(-i\Delta\beta z)$$
(6.2)

$$\frac{dA_3}{dz} = i\gamma(|A_3|^2 + 2|A_1|^2 + 2|A_2|^2)A_3 + i\gamma A_2^* A_1^2 exp(-i\Delta\beta z)$$
(6.3)

where the 1, 2 and 3 indices refer to the pump, signal and idler respectively, and $\Delta\beta = -2\beta(\omega_1) + \beta(\omega_2) + \beta(\omega_3)$. The value of n_2 determined at $\lambda = 1550$ nm and a frequency of ω_1 will be used to evaluate γ .

Note the difference between the situation here and that of Chpt. 4: here the modes are in the same spatial mode with different frequencies, while in Chpt. 4 the modes had the same frequency but different spatial modes. The most common configuration for DFWM is with all of the modes in either the fundamental TE or TM mode. This scheme has been thoroughly investigated both theoretically and experimentally in multiple material systems [15] including AlGaAs [12, 14, 21, 54, 55, 57, 58, 61], with some experimental demonstrations in AlGaAsOI [23, 24]. The full-vectorial model presented in this thesis is not significantly different than the commonly used CW DFWM model [26], however typically a scalar mode approximation is used, which tends to underestimate the magnitude of γ (see Chpt. 5).

It is common to assume that the pump power is much higher than the signal and idler powers: $|A_1|^2 = P_1 >> |A_2|^2$, $|A_3|^2$, so the terms proportional to $|A_2|^2$ and $|A_3|^2$ can be neglected. This simplifies the system of equations and allows an analytic solution to be found. Otherwise, the full system of equations can be solved numerically. The linear waveguide loss due to scattering, substrate leakage loss, etc. can also be added heuristically to give:

$$\frac{dA_1}{dz} = -\frac{\alpha}{2}A_1 + i\gamma P_1 A_1
\frac{dA_2}{dz} = -\frac{\alpha}{2}A_2 + i2\gamma P_1 A_2 + i\gamma A_3^* A_1^2 exp(-i\Delta\beta z)
\frac{dA_3}{dz} = -\frac{\alpha}{2}A_3 + i2\gamma P_1 A_3 + i\gamma A_2^* A_1^2 exp(-i\Delta\beta z)$$
(6.4)

where α is the linear loss coefficient. Writing $\omega_2 = \omega_1 + \Delta \omega$ and $\omega_3 = \omega_1 - \Delta \omega$, the phase mismatch $\Delta \beta$ can be Taylor expanded about ω_1 :

$$\Delta\beta = -2\beta(\omega_1) + \beta(\omega_1 + \Delta\omega) + \beta(\omega_1 - \Delta\omega) = \beta_2 \Delta\omega^2 + \dots$$
(6.5)

where $\beta_2 = d^2 \beta(\omega)/d\omega^2$ evaluated at ω_1 . To phase match the process, it is required that $\beta_2 \approx 0$ at the pump frequency.

A figure of merit for a wavelength conversion process is the conversion efficiency $\eta = |A_3(L)|^2/|A_2(0)|^2$, where L is the device length. For a phase-matched process where $\Delta\beta \approx 0, \eta$ is given by [21]:

$$\eta = \frac{|A_3(L)|^2}{|A_2(0)|^2} = (\gamma P_1 L_{eff})^2 e^{-\alpha L}$$
(6.6)

where the effective length L_{eff} is given by $L_{eff} = (1 - exp(-\alpha L))/\alpha$, and P_1 is the

initial pump power. The maximum conversion efficiency obtainable η_{max} can be found by taking the derivative of Eq. (6.6) and setting it to zero to find the optimal waveguide length $L_{opt} = ln(3)/\alpha$. Inserting this into Eq. (6.6) gives [62]:

$$\eta_{max} = \frac{3}{27} \left(P_1 \frac{\gamma}{\alpha} \right)^2 \tag{6.7}$$

6.2 AlGaAsOI Waveguide

The DFWM performance in an AlGasOI waveguide will now be predicted using the fullvectorial model. Plotted in Fig. 6.1 is the calculated β_2 and γ for the fundamental TE mode at $\lambda = 1550$ nm of an AlGaAsOI with w = 450 nm and various values of h. From this figure it can be seen that the phase-matching condition is achieved for the TE₀₀ mode for a waveguide with w = 450 nm and h = 260 nm.



Figure 6.1: Calculated γ and β_2 evaluated for TE₀₀ mode at a wavelength of 1550 nm for an AlGaAsOI waveguide with w = 450 nm and varying h.

The fourth order dispersion terms β_4 may become relevant when $\beta_2 \approx 0$, and should be considered for DFWM processes with larger wavelength bandwidths. Higher order phase-matching using more terms in the Taylor expansion of β has been demonstrated experimentally for the AlGaAsOI system [24].

Take the waveguide dimensions to be w = 450 nm, h = 260 nm to minimize β_2 , the initial pump power to be $P_1 = 1$ W and the pump wavelength to be 1550 nm. For this waveguide geometry, the NLC is calculated to be $\gamma = 686$ W⁻¹m⁻¹ (see Fig.6.1).

To estimate the device performance the linear loss will be approximated using previous experimental results to be $\alpha \approx 2 \text{ dB/cm}$ [63] for the TE₀₀ mode of an AlGaAsOI
waveguide with w = 450 nm.

The η for different propagation lengths L is calculated using Eq. (6.6) and the results are shown in Fig. 6.2 a). An η_{max} of -10.3 dB is predicted at a distance of L = 1.3 mm for this waveguide. The calculated maximum conversion efficiency η_{max} as a function of P_1 for this waveguide geometry at a pump wavelength of 1550 nm is shown in Fig. 6.2 b).

These results show that high conversion efficiencies could potentially be achieved in AlGaAsOI waveguides due to the high confinement, control over dispersion to ensure phase-matching, and low losses.



Figure 6.2: The calculated conversion efficiency η as a function of waveguide length L for an AlGaAsOI waveguide with w = 800 nm, h = 250 nm, and a pump wavelength of $\lambda_p = 1550$ nm. Perfect phase-matching was assumed.

Unlike conventional nanowire AlGaAs waveguides, it is possible to phasematch this process for TM modes in AlGaAsOI due to the enhanced confinement in the vertical direction. Note, however, that at a waveguide orientation of $\theta = \pi/4$ the TE₀₀ mode will have a higher γ than the TM mode with the same mode profile due to the anisotropy of the AlGaAs $\chi^{(3)}$ tensor (see Chpt. 3).

6.3 Plasmonic Slot Waveguides

Wavelength conversion in a class of waveguides called plasmonic slot waveguides (PSW) will now be considered. Typical dielectric or semiconductor waveguides cannot have mode areas below the diffraction limit. If the waveguide core area is reduced below this limit, the mode profile will spread out beyond the core into the cladding, as discussed in Chpt. 3.

6.3.1 Plasmonic Waveguide Geometry

This limitation can be bypassed through the use of plasmonic waveguides, involving an interface between a dielectric/semiconductor and a metal [64]. In particular, the PSW configuration where a semiconductor is sandwiched between two metal layers allows for very small waveguide mode areas. An example of a cross-section of such a waveguide is shown in Fig. 6.3. Here I have used the AlGaAsOI platform, where instead of a silicon dioxide cladding a layer of metal has been deposited on top of the waveguide core to form the PSW.



Figure 6.3: Cross-section in the x - y plane of a typical AlGaAs PSW.

Studies of third-order nonlinear effects in PSWs, including those using a full-vectorial approach, have been performed [62, 65, 66] however generally silicon or nonlinear polymers have been used as the core material. They have also been recently used to perform wavelength conversion for the first time [67]. To the best of our knowledge, no investigation of wavelength conversion in PSW has been performed with AlGaAs as the core material. Because of the abrupt index changes and high confinement of the waveguide it is reasonable to expect a full-vectorial model will be necessary to model nonlinear processes in a PSW. In this section, I will apply the full-vectorial theory to this type of waveguide to predict its wavelength conversion performance.

Note that the fact that the waveguide modes are lossy due to the complex refractive index of the metal. This complicates the full-vectorial theory, as some of the assumptions made in the derivation no longer apply. Namely, the transverse components can no longer be assumed to be purely real and the e_z component cannot be taken to be purely imaginary. As a result, expressions such as Eq. (3.9) no longer apply.

However, simulations show the $\text{Im}(e_x)$, $\text{Im}(e_y)$ and $\text{Re}(e_z)$ are negligible compared to the magnitudes of these components. We will therefore use our derived NLCs as they are in analyzing the PSW nonlinear performance. See [62] for more details on a derivation of full-vectorial nonlinear propagation equations for plasmonic waveguides.

6.3.2 Nonlinear Performance

The small mode area in a PSW results in very strong nonlinear effects. However, due to absorption in the metal, these waveguide also have very high linear losses, on the order of thousands of dB/cm. These losses limit the effective length of nonlinear plasmonic devices. However, with a short device length the effects of phase-matching become negligible.

As for the AlGaAsOI waveguides, the mode profiles and characteristics of the PSW modes can be calculated via finite element simulations. For narrow (w < 150 nm) PSWs it is possible for there to exist a fundamental TE₀₀ mode and a second order TE₀₁ mode at $\lambda = 1550$ nm (see Fig. 6.4).



Figure 6.4: Normalized profiles of the components of the TE₀₀ and TE₀₁ modes of a PSW with an AlGaAs core, with w = 50 nm and h = 250 nm at $\lambda = 1550$ nm.

It will be assumed that only the fundamental mode is excited when light is coupled into the plasmonic waveguide, though whether this holds true will depend on which coupling mechanism used. I will therefore be mainly interested in the case where there is a single spatial mode. The NLC will therefore take the form of Eq. (3.10).

Due to the complex permittivity of the metal, the propagation constant β will also be complex. This results in a linear absorption loss with coefficient α . As would be expected, a smaller waveguide core will result in a higher γ . However, reducing the size of the waveguide also increases α , which reduces the effectiveness of wavelength conversion devices (see Eq. (6.7)). The trade-offs between γ and α must be considered when designing nonlinear PSW devices.

In Fig. 6.5, $\gamma(\theta = \pi/4)$, α , n_{eff} , n_g/n_{core} , $\Delta\gamma$ and f_z of the fundamental TE mode of the PSW, all evaluated at a wavelength of $\lambda = 1550$ nm, are plotted as functions of waveguide cross-section. Gold was used as the metal. Note also that the losses here only account for absorption losses and not, for example, scattering losses due to roughness at the interface of the metal and the AlGaAs core.

It can be seen that, while both γ and α increase with decreasing w, overall there will be an improvement in γ/α . Therefore it is desirable to create a PSW with as narrow a width as possible. This is in agreement with other similar studies [62]. The width will most likely be limited by fabrication technology as the w : h aspect ratio cannot be made arbitrarily small. However, the height of the AlGaAs layer must also be large enough that the mode is largely contained within the waveguide core for a non-plasmonic waveguide with the same h, otherwise it may be difficult to efficiently couple the light into the PSW. This restricts the height of the waveguide to around h > 250 nm. Assuming an aspect ratio of $w : h \approx 1 : 5$, the width is limited to w > 50 nm.

From Fig. 6.5 c), the effective index, unlike the AlGaAsOI waveguide, is higher than the core index n_{core} . The group index is also high, reaching up to approximately $1.7n_{core}$. It can also be seen that, despite the small core size and high confinement, f_z is relatively low compared to the AlGaAsOI waveguide. $\Delta \gamma$ is high due to the fact that this is a TE mode, and does not change much with reducing waveguide width because of the small $|e_z|$ component.

The low f_z suggests that the mode profile mainly consists of the e_x component. Due to this, a scalar approximation for γ could possibly be accurate for the PSW geometry. Plotted in Fig. 6.6 are the various NLCs at $\lambda = 1550$ nm described in Chpt. 5 for the fundamental TE mode of a PSW of height h = 250 nm with $\theta = 0$. The scalar NLCs underestimate the full-vectorial γ , by a factor of more than 2 for $w \approx 50$ nm. Clearly they are not suitable for estimating the NLCs of plasmonic slot waveguides, despite the low magnitude of e_z . The full-vectorial γ will therefore be used to predict the performance of the PSW for DFWM.



Figure 6.5: Various properties of the fundamental PSW mode at a wavelength of 1550 nm. The plasmonic metal was gold, and the waveguide height h = 250 nm. a) Nonlinear coefficient γ . b) Absorption loss α . c) Effective index n_{eff} . d) Group index divided by core refractive index n_g/n_{core} . e) Transverse mode fraction f_z . d) Change in NLC with angle $\Delta\gamma$.

From these parameters, the conversion efficiency of a DFWM process in the quasi-CW approximation can be estimated using Eq. (6.7). η_{max} as well as the optimal length L_{opt} as a function of w are shown in Fig. 6.7. The initial pump power was chosen to be $P_1 = 1$ W.

This results in a η_{max} of around -42 dB, which is lower than that predicted for the AlGaAsOI waveguide. However, it is achieved at a much shorter distance of around 1.7 microns, which allows for denser integration on chip. Also, due to the short propagation distances phase matching is irrelevant, so potentially third order nonlinear processes that would not otherwise be possible in nonplasmonic AlGaAs waveguides due to phasematching constraints could be achievable in PSWs.



Figure 6.6: Calculated values of the various NLCs for the fundamental PSW mode at a wavelength of 1550 nm. The plasmonic metal was gold, and the waveguide height was h = 250 nm.

6.4 Conclusion

In this chapter, application of the full-vectorial model to AlGaAs waveguide wavelength conversion devices was investigated. For the case of DFWM where all the modes are in the same spatial mode, the large γ and possibility for phase-matching in AlGaAsOI waveguides were demonstrated. A maximum conversion efficiency η_{max} of -10.3 dB at a pump power of 1 W and a waveguide length of L = 1.3 mm was predicted for an AlGaAsOI waveguide.

The performance of a PSW wavelength conversion device was also estimated using the full-vectorial model. A maximum conversion efficiency of -42 dB achieved at an optimal device length of 1.7 microns was predicted for a PSW with a 50 nm wide AlGaAs core.



Figure 6.7: Calculated values of a) η_{max} and b) L_{opt} of the fundamental PSW mode at a wavelength of 1550 nm. The plasmonic metal was gold, and the waveguide height was h = 250 nm.

Chapter 7

Conclusion

In this chapter potential directions for future research are proposed and the results of this thesis are summarized.

7.1 Future Work

As the work in this thesis is purely theoretical, experimental verification of the results presented here is necessary. The accuracy of the full-vectorial model is highly dependent on material parameters such as n_2 , σ and δ . Therefore it would be useful to perform experiments determining these factors to higher accuracy, in particular the anisotropy parameters σ and δ which have not been studied in many years. In fact, the theory presented in this thesis may be useful for higher accuracy measurements of these parameters using nonlinear experiments in high-confinement AlGaAsOI waveguides.

There are many ways the theoretical investigations in this thesis could be extended, for example by using different mode combinations or waveguide geometries. A suspended waveguide, where an AlGaAs core is completely surrounded by air, would have a higher degree of confinement than the AlGaAsOI waveguide, making a full-vectorial approach even more important for properly evaluating the waveguide's nonlinearity. Removing the SiO₂ cladding of an AlGaAsOI waveguide would have a similar effect, in particular for TE modes.

The theory presented here could also be used to investigate waveguide fabricated on wafers with growth directions other than [001]. Due to the anisotropy of the $\chi^{(3)}$ tensor the highest nonlinearity is achieved by directing the electric field away from the crystal axis, for example in the [111] direction. This can be achieved with a wafer grown in the [111] direction. Investigating the impact this would have on the NLCs would only require changing the rotation matrix used to define the $\chi^{(3)}$ tensor.

Due to the high absolute value of σ in AlGaAs some NLCs, particularly those involving modes with high e_x components, have a strong dependence on the orientation of the waveguide propagation direction with respect to the crystal axis, θ . The variation of the NLCs with θ has potentially interesting applications. For example, this variation can be used to quasi-phasematch broadband FWM processes in ring resonators, as suggested in [45]. The high predicted values of $\Delta \gamma_{1122}$ for some mode combinations in particular suggest that this method could be used to quasi-phasematch intermodal FWM schemes that would otherwise be difficult to phasematch. The periodic modulation of the NLCs may also have an impact on other nonlinear processes in waveguide ring resonators, for example the dynamics of dispersive Kerr solitons [68].

The results for the NLCs could be used in an extended model which includes various other effects influencing pulse propagation in high-confinement waveguides, such as dispersion, TPA, free carrier effects, and Raman scattering. Though the theory for these effects has been developed and investigated for SOI waveguides (see [28]), the material parameters involved will be different for AlGaAs.

7.2 Summary

In this thesis a full-vectorial theory for nonlinear mode propagation was used to derive expressions for the NLCs for modes in high-confinement AlGaAs waveguides. The results can be applied to situations involving an arbitrary number of modes with different central frequencies and spatial profiles, with no assumptions made about the electric field components involved or the orientation of the waveguide with respect to the crystal lattice. The unique characteristics of the AlGaAs susceptibility tensor were introduced and included in the theory.

Explicit expressions for the single-mode (SPM) and two-mode (XPM and FWM) NLCs based on the mode profile components were derived. NLCs for various mode combinations were calculated via simulation, and their dependence on the geometric parameters width w, height h and orientation θ of an AlGaAsOI waveguide were investigated. It was found that the NLCs' dependence on θ varied significantly based on the strength of the various electric field components of the modes involved. For the single-mode NLC γ it was found that the θ dependence was proportional to the integral of $(|e_x|^2 - |e_z|^2)^2$. This means that increasing the confinement of the AlGaAsOI waveguide, and therefore increasing $|e_z|$, decreased the θ dependence of the single-mode NLC of TE modes, while the opposite is true of TM modes. The XPM NLC γ_{1212} was found to have a relatively small negative dependence on θ when considering the interaction between the TE₀₀ and TM_{00} or the TE_{00} and TE_{10} modes. The FWM NLC γ_{1122} , on the other hand, has a much stronger dependence on θ , increasing by up to a factor of 3 for the TE_{00} and TE_{10} modes.

The predictions of the full-vectorial model were compared to those of other scalar nonlinear theories for AlGaAsOI and AlGaAs nanowire waveguides. It was found that the scalar theories tend to underestimate the single-mode NLC γ for the fundamental TE and TM modes of AlGaAsOI waveguides. In particular the commonly used γ^{II} was found to poorly approximate the full-vectorial NLC. The scalar NLCs were found to be more accurate for AlGaAs nanowire waveguides due to the lower confinement in the vertical direction. Out of the three scalar NLCs considered, γ^{IV} was found to be the best approximation for the full-vectorial theory in general.

The application of the full-vectorial model to designing and predicting the performance of AlGaAs waveguide wavelength conversion devices was demonstrated, for both AlGaAsOI and PSW geometries.

In total, the work presented in this thesis permits a deeper understanding of thirdorder nonlinear effects in high confinement AlGaAs waveguides, in particular the recently developed AlGaAsOI scheme. This understanding will allow for more accurate modeling and optimization of nonlinear devices in this unique material system.

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