Photoelastic Waveguides
in
Bulk Silicon
and
$\text{Si}_{1-x}\text{Ge}_x$ Heterostructures

by

Erik Lea

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Abstract

A theoretical and experimental investigation into the characteristics of photoelastic optical waveguides in bulk silicon and Si\textsubscript{1-x}Ge\textsubscript{x}/Si heterostructures is presented. This is the first experimental demonstration of this type of waveguide in these material structures. The bulk silicon structures are also the first demonstration of channel waveguides defined using only photoelastic confinement.

The photoelastic constants of silicon and Si\textsubscript{1-x}Ge\textsubscript{x}, which give the change in refractive index with strain, are calculated from the strain-induced shifts in the energy band structure of silicon and germanium which modifies their extinction coefficient, from which the strain-induced refractive index changes are found from the Kramers-Krönig relations. A finite element model of the waveguide structures is presented which uses the calculated photoelastic constants to determine the refractive index profiles of the waveguides. Subsequently, finite difference calculations are used to calculate the optical mode profiles of the waveguides.

Photoelastic waveguides are fabricated by depositing SiN\textsubscript{y} stressor films onto bulk silicon and Si\textsubscript{1-x}Ge\textsubscript{x}/Si heterostructures which are subsequently cleaved and polished to produce waveguide facets before narrow stressor stripes are defined from the SiN\textsubscript{y} films using photolithography and wet etching. The characteristics of the waveguides are investigated at wavelengths of 1.15\textmu m and 1.523\textmu m.

Measurements show that there is always one guiding region outside each edge of the stressor stripe. The Si\textsubscript{1-x}Ge\textsubscript{x}/Si heterostructures also allow a third mode to be confined under the centre of the stressor stripe, and the relative intensity and the distance between the guided modes is controlled by the stripe width, in good accordance with the modelling results. These structures are interesting in that up to three guiding regions can be defined by the deposition of one stressor stripe on the waveguide surface, which provides a particularly simple and compact way of fabricating waveguide couplers.

An interferometer is used to study the force generated by the SiN\textsubscript{y} stressor layers. It is shown that the as-deposited stressors produce low and poorly defined stresses, although significant forces of up to 2-3-10\textsuperscript{6} dyn/cm are measured after rapid thermal annealing of the structures. Annealing of photoelastic waveguides in bulk silicon show a corresponding increase in photoelastic confinement which produces waveguides with excess losses of down to 4.3 dB/cm. Photoelastic waveguides in Si\textsubscript{1-x}Ge\textsubscript{x}/Si heterostructures, due to the additional confinement from the heterojunction, are reported with zero excess losses.

At 1.15\textmu m, the band-edge absorption increases the waveguide propagation losses by up to several dB/cm, and the waveguides show multimode behaviour, making these structures unsuitable for applications at this wavelength. At 1.523\textmu m, however, measurements show low excess propagation losses and single-mode behaviour, and they exhibit a low degree of birefringence.

The simple fabrication process and compact design of these structures make them appropriate for optoelectronic integration, and several possible applications for photoelastic waveguides in optical devices are suggested.
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Chapter 1

Background and Review

The increase in demand for information brought about by advances in the media, computer technology and the internet is followed by an increase in the capacity of communication networks. Fibre-optic cables, due to their very high capacity, are currently being employed in highly trafficked communication links, and all-optical networks are expected in 1998, with terabit systems predicted in commercial use by the turn of the century [1, 2]. With the development of optical communications, the information technology will become increasingly dependent on optical signal processing, as is indicated by the increasing worldwide optoelectronics market with sales of around $7 billion in 1997 [3].

As the information transfer in communication systems increases, it will be of interest to perform both optical and electronic processing on the same substrate, in so-called optoelectronic integrated circuits, as this would be potentially cheaper, more integrated, smaller and faster. Practically, the base for any integrated electronics will be silicon, due to the present technology, existing processing equipment, and cost. Although simple silicon-based optoelectronic integrated circuits have been marketed [4], optical switching and light emission are generally realised in other materials, such as GaAs and InP [5, 6], due to their physical properties. Although methods exist for integrating different materials onto a single substrate [7, 8], they often require significant modification of the surface topography, and processing steps which can be inappropriate for integration with electronic circuitry. It would therefore be advantageous for optoelectronic integration if silicon-based optical circuitry could be made using only standard silicon processing technology. Recent advances in silicon-based optical switching [9] and light emission [10, 11] suggest that all-silicon optoelectronic circuits may become practical. In particular, the development of Si$_{1-x}$Ge$_x$ technology, which is compatible with standard silicon processing, poses interesting opportunities for optoelectronics.

This project presents a study into integrated optical waveguides, which guide light around optical circuits, in bulk silicon and Si$_{1-x}$Ge$_x$/Si heterostructures. In this chapter an evaluation of silicon and Si$_{1-x}$Ge$_x$ as a base for integrated optics is presented, and a comparison is made of different waveguide technologies to determine which is the most appropriate for optoelectronic integration. In section 1.4 the specific aims of the project are established based on the qualitative and quantitative evaluation in this chapter. Chapter 7 concludes on whether the findings from the investigation are of practical use for optoelectronic integrated circuits in silicon and Si$_{1-x}$Ge$_x$, and presents suggestions for further investigations in the field.
1.1 Evaluation of Silicon-Based Materials for Integrated Optics

Silicon was long a disregarded material for use in optical engineering, due especially to its indirect energy bandgap and cubic symmetry, providing poor prospects for active silicon devices. However, some silicon-based optics has been investigated during the last decade, and with interesting results [12]. Two prospective silicon bases which have been given much attention are Silicon-On-Insulator (SOI) structures, for instance silicon on SiO$_2$, and Si$_{1-x}$Ge$_x$ alloys. They have their respective advantages, and can well be combined [13].

SOI on the one hand, isolates and insulates the top silicon layer from the substrate. This provides an excellent structure for VLSI. For optoelectronics, the structure has very high dielectric isolation, with the SiO$_2$ layer and the silicon layer having refractive indices of respectively 1.5 and 3.5 in the near infra-red, and it is thus in principle good for waveguiding. One consideration though may be that for VLSI, the top silicon layer should ideally be thin, i.e. about 0.1µm, while for waveguiding, it is typically at least a few microns. Nevertheless, both low-loss waveguides [14, 15, 16] and devices [17, 13, 18] have been reported in SOI structures.

Si$_{1-x}$Ge$_x$, on the other hand, is interesting in terms of material properties. The germanium content of the alloy can be continuously varied, thus allowing alloy characteristics such as energy band gap and lattice constant to be precisely controlled. This allows a great amount of freedom when specifying optical cut-off wavelengths, and when designing strained devices. The energy band gaps of silicon and germanium are 1.11eV and 0.68eV, respectively. The compound energy gap of bulk Si$_{1-x}$Ge$_x$ will lie between these two values. This corresponds to a wavelength range of 1.1–1.8µm, covering the two minimum absorption windows in commonly available silica fibres at 1.3µm and 1.55µm [19, 20], making Si$_{1-x}$Ge$_x$ alloys interesting for optical communication. Varying the germanium content thus allows the alloy to be either transparent or absorbent. Since 1986, there have been numerous reports on Si$_{1-x}$Ge$_x$ optoelectronics, reporting waveguiding properties [21, 22, 23, 24] and detectors [25, 26, 27, 28, 29]. The recent demonstration of silicon-based modulators [30, 31] and switches [9, 32, 33] as well as experimental [10, 11, 34] and theoretical reports [35, 36] on light emission has also strongly improved the prospects for silicon-based integrated optics.

VLSI will normally be made on crystalline silicon. Even though not all devices require the crystallinity, the research into strained devices and quantum wells promises a higher performance in crystalline than in amorphous circuits [37, 38]. Si$_{1-x}$Ge$_x$ is one of the few materials which can practically be grown on a silicon substrate, without relaxing the crystal due to too high strain. In electronic devices, Si$_{1-x}$Ge$_x$ has already proven to have performance characteristics above those of pure silicon [39]. Because the alloy composition can be varied continuously, both thick layers of low germanium content and low strain, and strained superlattices, with periodically varying alloy composition, can be grown straight onto a crystalline silicon substrate. Only a few other commonly known optical materials, such as GaP and AlP, could do this without creating a too high strain. Other materials would require some hybrid interface between the materials, or accept a defaulting crystal region at the material junctions.

Given the recent progress in active silicon devices, silicon now appears as a much more potential material for optical applications than previously. Particularly in conjunction with Si$_{1-x}$Ge$_x$ alloys, the possibilities in strain design, useful wavelength range and integration with silicon VLSI pose interesting options for optoelectronics.
Apart from the material properties, it is useful for the integration with VLSI with an optical technology which leaves the surface intact, as this simplifies the further processing of the structure, and allows the crystal to remain strained. In section 1.2 different optical waveguide technologies are compared in terms of their ease of fabrication and appropriateness for integration into optoelectronic circuitry.

1.2 Waveguides in Si and Si$_{1-x}$Ge$_x$ Structures

Planar waveguides, in which light is confined vertically, but not horizontally, are commonly grown epitaxially by molecular beam epitaxy (MBE) or chemical vapour deposition (CVD). For integrated use, however, waveguides should also have horizontal confinement. Si$_{1-x}$Ge$_x$ channel waveguides have normally been made by etching CVD-grown epitaxial layers, producing strips or ribs. While MBE or CVD are likely to remain the favoured methods for making the initial planar layers, horizontal confinement can be created in several ways. Some considerations about these technologies are presented below.

**Etched Rib Waveguides**

Rib waveguides are commonly made by etching into a planar waveguide. Several rib waveguides have been reported in silicon and Si$_{1-x}$Ge$_x$ based structures, with losses of down to 0.5dB/cm. Figure 1.1 shows some of the Si$_{1-x}$Ge$_x$ based waveguides which have been investigated.

![Rib waveguides in Si$_{1-x}$Ge$_x$ structures](image)

Figure 1.1 Rib waveguides reported in Si$_{1-x}$Ge$_x$. All waveguides were grown on silicon substrates. The propagation losses reported by (a) Splett et al. [40], (b) Liu and Prucnal [22] and (c) Pesarcik et al. [23] were 3-5dB/cm, 2.5dB/cm and 0.5dB/cm, respectively, at ~1.3μm.

This technology allows great freedom in defining the width and height of the waveguide, which controls the optical mode profiles, and it is in principle a simple fabrication method. Nevertheless, the deep etching of the material and the requirement for a planar layer of several microns in thickness can be inappropriate for the processing of other components on the same substrate. An alternative to the rib structure, called an optical stripline or strip-loaded waveguide is shown in figure 1.2, where a strip is deposited onto a planar layer of higher refractive index to increase the effective refractive index under the strip. This structure is useful in that it does not require etching of the guiding layer, and it has been used to fabricate waveguides in GaAs [41, 42] and glass [43]. However, unless
Figure 1.2 Strip-Loaded Waveguide. This structure differs from the rib waveguides in that the protruding rib is of a lower refractive index, so that the guiding layer itself is not etched. The guiding layer underneath the strip sees a higher effective refractive index due to the strip, which can be used to define channel waveguides, as demonstrated in GaAs by Blum et al. [41]. Strip loading has also been employed together with rib waveguides, as shown in figure 1.1(c).

the deposited strip is relatively thick, these waveguides are likely to have poor lateral confinement. For optoelectronic integrated circuits, it can be more suitable with a waveguide technology which does not require deep etching or thick deposited layers, as is the case for ion implanted, photoelastic and indiffused waveguides.

Ion Implanted Waveguides

Ion implanted guides have been reported in several materials [44], with very low propagation losses, including several silica based guides, with losses of ~0.2 dB/cm [45, 46]. Regarding the field profile of the light beam, ion implantation would allow for very high flexibility in designing the shape of the guided mode. Not only would it give a naturally smooth transition between the maximum doped location and its surroundings; it would also allow very precise profiling both horizontally and vertically.

Practically, however, implanting germanium into silicon may be difficult. Assuming a rather high implantation energy, 2MeV, the projected range of germanium would still be only about 1.5μm 1, which is rather shallow. Higher energies, or double charging of the ions would give a somewhat longer range, but considering that most VLSI circuitry today can easily be produced with much lower energy implanters, it is unlikely that optical devices requiring several MeV will be of commercial interest.

There is still the interesting possibility of using implantation to screen off a region in a guiding layer, as shown in figure 1.3. In this case, the guide itself will not be implanted, but rather the surrounding areas would be doped by an element reducing its refractive index. In this way, the doping would not need to be very deep, although it could only be used together with a planar waveguide structure. Alternatively, waveguides could be defined from the implantation damage from lighter ions, which would require lower implantation energy, as has been demonstrated in quartz [45], though damaging the crystal

1 Calculated using the implantation modelling program SUSPRE.
Implanted confining areas (Low refractive index)

Guiding layer (High refractive index)

Figure 1.3 Possible structure for an optical channel waveguide, confined laterally by ion implantation. By doping the low index areas rather than the guide itself, the projected implantation-range (depth) would not need to be very great.

layer restricts the design of other components in the vicinity of the waveguide. It is possible, however, to define waveguides without growing planar layers, without etching the surface and without destroying the crystallinity of the structure, as has been shown with germanium-indiffused silicon waveguides.

Ge-Indiffused Silicon Waveguides

A simple method of defining waveguides in silicon is by depositing a stripe of germanium on top of a silicon substrate, and diffusing germanium into the substrate by annealing the structure, thus creating a channel of Si$_{1-x}$Ge$_x$ underneath the stripe, as shown in figure 1.4. Several reports of low-loss waveguides using this method have been published [47, 48, 49], and they have been integrated into both passive [49] and active [9, 32] devices. These waveguides are in principle useful for optoelectronic integration, however, the reported annealing times to diffuse the germanium into the silicon are of the order of 60 hours, which does not seem commercially viable.

Photoelastic Waveguides

Photoelastic technology is another alternative for generating channel waveguides which does not require doping or damaging of the crystal and which leaves the material surface intact. By introducing strain into the guiding layer, the refractive index is modified via the photoelastic effect, which can be used to define waveguides.

A simple method for inducing strain locally in a waveguide structure is by depositing a stressor layer onto a planar waveguide structure at a high temperature, which on cooling to room temperature generates strains into the waveguide structure due to the difference in thermal expansion between the stressor layer and the guiding layer. A possible photoelastic waveguide structure is shown in figure 1.5, where a Si$_{1-x}$Ge$_x$/Si heterostructure defines the planar waveguide, and a stressor stripe has been defined from a deposited SiN$_y$ layer. Although Si$_{1-x}$Ge$_x$ has not previously been used for photoelastic waveguides, the same basic waveguide structure has been investigated in GaAs-based planar structures [50, 51].
Si$_{1-x}$Ge$_x$ stripe diffusion source

Figure 1.4 Ge-Indiffused Silicon Waveguide. By depositing a stripe of Si$_{1-x}$Ge$_x$ onto a silicon substrate and subsequently annealing the structure at high temperatures, germanium atoms diffuse into the silicon to create an indiffused channel waveguide. This type of waveguide has been reported by Schmidtchen et al. [48] with a reported maximum germanium content in the channel of up to 10%, and a diffusion depth of 1.55\(\mu\)m. The diffusion source, which is generally of high germanium content, is normally left on the surface after the diffusion. Even though losses of 0.3dB/cm have been reported for these waveguides, the reported annealing times to diffuse the germanium into the silicon are of the order of 60 hours at 1200°C and above, which does not seem commercially viable.

Photoelastic waveguides will have naturally smooth transitions between regions of different refractive index, eliminating the problem with rough sidewalls. However, the maximum strain, and thus the maximum change in refractive index would always be at the interface between different materials, or between regions of different alloy compositions, thus always guiding along, or close to, junctions, which slightly reduces the design flexibility of the technique. On the other hand, very simple waveguides can be made by common deposition methods, making the technique cheap and simple. If the photoelastic confinement is strong enough, it should in principle be possible to define channel waveguides without the additional confinement of planar structures; however, such purely photoelastic structures have not yet been reported.

Several interesting photoelastic devices have been produced, and the technology has been investigated for its effect in waveguides [52, 50, 51, 53], lasers [54, 55, 56] and modulators [57, 58, 59]. There has also been one report on photoelastic confinement in a SiO$_2$/Si/SiO$_2$/Si heterostructure [60], although neither bulk silicon nor Si$_{1-x}$Ge$_x$ based structures have been investigated for photoelastic applications.
Figure 1.5 **Photoelastic waveguide structure** using a SiN$_y$ stressor stripe to generate strains into a Si$_{1-x}$Ge$_x$ planar waveguide. The strain-induced refractive index changes could be used to define channel waveguides. Although photoelastic waveguides have not been reported in Si$_{1-x}$Ge$_x$, the same basic waveguide structure has been investigated in GaAs-based structures.

1.2.1 **Comparing different waveguide technologies**

While CVD or MBE will probably remain the favoured method for creating planar structures, ion implantation, etching of strips and ribs, indiffusion and photoelastic techniques may all be used for horizontal confinement. It is the purpose of this section to decide on which is the most appropriate waveguide technology, not in terms of their reported merit, but rather by considering their appropriateness for optoelectronic integration.

Firstly, it is useful if the material surface remains intact, since this simplifies the device interconnection and further processing of the circuit. Etched rib waveguides are not useful in this respect, since they typically require etching of the guiding layer down to depths of several microns, while electronic devices typically have vertical dimensions of around 0.1$\mu$m. Secondly, etched waveguides, as well as ion-implanted waveguides, affect the strain in the guiding layer, either by changing the surface topology or by amorphising the material, which sets restrictions on the design of strained devices in the vicinity of the waveguides. Amorphising the material can also have a strong effect on both optical absorption and the carrier mobility, which is undesirable.

Since epitaxial planar layers of thickness $\sim$0.1$\mu$m are often used for VLSI, and multilayer structures are increasingly being investigated to optimise the parameters of optical devices, a third important issue is that waveguide technologies should not restrict the design of other devices based on such planar layers. Photoelastic waveguides seem particularly useful in this respect, since they have been fabricated both in buried planar layers and in surface layers. They could in principle also be fabricated without any planar structure, or below a thin surface layer used for VLSI, although this has not yet been demonstrated. Ge-indiffused guides could also be useful, although the rather significant annealing needed for the waveguide indiffusion will clearly also affect other structures, such as Si$_{1-x}$Ge$_x$/Si superlattices, which is an obvious drawback. Ion-implanted guides...
of the type shown in figure 1.3 could not be made without a thick planar layer, although they could guide underneath a thin surface layer, which is also the case for etched ribs. In conjunction with multilayers, however, etched ribs and ion-implanted guides could be difficult to fabricate. By using ion implantation to amorphise the crystal layers, however, waveguides could be fabricated both with and without planar layers.

Finally, the speed and ease of fabrication are important factors if a waveguide technology is to be attractive for commercial applications. In this respect, etched waveguides are rather simple structures which can be fabricated with one step of standard photolithography and etching. Ion implanted waveguides are in principle suitable for fabrication together with VLSI, although rather high implantation energies are required, which could make it unattractive for practical applications. Ge-indiffused silicon waveguides are based on simple deposition and etching, however, the reported annealing times of around 60 hours at 1200°C and above probably rules it out for use in commercial applications. Photoelastic waveguides, on the other hand, need only to define a stressor stripe on top of the guiding layer, making this a particularly simple technology. It is interesting that the deposition of a stripe of dielectric onto the guiding layer such as shown in figure 1.5 is also an integral part of making both the etched ribs and the indiffused waveguides.

Based on the considerations presented here, photoelastic waveguides of the type shown in figure 1.5 seem the most appropriate technology for optoelectronic integration and fabrication: It leaves the material surface intact and requires no doping or damaging of the guiding layer, it uses standard processing technology, no long-term annealing is needed and it can be used together with planar layers. However, for the waveguides to be useful for practical applications, the optical properties, in particular losses and optical mode profiles, must be appropriate. Whether photoelastic waveguides are indeed possible to fabricate in bulk silicon and Si$_{1-x}$Ge$_x$/Si heterostructures can only be determined by an experimental investigation, although there has been one report on horizontal photoelastic confinement in a SiO$_2$/Si/SiO$_2$/Si heterostructure [60], suggesting that such waveguide structures are feasible.

Before investigating these waveguide structures further, it is useful for the understanding of the project with a further review of photoelastic waveguiding, as well as waveguiding in Si$_{1-x}$Ge$_x$/Si heterostructures. This will give an indication of what to expect from the investigation, and it may reveal interesting aspects of photoelastic waveguiding which have not been considered previously, so that more specific aims can be set for the project.

### 1.2.2 Attenuation in Si and Si$_{1-x}$Ge$_x$/Si Heterostructures

While the study of photoelastic waveguides in bulk silicon and Si$_{1-x}$Ge$_x$ is a new field, there are numerous reports of other types of waveguide in these materials. These measurements are useful in indicating the level of propagation losses which is achievable. They also serve as a yardstick for the photoelastic waveguides, which will have to be as low loss as other types of waveguide to be of interest for practical applications. The one reference to photoelastic waveguides in SiO$_2$/Si/SiO$_2$/Si heterostructures is not seen as representative for photoelastic waveguides in silicon, since it is really just a planar waveguide using photoelastic confinement to limit a planar mode.

The minimum bandgap energy of silicon is 1.11eV, corresponding to a wavelength of approximately 1.1μm. At shorter wavelengths the optical absorption is very high, such that waveguiding becomes impractical. In Si$_{1-x}$Ge$_x$, the minimum wavelength increases with germanium content. Reports on waveguiding in Si$_{1-x}$Ge$_x$ therefore typically start...
at 1.15\mu m, which is just above the minimum bandgap of silicon, and goes up to \sim 1.3\mu m and \sim 1.55\mu m, corresponding to the minimum absorption windows in common optical communication fibres.

Table 1.1 presents a number of reported propagation losses in silicon and Si_{1-x}Ge_x waveguides, indicating both the growth method of the planar layer and the waveguide technology. Notice that the pure silicon waveguides are also fabricated from planar structures, such as SOI, even though the substrate is silicon. It is found that the propagation losses at 1.15\mu m is generally at least a few dB/cm, showing the effect of the minimum energy bandgap. However, for wavelengths of 1.3-1.55\mu m, there are several reports of losses well below 1dB/cm, demonstrating the low-loss potential of the material.

<table>
<thead>
<tr>
<th>Reference</th>
<th>Growth Method</th>
<th>Germanium content x</th>
<th>Wavelength</th>
<th>Minimum reported loss</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fischer et al. (1996) [14]</td>
<td>BE-SOI</td>
<td>0%</td>
<td>1.3\mu m</td>
<td>0.1dB/cm</td>
</tr>
<tr>
<td>Yu et al. (1995) [60]</td>
<td>BE-SOI</td>
<td>0%</td>
<td>1.53\mu m</td>
<td>1.5dB/cm</td>
</tr>
<tr>
<td>Rickman et al. (1994) [15]</td>
<td>SIMOX-SOI</td>
<td>0%</td>
<td>1.15\mu m</td>
<td>&lt;3dB/cm</td>
</tr>
<tr>
<td>Rickman et al. (1994) [61]</td>
<td>SIMOX-SOI</td>
<td>0%</td>
<td>1.523\mu m</td>
<td>0.0\pm0.5dB/cm</td>
</tr>
<tr>
<td>Splett et al. (1994) [62]</td>
<td>'Standard epitaxial Si'</td>
<td>0%</td>
<td>1.3\mu m</td>
<td>&lt;1.5dB/cm</td>
</tr>
<tr>
<td>Zinke et al. (1993) [16]</td>
<td>BE-SOI</td>
<td>0%</td>
<td>1.3\mu m</td>
<td>&lt;0.5dB/cm</td>
</tr>
<tr>
<td>Kesan et al. (1991) [13]</td>
<td>MBE</td>
<td>0%</td>
<td>1.3\mu m</td>
<td>1-2dB/cm</td>
</tr>
<tr>
<td>Splett et al. (1990) [40]</td>
<td>MBE</td>
<td>1%</td>
<td>1.3\mu m</td>
<td>3-5dB/cm</td>
</tr>
<tr>
<td>Liu &amp; Prucnal (1992) [22]</td>
<td>RTPCVD</td>
<td>1.0%</td>
<td>1.3\mu m</td>
<td>2.5\pm1dB/cm</td>
</tr>
<tr>
<td>Posarcik et al. (1992) [23]</td>
<td>CVD</td>
<td>1.2%</td>
<td>1.32\mu m</td>
<td>0.5dB/cm</td>
</tr>
<tr>
<td>Splett et al. (1994) [25]</td>
<td>MBE</td>
<td>2%</td>
<td>1.3\mu m</td>
<td>2.6-2.7dB/cm</td>
</tr>
<tr>
<td>Yang et al. (1993) [63]</td>
<td>CVD</td>
<td>1.3%</td>
<td>1.523\mu m</td>
<td>4.2dB/cm</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2.3%</td>
<td>1.523\mu m</td>
<td>2.5dB/cm</td>
</tr>
<tr>
<td></td>
<td></td>
<td>10%</td>
<td>1.15\mu m</td>
<td>10.5dB/cm</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1.3\mu m</td>
<td>1.9dB/cm</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1.523\mu m</td>
</tr>
<tr>
<td>Soref et al. (1990) [21]</td>
<td>CVD</td>
<td>10%</td>
<td>1.3\mu m</td>
<td>1.9dB/cm</td>
</tr>
<tr>
<td>Weiss et al. (1992) [64]</td>
<td>CVD</td>
<td>10%</td>
<td>1.15\mu m</td>
<td>8dB/cm</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1.523\mu m</td>
</tr>
<tr>
<td>Schüppert et al. (1989) [47]</td>
<td>Indiffusion</td>
<td>27%</td>
<td>1.3\mu m</td>
<td>&lt;4dB/cm</td>
</tr>
<tr>
<td>Schmidtchen et al. (1992) [48]</td>
<td>Indiffusion</td>
<td>70%</td>
<td>1.3\mu m</td>
<td>0.3dB/cm</td>
</tr>
</tbody>
</table>

Table 1.1 Propagation losses measured in Si_{1-x}Ge_x waveguides, demonstrating their potential for low-loss waveguiding. Notice that the waveguides made by Yu et al. [60] are made from a SiO_2/Si/SiO_2/Si heterostructure, and make use of photoelastic horizontal confinement. This reference is not seen as representative for photoelastic waveguides in silicon, since it is really just a planar waveguide using photoelastic confinement to limit a planar mode. Notice also that the indiffused guides by Schüppert et al. and Schmidtchen et al. have indiffused channels of lower germanium content beneath the deposited strip of high (27% and 70%) germanium content. See figure 1.4.
Poor crystal quality can significantly increase these waveguide losses. In $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ heterostructure waveguides, the crystal quality depends on the strain in the $\text{Si}_{1-x}\text{Ge}_x$ guiding layer, which increases with germanium content, because excessive strain will cause the crystal to relax along the heterojunction, and crystal dislocations can propagate into the guiding layer, thus increasing the propagation losses. It is noticeable how all the waveguides reported in table 1.1 have relatively low germanium content. Section 1.2.3 discusses the lattice mismatch and strain set up due to the $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ heterojunction.

### 1.2.3 Lattice Mismatch and Strain

If germanium is grown onto a silicon substrate, there will be a lattice mismatch at the boundary between the materials due to their different lattice constants. Assuming a rigid silicon substrate, the strain $\varepsilon$ required to match the germanium layer to the silicon lattice is found from

$$a_{\text{Si}} = a_{\text{Ge}} (1 + \varepsilon)$$

$$\varepsilon = \frac{a_{\text{Si}} - a_{\text{Ge}}}{a_{\text{Ge}}}$$

(1.1)

where $a_{\text{Si}}$ is the lattice constant of silicon, and $a_{\text{Ge}}$ is that of germanium. Bulk silicon and bulk germanium have lattice constants of 5.430Å and 5.658Å, respectively, giving a lattice mismatch of $\frac{5.430\text{Å} - 5.658\text{Å}}{5.658\text{Å}} = -4.03\%$. The negative sign indicates that the germanium film is under compressive strain. Any $\text{Si}_{1-x}\text{Ge}_x$ film grown onto a silicon substrate will therefore see a lattice mismatch corresponding to a strain in the range $0 \leftrightarrow -4.03\%$. As will be calculated in chapter 3, some of this strain is actually absorbed by the substrate, since it is not perfectly rigid.

When the thickness of the strained layer is less than a certain value, known as the pseudomorphic or critical layer thickness, all the strain will be accommodated by the materials. Once this thickness is exceeded, however, the strained material will begin to relax by defaulting in the heterojunction area. Since this will affect both the refractive index and the energy bandgap, and since the crystal damage can affect the propagation losses of waveguides, it is useful to know the critical layer thickness of $\text{Si}_{1-x}\text{Ge}_x$ on silicon, and how it changes with germanium content.

People and Jackson [65] give a good review of the different theories for calculating the pseudomorphic thickness. The ambiguous aspect is which theory to use in any particular case. Figure 1.6, taken from People and Jackson, does present rather inconsistent data. This indicates the high reliance the critical layer thickness has on the production specifics, typically growth method, temperature and subsequent processing. Several people have studied strained and relaxed layers and the strain mechanisms in them [37, 66], but as yet no completely satisfactory data or theory exist.

Some useful additional data from Yang et al. [63] show that an 8μm thick $\text{Si}_{0.9}\text{Ge}_{0.1}$ layer grown epitaxially on (100) silicon had few dislocations, and these were concentrated around the $\text{Si}_{0.9}\text{Ge}_{0.1}/\text{Si}$ interface. For 10μm thick layers containing 1.3% and 2.3% germanium, there appeared to be no dislocations at all.

In a silicon-based system, $\text{Si}_{1-x}\text{Ge}_x$ turns out to be the ultimate optical material in terms of strain. Firstly, because the alloy composition is continuously variable, the strain can be designed to lie anywhere in the range $0 \leftrightarrow -4.03\%$. Secondly, most other materials have too large lattice constants. Therefore, strained epitaxial layers of practical thickness
Figure 1.6 Critical layer thickness of $\text{Si}_{1-x}\text{Ge}_x$ grown on (100) silicon as a function of germanium content, taken from People and Jackson [65], presenting various models for single-layer critical layer thickness, along with experimental data. This indicates the high reliance of the critical layer thickness on the production specifics, typically growth method, temperature and subsequent processing.

Figure 1.7, taken from Pearsall [67], shows the lattice constants of many common optical materials.

Most reports on strain and strained layers assume epitaxial layers grown by MBE or CVD, and only one-dimensional growth. Two- and three-dimensional structures, however, represent a much more intricate setting for the strain. Photoelastic waveguides, using strain-induced changes in the refractive index to define waveguides, therefore need a more detailed description of the waveguide strains. Section 1.3 explains in general terms how a three dimensional strain tensor can be used to calculate the refractive index profiles in photoelastic waveguides, and goes on to review some useful waveguides and devices based on photoelastic technology.

### 1.3 Photoelastic Waveguiding

The principle idea of optical waveguiding is to increase the refractive index in a small region of the structure, and so confine light within this region. In photoelastic waveguides the refractive index increase is generated by introducing strain into the structure. Before studying these structures further, it is important with a basic understanding of the three-dimensional state of strain and the photoelastic effect in crystals.
1.3.1 The Strain Tensor

Strain describes the relative change in dimensions of an object, which may be caused by mechanical, electrical or thermal influences. In photoelastic waveguides, it is important to consider the strains in three dimensions, which are generally different. Figure 1.8 illustrates the nine components of the general strain tensor, which together completely describe an arbitrary deformation of an object. The directions and notations of the strains are consistent with Nye [68], although the reference to crystal axes are specific for this project. A few definitions and details are needed for a consistent description of the photoelastic waveguides investigated here:

- Tensile strains or elongation along a direction are described as positive strains, while compressive strains are negative.

- In general, the strains have two suffixes, the first one showing the direction of the displacement, the second being the axis normal to the plane affected by strain. The component $\varepsilon_{xy}$ therefore gives the displacement in the x direction seen by the plane normal to the y axis. The components with two different suffixes are known as shear strains.

- In this project the main axes of the strain tensor are denoted by x, y and z and they are, unless otherwise specified, coincident with the [100], [010] and [001] axes of the crystals.

- The strain tensor is defined on an infinitesimally small volume, and is in general different at every location of a waveguide.

- The strains $\varepsilon_{xy}$ and $\varepsilon_{yx}$ are equal. Similarly, $\varepsilon_{xx} = \varepsilon_{zz}$ and $\varepsilon_{yz} = \varepsilon_{zy}$. There are therefore only six independent components of the tensor.
Figure 1.8 The strain tensor. For a cube with its edges parallel to three mutually perpendicular axes \( x, y \) and \( z \), an arbitrary deformation can be defined in terms of the strain tensor \( \varepsilon_{ij} \) where \( i,j = x, y \) or \( z \), so that there are nine possible strain coefficients. In general, the strains have two suffixes, the first one showing the direction of the displacement, the second being the axis normal to the plane affected by strain. In this project, the axes \( x, y \) and \( z \) are, unless otherwise specified, parallel to the \([100], [010] \) and \([001] \) crystal axes of the waveguides.

- A few references are made to stresses, which represent the force per unit area at some location. The stress tensor is defined on the same axes and with the same positive directions as the strains.

Due to the symmetry of the strain tensor, it is common to use an abbreviated notation with only one suffix, as illustrated in figure 1.9, which reduces the number of coefficients needed for further tensor operations. Given the strain tensor, the strain-induced refractive index can be calculated from photoelastic theory.

1.3.2 Photoelastic Theory

According to photoelastic theory [68], the strain-induced refractive index changes in a crystal can be found from the change in the relative dielectric impermeability tensor \( B_m \), which is a function of the strain tensor \( \varepsilon_n \):

\[
\Delta B_m = p_{mn} \varepsilon_n \quad (m, n = 1, 2, \ldots, 6)
\]

where \( p_{mn} \) are the elasto-optical photoelastic constants. In this project they will be referred to only as photoelastic constants. The use of abbreviated tensor notation for both \( B_m \),...
Two-suffix Notation

\[
\begin{bmatrix}
\varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\
\varepsilon_{21} & \varepsilon_{22} & \varepsilon_{23} \\
\varepsilon_{31} & \varepsilon_{32} & \varepsilon_{33}
\end{bmatrix}
\]

One-suffix Notation

\[
\begin{bmatrix}
\frac{1}{2} \varepsilon_6 \\
\frac{1}{2} \varepsilon_5 \\
\varepsilon_2 \\
\frac{1}{2} \varepsilon_4 \\
\frac{1}{2} \varepsilon_6
\end{bmatrix}
\]

Figure 1.9 Abbreviated Tensor Notation. Of the nine components of the strain tensor, only six components are independent. In the strain tensor in figure 1.8, it can be shown [68] that \( \varepsilon_{xy} = \varepsilon_{yx} \), \( \varepsilon_{xz} = \varepsilon_{zx} \) and \( \varepsilon_{yz} = \varepsilon_{zy} \). Therefore, given a general strain tensor \( \varepsilon_{ij} \) where \( i, j = 1, 2 \) or \( 3 \), it is common to use a one-suffix notation \( \varepsilon_n \) where \( n = 1, 2, \ldots, 6 \), which relates to the original tensor as shown above. It is then possible to present the tensor as a column matrix, as shown on the right, which reduces the number of coefficients needed for further tensor operations.

and \( \varepsilon_n \) reduces the number of photoelastic constants from 81 to 36, although in cubic crystals such as silicon and germanium, the symmetry of the crystal reduces the number of independent photoelastic constants further to only three. These are \( p_{11} \), \( p_{12} \) and \( p_{44} \).

The refractive indices \( n_x \), \( n_y \) and \( n_z \) seen along the \( x \), \( y \) and \( z \) directions in an unstrained cubic crystal are all equal, and are found from the relative dielectric impermeability:

\[
\begin{align*}
n_x &= \frac{1}{\sqrt{B_x}} \\
n_y &= \frac{1}{\sqrt{B_y}} \\
n_z &= \frac{1}{\sqrt{B_z}}
\end{align*}
\]  

(1.3)

In section 2.2, equations 1.2 and 1.3 are applied to a three-dimensional strain tensor oriented as described in figure 1.8 to give detailed expressions for the strain-induced refractive index. It is important to notice that as well as having an anisotropic strain with six independent strain components at every location in a waveguide, the crystal itself is anisotropic, and will set up a different refractive index profile for the same strain conditions applied along different crystallographic axes. For instance, if the photoelastic waveguide structure in figure 1.5 were grown on a (100) substrate, stressor stripes oriented along the [100] and [110] axes would generate virtually the same strains, although the strain-induced refractive index profiles could be very different, depending on the photoelastic constants. In chapters 2 and 3, the photoelastic constants for \( \text{Si}_{1-x}\text{Ge}_x \) are calculated and used in the modelling of photoelastic waveguides.
1.3.3 Photoelastic Waveguides

In section 1.2.1 a comparison was made of different waveguide technologies, and photoelastic waveguiding was found to be the most appropriate technology in terms of optoelectronic integration and fabrication. If well-confined waveguides could be realised by simply depositing a stressor stripe onto a Si$_{1-x}$Ge$_x$/Si heterostructure as shown in figure 1.5, this would present a very appropriate waveguiding structure for use in optoelectronic circuits, which it would be useful to investigate. If waveguides could be realised even without the need for a planar layer, by depositing a stressor stripe directly onto bulk silicon, then that would present a particularly cost-effective technology, although such purely photoelastic waveguides have not yet been reported in any material.

Photoelastic waveguides of the type shown in figure 1.5 have previously been reported by Westbrook et al. [51] in GaAs-based structures, as shown in figure 1.10(a). Similar structures have also been reported with buried planar structures by Yu et al. [69], as shown in figure 1.10(b). The horizontal confinement in these structures is generated by the stressor stripe, which exerts a force onto the planar structure, which in turn introduces strains and strain-induced refractive index changes into the guiding layer. Depending on the photoelastic constants of the guiding layer as well as the nature of the stressor stripe, guiding regions can be defined either at the stripe edges or under the centre of the stripe. In a report by Westbrook et al. [50], three separate modes were measured under a single stressor stripe, one being under the middle of the stripe and one at each edge. It was also demonstrated [51] that the number of guided modes depend on the stripe width. Since this is a particularly simple and compact technology for fabricating couplers, it is peculiar that photoelastic couplers have not been investigated further.

With reference to GaAs based structures, it seems a fuller understanding of the guiding regions in photoelastic waveguides is needed. For instance, waveguides of the type shown in figure 1.10(a) were reported to support both TE and TM polarised modes, while the one in figure 1.10(b) was found to be highly birefringent, even though calculations predict fairly similar photoelastic confinement for TE and TM polarised light. These calculations, however, are based on previously reported photoelastic constants, which strongly affect the calculated results. For the study of photoelastic waveguides in bulk silicon and Si$_{1-x}$Ge$_x$/Si heterostructures, both the photoelastic constants and the refractive index profiles will be investigated, so as to give a thorough understanding of both the planar layer and the effect of the stressor stripe.

One way of defining photoelastic waveguides is by high temperature deposition of a stressor layer, such as a dielectric or metal film, onto a guiding layer. On cooling to room temperature, strain is introduced into the guiding layer due to the different thermal expansion of the stressor and the guiding layer. Depending on the deposition conditions, the deposited films may also generate non-thermal stresses [70], which can be useful in defining photoelastic waveguides. Alternatively, a stressor can be generated by chemical reactions induced between a deposited film and the planar structure. For instance, in the waveguide structure in figure 1.10(b) a Ni$_2$GaAs stressor layer was generated by annealing a Ni layer sputtered onto GaAs [69]. Although all these stressor technologies have all been demonstrated in GaAs [55, 69, 71], generating stressors by chemical reactions in silicon and Si$_{1-x}$Ge$_x$ may be difficult, since they are chemically fairly stable materials.

Photoelastic waveguides have the advantage of a naturally smooth transition between regions of different refractive index, which avoids scattering and losses due to rough sidewalls. Table 1.2 presents propagation losses reported in various photoelastic waveguides,
Figure 1.10 *Photoelastic waveguides in GaAs-based structures* have been reported both with a stressor stripe deposited onto a simple surface planar waveguide, as shown in (a) [51], and in buried waveguides, as shown in (b) [69]. In the buried layers, only one guiding region has been reported which is located under the centre of the stressor stripe, while the surface layers could define up to three separate guiding regions with one stripe.

Showing that these structures are appropriate for low-loss waveguiding. It is therefore likely that photoelastic waveguides in silicon and Si_{1-x}Ge_{x} will be low-loss, since other types of waveguides in these materials have already been demonstrated with low losses, as shown in table 1.1.

Notice the difference in table 1.2 between photoelastic waveguides in planar surface layers and in buried layers. In the surface layers, the photoelastic confinement significantly affects both the vertical and horizontal profiles of the guided modes, and has been used to define several guiding regions [50, 51]. In the buried layers, the photoelastic confinement has in general been used to limit a planar mode [73, 71, 60]. Pure photoelastic waveguides, having no additional confinement from planar structures, have as yet not been reported.

In addition to its use in photoelastic waveguiding, the photoelastic effect has been used to explain the guiding mechanisms in lasers [55, 56]. There have also been reports on couplers [72, 57], polarisers [60, 69], modulators [50] and switches [58] using photoelastic guiding as the main method of confinement. These reports, together with the waveguide results in table 1.2 demonstrate the feasibility of photoelastic waveguiding. If this technology could be applied usefully in bulk silicon and Si_{1-x}Ge_{x}/Si heterostructures, it would present a simple, low-cost solution for the fabrication of waveguide based devices in optoelectronic integrated circuits.
Table 1.2 Losses reported for photoelastic waveguides show that these waveguide structures are potentially low-loss. Excess losses of due to photoelastic confinement of $<1\text{dB/cm}$ have also been reported[69], and it is claimed that the losses in photoelastic waveguides are in principle just material losses [73]. The lowest losses are made in buried structures, however, and could be higher in other types of photoelastic waveguide.

### 1.4 Aims of the Project

This review has investigated aspects of optical waveguiding in silicon-based structures, with particular attention to $\text{Si}_{1-x}\text{Ge}_x$ alloys, with the objective of finding a waveguide technology which is suitable for optoelectronic integration. Silicon and $\text{Si}_{1-x}\text{Ge}_x$ were investigated due to their appropriateness for integration with VLSI. Given the progress over the last decade on low-loss waveguides as well as passive and active devices they now appear as much more potential materials for optical applications than previously. After a comparison of different waveguide technologies, photoelastic waveguides were chosen as the most appropriate in terms of fabrication and optoelectronic integration. They have also been demonstrated as suitable for low-loss waveguiding, although they have not yet been reported in bulk silicon or $\text{Si}_{1-x}\text{Ge}_x$ structures.

Based on this review, the study of photoelastic waveguides in bulk silicon and $\text{Si}_{1-x}\text{Ge}_x$ appears as an interesting investigation with potential applications in optoelectronic integrated circuitry. The main aims of this project are therefore chosen to be:

1. To investigate whether photoelastic waveguides can be fabricated in bulk silicon. This is novel in that photoelastic waveguides have never been reported without additional confinement from planar structures. Such purely photoelastic waveguides would provide a particularly cheap and simple waveguide technology.

2. To investigate whether photoelastic waveguides can be fabricated in $\text{Si}_{1-x}\text{Ge}_x$, which has also never been investigated. Practically, these waveguides will be fabricated in $\text{Si}_{1-x}\text{Ge}_x$/Si heterostructures, since much of the usefulness of $\text{Si}_{1-x}\text{Ge}_x$ is that it can be grown on silicon substrates. These waveguides will therefore be introduced into a planar waveguide structure, in contrast to the waveguides fabricated in bulk silicon. The effect of the planar waveguide can then be evaluated from the difference between the two waveguide structures.

3. To investigate the propagation losses of the waveguides. If it turns out that the waveguides can be fabricated, it is important that they have low propagation losses if they are to be seen as a real alternative to other types of waveguide. This aim can be regarded as a study of the practical potential of the waveguides, in contrast to the first two aims, which define investigations into new waveguide structures.
These are the overall aims of the project. During the course of the investigation, several other aspects of these waveguides structures will also be investigated. These include a study of the photoelastic constants of Si$_{1-x}$Ge$_x$, detailed descriptions of the optical profiles of the waveguides and fabrication and characterisation of stressor layers. It is difficult to set up specific aims for all expected activities at the outset of the project. However, it is possible to set up a work plan wherein which the main tasks of the project are outlined.

The project is concerned with the modelling of photoelastic waveguides and the optical properties of the relevant materials. The project therefore starts off in chapter 2 with a calculation of the refractive indices, photoelastic constants and inherent losses of Si$_{1-x}$Ge$_x$. Chapter 3 presents a study of the strains, refractive index profiles and optical modes of the waveguides. Based on these calculations, the expected waveguide characteristics are outlined in terms of the system variables, giving a guideline to the subsequent fabrication and experimental investigation. Chapter 4 goes on to specify the waveguide fabrication and characterisation, together with a detailed description of the measurement equipment. The reasons for the particular equipment set-up are also explained. In chapter 5, measurement results are presented, showing the optical mode profiles and propagation losses, as well as the effect of system variables. Chapters 6 and 7 discuss and conclude on the work and results from the project, together with a presentation of issues which could usefully be investigated further.
Chapter 2

Optical Properties of $Si_{1-x}Ge_x$

This chapter presents calculations of the refractive index, photoelastic constants and inherent losses of $Si_{1-x}Ge_x$ alloys, which are required for the modelling of the photoelastic waveguides presented in chapter 3.

2.1 The Refractive Index of $Si_{1-x}Ge_x$

The refractive index of $Si_{1-x}Ge_x$ alloys is a function of alloy composition, silicon and germanium energy band structures, and strain 1. Two particular effects are of interest in this project, namely the shift of the energy band edges with strain, which affects the optical losses, and the related photoelastic effect, which gives the change in the real refractive index with strain.

A refractive index model for $Si_{1-x}Ge_x$ using the energy bandgap as an interpolation factor was previously proposed by Lareau et al. [74]:

$$n(Ge_xSi_{1-x}) = n(Si) + [n(Ge) - n(Si)] \frac{[E_g(Si) - E_g(x)]}{[E_g(Si) - E_g(Ge)]}$$  \hspace{1cm} (2.1)

where $n(Ge)$ and $n(Si)$ are the bulk refractive indices, $E_g(Ge)$ and $E_g(Si)$ are the bulk band gap energies of germanium and silicon, respectively, and $E_g(x)$ is the bandgap of the $Si_{1-x}Ge_x$ alloy, as a function of germanium content $x$.

According to Namavar and Soref[24], this equation, often known as the Red-shift equation, gave a fairly good fit to their waveguide mode measurements. Compared to ellipsometric measurements of unstrained $Si_{1-x}Ge_x$ by Humlicek [75], however, the refractive index change with germanium content according to the Red-shift equation can be several times that found experimentally. Also, when used to calculate the effect of induced strain, even bulk silicon would depend upon germanium data, which is obviously wrong. Finally, only the minimum bandgap is considered, while it is well known that the refractive index depends strongly upon higher energy transitions [75].

While the changes in energy bands do not relate simply to the real refractive index, their effect on the extinction coefficient is much better understood [76]. Given the modified extinction coefficient, the real refractive index is found from the Kramers-Krönig

1There are also other factors affecting the refractive index, in particular temperature and electric and magnetic fields. These effects are not considered in this project, since all measurements are made at room temperature, and there are no applied fields.
Figure 2.1 Experimental extinction coefficient data for bulk silicon (solid line) [78] and bulk germanium (dashed line) [79]. The characteristic peaks indicated correspond to the direct transitions listed in Table 2.1. The strong $E_2$ transitions in both materials at 4.4eV lie close to the $E_0(Si)$ peak at 4.1eV here, and have not been labelled explicitly, although they are quite distinct on a higher magnification.

2.1.1 The Extinction Coefficient of Silicon and Germanium

For unstrained silicon and germanium, experimental data for the extinction coefficients exist over a wide range of energies. Figure 2.1 presents measured data taken over several orders of magnitude of energy, starting from the energy band edge. Above and below this energy range, the extinction coefficient is small, and has little influence upon the real refractive index. For the purpose of the model presented here, it will be assumed to be zero outside this energy range.

Apart from the minimum energy band gap, which is indirect for both silicon and germanium, there are strong direct transitions which appear as characteristic peaks on the extinction coefficient curves in Figure 2.1. They correspond to the direct energy gaps or critical points listed in Table 2.1.

It will be assumed here that for small shifts in the energy bands, the general shape of the extinction coefficient curve stays the same as a function of energy, although it scales linearly between the characteristic peaks as they shift in energy. These strain-induced
Table 2.1 Energy gaps in silicon and germanium. The direct transitions $E_0$, $E_1$ and $E_2$ are energy minima in the reciprocal lattice of silicon and germanium, and are seen as characteristic peaks in the extinction coefficient curve in Figure 2.1. All transitions have a definite location in the reciprocal lattice, as shown in the table, which determines how they are shifted under the influence of strain, as calculated in section 2.1.2. The minimum energy gap $E_0(Si)$ in silicon and $E_0(Ge)$ in germanium are both indirect, and do not have a strong influence on the extinction coefficient, but they strongly affect the optical absorption, as calculated in section 2.3. Below the minimum energy gaps, the extinction coefficient is very small and the material becomes transparent. The data are taken from: (a) Braunstein et al. [80], (b) Cardona et al. [81], (c) Cardona et al. [82] and (d) Pickering et al. [66].

<table>
<thead>
<tr>
<th></th>
<th>Location in Reciprocal Space</th>
<th>Si</th>
<th>Ge</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_0(Si)$</td>
<td>along [100]</td>
<td>1.1(6)</td>
<td></td>
</tr>
<tr>
<td>$E_0(Ge)$</td>
<td>along [111]</td>
<td></td>
<td>0.65(6)</td>
</tr>
<tr>
<td>$E_0$ at $k=0$</td>
<td></td>
<td>4.1(6)</td>
<td>0.8(6)</td>
</tr>
<tr>
<td>$E_1$</td>
<td>along [111]</td>
<td>3.4(6)</td>
<td>2.1(6)</td>
</tr>
<tr>
<td>$E_2$</td>
<td>along [100]</td>
<td>4.4(6)</td>
<td>4.4(6)</td>
</tr>
</tbody>
</table>

energy shifts are calculated in section 2.1.2, and are used in section 2.1.3 to modify the extinction coefficient from which the photoelastic constants are found.

This approach does not consider fully the effect of energy band splitting along the different crystal directions, since bulk data is used. However, it is used here as a useful approximation for small shifts in the energy gaps.

2.1.2 Strain-Induced Changes in the Energy Band Structure of Silicon and Germanium

The important features of the extinction coefficient are the extinction cut-off, defined by the minimum bandgap, which is indirect for both silicon and germanium, and the direct transitions $E_0$, $E_1$ and $E_2$ as indicated in figure 2.1. While there are higher energy transitions, figure 2.1 shows that they are weaker. They will also have a relatively smaller effect on the real refractive index in the infrared region, as explained in section 2.1.3.

The strain-induced changes in the respective energy gaps can be broken down into shifts in the valence band $\Delta E_v$, and in the conduction band $\Delta E_c$. These band shifts can be further broken down into a hydrostatic component, which gives the average shift of energy bands for that transition with hydrostatic strain or volume change, and a uniaxial component, which causes a splitting of degenerate bands around the average value.

The Strain-Induced Shift of the Valence Bands can be found according to Pikus and Bir[83] around $k=0$ when deformed according to a strain tensor $\epsilon$ from

$$\Delta E_v = a \frac{1}{15} \epsilon^2 \pm \sqrt{\frac{1}{2} b^2 [(\epsilon_{xx} - \epsilon_{yy})^2 + c.p.]} + d^2 [\epsilon_{xy} + c.p.]$$

(2.2)

where $a$, $b$ and $d$ are deformation potentials, $\frac{1}{15} \epsilon$ is a unit tensor, $\epsilon_{ij}$ are the components of the strain tensor, and c.p. stands for a cyclic permutation of x, y and z. This gives the...
shift of the two top (J=3/2) valence bands. The change in the absorption band edge will be calculated from the uppermost of the bands, since it corresponds to the lowest energy gap. This transition is also stress-isotropic [84] and will be assumed to account for the E₀ gaps in all directions.

The Strain-Induced Shift of the Conduction Bands for silicon and germanium can be explained in terms of a dilational deformation potential Ξ_d and a uniaxial deformation potential Ξ_u only, according to Herring and Vogt[85]. According to Balslev [86], the energy shift ΔE_cᵢ of a conduction band valley i, when deformed according to a strain tensor ε, is given by

\[ \Delta E_c^{i} = \left[ \Xi_d \mathbb{1} + \Xi_u (\alpha_i \alpha_i) \right] : \varepsilon \] (2.3)

where \( \mathbb{1} \) is a unit tensor, \( \alpha_i \) is a unit vector parallel to the k vector of the valley i, and { } denotes a dyadic product. For valleys along the [100] direction, i.e. the E₂ direct gap and the silicon indirect transition, the energy band shift will then be

\[ \Delta E_c^{(100)} = \Xi_d (\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) + \Xi_u \varepsilon_{(100)} \] (2.4)

where \( \varepsilon_{(100)} \) is the strain in the (100) direction. For valleys along the [111] direction, which are the E₁ direct gap and the germanium indirect transition, the band shift will be

\[ \Delta E_c^{(111)} = \Xi_d (\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) + \frac{2}{3} \Xi_u (\varepsilon_{xy} + \varepsilon_{yz} + \varepsilon_{zx}) \] (2.5)

For other [111] directions, the shifts are similar, but with appropriate sign changes according to the direction of the valleys. Valence band shifts around \( \mathbf{k} = 0 \) are given by equation 2.2, while for the E₁ and E₂ transitions, the uniaxial component of the valence band shift has been included in the uniaxial deformation potential \( \Xi_u \) in table 2.2.

Hydrostatic Deformation Potentials for the conduction or valence bands are difficult to calculate or measure separately [87]. It is therefore normally given as the relative change between the average valence band and the average conduction band shifts. From equations 2.2 and 2.3 the hydrostatic component of the bandgap change is

\[ \Delta E_g^{av} = \Delta E_c^{av} \div \Delta E_v^{av} = \left[ \Xi_d + \frac{1}{3} \Xi_u - a \right] \mathbb{1} : \varepsilon \]

\[ \Delta E_g^{av} = \left[ \Xi_d + \frac{1}{3} \Xi_u - a \right] \left( \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz} \right) \] (2.6)

where \( \left( \Xi_d + \frac{1}{3} \Xi_u - a \right) \) is the hydrostatic deformation potential of the entire gap, and \( av \) denotes the average band shift. Deformation potentials for all transitions are listed in table 2.2.

Using equations 2.2 through 2.6, the strain-induced energy shifts of the minimum indirect bandgap as well as the direct transitions E₀, E₁ and E₂ are now known for any given strain tensor. These energy shifts are used in section 2.1.3 to modify the extinction coefficient data in figure 2.1, from which the photoelastic constants are found.
Table 2.2 Deformation potentials for silicon and germanium. Notice that the $E_1$ and $E_2$ potentials relate to the entire band gap, so there are no separate terms for the valence band contribution as there is for all transitions from $k=0$.

### 2.1.3 Kramers-Krönig Relations

According to the Kramers-Krönig relations [77], the real refractive index $n(E)$ at an energy $E$ relates to the extinction coefficient $k(E)$ as follows:

$$n(E) - 1 = \frac{2}{\pi} P \int_0^\infty \frac{E'k(E')}{(E')^2 - E^2} dE'$$

where $P$ is the Cauchy integral [77]:

$$P \int_0^\infty \equiv \lim_{x \to -\infty} \left( \int_0^{E' - x} + \int_{E' + x}^\infty \right)$$

The extinction coefficient data in figure 2.1 were divided into sections, and polynomials up to the tenth order were fitted to each section, giving an R-squared fit of above 0.995 for each section. On applying equation 2.7, the spectral refractive index curves of silicon and germanium are found as shown in figure 2.2.
Each section of the extinction coefficient can now be modified to account for small changes in the energy gaps. For a general section of the curve going from $E_a$ to $E_b$, as shown in figure 2.3, a change in energy at the respective endpoints of $\Delta E_a$ and $\Delta E_b$ is incorporated into the extinction coefficient $k(E)$ through a linear shift and scaling of the energy variable:

$$k(E) \Rightarrow k(E') = k([E + \Delta E_a] \left[1 + \frac{\Delta E_b - \Delta E_a}{E_b - E_a}\right])$$

(2.9)

where the scaling and shift of each section may be different and depends on the strain-induced energy changes calculated in section 2.1.2.

Since the extinction coefficient is a linear function of the number of free electrons in the crystal, and since silicon and germanium have similar band structures, it will be assumed that the extinction coefficient of any $Si_{1-x}Ge_x$ alloy can be found from a linear interpolation of the silicon and germanium values. The refractive indices of $Si_{1-x}Ge_x$ alloys are then found from

$$n_{Si_{1-x}Ge_x}(E) - 1 = \frac{2}{\pi} \left[ (1 - x) P \int_0^{\infty} \frac{E'k_{Si}(E')}{(E')^2 - E^2} dE' + x P \int_0^{\infty} \frac{E'k_{Ge}(E')}{(E')^2 - E^2} dE' \right]$$

(2.10)

which turns out to be a linear interpolation of the refractive indices. It is clear from the denominators in equation 2.10 that the refractive index depends most strongly on...
2.2 Photoelastic Constants

The extinction coefficients can now be modified according to equation 2.9 using the strain-induced energy shifts given by equations 2.2 through 2.6 and the deformation constants in table 2.2, from which a modified refractive index is found using the Kramers-Kröning relations.

In this project it is of interest to determine the strain-induced refractive index change along the [100] axes of the crystal, which are given by the photoelastic constants $p_{11}$ and $p_{12}$. The refractive indices can be found from the change in relative impermeability $B$, which for a cubic crystal depends on the applied strain as follows [68]:

\[
\begin{pmatrix}
\Delta B_1 \\
\Delta B_2 \\
\Delta B_3 \\
\Delta B_4 \\
\Delta B_5 \\
\Delta B_6
\end{pmatrix}
= \begin{pmatrix}
B_1 - B^0 \\
B_2 - B^0 \\
B_3 - B^0 \\
B_4 \\
B_5 \\
B_6
\end{pmatrix}
= \begin{pmatrix}
p_{11} & p_{12} & p_{12} & 0 & 0 & 0 \\
p_{12} & p_{11} & p_{12} & 0 & 0 & 0 \\
p_{12} & p_{12} & p_{11} & 0 & 0 & 0 \\
0 & 0 & 0 & p_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & p_{44} & 0 \\
0 & 0 & 0 & 0 & 0 & p_{44}
\end{pmatrix}
\begin{pmatrix}
\epsilon_{11} \\
\epsilon_{22} \\
\epsilon_{33} \\
2\epsilon_{23} \\
2\epsilon_{31} \\
2\epsilon_{12}
\end{pmatrix}
\]
Table 2.3 Calculated photoelastic constants for Si and Si$_{1-x}$Ge$_x$ alloys. The values are the average for positive and negative strains in the range 0.001 to 0.01.

<table>
<thead>
<tr>
<th></th>
<th>Si</th>
<th>Si$<em>{0.987}$Ge$</em>{0.013}$</th>
<th>Si$<em>{0.950}$Ge$</em>{0.050}$</th>
<th>Si$<em>{0.900}$Ge$</em>{0.100}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1.15µm</td>
<td>1.523µm</td>
<td>1.15µm</td>
<td>1.523µm</td>
</tr>
<tr>
<td>$p_{11}$</td>
<td>0.37</td>
<td>0.36</td>
<td>0.38</td>
<td>0.37</td>
</tr>
<tr>
<td>$p_{12}$</td>
<td>0.48</td>
<td>0.43</td>
<td>0.48</td>
<td>0.44</td>
</tr>
</tbody>
</table>

Given strain components defined along the x, y and z axes, as in figure 1.8, the refractive indices can be approximated according to Nye [68] from equations 1.3:

\[
\begin{align*}
\Delta n_x &= -\frac{n_0^3}{2} \Delta B_{xx} = -\frac{n_0^3}{2} (\epsilon_{xx} p_{11} + \epsilon_{yy} p_{12} + \epsilon_{zz} p_{12}) \\
\Delta n_y &= -\frac{n_0^3}{2} \Delta B_{yy} = -\frac{n_0^3}{2} (\epsilon_{xx} p_{12} + \epsilon_{yy} p_{11} + \epsilon_{zz} p_{11}) \\
\Delta n_z &= -\frac{n_0^3}{2} \Delta B_{zz} = -\frac{n_0^3}{2} (\epsilon_{xx} p_{12} + \epsilon_{yy} p_{12} + \epsilon_{zz} p_{11})
\end{align*}
\]

Using equations 2.11 through 2.13, the photoelastic constants are now found from the refractive index model. By applying the energy shifts projecting along the x, y and z directions, respectively, values for $p_{11}$ and $p_{12}$ were calculated at wavelengths of 1.15µm and 1.523µm, and are listed in table 2.3 for several compositions.

The calculated constants in table 2.3 are the averages for positive and negative strains from 0.001 to 0.01, which is the range of interest for photoelastic waveguides, as will be seen in chapters 3 and 5. For only positive or only negative strains, the calculated constants are consistent to within 5%, while averaging for both positive and negative strains, there is a tolerance of around ±25%, with the value for positive strains always being higher. Given the complex strains set up within a photoelastic waveguide, however, average values for positive and negative strains are used in this project.

It is appropriate to mention here that the photoelastic constants refer to regions of homogeneous strain, due to their dependence on the energy band structure. In some parts of the waveguides investigated here, the strain changes quite abruptly. However, it will be assumed that for any atom in the structure, only the nearest few neighbouring atoms will have any significant effect on the energy band structure, and being within a few nanometres of each other, they will experience a fairly constant level of strain.

Some experimental values exist for the photoelastic constants of bulk silicon and germanium at 10.6µm, but they are smaller than the values predicted by this model. This seems to be because the constants were determined by uniaxial stress measurements. On applying a uniaxial stress $\sigma_{xx}$ in the x direction, strains are set up in both the x, y and z directions,
Table 2.4 Photoelastic constants compared to experimental data at 10.6\,\mu m. The calculated values show the range of constants corresponding to positive and negative strains in the range 0.001 to 0.01. The values of 0.154 for $p_{11}$ and 0.126 for $p_{12}$ were presented in the reference as negative, but they were calculated from negative piezo-optic constants $q_{ij}$, which should give positive values [101], as shown here.

\begin{tabular}{|c|c|c|c|}
\hline
 & Si & Ge \\
\hline
 & Calculated & Experimental & Calculated & Experimental \\
\hline
$p_{11}$ & 0.106-0.194 & 0.092 [98] & 0.212-0.227 & 0.154 [99], 0.27 [100] \\
$p_{12}$ & Not observed & 0.093-0.133 & 0.126 [99], 0.235 [100] & \\
\hline
\end{tabular}

\[ \sigma_{xx} = \varepsilon_{xx} E = -\frac{\varepsilon_{yy} E}{\nu} = -\frac{\varepsilon_{zz} E}{\nu} \] (2.15)

where $E$ is Young’s modulus and $\nu$ is Poisson’s ratio, which are given in appendix A. Photelastic constants were calculated for both positive and negative strains $\varepsilon_z$ from 0.001 to 0.01, including the two perpendicular strains $\varepsilon_{yy} = -\nu\varepsilon_{xx}$ and $\varepsilon_{zz} = -\nu\varepsilon_{xx}$. The results are given in table 2.4 together with experimental data.

While the experimental data have a significant spread, they are comparable to the calculated values. Measurement data for $p_{12}$ for silicon have not been found, but a value of $-0.02$ can be calculated from piezo-birefringence data [95] at 2.25\,\mu m, in strong disagreement with the value of 0.22 calculated from the model. Values of $p_{11}$ and $p_{12}$ of respectively $-0.101$ and 0.0094 have also been calculated [96] from piezo-optic data recorded at 1.15\,\mu m [97], again in disagreement with the values calculated here. The reason for this large difference is not clear. However, given the reasonable agreement with $p_{11}$ for silicon at 10.6\,\mu m and both $p_{11}$ and $p_{12}$ for germanium, the model will be assumed correct.

### 2.3 The Strain-Induced Shift of the Absorption Band-Edge

The intrinsic absorption $\alpha_i(E)$ at an energy $E$ in a crystal is a function of the extinction coefficient $k(E)$ and is given by [77]

\[ \alpha_i(E) = \frac{4\pi E}{hc} k(E) \] (2.16)

where $h$ is Planck’s constant and $c$ is the velocity of light in a vacuum. In this calculation, however, there is no integration across the energy spectrum, as there is when using the Kramers-Krönig relations, so the linear interpolation of the extinction coefficients cannot be used.

Instead, it has been shown by Macfarlane and Roberts [102, 103] that the absorption of silicon and germanium can be well represented at low levels by a law of the form

\[ \alpha_i(E_{ph}) = A \left[ \frac{(h\nu - E_g + k\theta)^2}{e^{\theta/T} - 1} + \frac{(h\nu - E_g - k\theta)^2}{1 - e^{-\theta/T}} \right] \] (2.17)
where $E_{ph}$ is the photon energy, $E_g$ is the material bandgap, $k\theta$ is the energy characteristic of a phonon required in a transition across the indirect minimum bandgap, and $\theta$ is the equivalent temperature of the phonon, which equals the phonon energy divided by Boltzmann’s constant $k$. $A$ is a proportionality factor representing the probability of the emission and absorption of phonons. At energies below the minimum bandgap the material becomes transparent and the absorption can be very low, as demonstrated by the low loss waveguides in table 1.1. However, there can be considerable losses even in the transparent region due to free carriers and poor crystal quality.

Equation 2.17 gives the probability of a phonon absorption at energies above $E_g - k\theta$, given by the first term, and the probability of a phonon emission above $E_g + k\theta$, given by the second term. By fitting the equation to room temperature absorption data from Braunstein et al. [80] for bulk silicon and Si$_{957}$Ge$_{043}$, values of $A$ of respectively 3750 and 3250 were found to represent the data accurately.

Assuming that the absorption is given by the minimum bandgap, equation 2.17 can now be modified to account for the strain-induced shifts in the energy gaps. Figure 2.4 presents the calculated absorption of bulk silicon and Si$_{957}$Ge$_{043}$. The unstrained values correspond to the experimental data from Braunstein et al. [80], using their value of phonon equivalent temperature $\theta$ of 550K. In addition, the absorption is given for assumed uniaxial stresses of $10^9$ and $10^{10}$ dyn/cm$^2$, applied along the [100] direction. According to equation 2.15, this will set up strains of the order of 0.001-0.01. It will be shown later that strains of this magnitude can occur in photoelastic waveguides, indicating that the stress-induced shift of the absorption band edge can be significant. The stresses and strains in photoelastic waveguides will be investigated further in chapter 3, and their effect on the absorption will be investigated in more detail in section 3.2.2.

For bulk silicon, the absorption at 1.15$\mu$m, indicated by a vertical line in figure 2.4, is about 0.88/cm, or about 3.9 dB/cm in terms of waveguide losses. Practically, this means that the losses at 1.15$\mu$m will be at least 3.9 dB/cm above those at longer wavelengths, where there will be practically no phonon-assisted absorption. Due to the stresses in the photoelastic waveguides, this difference will be even greater, and will be considered further in section 3.2.2.

### 2.4 Free-Carrier Absorption

In addition to the phonon-assisted absorption close to the band edge, the losses generated by free carriers in the crystal may be significant and should be determined.

The materials used in this project are p-type silicon with an impurity concentration of less than $3 \cdot 10^{15}$/cm$^3$ and p-type Si$_{957}$Ge$_{043}$ with less than $6 \cdot 10^{14}$/cm$^3$. For p-type materials, the free carrier absorption $\alpha_{fc}$ is found as a function of free holes $N_h$ from [104]:

$$\alpha_{fc} = \frac{q^3 \lambda^2 N_h}{4\pi^2 c^3 \epsilon_0 \mu_h}$$  \hspace{1cm} (2.18)

where $q$ is the electronic charge, $\lambda$ is the wavelength of light, $c$ is the velocity of light in a vacuum, $\epsilon_0$ is the permittivity in a vacuum, $n$ is the refractive index, $m_h$ is the effective mass of the holes, and $\mu_h$ is the hole mobility. All physical constants are listed in appendix B.

Using an effective carrier mass for holes of $m_h = 0.16m_0$ [105], the absorption for silicon becomes respectively 0.005/cm and 0.009/cm at wavelengths of 1.15$\mu$m and 1.523$\mu$m. For
Figure 2.4 Square root of absorption vs photon energy for bulk silicon and Si$_{0.957}$Ge$_{0.043}$. The solid lines show the phonon-assisted absorption for unstrained crystals in the region around $1.15\mu$m, indicated by a thin vertical line. The dot-dashed and dashed lines refer to applied stresses of $10^9$ and $10^{10}$ dyn/cm$^2$, respectively.

Si$_{0.987}$Ge$_{0.013}$, the material properties will be marginally different, but with only a fifth of the impurity concentration, the free carrier induced losses will be even less.

2.5 Summary

This chapter presents a refractive index model, using the strain-induced shifts in the energy band structure to modify the experimental extinction coefficient data of silicon and germanium, from which the strain-induced refractive index changes are found from the Kramers-Krönig relations. The photoelastic constants $p_{11}$ and $p_{12}$, giving the change in refractive index with strain, have been calculated for several Si$_{1-x}$Ge$_x$ alloys, showing that they are similar in magnitude, and both lie in the range 0.36-0.51 for Si$_{1-x}$Ge$_x$ alloys of germanium content $x$ up to 10%.

The calculated photoelastic constants were compared to published experimental data. With the assumption that the published data did not consider the effect of transverse strains generated by a uniaxial stress, a reasonable correlation was found for all the constants, apart from the $p_{12}$ for silicon. In chapter 3 the calculated photoelastic constants are used to model the refractive index profiles and the optical modes of photoelastic waveguides in bulk silicon and Si$_{1-x}$Ge$_x$/Si heterostructures. It will be shown that a difference in sign or a significant difference in magnitude between $p_{11}$ and $p_{12}$ will strongly affect the predicted refractive index and modal pattern of the waveguide. In chapter 5, photoelastic waveguides in bulk silicon and Si$_{1-x}$Ge$_x$/Si heterostructures will be investigated experimentally and compared to the modal patterns predicted by modelling, which will give a good estimation of the correctness of the calculated photoelastic constants.

The absorption level around the minimum bandgap energy was calculated for bulk
silicon and bulk Si$_{0.957}$Ge$_{0.043}$, predicting that the optical losses around 1.15μm will be at least 3.9dB/cm above those at 1.523μm. Similar calculations have been made previously for bulk (unstrained) Si$_{1-x}$Ge$_x$ alloys [80, 63]. In chapter 3, the effect of strain is included in the absorption calculation, showing that the strain-induced changes in the energy band structure can significantly affect the optical losses around the band-edge energy.
Chapter 3

Modelling of Strain, Refractive Index and Optical Mode Patterns in Photoelastic Waveguides

In photoelastic waveguides, the guiding regions are produced by introducing strain into the structure to locally modify the refractive index. The strain is generated here by depositing a SiNy stressor stripe onto a planar waveguide structure of bulk silicon or a Si$_{1-x}$Ge$_x$/Si heterostructure. This chapter investigates these strains and the corresponding strain-induced refractive index profiles, as well as the optical mode profiles of the waveguides.

The waveguide structures are as shown in figure 3.1, where the main design variables are the stressor stripe width, height and deposition temperature, and the Si$_{1-x}$Ge$_x$ layer thickness and germanium content. The strain profiles in the waveguides are made up from the thermal and lattice mismatch between the Si$_{1-x}$Ge$_x$ layer and Si substrate, and the thermal mismatch strains generated around the edges of the deposited stripe. These strains will be referred to in the following investigations as substrate thermal strains, substrate mismatch strains and stripe strains, respectively.

The strains and refractive indices are investigated by finite element analysis. While the shape and size of the guiding regions are easiest to evaluate analytically, finite element modelling allows the waveguide structure to be analysed with fewer assumptions, so that effects such as substrate bending, stress distribution and stressor edge imperfections, can be considered. Finite difference calculations are used to evaluate the optical fields, from which waveguide coupling losses and guiding characteristics are found.

3.1 Finite Element Analysis

In finite element analysis, a physical structure is divided into a number of elements, and numerical solutions to structural problems are calculated at discrete nodes within each element. This type of analysis allows investigations of physical settings where the mathematical expressions of the loads are not known.

In photoelastic waveguides, the main structural load is the stressor edge force, the effects of which can be modelled analytically. Finite element analysis is used in this project to create a more precise model of the waveguide, incorporating the joint effects of a stressor stripe and a Si$_{1-x}$Ge$_x$/Si heterojunction, while also including structural imperfections.
3.1.1 Modelling and Meshing the Waveguide Structure

The aim of the modelling is to determine the strain and strain-induced refractive index profiles in photoelastic waveguides in bulk silicon and Si_{1-x}Ge_{x}/Si heterostructures, as a function of stressor geometry and deposition temperature and Si_{1-x}Ge_{x} layer thickness and composition. ANSYS [106], a commercial finite element simulation package, is used to model the waveguide structures, using standard ANSYS functions to calculate the strains. Using the ANSYS Parametric Design Language, a macro program is written to access these strains and calculate the strain-induced refractive index change for each element. The refractive indices are output in a matrix form from which optical fields are found from finite difference calculations as presented in section 3.4.

The waveguide was modelled in ANSYS for the strain calculations as a two-dimensional structure with a geometry and directions as shown in figure 3.1. Mechanical properties, as presented in table 3.1, were specified for each layer. All mechanical data (thermal expansion coefficient, Poisson's ratio, Young's Modulus) were based on experimental data, and were assumed isotropic. Subsequently, the model was split up into a mesh of elements, as shown in figure 3.2, with elements of size 0.5μm by 0.5μm around the stressor stripe, where the strain changes are greatest, and increasing in size towards the bottom of the substrate. Around the edges of the stripe, due to the great stresses and strain changes,
Figure 3.2 Finite element mesh for the structural analysis of the photoelastic waveguides. The model includes a substrate of 500μm by 400μm, and a guiding layer of thickness up to 8μm, which can be modelled as any Si_{1-x}Ge_{x} alloy or bulk silicon. In the area around the stressor stripe, the elements are all of size 0.5μm by 0.5μm, apart from very close to the stressor edge, where they are as small as 0.25μm by 0.25μm. The stressor stripe pictured in this particular mesh is 9μm wide and 1μm thick.

The mesh was made even finer, with elements as small as 0.25μm, to improve the accuracy of the results. This meshing into elements introduces a structural quantising error, which is calculated by ANSYS, and lies between 1.8% and 2.4% for the main part of the guiding region for all cases investigated with the model. Without the additional meshing at the stripe edge, the quantising error can be up to 5% higher.

A 400μm thick and 500μm wide substrate is included in the model to determine the effect of the silicon substrate on the strain profile in the structure. Earlier work on Si_{1-x}Ge_{x}/Si heterojunctions has assumed a rigid substrate [107], which essentially replaces the substrate with forces along the Si_{1-x}Ge_{x}/Si interface. However, since the Si_{1-x}Ge_{x} layer modelled here contains only a few per cent germanium, its mechanical properties are very similar to that of pure silicon so that any strain between the Si_{1-x}Ge_{x} and Si will be distributed into both materials in the vicinity of the junction. A model incorporating the physical effects of the substrate is therefore a more realistic representation than the rigid substrate approximation used previously.

Figure 3.2 represents a slice through the structure somewhere along the waveguide,
Table 3.1 Mechanical data used in the strain calculations. Young's Modulus $E$, Poisson's ratio $\nu$, thermal expansion coefficient $\alpha$ and lattice constant $a$ are based upon experimental data. All assumptions and references are presented in appendix A. A linear interpolation of the silicon and germanium bulk data is used for the Si$_{1-x}$Ge$_x$ alloy values.

<table>
<thead>
<tr>
<th></th>
<th>Si</th>
<th>Si$<em>{0.98}$Ge$</em>{0.013}$</th>
<th>Si$<em>{0.95}$Ge$</em>{0.05}$</th>
<th>Si$<em>{0.90}$Ge$</em>{0.10}$</th>
<th>Ge</th>
<th>SiN$_x$</th>
<th>Unit</th>
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</thead>
<tbody>
<tr>
<td>$E$</td>
<td>1.30</td>
<td>1.30</td>
<td>1.29</td>
<td>1.27</td>
<td>1.02</td>
<td>0.913</td>
<td>10$^{12}$ dyne/cm$^2$</td>
</tr>
<tr>
<td>$\nu$</td>
<td>0.278</td>
<td>0.278</td>
<td>0.278</td>
<td>0.278</td>
<td>0.273</td>
<td>0.17</td>
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<tr>
<td>$\alpha$</td>
<td>3.29</td>
<td>3.35</td>
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<td>3.77</td>
<td>8.12</td>
<td>1.5</td>
<td>10$^{-6}$/K</td>
</tr>
<tr>
<td>$a$</td>
<td>5.430</td>
<td>5.433</td>
<td>5.441</td>
<td>5.453</td>
<td>5.658</td>
<td></td>
<td>Å</td>
</tr>
</tbody>
</table>

where both the stripe stresses and the stripe strains in the direction of the waveguide, or the $z$-direction, are essentially zero due to the symmetry of the structure. The model is defined specifically to have plane strain and plane stress in the $xy$ plane. All stresses and strains referred to in these investigations, and all refractive index and field calculations based upon them, will therefore refer only to the $x$ and $y$ directions. Close to the facets, the stresses and strains in the $z$ direction become significant. As will be shown later, however, stress acting upon the surface of a silicon crystal will generate significant strains only about 150$\mu$m into the material. A practical waveguide, which is at least a few millimetres in length, is therefore well represented by this model.

Having modelled and meshed the structure, including material properties and stress and strain boundary conditions, ANSYS is given a temperature difference, which in most calculations here will be from 300°C to room temperature, to simulate the sample cooling down after deposition. Using the specified thermal expansion coefficient for each material, a thermal mismatch is found at the material interfaces, with a corresponding displacement throughout the structure, which is calculated at eight points within each element. From the displacements, ANSYS calculates the stresses and strains, the results of which are presented later in the chapter.

In calculating the strains, it is assumed that the crystals remain strained, and that there is no relaxation along the junctions. By modelling a Si$_{1-x}$Ge$_x$ layer thickness of $<8\mu$m and a germanium content of $<10\%$, the Si$_{1-x}$Ge$_x$ layer can be expected to remain strained. However, with greater Si$_{1-x}$Ge$_x$ layer thicknesses or germanium content, the mismatch at the Si$_{1-x}$Ge$_x$/Si junction will exceed the critical limit and the crystal will relax. Theoretical [65] and experimental results on strained epitaxial layers [63] support this assumption.

### 3.1.2 Substrate Strains

The substrate strains, in contrast to the stripe strains, are not well represented by this model and require some modification. Firstly, they are biaxial in nature, as they are generated by the plane stress in the Si$_{1-x}$Ge$_x$/Si heterojunction. Secondly, the greatest component of the substrate strains is the lattice mismatch which is not considered in the model.
Accounting for the Biaxial State of Stress at the Si$_{1-x}$Ge$_x$/Si Heterojunction

The substrate strains, as calculated by the model in figure 3.2, assumes a uniaxial stress along the Si$_{1-x}$Ge$_x$/Si interface. This is because a two-dimensional model simultaneously involves the essentially uniaxial stresses from the stressor stripe and the biaxial stresses at the heterojunction. The stress in the x-direction along the heterojunction must be correct, however, since it corresponds to the thermal mismatch between the Si$_{1-x}$Ge$_x$ layer and the silicon substrate. It must also equal the substrate stress in the z-direction.

For a purely uniaxial stress $\sigma_{xx}$ applied in the x-direction, the corresponding strains in the x and y directions are

$$
\varepsilon_{xx} = \frac{\sigma_{xx}}{E}, \\
\varepsilon_{yy} = \frac{-\nu\sigma_{xx}}{E}
$$

(3.1)

where $\varepsilon$ is the strain and $E$ is Young's Modulus. These are the values found by ANSYS in the two-dimensional model. For biaxial stresses in the plane of the junction, the stresses $\sigma_{xx}$ and $\sigma_{zz}$ are identical, so the strains are given by

$$
\varepsilon_{xx} = \frac{\sigma_{xx} - \nu\sigma_{zz}}{E} = \frac{(1-\nu)\sigma_{xx}}{E}, \\
\varepsilon_{yy} = \frac{-\nu(\sigma_{xx} + \sigma_{zz})}{E} = \frac{-2\nu\sigma_{xx}}{E}
$$

(3.2)

Therefore, to modify these substrate strains to account for the biaxial stress at the Si$_{1-x}$Ge$_x$/Si heterojunction, they need only be scaled by factors of $(1 - \nu)$ and 2, respectively. Since the Si$_{1-x}$Ge$_x$ layer is only a few microns thick, the substrate strains are virtually constant throughout the layer, so the scaling takes the form of a linear shift of the strains. The stripe strains overlay the substrate strains according to the superposition principle, and are not affected by a linear shift of the substrate strains.

Lattice Mismatch Strains

ANSYS is not set up to calculate the lattice mismatch between the Si$_{1-x}$Ge$_x$ layer and the silicon substrate, but it can calculate thermal stresses, given a thermal expansion coefficient for each material and an assumed temperature difference. The lattice mismatch can then be accounted for by adding a dummy thermal expansion coefficient to the Si$_{1-x}$Ge$_x$ layer.

The Si$_{1-x}$Ge$_x$ layer is grown at an elevated temperature, and therefore it will have both a thermal and a lattice mismatch. Assuming a rigid silicon substrate, the strain $\varepsilon_{lattice}$ required to match the Si$_{1-x}$Ge$_x$ layer to the silicon lattice is found from

$$
a_{Si}(1 + \alpha_{Si}\Delta t) = a_{SiGe}(1 + \alpha_{SiGe}\Delta t)(1 + \varepsilon_{lattice})
$$

(3.3)

and

$$
\varepsilon_{lattice} = \frac{a_{Si}(1 + \alpha_{Si}\Delta t)}{a_{SiGe}(1 + \alpha_{SiGe}\Delta t)} - 1
$$

(3.4)

where $\Delta t$ is the difference between growth and room temperature, $a_{Si}$ and $a_{SiGe}$ are the lattice constants at room temperature, and $\alpha_{Si}$ and $\alpha_{SiGe}$ are the thermal expansion coefficients for Si and Si$_{1-x}$Ge$_x$, respectively. Notice that while the thermal expansion
coefficients are actually functions of temperature, their average values are used throughout this project.

Using the lattice constants and thermal expansion coefficients listed in table 3.1, it is found that the thermal effects account for no more than about 5% of the lattice mismatch strain. By representing the strain $\varepsilon_{\text{lattice}}$ as a thermal expansion $\alpha_{\text{lattice}} \Delta t$, the strain at room temperature becomes

$$\text{Total strain} = \alpha_{\text{lattice}} \Delta t + (\alpha_{\text{SiGe}} - \alpha_{\text{Si}}) \Delta t$$  (3.5)

Although this value of strain is based on the assumption of a rigid substrate, it gives a good approximation to the mismatch at the heterojunction. When modifying the thermal expansion coefficient in the model, ANSYS will only see a thermal mismatch at the heterojunction, and the strains will be calculated correctly into both the silicon and the Si$_{1-x}$Ge$_x$ layer. It is found from equations 3.4 and 3.5 that the real thermal mismatch is opposite in sense to the lattice mismatch, so the calculated strain in the Si$_{1-x}$Ge$_x$ layer will be slightly less than that due to the lattice mismatch.

To account for the lattice mismatch, $\alpha_{\text{lattice}}$ is added to the Si$_{1-x}$Ge$_x$ thermal expansion coefficient. However, to prevent a gross overestimate of the stripe strains, $\alpha_{\text{lattice}}$ must also be added to the thermal expansion coefficient of the stripe. In this way, the difference in thermal expansion remains the same between the Si$_{1-x}$Ge$_x$ and the stripe.

### 3.2 Strain Profiles in Photoelastic Waveguides

The strains in the photoelastic waveguides investigated here comprise of the substrate strains, which are due to the lattice and thermal mismatch at the Si$_{1-x}$Ge$_x$/Si heterojunction, and the stripe strains, which are due to the thermal mismatch between the Si$_{1-x}$Ge$_x$ and Si$_N$ layers. These two categories of strain are different in nature in that the substrate strains are approximately constant along the guiding layer in all directions, while singularities occur at the edges of the Si$_N$ stripe, which result in significant strain variation around the stripe edges. The shape and size of the guiding regions will therefore depend upon the stripe strains, while the substrate strains may be considered to represent a 'background level' which changes with the germanium content of the Si$_{1-x}$Ge$_x$ layer.

This section discusses the characteristics of these strains and examines the effects of the waveguide geometry, Si$_{1-x}$Ge$_x$ composition and deposition temperature, starting with an analysis of a simple stressor stripe on a bulk silicon substrate.

#### 3.2.1 Silicon Waveguides

The waveguide structure, as shown in figure 3.2, is modelled in ANSYS with plane stress as well as plane strain in the xy plane, so that all stresses and strains in the direction of the waveguide are zero. Figure 3.3 presents the strains in the lateral (x) and vertical (y) directions for bulk silicon photoelastic waveguides of different stripe widths. It is seen that there are characteristic strain profiles focussed around the stripe edges which do not change much with stripe width but which are significantly different in the x and y directions.

The strain profiles are given for the same absolute strain values for all plots, illustrating that as the stripe width becomes narrower, the strain changes become increasingly steep. For a waveguide with a 3$\mu$m wide stripe, figure 3.3 shows that the lateral strain regions
Lateral (x) strains | Vertical (y) strains
---|---

Figure 3.3 Strains in bulk silicon photoelastic waveguides as calculated by ANSYS from the model in figure 3.2. The strains are plotted for stripe widths of 3μm (top), 6μm (middle) and 9μm (bottom), showing that the characteristic strain profiles around the stripe edges do not change much with stripe width, but they are significantly different for the lateral (x) and vertical (y) directions. Contour lines are plotted for strains from \(-3\times10^{-5}\) to \(3\times10^{-5}\), in steps of \(0.5\times10^{-5}\). Negative or compressive strains are presented as thin contours. The box around the plots, which does not represent any physical boundary, corresponds to the middle 32μm section of the top 8μm of the top of the silicon. All cases are calculated for a 0.5 μm thick SiNx stressor stripe deposited at 300°C.

extend about 4μm beyond the stripe. There are regions of lower strain, of the same shape and size as those plotted for the wider stressor stripes. The strain regions outside the stripe edges therefore only change in magnitude, and not in shape, in contrast to the middle region, where the strain maximum moves upwards with decreasing stripe width, becoming increasingly confined, which is particularly apparent for the vertical strains.

The maximum strains in figure 3.3 do not seem to be quite coincident with the edges of the stressor stripes drawn on top of the plots. There are increasingly small regions of higher strains which focus around the stripe edges. These regions have not been included in figure 3.3 for the sake of clarity, but they have been considered when calculating the strain-induced refractive index changes and the optical field profiles later in this chapter.

It is useful at this point to consider the analytical expressions for stresses generated by an ideal concentrated load line acting on the silicon surface, as shown in figure 3.4. According to Durelli et al. [108], the stresses \(\sigma\) in the x and y directions due to an applied force \(F\) are given by

\[
\sigma_{xx} = -\frac{2F}{\pi} \frac{x^3}{(x^2 + y^2)^{3/2}}
\]

\[(3.6)\]
Figure 3.4 Comparison of strains calculated by ANSYS and by the analytical expressions. Both figures show the lateral strains generated by a 4μm wide stressor stripe. In the analytical model the edge forces, indicated here as arrows pointing outwards from the stripe edges, are assumed to be represented by two perfect load lines, which gives an answer fairly similar to ANSYS. There are small differences in the strains in the region underneath the stripe, which cannot be changed by varying the edge force F. These differences represent the fact that the stripe edges, when the material compliance is considered, do not represent perfect load lines. The boxes around the plots represent the top 4μm of the middle 32μm of the silicon waveguide, and the stressor modelled in ANSYS is a 1μm thick SiNx stripe. Notice that the vertical scale has been stretched to present the stresses more clearly.

\[ \sigma_{yy} = -\frac{2F}{\pi} \frac{xy^2}{(x^2 + y^2)^2} \]  

(3.7)

with corresponding strains

\[ \varepsilon_{xx} = \frac{\sigma_{xx} - \nu \sigma_{yy}}{E} \]  

(3.8)

\[ \varepsilon_{yy} = \frac{\sigma_{yy} - \nu \sigma_{xx}}{E} \]  

(3.9)

where \( E \) is Young’s Modulus and \( \nu \) is Poisson’s ratio. In figure 3.4, the strains in the x direction for a 4μm wide stripe on bulk silicon, as calculated by ANSYS, are presented together with the strains found from equations 3.6 through 3.8, assuming load lines as shown coinciding with each of the stripe edges. The two sets of strain profiles are similar in shape, indicating that the assumption used by Kirkby et al. [55] and Benson et al. [58], that the stripe stresses can be seen as a load line at each stripe edge, is good. However, according to equations 3.6 and 3.7, the only variable affecting the stresses, and therefore also the strains, is the edge force \( F \). For any given stripe width, the strain profiles are therefore constant, and can only change in magnitude. The difference between the two models seen in the region under the middle of the stripe will therefore not change with the edge force.

The similarity in the strain profiles generated by the ANSYS model and the analytical expressions indicate that the stresses are generated by the stripe edges, while the difference between the stress profiles indicates that the edge force is not an ideal load line. Since the stressor has a finite thickness, it makes sense that the generated edge force is not actually focussed into a line, but rather that it is distributed within the edge region, as a function of stressor thickness and edge angle. It is therefore appropriate in this project to consider...
whether the stripe thickness and edge angle has any significant effect on the strain profiles. ANSYS is an appropriate tool for this investigation, since the stripe geometry can easily be changed, and accurate numerical results can be found without knowing the analytical form of the stress and strain distributions.

Variations in the Stressor Stripe Geometry

The stressor stripes investigated in this project will be defined from deposited SiNy films using standard photolithography and wet etching, as explained in section 4.2. Practically, when etching the stripes, the photoresist pattern may be undercut, so the stripe edge will slant inwards or outwards, which may have an effect on the edge force.

The model in figure 3.2 is again used to calculate the strains in the waveguide structure for stressor stripes with edges at an angle. Apart from the change in the stripe, all modelling parameters remain as before. Assuming a temperature reduction from 300°C to 20°C, and varying the angle of the stripe edge from -70° to +70°, the lateral strains vary as shown in figure 3.5.

It is seen that these fairly large changes in the edge angle have only a marginal effect on the strain profiles, which are given for the same absolute strain values in all the plots. By close inspection, the strain regions outside the stripe edges are found to grow very slightly as the edge slopes outwards, showing that the mechanical strength of the stripe improves around the edges, and so increases the edge force slightly. Conversely, as the edges slope inwards, as shown in the top plot of figure 3.5, there is a slight spread between the contours just underneath the stripe edges, showing that the edge force becomes less confined. However, the overall effect of the edge angle on the strain profiles is minimal, so that the results from the model in figure 3.2 will be assumed to represent the sample well, even for samples where the edge has been etched at an angle.

An increase in the stripe thickness, on the other hand, will increase its mechanical strength, and the edge force and all strains and stresses increase accordingly. For the waveguide modelled in figure 3.5, an increase in the stripe thickness from 0.5μm to 1.0μm has little effect on the shape of the profiles, apart from increasing the strains by a factor of around 1.55.

The Effect of Deposition Temperature

The strains induced by the stressor stripe are all thermal mismatch strains. For a stressor film with a thermal expansion coefficient $\alpha_{SiN}$, a temperature difference of $\Delta t$ will induce a linear thermal expansion in the film of $\alpha_{SiN}\Delta t$. Similarly, a silicon layer of thermal expansion coefficient $\alpha_{Si}$, will expand by $\alpha_{Si}\Delta t$. For a SiNy stressor film deposited onto a silicon substrate, the strain $\varepsilon$ needed in the stressor film to match it to the silicon is

$$
\varepsilon = \frac{(1 + \alpha_{Si}\Delta t)(1 + \varepsilon) - (1 + \alpha_{SiN}\Delta t)}{(1 + \alpha_{SiN}\Delta t)}
$$

$$(\alpha_{Si} - \alpha_{SiN})\Delta t
$$

This mismatch strain, depending on the waveguide geometry and the relative material strengths, gives rise to the edge forces generated by stressor stripes made from the SiNy film.
Figure 3.5 Lateral (x) strains in bulk silicon waveguides, showing the effect of varying the angle of the stressor stripe edge. By varying the stressor edge angle from 70° inwards sloping, shown in the top plot, to 70° outwards sloping, as shown in the bottom plot, the effect on the strains is seen to be marginal. Contour lines are plotted for strains from $-3 \times 10^{-5}$ to $3 \times 10^{-5}$, in steps of $0.5 \times 10^{-5}$. Negative or compressive strains are presented as thin contours. The box around the plots, which does not represent any physical boundary, corresponds to the middle $32\mu m$ section of the top $8\mu m$ of the top of the silicon. All cases are calculated for a $0.5 \mu m$ thick SiN$_y$ stressor stripe deposited at $300^\circ C$.

film, which in turn generate the stress and strain profiles presented in this chapter. From equation 3.10 the mismatch is seen to increase nearly linearly with the change in temperature, which also implies a near linear increase in the edge force and in all the induced strains and stresses. It should be noted that the thermal expansion coefficients are functions of temperature, but constant average values have been used for all calculations in this project.

It is important at this point to consider the inherent assumptions in the modelling, and to see whether they are appropriate to characterise the performance of a real waveguide. Three of these assumptions could be significantly different for the model and real samples, and are listed below.

1. **Adhesion at the material interface.** In the ANSYS model, the materials are defined to be in perfect contact at some starting 'deposition' temperature, and the structure then cools to $20^\circ C$, with no relaxation considered at the material interface. It is not certain that the deposited stressor film adheres perfectly to the silicon, nor
is it given that the material properties during the deposition and cooling of the film are well represented by the constant stiffness and thermal expansion values used in ANSYS. Also, for some temperature difference, $\Delta t$, the stresses at the material interface will be become excessive, resulting in relaxation along the interface.

2. **Annealing effects.** After deposition of the stressor film, annealing the structure at higher temperatures could be a useful method to increase the thermal mismatch, and so increase all induced strains. Whether or not this is possible depends on whether the stressor film regrows at the annealing temperature. The annealing may also affect the mechanical properties of the stressor layer, which may further change the level of the strain. An understanding of the effects of annealing on the stressor film is useful even when it is not required for the waveguides themselves, because the waveguides will eventually be integrated with other optical circuitry, some of which is likely to need annealing during fabrication.

3. **Intrinsic stress at the material interface.** The modelling and discussion so far has only considered the thermal mismatch between the stressor and the silicon, and this effect will always be present. However, it is well known that there may be a significant amount of 'inherent' stress in the stressor film, depending on the various deposition parameters, which may or may not be affected by subsequent annealing [70, 109].

While according to modelling, all stresses and strains induced by the stressor stripe will increase nearly linearly with increasing deposition temperature, the real physical effects need to be investigated experimentally. In chapters 4 and 5, the stressor films used in this project are investigated by interferometric measurements, showing the effect of film thickness and annealing on the induced stress and strain.

3.2.2 **Si$_{1-x}$Ge$_x$ Photoelastic Waveguides**

The Si$_{1-x}$Ge$_x$ photoelastic waveguides are essentially the same as the bulk silicon structures in terms of the stripe strains. In addition to the stripe strains, there are the thermal and lattice mismatch strains, or substrate strains, due to the Si$_{1-x}$Ge$_x$/Si heterojunction, which are constant everywhere in the plane of the junction. Since the Si$_{1-x}$Ge$_x$ layer is very thin, of the order of a few microns, the substrate strains are also virtually constant in the vertical (y) direction. As mentioned in section 3.1.2, the substrate strains are mostly lattice mismatch strains, and are therefore not a strong function of temperature.

Figure 3.6 shows the lateral (x) strains in a 4$\mu$m thick Si$_{0.987}$Ge$_{0.013}$ layer on silicon, without a stressor layer, drawn through the Si$_{1-x}$Ge$_x$ layer and into the substrate. The change in strain level through the Si$_{1-x}$Ge$_x$ layer was calculated to be about 0.05% using ANSYS, which is virtually constant. The strain at the top of the silicon substrate is only about 5% of that seen in the Si$_{1-x}$Ge$_x$ layer, but it decays slowly into the substrate, and reaches zero after about 150$\mu$m, taking up much of the strain energy $^1$ from the junction. With a rigid substrate, the strain in the Si$_{1-x}$Ge$_x$ layer would be -0.055% according to equation 3.5, rather than the -0.035% found by ANSYS. Therefore, even if the absolute value of strain in the substrate is very low, the substrate does consume about a third of the total strain energy. For Si$_{1-x}$Ge$_x$/Si heterojunctions of germanium content x in the

$^1$The strain energy is the work needed to produce a given level of strain [68].
The substrate strains due to the thermal and lattice mismatch at the Si$_{1-x}$Ge$_x$/Si heterojunction calculated by ANSYS are about two thirds of the value calculated for a rigid substrate. Assuming a rigid silicon substrate, the lateral strains in a Si$_{0.987}$Ge$_{0.013}$ layer should be around -0.055%, but is found to be only -0.035% for a 4µm thick layer, with the rest taken up by the substrate. While the substrate strain is only 0.0017% at the interface, it reaches zero strain only after about 150µm, and takes up a considerable amount of strain energy.

Figure 3.6 The substrate strains due to the thermal and lattice mismatch at the Si$_{1-x}$Ge$_x$/Si heterojunction calculated by ANSYS are about two thirds of the value found from equation 3.5. This is also the case for the strains in the y and z directions.

These results show that the strains in the Si$_{1-x}$Ge$_x$ layer are virtually constant throughout the layer, which was a requirement for the corrections made to the substrate strains, as explained in section 3.1.2. Also, the substrate strains decay to zero after about 150µm, suggesting that the ANSYS model can correctly assume that there are no stresses or strains in the z direction, apart from in the 150µm regions next to the facets, where the model becomes increasingly inaccurate.

The compound strains in photoelastic waveguides in Si$_{1-x}$Ge$_x$/Si heterojunctions are similar to those in bulk silicon with respect to the stripe strains, while they are shifted by a virtually constant level of strain induced by the heterojunction. Using equation 2.12 and photoelastic constants from table 2.3, it is found that the total strain-induced refractive index shift in the Si$_{1-x}$Ge$_x$ layer and the top of the silicon substrate will never exceed more than about 2.5% of the refractive index step at the Si$_{1-x}$Ge$_x$/Si junction. The substrate strains therefore have a negligible effect on the waveguide confinement. However, they may have a considerable effect on the position of the absorption band-edge, as considered in section 2.3, which will affect the waveguide propagation losses around 1.15µm.

It is seen from figure 3.3 that for a 0.5µm thick stressor stripe deposited at 300°C the stripe strains do not exceed -3 · 10^{-5}, apart from very close to the stripe edge. Even for a 700°C deposition temperature, this is only 20% of the substrate strains in a Si$_{0.987}$Ge$_{0.013}$ layer grown on silicon. For Si$_{1-x}$Ge$_x$ layers with a germanium content of 1.3% or greater, the strain-induced shift of the absorption band-edge in most of the structure can therefore be approximated by the substrate strains only. Figure 3.7 presents the phonon-assisted losses at 1.15µm photon wavelength calculated from equation 2.17 for different Si$_{1-x}$Ge$_x$ alloys, showing that the strain can add considerably to the absorption level. A linear interpolation and extrapolation of the bandgap data for bulk silicon and Si$_{0.957}$Ge$_{0.043}$ from Braunstein et al. [80] were used in finding the losses.
Figure 3.7 Strain-Induced Shifts in the Absorption Band-Edge at 1.15μm, corresponding to the substrate strains calculated by ANSYS. The unstrained or bulk absorption values are plotted as rings, and the strained values are plotted as diamonds. For a Si₀.₉₇Ge₀.₀₁₃ layer grown on silicon the losses increase from 4.9dB/cm to 5.9dB/cm due to the substrate strains, while for higher germanium contents, both the bulk losses and the strain-induced losses grow substantially, making them rather unsuitable for waveguiding at this wavelength.

3.3 Refractive Index Profiles

In photoelastic waveguides in bulk silicon, the dielectric confinement is due to the strain-induced refractive index change and the dielectric boundary at the silicon/air interface. Photoelastic waveguides within Si₁₋ₓGeₓ/Si heterostructures have the additional confinement due to the Si₁₋ₓGeₓ/Si dielectric boundary.

3.3.1 Pure Photoelastic Confinement in Bulk Silicon Waveguides

Given a strain tensor defined as in figure 1.8, the photoelastic contribution to the refractive index is given by equations 2.12 through 2.14. For a photoelastic waveguide oriented as shown in figure 3.1, where the stressor stripe is oriented along the [100] axis on a (100) substrate, the strains in the direction of the waveguide are zero in most of the structure, and the refractive index profiles in the x and y directions are therefore given by

\[ \Delta n_x = -\frac{n_0^3}{2} \Delta B_{xx} = -\frac{n_0^3}{2} (\varepsilon_{xx} p_{11} + \varepsilon_{yy} p_{12}) \] (3.11)

\[ \Delta n_y = -\frac{n_0^3}{2} \Delta B_{yy} = -\frac{n_0^3}{2} (\varepsilon_{xx} p_{12} + \varepsilon_{yy} p_{11}) \] (3.12)

While the strain profiles are significantly different in the x and y directions, the photoelastic constants \( p_{11} \) and \( p_{12} \) according to table 2.3 are similar in magnitude, predicting
It is seen that the refractive index in the lateral and vertical directions are very similar, predicting a low degree of birefringence. The box around the plots, which does not represent any physical boundary, corresponds to the middle 32 µm section of the top 8 µm of the top of the silicon. All cases are calculated for a 0.5 µm thick SiNy stressor stripe deposited at 300°C.

Photoelastic waveguides have been reported by Yu et al. [60] in a silicon-based structure with significant birefringence. However, they were oriented with the stressor stripe along the [110] direction, which has different photoelastic characteristics to the [100] direction. If the x and z axes for the waveguide in figure 3.1 were rotated by 45° towards the [110] crystallographic direction the refractive indices would be [55, 68]

\[
\Delta n_x = -\frac{n_0^3}{2}(\varepsilon_{xx}P_{11} + \varepsilon_{yy}P_{12}) + \varepsilon_{yy}P_{11}
\]

\[
\Delta n_y = -\frac{n_0^3}{2}(\varepsilon_{xx}P_{12} + \varepsilon_{yy}P_{12})
\]

Yu et al. [60] calculated the refractive index profiles in their waveguide structures using values of the photoelastic constants $P_{11}$, $P_{12}$ and $P_{44}$ of -0.101, 0.0994 and -0.051, respectively. The calculations show a strong birefringence, in accordance with measurements. Using these values of photoelastic constants the refractive index profiles in the
Lateral (x) Refractive Index Profiles

Vertical (y) Refractive Index Profiles

Figure 3.9 Refractive index profiles in bulk silicon photoelastic waveguides oriented along the [110] direction for a 6μm wide stressor stripe with the same strains as in figure 3.3. Negative refractive index changes are shown as thin lines. The box around the plots corresponds to the middle 32μm section of the top 8μm of the top of the silicon. These profiles were calculated with the photoelastic constants used by Yu et al. [60], and are seen to be highly birefringent, in correspondence with waveguide measurements. However, these photoelastic constants also predict strong birefringence for photoelastic waveguides oriented along the [100] direction.

lateral (x) and vertical (y) directions for a waveguide with a 6μm wide stripe with the same strains as in figure 3.3 are as shown in figure 3.9. The lateral refractive index profiles are now significantly different from in figure 3.8. However, with these photoelastic constants, the calculated refractive index profiles for waveguides oriented along the [100] axis also show strong birefringence. This is because this value of $p_{11}$ is much greater in magnitude than $p_{12}$, making the lateral refractive index profiles similar in shape to the lateral strains, and the vertical refractive index profiles similar to the vertical strains, as given by equations 3.11 and 3.12.

The refractive index profiles predicted using the photoelastic constants calculated in chapter 2 are distinctly different from those found with the photoelastic constants used by Yu et al. [60]. This difference will be referred to when evaluating the experimental results in chapter 5, since the sign and relative magnitude of the photoelastic constants will define the guiding regions and birefringence of the waveguides, giving an indication of the real values of the photoelastic constants. However, the constants calculated in chapter 2 will be assumed correct for the further analysis in this chapter.

The Effect of Stressor Stripe Geometry and Deposition Temperature

Figure 3.8 shows that the contours corresponding to a given level of refractive index change become larger with increasing stripe width. This trend reflects the overlap of the strains generated by the two stripe edges, which becomes negligible for further increases in the stripe width.

In figure 3.10(a), the lateral (x) refractive index in the vicinity of the stressor edge is plotted at a depth of 1μm, for stressor stripes of widths from 3μm to 18μm. The horizontal scale has been shifted such that the maxima of the curves coincide, and the value 0 corresponds to the point directly below the stressor edge. Each curve represents an increase in stripe width of 3μm, showing that increases in stripe width of more than about 9μm have very little effect on the refractive index. Figure 3.10(b) presents the same refractive indices plotted vertically through the structure 0.5μm outside the stripe edge, corresponding to the maximum in figure 3.10(a).

A change in deposition temperature, on the other hand, should give a nearly linear change in the edge force and the corresponding strains, which will increase the refractive
Figure 3.10 Lateral (x) refractive index under the right edge of the stressor stripe. Figure (a) shows the refractive index plotted horizontally at a depth of 1μm, for stripe widths of 3μm to 18μm, in steps of 3μm. The plots have been adjusted so that 0 corresponds to the point just under the stripe edge for all the curves. In figure (b), the same refractive indices are plotted vertically through the structure 0.5μm outside the stripe. Both graphs show a gradually smaller increase in refractive index with increasing stripe width. Notice that very close to the stripe edge, there are refractive index changes of several times 0.001, but these values are only seen in a very limited region.

index changes linearly, according to equations 3.11 and 3.12. Figure 3.11(a) shows the lateral refractive index in the vicinity of the stressor edge plotted at a depth of 1μm, corresponding to figure 3.10(a), for a 3μm wide stressor stripe deposited at temperatures of 300°C to 700°C, showing a practically linear increase with deposition temperature. Figure 3.11(b) shows the same refractive indices plotted vertically through the structure 0.5μm outside the stripe edge, corresponding to the maximum in figure 3.11(a). In a real waveguide the strains depend on the adhesion at the stressor/silicon interface, intrinsic interface stress and may be affected by annealing, as mentioned in section 3.2.1, giving the refractive indices a different thermal response than predicted in figure 3.11. The experimental investigation of stressor films and waveguides in chapter 5 will determine how well the waveguides follow the response indicated in figure 3.11.

3.3.2 Guiding Regions in Various Structures

In the refractive index plots in figure 3.8, there is a region of high refractive index under each edge of the stressor stripe, which could be used for waveguiding if the confinement is sufficiently large. Guiding in these regions has been investigated previously in GaAs-based structures [50, 58].

For waveguides oriented along the [110] directions, figure 3.9 shows that the lateral refractive index regions at the stripe edges penetrate the structure quite deeply, and they have been used to 'clip off' a guiding region in buried planar structures [60, 69]. As evident
Refractive Index Refractive Index

![Graph (a)](image-a)

![Graph (b)](image-b)

Figure 3.11 Lateral (x) refractive index under the right edge of a 3μm wide stressor stripe, showing the effect of stressor deposition temperature. Figure (a) shows the refractive index plotted horizontally, at a depth of 1μm. In figure (b) the corresponding refractive indices are plotted vertically through the structure 0.5μm outside the stripe. Both graphs present curves for deposition temperatures of 300°, 400°, 500°, 600°, and 700°ZL.

From equations 3.6 and 3.7, it is clear that by changing the direction of the edge forces, all stresses and strains should become identical, but opposite in sense. The region of low refractive index under the stressor stripe would then be a potential guiding region. Such a change in the edge force could be made either by using a stressor material of higher thermal expansion than the guiding region or by etching a gap in the stressor layer, rather than making a stripe, as is shown in figure 3.12. Studies of the forces from stressor layers have been reported several times, but they all refer to guiding structures oriented along the [110] direction [73, 60, 55].

There are two guiding schemes which have not been investigated previously. One of them is to guide in the regions around the stressor edges without the additional confinement of a heterostructure. This would show whether photoelastic confinement on its own would be sufficient for optical guiding, which was stated in chapter 1 as one of the main aims of the project. Another possibility, which is not immediately obvious from this investigation of the refractive index profiles, is that the region of low refractive index under the centre of the stripe becomes a guiding region when the two regions at the stressor edges are subjected to a Si1−xGex/Si heterojunction. This will become clear in the following section, where finite difference calculations are used to study the optical modes of the waveguides.
3.4 Modal Intensity Profiles in Photoelastic Waveguides

Having calculated the refractive indices in section 3.3, the optical field and intensity profiles in the guiding regions can be found. With the refractive indices already stored in a matrix form, as generated by the ANSYS model, an appropriate technique for calculating the field profiles is that of finite differences. It would have been ideal to have an analytical solution to the field equations, as this would give useful information about polarisation and wavelength dependences, and possible higher order modes; this was attempted, using stress profiles based on equations 3.6 and 3.7, but it was not successful due to the mathematical complexity of the problem. ANSYS also has a facility for calculating electric scalar potentials within a structure with a given refractive index distribution. A model, similar to that shown in figure 3.2 was set up for field calculations in ANSYS. The results, however, seem not to consider duly the refractive index changes throughout the structure. The ANSYS model was therefore abandoned in favour of the finite difference method presented below.

This section explains the finite difference method and presents field and intensity profiles for the waveguides, showing how the profiles depend on the waveguide design. The results are also used to calculate the coupling mismatch losses, which are used together with the intensity profile plots in chapter 5 to evaluate the experimental results from the waveguides.

3.4.1 Finite Difference Calculations of Optical Field Profiles

The physical problem to be solved is that of fitting the electrical field in the xy plane, \( E(x, y) \), to the refractive index \( n(x, y) \) in the waveguide according to the wave equation [110]

\[ \left( \frac{d^2}{dz^2} + \frac{d^2}{dx^2} \right) E(x, y) + \left( \frac{\omega}{c} n(x, y) \right)^2 E(x, y) = 0 \]

(3.15)

where \( \omega \) is the angular frequency of light, and \( c \) is the velocity of light in a vacuum. Since the refractive index is not constant, the fields must also be compensated to account for
Figure 3.13 Matrix structure used for the finite difference calculations. A rectangular matrix, 65 points wide and 33 points high, with a distance $h$ of 0.5$\mu$m between all the points, was defined to represent the top 12$\mu$m of the middle 32$\mu$m of the waveguide structure, as well as the 4$\mu$m of air above it. Every point in the matrix also corresponds to a corner node of an element in the ANSYS model, allowing the refractive index data to be loaded into a matrix straight from ANSYS.

reflections within the structure, as explained later.

Following Forsythe and Moler [111], if the electric field is specified as a two-dimensional matrix of discrete points, as shown in figure 3.13, the double differentials in equation 3.15 can be approximated accurately by

$$
\frac{d^2}{dx^2} E(x, y) = \frac{E(x - h, y) - 2E(x, y) + E(x + h, y)}{h^2}
$$

$$
\frac{d^2}{dy^2} E(x, y) = \frac{E(x, y - h) - 2E(x, y) + E(x, y + h)}{h^2}
$$

where $h$ is the distance between the points in the field matrix. This approximation reduces equation 3.15 from a partial differential problem to a simple algebraic calculation.

A field matrix, 65 points wide and 33 points high, is defined for these calculations. The matrix represents the middle 32$\mu$m section of the top 12$\mu$m of the waveguide structure, and 4$\mu$m of the air above it. A constant distance $h$ of 0.5$\mu$m between all the points is used, corresponding to the element corner nodes in the ANSYS model. Another matrix of the same dimensions contains the refractive index values calculated by ANSYS. The stressor stripe, having a refractive index of about 2.05, is not included as a dielectric structure.

As well as fitting the electric fields to the refractive index profiles using equation 3.15, the effect of the variation of the refractive index in the structure must be accounted for. It will be assumed that within the waveguide structure, the fields at two adjacent points $A$ and $B$ with different refractive indices $n_A$ and $n_B$, will have a flow of the field when going from $A$ to $B$ according to the Fresnel formulae for reflection $r_{AB}$ and transmission $t_{AB}$ for normal incidence on a dielectric boundary [110].
\[
\begin{align*}
    r_{AB} &= \frac{n_A - n_B}{n_A + n_B} \\
    t_{AB} &= \frac{2n_A}{n_A + n_B}
\end{align*}
\] (3.18)
(3.19)

In the air above the waveguide, where the refractive index at every point is set to unity, the field only depends on equation 3.15. The boundary conditions for the field are defined here to be zero at the top of the air region, and equal to that calculated for the waveguide along the top of the waveguide.

The finite difference calculation is performed with Maple V version 3, which is a commercial mathematical analysis computer package. By performing the Fresnel reflection correction and calculating equation 3.15 alternately, on every point in the matrix, a solution for the field is reached within about two cycles. Due to the constant flow represented by the Fresnel equations, the field is shifted and normalised, to keep the peripheral fields close to zero, and to prevent the numerical value of the field from overflowing during the calculations.

The finite difference calculation is performed with Maple V version 3, which is a commercial mathematical analysis computer package. By performing the Fresnel reflection correction and calculating equation 3.15 alternately, on every point in the matrix, a solution for the field is reached within about two cycles. Due to the constant flow represented by the Fresnel equations, the field is shifted and normalised, to keep the peripheral fields close to zero, and to prevent the numerical value of the field from overflowing during the calculations.

The results suffer from two weaknesses. Firstly, the field calculated for the air region does not settle at one unique value, but changes from cycle to cycle between a number of very similar solutions. This is because it is calculated from the absolute value of the field at the waveguide/air interface, without considering the differential of the field. Since the field in the air decays quickly towards zero above the waveguide structure, these differences have a negligible effect on the results. Secondly, successive repetition of the calculations based on the solved fields can set up waves between dielectric boundaries. While for the case of Si_{1-x}Ge_x/Si planar structures this may represent real modal solutions, this also happens for bulk silicon structures, since the model only represents the top 12μm of the structure, and the dielectric effect of the substrate is ignored.

In this investigation the intensity profiles are more useful than the field solutions themselves, since all plots, pictures and loss measurements relate specifically to the intensity. All modes and modal patterns discussed in the following investigation therefore refer to the intensity distribution in the waveguides, which is the square of the field values.

3.4.2 The Basic Optical Modal Patterns of Photoelastic Waveguides in Bulk Silicon and Si_{1-x}Ge_x/Si Heterostructures

Intensity profiles were investigated for photoelastic waveguides in bulk silicon based on the refractive index profiles calculated in the previous section. For the waveguides presented in figure 3.8, the corresponding intensity profiles are shown in figure 3.14. The transverse electric (TE) mode corresponds to light with its electric field polarised linearly along the x direction, and is calculated from the lateral (x) refractive index profiles. The transverse magnetic (TM) mode has its electric vector along the y direction, and is found from the vertical (y) refractive indices. For all stripe widths there are two well confined spots in the regions of high refractive index at the stripe edges. Figure 3.14 also shows regions of low light intensity, showing that the intensity profiles correspond well to the respective refractive index profiles in figure 3.8.

While there are always intensity peaks in the edge regions, the calculated intensity in the region underneath the stripe will change after a number of cycles and set up a pattern as shown in figure 3.15. This is because the finite difference model incorporates only the
Figure 3.14 Calculated intensity profiles in bulk silicon photoelastic waveguides at 1.523 µm, based on the refractive index profiles in figure 3.8. The pictures show the whole area included in the finite difference calculations, which includes the top 12 µm of the middle 32 µm of the waveguide, and 4 µm of the air above it. The important aspects of these intensity profiles are that they have two well confined guiding regions, and that they show a very low degree of birefringence. While the intensity is focused at the stripe edges, contours of lower intensity are included to show how the intensity distribution correlates with the refractive index profiles. The stressor stripe was not included in the finite difference calculations as a dielectric structure, but its width is indicated separately on each plot, to show its effect on the separation of the modes.
Figure 3.15 TE Intensity pattern in a bulk silicon waveguide at 1.523 μm set up after continual repetition of the finite difference calculation. While the two modes by the stripe edges as shown in figure 3.14 remain present, and do not change in character, the region between the edge modes sets up a pattern as shown between the top of the guiding layer and the bottom of the model. This pattern emerges because the bottom of the model is seen as a dielectric boundary, while in a real bulk silicon waveguide, most or all of the light under the stripe will couple into the substrate. The intensity pattern shown here is for a 3μm wide stressor stripe, while the effect occurs for all stripe widths and in both polarisations, but is more evident for the narrow stripes.

top region of the structure. In a real bulk silicon waveguide, the whole substrate will act as a highly multimode waveguide, so that most or all of the light under the middle of the stressor stripe is expected to couple into the substrate.

Photoelastic waveguides in Si_{1-x}Ge_{x}/Si heterostructures have a dielectric boundary at the heterojunction to prevent substrate coupling, and there will therefore be an additional confined mode under the middle of the stripe, between the edge regions. The calculated intensity profiles for photoelastic waveguides in a 4μm thick Si_{1-x}Ge_{x} layer on a silicon substrate are shown in figure 3.16. In addition to the edge guiding regions, there is now a distinct third mode under the centre of the stripe.

The predicted modes under each stripe edge and the one under the middle of the stripe will be referred to in the rest of this work as the edge modes and the middle mode, respectively. In the following sections, their characteristics will be investigated in terms of the waveguide variables, and the findings will be used in analysing the experimental data presented in chapter 5.

3.4.3 Controlling the Size of Edge Modes

The edge modes are seen to correspond well with the refractive index pattern around the stripe edges, which have been investigated earlier in this chapter. They can therefore be expected to have a similar dependence on the waveguide geometry and stressor deposition temperature.

A typical calculated edge mode is portrayed in figure 3.17. The intensity maximum tends slightly towards the stripe edge, where the refractive index is focussed. Since the refractive index edge region becomes wider and deeper with stripe width, as seen in figures 3.8 and 3.10, the mode size increases correspondingly. In figure 3.18 and 3.19 the width and depth of the edge modes, as read from the intensity plots, have been plotted.
Figure 3.16 Intensity profiles in photoelastic waveguides in Si$_{0.987}$Ge$_{0.013}$/Si heterostructures at 1.523 µm. The model used for these calculations incorporates a 4 µm thick Si$_{0.987}$Ge$_{0.013}$ layer, on top of an 8 µm silicon substrate and a 4 µm layer of air above the waveguide. The stressor stripe was not included in the finite difference calculations as a dielectric structure, but its width is indicated separately on each plot, to show its effect on the separation of the modes. It is seen that with the additional confinement provided by the heterojunction, there is now a confined mode under the middle of the stripe. This middle mode is most clearly defined for narrow stripe widths, and extends slightly further into the structure than the edge modes.
Figure 3.17 **TM Edge mode in a bulk silicon photoelastic waveguide with a 9\(\mu\)m wide stripe.** The edge mode, which is fairly similar for all stripe widths, is asymmetrical with its maximum tending slightly towards the stressor stripe, where the refractive index is highest. It is seen that the entire edge mode is defined within a region of approximately 6\(\mu\)m by 3\(\mu\)m.

as a function of stripe width. It is seen that there is very little difference between 1.15\(\mu\)m and 1.523\(\mu\)m wavelength plots. The TE and TM polarisations have distinct differences, but they never differ by more than 15%. As could be expected from the shape of the refractive index profiles in figure 3.8, the TM intensity profiles are both wider and less deep than the TE modes. As the stressor stripe becomes wider, both modes approach a limit in width and depth, which corresponds to the edge modes of a semi-infinite stressor stripe. The maximum widths of the TE and TM modes are around 2.1\(\mu\)m and 1.9\(\mu\)m, respectively, and the maximum depth is about 1.4\(\mu\)m for both polarisations. For stripe widths of 9\(\mu\)m, it is seen that the mode width and depth are already within 10% of their maximum value, and a further increase in stripe width will have little effect on the size and shape of the edge mode.

As the deposition temperature increases, the edge force also increases and generates greater refractive index changes. However, the refractive index profiles remain the same, as shown in figure 3.11. The width and depth of the edge modes should therefore remain practically constant. The edge modes for a bulk silicon waveguide with a 3\(\mu\)m stressor stripe were calculated for deposition temperatures from 300\(^\circ\)C to 700\(^\circ\)C, and their widths and depths were found to be constant to within 2% for all cases. It is expected that the substrate coupling, which is not considered in this model, will be reduced as the refractive index change increases, and this will be investigated experimentally in chapter 5.
Figure 3.18 The depth of the edge mode for TE and TM modes at 1.15\(\mu\)m and 1.523\(\mu\)m, calculated at half the maximum intensity. The depth is seen to vary little with wavelength, while the TE modes have a greater depth than TM modes. For wider stressor stripes, both TE and TM modes approach a maximum depth of around 1.4\(\mu\)m.

Figure 3.19 The width of the edge mode for TE and TM modes at 1.15\(\mu\)m and 1.523\(\mu\)m, calculated at half the maximum intensity. The depth is seen to vary little with wavelength, while the TM modes are somewhat wider than the TE modes. For wider stressor stripes, the modes reach a maximum width of about 1.9\(\mu\)m for the TE modes and 2.1\(\mu\)m for the TM modes.
3.4.4 Intensity Profiles in Si$_{1-x}$Ge$_x$/Si Photoelastic Waveguides

Photoelastic waveguides in Si$_{1-x}$Ge$_x$/Si heterostructures are similar to bulk silicon waveguides in terms of the edge modes. The addition of the middle mode shown in figure 3.16 is interesting in that it becomes relatively larger than the edge modes as the stressor stripe becomes narrow. For a 3$\mu$m wide stressor stripe on a Si$_{0.987}$Ge$_{0.013}$/Si heterostructure, the calculated TE intensity at a depth of 1.5$\mu$m is plotted in figure 3.20, showing three distinct modes, the middle mode being higher intensity than the edge modes. The relationship between the middle mode and the edge modes was calculated for various Si$_{1-x}$Ge$_x$ alloy contents and stripe widths, and is presented in figure 3.21.

The relative mode intensity is defined in figure 3.21 as the maximum intensity of the middle mode under the centre of the stressor stripe, divided by the maximum of the edge modes. These calculations predict that the middle mode becomes larger than the edge modes for narrow stressor stripes, and that all modes will have the same intensity for a stripe width of approximately 4.5$\mu$m. Figure 3.21 shows the relative mode intensity for TE modes, averaged for 4$\mu$m and 8$\mu$m thick Si$_{1-x}$Ge$_x$ layers, with 1.3%, 5.0% and 10.0% germanium. The error bars indicate the total spread in the relative mode intensity, showing that the effect of Si$_{1-x}$Ge$_x$ layer thickness and alloy content is marginal. This relationship is practically identical for TE and TM modes.

Since the relative size of the middle and edge modes is controlled by the stripe width, while the other waveguide parameters have little effect, this kind of structure may prove useful for coupling and splitting devices, since according to figure 3.21 the device can work as a two-arm or three-arm coupler depending only on the stripe width. For narrow stripes, there will be essentially one single guiding region, although the edge regions can never disappear completely, since the middle guiding region does not represent a confined region without the edge modes, as is evident from the refractive index profiles.
Figure 3.21 Relative intensity of middle mode to edge modes in photoelastic waveguides in Si$_{1-x}$Ge$_x$/Si heterostructures. The relative mode intensity is defined in this graph as the maximum intensity of the middle mode under the centre of the stressor stripe, divided by the maximum of the edge modes. It is predicted that the middle mode becomes larger than the edge modes for narrow stripe widths, and that all modes will have the same intensity for a stripe width of approximately 4.5\,\mu m. The curve shows the average value for TE modes with 4\,\mu m and 8\,\mu m thick Si$_{1-x}$Ge$_x$ layers, with 1.3%, 5.0% and 10.0% germanium. The error bars indicate the total spread in the relative mode intensity, showing that the effect of Si$_{1-x}$Ge$_x$ layer thickness and alloy content is marginal.

### 3.5 Calculating the Mode Mismatch

For the experimental investigation, photoelastic waveguides are fabricated corresponding to the ones investigated theoretically in this chapter. The losses are then measured, using end-fire coupling as explained in chapter 4. This coupling results in a loss due to the mismatch of the field of the input beam and the field set up inside the waveguide. Having found the waveguide modes, this mismatch can be calculated.

For a field $E_{\text{wg}}$ set up inside the waveguide, and a field $E_{\text{beam}}$ representing the beam incident on the waveguide facet, the normalised overlap integral is found from [112]

$$\text{overlap integral} = \frac{\int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} E_{\text{wg}} E_{\text{beam}} \, dx}{\sqrt{\int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} E_{\text{wg}}^2 \, dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} E_{\text{beam}}^2 \, dx}}$$

(3.20)

The waveguide field $E_{\text{wg}}$ was found from the finite difference calculations, and equals the square root of the intensity profile. Since the field is given as a matrix, it can be used to extract only the mode of interest, and define all others to be zero. This is shown in
Figure 3.22 Field profile of one of the guided edge modes used in calculating the coupling overlap mismatch. The edge mode profile is extracted from the field matrix used for the finite difference calculations, and is inserted into a matrix where all points outside the guided mode are defined to be zero. By assuming that the input beam profile is Gaussian and is given by equation 3.21, the overlap mismatch is given for any beam size and offset by equation 3.20.

\[ E_{\text{beam}} = e^{-\frac{\left( (x-\Delta x)^2 + (y-\Delta y)^2 \right)}{W_{\text{beam}}}} \]  

where \( W_{\text{beam}} \) is the 1/e width of the field, and \( \Delta x \) and \( \Delta y \) are the beam offsets in the x and y directions, respectively. From equation 3.20, the overlap can now be found for any input beam width and location. Solving equation 3.20 for analytical functions can become awkward due to the integrals. For discrete points in a matrix, the problem reduces to simple arithmetic operations and summation across the matrix.

Figure 3.23 shows the calculated mode mismatch losses in dB for edge modes as a function of input beam width. The input beam width has a significant effect on the coupling mismatch, and can generate considerable losses. Beam offsets up to 0.3\( \mu \)m have only marginal influence on the coupling losses, and are greatest for a narrow beam width (2.7\( \mu \)m), where it can reach 0.1dB. The offset value of 0.3\( \mu \)m corresponds to the tolerance in horizontal and vertical movement of the micropositioning equipment used to focus the light onto the waveguide, as explained further in chapter 4. The difference between edge modes for various stripe widths affects the coupling losses by only around 0.01dB.
3.6 Fresnel Reflections

At every dielectric boundary, there will be reflections depending on the angle of incidence and on the refractive indices on both sides of the boundary. On coupling light from air into a waveguide of refractive index 3.505, assuming a normal incidence, there will be a field reflection at the waveguide according to the Fresnel reflection equation 3.18 of

$$r_{\text{Air/Si}} = \frac{1.0 - 3.505}{1.0 + 3.505} = -0.556 \quad (3.22)$$

The square of the reflection gives the reflectance $R_{\text{Air/Si}} \ [110]$, which is the amount of energy reflected on coupling. For 1.15\(\mu\)m and 1.523\(\mu\)m the reflectances are 0.319 and 0.308, respectively, corresponding to losses of 1.67\(\text{dB}\) and 1.60\(\text{dB}\), respectively. These values are identical for TE and TM polarised light, and are practically the same on coupling from air into $\text{Si}_{0.987}\text{Ge}_{0.013}$. 

Figure 3.23 Waveguide coupling losses due to the mismatch between the field profile of the input beam and the guided mode in an edge mode as calculated from equation 3.20. Notice that the beam width refers to the full width at half of the maximum intensity, which corresponds to the $1/e$ field width used in equation 3.21.
3.7 Summary

This chapter has investigated the strains, the strain-induced refractive index profiles and the intensity profiles set up in photoelastic waveguides in bulk silicon and \( \text{Si}_{1-x}\text{Ge}_x/\text{Si} \) heterostructures. The modelling shows that the characteristics of the waveguides are determined mainly by the stressor stripe width and the stressor edge force and that there will be one guiding region just outside each stripe edge, although the presence of the \( \text{Si}_{1-x}\text{Ge}_x/\text{Si} \) heterojunction allows a third mode to be supported between the two edge modes.

It was found that the strain profiles are distinctly different for the lateral (\( x \)) and the vertical (\( y \)) directions, but that the strain-induced refractive index profiles for photoelastic waveguides in (100)-grown bulk silicon and \( \text{Si}_{1-x}\text{Ge}_x/\text{Si} \) heterostructures with stressor stripes oriented along the [100] crystallographic axes are similar for both polarisations, since the photoelastic constants \( p_{11} \) and \( p_{12} \) are similar in magnitude. Other reported photoelastic constants predict a very different guiding pattern. The experimental investigation of the waveguides will show whether the calculated photoelastic constants are correct in terms of sense and relative magnitude.

The calculations here predict that photoelastic guiding in bulk silicon is possible without the additional confinement from a planar structure, and that there will be two modes, one at each stripe edge. The mode width and depth of the edge modes were calculated, showing that the width converges towards approximately 1.9\( \mu \)m for TE modes and 2.1\( \mu \)m for TM modes. Both polarisations have a maximum depth of about 1.4\( \mu \)m. Although the guiding regions are well confined, the model does not consider the whole silicon substrate, and it is not clear from these calculations how much energy would be coupled into the substrate. In chapters 4 and 5 the fabrication and characterisation of photoelastic waveguides in bulk silicon are described to determine how well this model describes the actual waveguide performance.

By defining photoelastic waveguides in a \( \text{Si}_{1-x}\text{Ge}_x/\text{Si} \) heterostructure, a middle mode appears between the edge modes, and the modelling predicts that the middle mode increases relative to the edge modes as the stressor stripe becomes narrower, with all modes having approximately the same peak intensity for a 4.5\( \mu \)m wide stripe.

It was also predicted that the substrate strains in \( \text{Si}_{1-x}\text{Ge}_x/\text{Si} \) heterostructures will increase the phonon-assisted absorption around the band-gap energy. For a Si\( \text{Ge}_{0.013} \) layer on a silicon substrate, the strain-induced shift of the absorption band-edge will increase the optical propagation losses from the bulk or unstrained value of 4.9dB/cm to 5.9dB/cm at 1.15\( \mu \)m, compared to 3.9dB/cm in bulk silicon.

In chapters 4 and 5 photoelastic waveguides are produced in Si\( \text{Ge}_{0.013} \)/Si heterostructures, to investigate whether a middle mode exists, and whether it changes in intensity relative to the edge modes, according to the modelling, and whether the Si\( \text{Ge}_{0.013} \) samples have relatively higher losses at 1.15\( \mu \)m than at 1.523\( \mu \)m compared to bulk silicon waveguides, due to the phonon-assisted absorption around the band-gap energy.
This chapter describes the fabrication of the waveguides investigated in chapter 3, and explains why and how measurements were performed to characterise them. The aim of the experimental investigation is to check whether waveguides can be produced to yield losses and modal properties according to the modelling. An interferometric method to study the mechanical properties of stressor films is also explained. Results from these measurements are presented in chapter 5.

The fabrication of the waveguides involves depositing the stressor films onto the Si$_1$$_x$Ge$_x$/Si heterostructure, defining stripes by masking and etching the stressor film, and preparing the end facets. Each process will be explained in this chapter.

4.1 Sample Description and Design Variables

The basic waveguide structure investigated in this project is shown in figure 4.1. The height and width of the Si$_{Ny}$ stressor stripe and the thickness and germanium content $x$ of the Si$_{1-x}$Ge$_x$ guiding layer, as well as the stressor deposition temperature, are the main design variables of the waveguide.

It was concluded in chapter 3 that the characteristics of photoelastic waveguides are determined mainly by the stripe width and the generated edge force. According to the modelling, the edge force represents the difference in thermal expansion between the stressor layer and the Si$_{1-x}$Ge$_x$ guiding layer, and their relative mechanical strength. However, as mentioned in section 3.2.1, the inherent assumptions in the modelling of the waveguide strains may differ significantly from the physical effects in a real waveguide, and these need to be investigated experimentally.

This chapter describes the deposition of Si$_{Ny}$ films and explains how the forces generated by the films are calculated from the sample curvature, which is found by interference measurements. The measurement results, showing the effect of annealing and stressor film thickness, are presented in chapter 5, and are correlated with waveguide modelling and measurement results.

Photoelastic waveguides are fabricated with different stripe widths to show the effect on the size of the edge modes and the relative intensity of the middle mode to the edge modes, according to the modelling results in chapter 3. The stressor edge angle was predicted by modelling to have only marginal influence on the induced strains, and is not
investigated experimentally.

In this investigation, it is not of interest to investigate the effects of Si$_{1-x}$Ge$_x$ composition, since this is already well documented [80, 63]. It therefore makes sense to use only one Si$_{1-x}$Ge$_x$ composition for all measurements, so the strain-induced effects can be studied separately from the compositional effects, and measurements can be made for different strains in the same waveguide. A germanium content $x$ of 1.3% has been chosen for the Si$_{1-x}$Ge$_x$ layers, since strained layers in excess of 10nm can be grown on silicon, without the strong strain-induced shift of the absorption band-edge predicted for higher germanium contents, as shown in figure 3.7.

### 4.2 Deposition of SiN$_y$ Stressor Films

Silicon nitride stressor films were deposited by plasma-enhanced chemical vapour deposition (PECVD), where silane (SiH$_4$) and ammonia (NH$_3$) react to form the film. The deposition was performed at 300°C, generating a non-stoichiometric plasma nitride SiN$_y$, rather than a stoichiometric Si$_3$N$_4$.

Before deposition, the silicon and Si$_{1-x}$Ge$_x$ wafers were cleaned in trichloroethylene, acetone and isopropanol, one minute in each bath. Subsequently, the wafers were given a 45 seconds etch in 10% buffered hydrofluoric acid (HF) and a rinse in de-ionised water, and were placed in the PECVD deposition chamber immediately after the etch. This procedure was performed to remove the native oxide from the specimen, so the stressor film could be deposited onto the actual guiding layer. A native oxide grows on the surface of the wafer due to the reaction between the silicon and the ambient air, and is of the order of a few nanometres thick. The buffered HF has an etch rate of about 40nm/min on SiO$_2$, but has virtually no effect on crystalline silicon, and is therefore appropriate for this purpose.
SiNy films were deposited to nominal thicknesses of 300, 600 and 900nm, with a nominal refractive index of 2.05. Deposited 3" wafers were characterised using a PLASMOS ellipsometer, which allows automatic raster-mapping of the entire wafer, giving a variation in thickness across the wafers of 7-12%, while for a typical waveguide specimen, the variation was of the order of 1% or less. The refractive index of all films was in the range 1.95-2.14, while for any waveguide sized specimen it was constant to within ±0.01.

Notice that the only purpose of the ellipsometer mapping of the wafers is to evaluate the uniformity of the film, which will be referred to when calculating the stressor stripe edge force from the interferometer measurements in section 4.3. The absolute values of thickness and refractive index are not required other than as reference values.

4.3 Characterisation of Stressor Films by Interferometry

The deposition of a stressor film on a silicon wafer causes the wafer to bend slightly. This section describes how the sample curvature is measured by interferometry, and calculates the edge force of a stressor stripe made from the film. Results from these measurements are presented in chapter 5, and they are used to evaluate the guiding properties of photoelastic waveguides in bulk silicon.

Interferometer Set-Up

An interferometer was set up for measuring the curvature induced in silicon samples by thin SiNy stressor films deposited by PECVD. These stressor films generate a biaxial stress in the substrates, giving the samples a spherical curvature. A study of such a spherical surface can be made by placing the sample next to another spherical surface, such as a lens, as shown in figure 4.2. This creates a layer of air between the sample and the lens. Using a red helium-neon (HeNe) laser to excite the system, the light is set up between the sample and the lens, giving multiple reflections in the air gap between them resulting in light being reflected back through the lens at different angles, thus setting up an interference pattern which can be viewed through the camera. Each fringe in the interference pattern corresponds to light having traversed the air gap twice, thus representing twice the distance between the sample and the lens. If the fringes can be read accurately down to \( \frac{\lambda}{10} \), then the apparatus in figure 4.2, using red light of a wavelength \( \lambda = 0.632\mu m \), should be able to detect changes in the air gap down to \( \frac{\lambda}{20} = 31.6nm \).

This particular set-up is useful in that it allows small samples to be placed face down on the lens, with no additional clamping or sticking to interfere with the readings. It is also designed to be used together with the equipment set up for waveguide measurements as explained in section 4.6.2, since the light source and camera are already set up, as shown in figure 4.13, so it can be transformed into an interferometer apparatus within a matter of minutes.

Each fringe in the pattern set up by the interferometer represents twice the width of the air gap between the sample and the lens, which can be calculated from figure 4.3 using standard theory [113]. On the right side of the figure, a perpendicular is dropped from a general point \( P_{\text{lens}} \) on the lens surface onto the centre line, giving a distance \( cd \) for any distance \( x \) from the centre line. For a general arc of radius \( R \), as shown on the right, \( y \) relates to the distance \( x \) from the centre line:

\[
R^2 = x^2 + (R - y)^2
\] (4.1)
Figure 4.2 Interferometer set-up used for bending measurements. Using a red HeNe laser to excite the system, reflections are set up between a sample and the lens, which are of slightly different curvature. The interferometric fringe pattern which appears on the camera is then an examination of the air gap between the sample and the lens. Since both the lens and the sample are spherically curved around their point of contact, they will produce a circular ring pattern, which is a function of their respective curvatures. In addition to the equipment shown on the picture, micropositioning tools were used to control the direction of the input beam and the position and inclination of the lens.

\[
\begin{align*}
    y &= \frac{x^2 + R^2 - 2Ry + y^2}{2R} \\
    &\approx \frac{x^2}{2R}
\end{align*}
\]

From figure 4.3, the width of the air gap \( \delta \) between two points \( P_{\text{sample}} \) and \( P_{\text{lens}} \) is found from

\[
\delta = ac - \frac{x_{\text{sample}}^2}{2R_{\text{sample}}} + \frac{x_{\text{lens}}^2}{2R_{\text{lens}}}
\]

where the distance from the centre line \( x_{lens} \) for the lens and \( x_{sample} \) for the sample are almost the same for large radii. Since the air gap \( \delta \) represents half a wavelength, or multiples thereof, the distance \( x \) from the centre line can now be written as a function of the number of wavelengths \( n \).

\[
ac + \frac{x^2}{2} \left( \frac{1}{R_{\text{lens}}} - \frac{1}{R_{\text{sample}}} \right) = \frac{n \lambda}{2}
\]
Figure 4.3 The interferometer in figure 4.2 works by setting up light between the sample and the lens, thus generating a fringe pattern, as shown in figure 4.4. This pattern is an examination of the air gap between the sample and the lens, and can be calculated from their geometry, as shown on the left. The change in the width of the gap $\delta$ compared to its value $ac$ at the centre line is found as a function of $x$, the distance from the centre line, and radius $R$, as illustrated on the right, corresponding to equation 4.1.

\begin{equation}
\downarrow \quad x^2 = \frac{\lambda}{\frac{1}{R_{\text{lens}}} - \frac{1}{R_{\text{sample}}}} n + \frac{2ac}{\frac{1}{R_{\text{lens}}} - \frac{1}{R_{\text{sample}}}} \quad (4.3)
\end{equation}

Equation 4.3 gives a linear relation between $x^2$ and $n$, the slope of which can be calculated from the interferometric ring pattern set up on the camera in the apparatus in figure 4.2. The distance $ac$ is constant with fringe number, resulting in an offset from zero.

As an example, the ring pattern shown in figure 4.4 was generated using the interferometer in figure 4.2 and a silicon sample covered by a 0.6µm thick SiNy film, causing the silicon to bend very slightly. A video graphics card from Parallax Graphics with software capable of storing the image from the camera was used with the interferometer, allowing the fringe pattern to be recorded on a computer file exactly as seen by the camera.

The diameter of the rings or fringes can now be readily extracted from the saved interference pattern. Since the saved interference patterns are pixelised, the diameters can be determined from the pixel coordinates. It is easy from these coordinates to ensure that the readings are taken through the centre of the rings, and that they are taken completely horizontally. In principle, since the lens and sample are spherical around their point of contact, the fringes should be perfectly circular. Through misalignment of the interferometer, however, the ring pattern saved from the camera may be slightly elliptical. By always taking the readings horizontally through the centre of the rings, such disturbances in the image will not affect the readings.

The fringe diameters from figure 4.4 are plotted in figure 4.5 for the first ten fringes together with the corresponding data from a flat reference sample. Squaring the radii from
Figure 4.4 Ring pattern generated by the interferometer in figure 4.2. The pattern represents the layer of air between the sample and the lens, and is circular because both the sample and the lens have spherical curvature. A screen-grabbing tool was used to read the picture data directly from the camera to a computer file, allowing the rings subsequently to be examined to the nearest pixel generated by the camera.

Figure 4.5 gives a highly linear relationship between $x^2$ and $n$ as shown in figure 4.6. With the particular interferometer geometry and lens chosen for these experiments, the smallest number of pixels between fringes for any sample in this project was about twenty. The practical reading accuracy is within ±1 pixel for the diameter readings, and the correlation coefficient between the experimental data for the ten first fringes and a straight line fit was above 0.999 for every measurement in this project. This accuracy will be taken to account for the pixel quantisation error, the reading uncertainty, and differences between the experimental set-up and theory, such as imperfections in the lens and deviations to the beam path.

Figure 4.5 The diameter of the fringes can be found accurately from the interference patterns saved as video images from the camera. Here the diameter of the first ten fringes from the image in figure 4.4 are plotted as stars together with the corresponding data from a flat reference sample, shown as circles.

Figure 4.6 Plotting the square of the radii of the samples in figure 4.5 versus fringe number, one obtains a straight line, whose slope is given by equation 4.3. Having found the slope $\gamma$ from both sets of measurements, the sample curvature relative to the reference sample is found from equation 4.7.
A value for the slope of the $\frac{3^2}{n}$ curve can now be found for every sample, and the corresponding sample radius can be found from equation 4.3. Setting $ac$ equal to zero and using $\gamma$ as the slope of the $\frac{3^2}{n}$ curve,

$$\frac{1}{R_{\text{tens}}} - \frac{1}{R_{\text{sample}}} = \frac{\lambda}{\gamma}$$

$$R_{\text{sample}} = \frac{1}{R_{\text{tens}} - \frac{\lambda}{\gamma}} = \frac{R_{\text{tens}} \gamma}{\gamma - R_{\text{tens}} \lambda}$$

For a completely flat reference sample, the radius $R_{\text{ref}}$ is infinite, and $R_{\text{tens}}$ can be found from equation 4.5:

$$R_{\text{ref}} = \infty$$

$$\frac{1}{R_{\text{tens}}} - 0 = \frac{\lambda}{\gamma_{\text{ref}}}$$

$$R_{\text{tens}} = \frac{\gamma_{\text{ref}}}{\lambda}$$

where $\gamma_{\text{ref}}$ is the slope of the flat reference sample. Inserting equation 4.6 into equation 4.5,

$$R_{\text{sample}} = \frac{\gamma_{\text{ref}} \gamma_{\text{sample}}}{\lambda} \frac{1}{\gamma_{\text{sample}} - \gamma_{\text{ref}}}$$

The readings taken from the fringe patterns, from which the $\gamma$ values are extracted, are given in pixels, however, and must be converted to absolute distance to give an absolute value of curvature. This is because a bi-convex lens, rather than planar-convex one, was used in the interferometer to allow an extra degree of freedom in focussing the image.

Converting the data to absolute values is most easily done by measuring the radius of the lens, which equals $\frac{2\gamma_{\text{ref}}}{\lambda}$, and inserting it into equation 4.7. The lens has a significantly smaller radius than the samples, allowing accurate measurement of its radius by reflecting light off its surface.

Measurement of the Interferometer Lens Radius

The lens was set up on a micropositioning stage and a narrow beam of light was shone onto it. By moving the lens in small steps the curvature of the lens was found by measuring the movement of the reflected beam. According to figure 4.7, the movement of the reflected beam represents twice the change in the surface normal.

By recording the movement $x$ in the reflected beam a distance $d$ from the lens, as a function of the travel $y$ of the lens, the lens radius $R_{\text{lens}}$ is found from figure 4.7 to be

$$\frac{x/2}{d} = \frac{y}{R_{\text{lens}}}$$

$$R_{\text{lens}} = \frac{2yd}{x}$$

For a number of readings across the lens, recorded at distances $d$ of $\frac{1}{2} - \frac{1}{2}$ m from the lens, $2yd$ is plotted versus $x$ in figure 4.8, giving a lens radius of 105.9 mm.
Calculating The Edge Force

For a silicon substrate with a thin SiNy film, the force $F$ generated by the film relates to the film stress $\sigma_{film}$ and thickness $t$, which are found from the radius of curvature $R$ of the substrate [55, 114]

$$F = \sigma_{film}t = \frac{ET^2}{6R(1-\nu)}$$

(4.9)

where $E$ is Young's modulus, $T$ is the thickness of the substrate, and $\nu$ is Poisson's ratio. By opening a gap in the film, a force $F = \sigma_{film}t$ is generated by the film edge [55]. This force corresponds to the stripe edge force shown in figure 3.4.

The thicknesses of the deposited SiNy films were found using a PLASMOS ellipsometer. For a typical waveguide specimen, the variation in thickness was of the order of 1% or less. The edge force calculated from waveguide-sized specimens could therefore be assumed to be virtually constant for any one sample. Since the edge force can be calculated directly from bending measurements, it is clear that the absolute film thickness is not required other than as a reference value.

Readings & Accuracies

The accuracies of the curvature measurements depend upon the accuracies given for the radius of the flat reference surface, $R_{ref}$, and that of the lens, $R_{lens}$.

From equation 4.8, the lens radius is given by $\frac{2yd}{x}$. The standard deviation on the slope, representing the spread of the measurements, is 1.1%, and the variables $y$ and $d$ could be
determined to better than 0.67%. Considering a range of three standard deviations on the slope, the overall accuracy becomes ±4.7%.

The reference surface is flat to \( \frac{\lambda}{20} \) at 0.632\( \mu \)m. For a surface of length \( L = 2.5\) cm, and a deviation \( h = \frac{0.632\mu m}{20} \) at the middle, the radius \( R_{ref} \) of curvature is found from [114]

\[
R_{ref} = \frac{L}{4} \left[ \frac{L}{2h} + \frac{2h}{L} \right] = 2472m
\]

Inserting this value into equation 4.4 instead of the assumed infinite radius introduces an error of around 0.004%. Additionally, the spread of the data will be calculated for each sample, and a three standard deviation accuracy will be used in equation 4.7 to account for the reading errors and pixelisation of the fringe patterns. The substrate thickness \( T \) is measured with a micrometer to an accuracy of 10\( \mu \)m. Since the samples are about 0.4\( mm \) thick, a 2.5\% accuracy on sample thickness will be included in equation 4.9.

The results from the interference measurements are presented and evaluated in chapter 5 together with the waveguide measurements.

### 4.4 Preparing the End Facets

According to the modelling in chapter 3, the cross-sections of the photoelastic waveguides studied in this project are of the order of 6\( \mu \)m by 3\( \mu \)m. Because of their structure, end-firing is the only practical method of coupling light into the guides. Therefore, it is required to prepare the end facets of the waveguides to optical quality across areas of only a few microns in each direction.

In previous work on GaAs-based photoelastic waveguides [58, 55], facets were cleaved along the (110) planes. Loss measurements were performed by repeatedly cleaving the specimen along the same direction. In theory, this method is ideal, in that it reveals perfect crystallographic planes, while it is quick to perform. In the current investigation, the waveguides are made from Si and Si\(_{1-x}\)Ge\(_x\)/Si heterostructures. These materials tend to cleave along the (100) planes, but the resulting facets are not of a high quality, as is required for waveguide coupling.

A number of methods were tried out in an attempt to improve the quality of the cleaved facets, including

1. **Chipping or cutting** the edge of the sample with various tools, such as scalpels, tungsten and diamond scribes and razor blades.

2. **Scribing the sample** along the whole intended cleaving line or parts of it, before cleaving or breaking.

3. **Sticking the sample to an elastic surface** and breaking it over various edges while under tension. Diverse sticky tapes were used as elastic surfaces.

4. **Using different carrier surfaces** to position the sample on before breaking, cutting or simply pressing against the carrier surface. Narrow edges of different radius, such as razor blades, paper clips and Biros, as well as flat surfaces of different hardness were tried out.
While it is possible to produce a good facet by cleaving, it is mostly not of the required quality. The facets also tend to become poorer as the sample becomes smaller, so that a cutback-and-repeat type measurement would not be practical. It should be mentioned that Yu et al. [60] claimed to have cleaved to optical quality a WNi/SiO₂/Si/SiO₂/Si heterostructure where the silicon guiding layer was 0.85μm thick, by lapping the structure down to less than 90μm thickness before cleaving. This method was not attempted here, although it is believed that thicker guiding layers which are not supported by SiO₂ layers may not cleave as reported by Yu et al.

Different polishing equipment was tested out with various mounting and polishing procedures, and it was found that the Planopol-2 polishing turntable could produce the required quality facets when used as explained in section 4.4.1.

4.4.1 The Planopol-2 Polishing Turntable

The Planopol-2 polishing turntable is an apparatus designed for the preparation of flat surfaces. By mounting the sample in a standard revolving sample clamp, it can be pressed against a rotating polishing disc, allowing different rotation speeds and pressures to be used. Various polishing surfaces can be attached to the disc, from silicon carbide papers of different grit size for coarse grinding, to silk pads prepared with fine diamond grains for fine polishing.

Mounting the Sample

To facilitate the polishing of the end facets of the specimen, the sample was mounted onto a Bakelite block which could be fixed into the Planopol-2 sample holder. Two glass slides were used, as shown in figure 4.9, to mount the sample sideways, allowing the end facet to be polished.

![Figure 4.9 The samples were mounted sideways between two glass slides on a Bakelite block, using black wax (not shown) to fix it into position, allowing the end facet, protruding slightly above the glass, to be polished.](image-url)
Figure 4.10 The waveguide facets should ideally be polished at 90° to the waveguide itself. Practically there will be tolerances on both the vertical angle $\theta_{in}$ and the horizontal angle $\alpha_{in}$ at the input facet, and similarly on the output facet. The mounting and polishing procedures presented here allow both angles to be controlled to within less than ±1°.

It is relatively simple to polish a flat surface. The problem when polishing a waveguide facet is that the guiding regions lie within the top few microns of the sample, where the polishing stresses become very high, and where polishing grit tends to accumulate, causing significant chipping of the facets.

The sample was mounted between the glass slides using black wax\(^1\) to give the sample mechanical support during polishing. When heated, the black wax liquifies sufficiently to place the glass slides in close contact with the sample, while on cooling, it solidifies enough to let only very little polishing grit accumulate in the wax next to the sample. Glass was chosen as a supporting medium because it will grind down at somewhat the same rate as silicon, so that the whole polished surface, i.e. the glass and the sample edge, remains flat during polishing.

As well as providing for an optical quality waveguide facet, this mounting procedure allows a good control of the angle between the facet and the waveguide. The angle in the vertical plane, $\theta_{in}$, and in the horizontal plane, $\alpha_{in}$, as indicated in figure 4.10, should ideally be 90°, but there will be a certain tolerance on both due to the polishing procedure.

The vertical angle, $\theta_{in}$, is determined by how straight the sample can practically be mounted between the glass slides. By mounting microslides, 7.5cm in length, between the glass slides, the deviation from normal was found to be less than ±1° by comparison with a metal set square.

After polishing one facet the sample is unmounted and turned around to polish the other facet. If the sample is not properly remounted, the two facets will not be perfectly parallel. Practically, by pressing the sample firmly against the Bakelite block while the wax is setting, the horizontal deviation will be minimal. All experimental results presented in chapter 5 are made on samples which were measured on a travelling microscope to have less than 0.5° between the facets. If care is not taken during remounting, however, this angle can easily become 5° or more.

\(^1\)W wax from APIEZON Products
Polishing Procedure

The samples are mounted such that they protrude slightly above the glass slides. This protrusion is then ground down manually on 220 grit silicon carbide paper until it is almost flush with the glass. After mounting the Bakelite blocks in a sample clamp on the Planopol-2, it is placed face down on the polishing disc. Using first silicon carbide paper of 1200 and 4000 grit, the facets are ground down to a fairly smooth finish. Subsequently, silk pads impregnated with 6μm and then 1μm diamond grains are used with an alcohol-based lubricant for a final polish. With good control of lubrication and by regular removal of polishing grit from the polished surface, facets of the required optical quality can be produced consistently. The measurement results presented in chapter 5 confirm that the waveguide facets allow coupling with little distortion and loss.

4.5 Defining the SiNy Stressor Stripes

It is required in this project to produce samples of the type shown in figure 4.1. Having deposited a stressor film as described in section 4.2, stripes of any width can be defined by standard photolithography and wet etching of the stressor film. However, while both preparing the facets and defining the stressor stripes could be done with relative ease, significant problems arise when defining both the facets and the stripes on the same sample, as explained in section 4.5.2.

4.5.1 Photolithography & Etching

The stressor stripes were defined using standard photolithography, which involves applying photoresist to the sample and spinning it into a thin film. By exposing the photoresist to ultraviolet light through a photo mask, the exposed resist becomes removable in photoresist developer, leaving only a pattern of resist corresponding to the photo mask. Subsequently, the areas of the SiNy film not covered by resist are etched away in a bath of 10% buffered hydrofluoric acid.

This procedure of masking and etching uses standard chemicals and equipment, and proved to be suitable for defining stressor stripes as narrow as 2μm, which are the finest features investigated in this project.

4.5.2 Edge Build-Up During Photolithography

As separate processes, both the facets and the SiNy stripes can be prepared as explained in sections 4.4 and 4.5.1. A problem arises in this project because the stripes must be defined all the way to the facet, as in figure 4.1.

During the photolithography, the spinning of the photoresist inevitably causes an accumulation of resist at the edges of the specimen, which makes it difficult to define the required pattern close to the specimen edge. Practically, on developing the resist, there will remain a stripe of resist around the edge of the sample, which prevents the stripes from being defined at the facets. On further developing the photoresist, it is possible to define the pattern close to the edge of the sample. However, this will also remove the pattern at the middle of the sample, where the resist is thinner.

\[\text{The grain diameter of the SiC paper is 1 inch divided by the grit value.}\]
This problem was first addressed by specifying the polishing procedure around the requirements of the photolithography.

1. By defining the stripes before preparing the facets, there would be no problem with edge build-up. This was attempted several times, but the SiNy stripes were invariably torn off the specimens close to the facets during polishing.

2. If the photoresist could be put down before the polishing, the facets could be polished, and the etch could be carried out afterwards, and again, there would be no problem with edge build-up. However, the photoresist can only withstand temperatures up to 100°C. At higher temperatures, the resist quickly carbonises, making it useless for photolithography. At 100°C the black wax used in mounting the sample for polishing is not sufficiently liquid to mount the specimen properly.

3. There are some epoxy based cold-setting resins which could be used to mount the sample for polishing, so that the photoresist could be put down before polishing. However, to remove the resins, one would need solvents, and possibly ultrasound, which would also remove the photoresist.

From these considerations, it is clear that the stripes must be defined after the facets. Several attempts were therefore made to improve the photolithographic process itself.

1. Two commercially available resists, AZ 4330 and AZ 1505 from Hoechst Celanese, were used together with hexamethyldisilazan vapour, which improves the adhesion of the resist to the sample. AZ 4330A, which is the more viscous resist, has a potential thickness range of 2.6μm to 4.0μm, while AZ 1505 has a thickness range of 0.36μm to 0.46μm. This significant difference in viscosity and potential thickness of the resist did not significantly affect the relative edge build-up.

2. Spinning speeds were varied in the range 300-800 revolutions per minute, for durations of 30-90 seconds to vary the film thickness. While this changed the overall thickness of the films, the relative amount of the edge build-up was not noticeably different.

3. The UV exposure and developing times were varied to better remove the exposed resist at the edges while leaving the stripe across the whole sample. While some improvement could be made with a long exposure time on the AZ 1505 films when spun above 600 rpm, it seemed generally impractical to define a stripe across a sample from facet to facet.

Given that the photolithography had to be performed after the polishing, and that there will practically always be a resist accumulation at the sample edges, a different method was attempted, in which the sample surface was extended beyond its edges after polishing, so as to effectively remove the edges from the sample. Section 4.5.3 explains this procedure in detail.
4.5.3 Overcoming Edge Build-Up by Surface Extension

On spinning the photoresist onto the sample, it accumulates at the sample edges. This accumulation can be avoided if the sample surface is extended past its edges using a supporting medium. By using a viscous liquid as a medium, it should be possible to achieve perfect contact with the facets while being flush with the surface. This has not been reported before to the best of my knowledge. It turns out that the same black wax used when polishing the facets is very well suited for this purpose.

Planar Mounting of Samples

Initially, the surface extension was performed by melting a small amount of black wax onto a silicon carrier plate, and then simply dropping the sample into the wax, as shown on the top of figure 4.11. The sample would then sink into the wax and the wax would be in close contact with the facets and flush with the surface. One problem with this method is that the sample is not always parallel with the carrier, because of the wax between them. During the UV exposure of the photoresist, this can cause a poor definition of the pattern, because the photomask is not in perfect contact with the sample.

This problem is avoided by placing the sample straight onto the carrier, and placing a small globule of wax next to each facet. The wax will then make contact with the entire facet by capillary action. With little practice, it is possible to extend sample surfaces suitably for the photolithography.

Figure 4.11 Planar mounting of the sample. The top two pictures show the initial method of surface extension, where black wax was melted onto a silicon carrier plate, shown in light grey, and the sample, shown in dark grey, was dropped into the wax. At the bottom, the sample is put directly onto the carrier, and black wax is deposited next to the facets, and runs into contact with the facets through capillary action. In this way the sample becomes parallel with the carrier, while in the initial method there could be a slight angle between the two, which could cause problems during the UV exposure of the photoresist.
Figure 4.12 SEM micrograph of the end facet of a Si$_{1-x}$Ge$_x$ waveguide prepared using the surface extension method portrayed in figure 4.11. The SiN$_x$ stripe is seen to extend across the Si$_{1-x}$Ge$_x$ surface (light), all the way to the facet (dark), similar to figure 4.1. The Si/Si$_{1-x}$Ge$_x$ junction is not visible on the micrograph. A 9µm mask was used when defining this stripe.

There are several reasons why black wax is used in this procedure. As well as being suitably viscous when mounting the sample, it becomes hard at room temperature, so the photoresist can be spun onto the sample. It does not react with the resist or the sample, and remains virtually solid at 100°C, at which temperature the photoresist is hardened or baked after being developed. The wax will also not react with the buffered hydrofluoric acid, so the whole sample with wax and carrier can be put in the etch. This is useful, because unmounting the sample at 150-200°C would destroy the resist. The sample is therefore unmounted after the etch, when the resist is no longer needed.

An example of a sample prepared using surface extension is shown in figure 4.12, where the stripe is seen to extend all the way to the facet.

4.6 Equipment Set-Up

Equipment was set up to characterise the waveguide propagation losses and the optical mode profiles. This section presents the considerations made while designing the equipment system.

4.6.1 Choice of Lasers and Wavelength Range

The wavelength range of interest for Si$_{1-x}$Ge$_x$ alloys is 1.1-1.8µm, as determined by the absorption edges of the bulk materials. Within this range, it would be useful to investigate the wavelengths corresponding to the low-loss windows of common optical fibres at 1.3µm and 1.55µm, as well as the region close to the silicon absorption edge at 1.1µm. This absorption edge is useful to characterise, both because it defines the lowest cut-off wavelength for Si$_{1-x}$Ge$_x$ alloys, and because it will be affected by both the alloy content and strain.

Standard helium-neon (HeNe) gas lasers exist with wavelengths of 1.15µm, just above the silicon cut-off, and 1.523µm. They are highly collimated, coherent, polarised and power stable units, making them appropriate and convenient for this project. Since the waveguide properties will be investigated for transverse electric and transverse magnetic polarisations, measurements can be made with a minimum of focusing optics and polarisers. Their power stability also provides for accurate and repeatable measurements.
4.6.2 Physical Arrangement

The equipment was set up as shown in figure 4.13 to allow measurement of waveguide losses as well as mode profiles. A number of considerations were made for each part of the arrangement, and are presented in turn in this section.

Alignment of the System

One main consideration when arranging the equipment was the alignment and controllability of the light beam. To allow good visual control of the light, a red (0.632\(\mu\)m) HeNe laser was set up and aligned with the IR laser beams as shown. A grating mounted on a rotation stage, marked H, was used to single out only one wavelength from the 1.15\(\mu\)m laser, which has a multimode output, and pellicle beamsplitters, marked G, were used to align the three wavelengths into one single beam. Pellicle beamsplitters were used because they are extremely thin, \(\leq 5\mu\)m, avoiding problems with ghost reflections. After travelling more than 1.3 m from the pellicle beamsplitters to the camera, having been reflected twice at F and E, and focussed through a set of objectives on the micro-positioning stage (\(\mu\)-POS), all wavelengths showed up in close proximity on the camera screen, which is of the order of 1.5 cm\(^2\). This close alignment is important in providing consistent measurements because...
1. On focussing, light which is not centred onto a lens will change in both shape and direction. Using the red light as a guide, the IR light beams can be controlled to within ±0.8 mm at the input objective at the micro-positioning stage. This tolerance is estimated from alignment and focussing tests.

2. It is of interest to characterise the same waveguides for both 1.15\mu m and 1.523\mu m. The close alignment allows measurements to be comparable for the two wavelengths.

3. Also, for the same wavelength, comparison can be made between different waveguides, or between a series of measurements on the same guide, using the same focussing conditions.

The Micro-Positioning Stage

The sample is mounted on the micro-positioning stage, shown as \mu-POS in figure 4.13. It consists of three separate parts, one for each of the objectives and one for the sample, as shown in figure 4.14. Each objective stage has three linear degrees of freedom, as shown. The sample stage in the middle can move in the vertical and lateral directions (not shown), and has additional freedom to pitch and rotate.

There is an accuracy of 0.3\mu m on the movement of the positioners, which equals roughly 15% of the half intensity width of an edge mode in a photoelastic waveguide, as predicted in chapter 3. A final degree of freedom is the positioning of the beam itself; the mirror at E in figure 4.13 is fixed onto a precision kinematic mount, allowing smooth and precise movement.
The numerical aperture of a lens is the sine of the angle $\alpha$ between the light of maximum deviation from the optical axis and the optical axis itself. The numerical aperture of a 10X objective will often lie around 0.20, and for a 40X objective it will be 0.60-0.65.

In a waveguide with refractive indices $n_{\text{core}} > n_{\text{intermediary}} > n_{\text{cladding}}$, the numerical aperture of the waveguide is the sine of the angle $\alpha_{\text{cladding}}$ corresponding to an angle $\theta_{\text{cladding}}$ of 90°, and can be calculated from the refractive indices $n_{\text{core}}$ and $n_{\text{cladding}}$. Light incident on the waveguide facet at a greater angle than $\alpha_{\text{air}}$ will be lost into the cladding. It is therefore important that the objective used for coupling light into the waveguide has a numerical aperture which is no greater than that of the waveguide.

Angular control of the mirror. This is to ensure that the light beams are well centred on the objective, so they will not exit the objective at an angle. Since the objective itself moves during focussing, this extra control is required. The distance from the mirror to the first objective was purposely made long, > 60cm, so that the change in the beam angle at $\mathbf{E}$ will appear practically as a linear shift at the objective.

**Choice of Microscope Objectives**

In photoelastic waveguides, the stressor edge force determines the strain-induced refractive index change, which controls the optical confinement within the guide. The confinement determines the maximum angle with which light can be coupled into the waveguide. It is important to choose an objective which can couple light within this angle.

The spread of light from an objective is given by its numerical aperture (N.A.), which equals the sine of the angle between the marginal ray (the ray with the greatest deviation from the optical axis) and the optical axis, as portrayed in figure 4.15. While the numerical aperture is a function of the shape and size of the lens, for practical objectives, the numerical aperture of a 10X objective will often lie around 0.20, and for a 40X objective it will be 0.60-0.65.

The numerical aperture of a waveguide is calculated from its refractive index distribution. For the waveguide shown in figure 4.16, internal reflection occurs when $\theta_{\text{cladding}}$ reaches 90°, so that according to Snell's law,

$$\sin(\theta_{\text{core}})n_{\text{core}} = \sin(\theta_{\text{cladding}})n_{\text{cladding}}$$

$$= \sin(90°)n_{\text{cladding}}$$

(4.11)
\[ \theta_{\text{core}} = \arcsin \left( \frac{n_{\text{cladding}}}{n_{\text{core}}} \right) \quad (4.12) \]

where the angles \( \theta \) and refractive indices \( n \) are defined as in figure 4.16. Above this value of \( \theta_{\text{core}} \), the light will be confined. From equation 4.11 it is also clear that any cladding of intermediary refractive index value will have no effect on the critical angle.

The angle \( \alpha_{\text{air}} \), corresponding to the critical angle \( \theta_{\text{core}} \), defines the greatest angle light can be coupled into, and the waveguide numerical aperture equals \( \sin(\alpha_{\text{air}}) \). It is given in terms of the waveguide refractive indices as follows:

\[
N.A. = \sin(\alpha_{\text{air}}) = n_{\text{core}} \sin \left[ 90^\circ - \theta_{\text{core}} \right] = n_{\text{core}} \sin \left[ 90^\circ - \arcsin \left( \frac{n_{\text{cladding}}}{n_{\text{core}}} \right) \right] = n_{\text{core}} \sqrt{1 - \left( \frac{n_{\text{cladding}}}{n_{\text{core}}} \right)^2} \quad (4.13)
\]

By expressing \( n_{\text{cladding}} \) as \( n_0 \), the bulk refractive index of the waveguide material, and \( n_{\text{core}} \) as \( n_0 + \Delta n \), where \( \Delta n \) is the refractive index change in the core, equation 4.13 becomes

\[
N.A. = (n_0 + \Delta n) \sqrt{1 - \left( \frac{n_0}{n_0 + \Delta n} \right)^2} \\
= (n_0 + \Delta n) \sqrt{\frac{n_0^2 + 2n_0 \Delta n + (\Delta n)^2 - n_0^2}{n_0^2 + 2n_0 \Delta n + (\Delta n)^2}} \\
\approx \sqrt{2n_0 \Delta n} \quad (4.14)
\]

where \( \Delta n \) is assumed to be much smaller than \( n_0 \). It is convenient here to have an analytical expression for the refractive index change \( \Delta n \) in a photoelastic waveguide. Using equations 3.6 through 3.9 to approximate the stripe strains, the strain-induced refractive index changes are found from equations 3.11 and 3.12:

\[
\Delta n_x = \frac{F n_0^3}{\pi E (x^2 + y^2)^2} (x^3 p_{11} - \nu x y^2 p_{12}) \quad (4.15)
\]

\[
\Delta n_y = \frac{F n_0^3}{\pi E (x^2 + y^2)^2} (x^3 p_{12} - \nu x y^2 p_{11}) \quad (4.16)
\]

Figure 4.17 presents the numerical aperture, given by equation 4.14, in the edge guiding region of a bulk silicon photoelastic waveguide for values of the edge force \( F \) of \( 5 \times 10^6 \), \( 10^6 \) and \( 5 \times 10^6 \) dyn/cm. The plots correspond to \( \Delta n_x \), which generally gives a smaller waveguiding region than \( \Delta n_y \). It is seen that with an objective with a numerical aperture of 0.2, it is possible to couple into a region >2\( \mu \)m wide with an edge force of \( 5 \times 10^6 \) dyn/cm, and this 'coupling region' increases with the edge force. An objective with a numerical aperture of 0.6, to couple into the same region, requires an edge force of about \( 5 \times 10^6 \) dyn/cm, which is a very strong force. In fact, the highest force generated by any of the stressor films investigated in chapter 5 is \( 3 \times 10^6 \) dyn/cm. It is therefore not practical to couple into the edge regions of these photoelastic waveguides using an objective with a numerical aperture of 0.6.
Figure 4.17 Numerical Aperture Profiles of Photoelastic Waveguides in Bulk Silicon. The plots give the solution to equation 4.14 for stressor edge forces of $5 \times 10^3$, $10^6$ and $5 \times 10^6$ dyn/cm based on the edge mode refractive index profiles in bulk silicon photoelastic waveguides. Each curve outlines the maximum region which can be coupled into using an objective of a given numerical aperture. It is seen that with an objective with a numerical aperture of 0.2, it is possible to couple into a region >2 $\mu$m wide with an edge force of $5 \times 10^5$ dyn/cm. Using an objective with a numerical aperture of 0.6, the edge force must be almost ten times greater to couple into the same region. The curve for a $5 \times 10^5$ dyn/cm edge force defines only a minute region with a numerical aperture of 0.6 and has not been explicitly labelled.

For the waveguide measurements presented in chapter 5 a 10X objective with a numerical aperture of 0.17 will be used to couple into the waveguides. At the waveguide output a 40X objective with a numerical aperture of 0.65 was found to give a good image of ~100 $\mu$m sections of the facet.

Controlling the Beam Width

The minimum width or spot size of the beam when focussed onto the waveguide facet is important, firstly because the mode mismatch losses depend strongly on the spot size, as calculated in figure 3.23, and secondly because the region which can be coupled into is limited, as shown in figure 4.17.

The minimum spot size was measured for the objectives by focussing the light through the input and output objectives, without any sample mounted between them, and onto the camera. By measuring the focussed beam width at half the maximum intensity and comparing it to the focussed output from a electron microscope aperture of 10 $\mu$m diameter, the 10X objective was found to have a 14.2 $\mu$m spot size, significantly greater than the 2.7 $\mu$m spot size of the 40X objective at the output facet. A large amount of the light will therefore not be confined unless the edge force is several times $10^6$ dyn/cm, as shown in figure 4.17.

The equipment set-up in figure 4.13 includes a mount for an expander lens at D to increase the beam width slightly to a few millimetres diameter at the input objective at the micropositioning stage. After careful choice and positioning of the expander lens, the
spot size (measured at half the maximum intensity) could repeatedly be focussed down to 4.2μm and 4.7μm with 1.15μm and 1.523μm light, respectively. This couples much more of the light into the waveguide, as is evident from figure 4.17 and will be used for all propagation loss measurements.

**Controlling Polarisation and Light Intensity**

The beams are linearly polarised as they exit the laser cavities. A half-wave plate was inserted into the beam at B in figure 4.13 to set the polarisation to any specified angle. Separate plates were used for the 1.15μm and 1.523μm light. By observing the red light reflection from the half-wave plate as it went back to E and F, the plate was always mounted at 90° to the light beam.

It was also often required to reduce the light intensity to protect the camera or to stay within the range of the photodetector. For this purpose neutral density filters were inserted at C. A special mount ensured that the filters were inserted normal to the light beam.

**Camera and Accessories**

The camera used is a Kestrel 25 from RT Labs, and is sensitive to light in the visible and near infrared spectrum. It is connected through a video analyser (Video Analyser 321 from Colorado Video Inc.) to a video monitor, where the image incident on the camera is displayed in real time. The analyser adds an intensity plot to the image, which can be set vertically or horizontally, and can be output on an X-Y plotter.

Additionally, the output from the monitor can be connected to a computer with Par­allax video processing equipment, which allows the monitor display to be stored as a computer image. However, the camera is much more sensitive to light at 1.15μm than at 1.523μm, making the plots recorded at 1.523μm more noisy than those at 1.15μm.

**'Tracer' - A digitising program for hard copies**

It is often required to change the scale of the axes on the intensity plots from the X-Y plotter, so that different plots can be compared on the same axes. Since the output from the analyser is analogue, a C++ program was written to digitise hard copies from the plotter. By first reading the plots with an optical scanner, the picture is saved as a portable bitmap file. The C++ program goes into the bitmap file and extracts the plot as X-Y tabular data. A listing of the program, named 'Tracer', is included in appendix C.

All the plots in chapter 5 have been generated from hard copies using Tracer and a data presentation computer program.

**4.6.3 Photodetector Diode Set-Up and Calibration**

The waveguide propagation losses will be found, as explained above, by end-fire insertion measurement. As well as positioning the equipment correctly, considering all angles, reflections and modal mismatch, the diode arrangement itself is important. Basically, the aim is to have a photodiode detecting the light incident upon it and outputting a value for the light intensity with high accuracy.

For this purpose, a germanium photodiode was set up as shown in figure 4.18. The following considerations were made for this diode arrangement:
1. **Reverse biasing of diode.** The total current in a photodiode is given by [115]

\[ I = I_{\text{photo}} + I_{\text{dk}} \left( e^{\frac{V_o}{kT}} - 1 \right) \]  

(4.17)

where \( I_{\text{photo}} \) is the photocurrent, \( I_{\text{dk}} \) is the dark current, \( V_o \) is the voltage across the diode junction, \( q \) is the charge of an electron, \( k \) is Boltzmann’s constant and \( T \) is the temperature in degrees Kelvin.

The photocurrent is linear with incident light irradiance \( I \) according to

\[ I_{\text{photo}} = \frac{\eta I_0 A q \lambda}{hc} \]  

(4.18)

and is additive to the diode current. Here \( \eta \) is the proton absorption quantum efficiency, \( A \) is the irradiated area of the diode, \( \lambda \) is the light wavelength, \( h \) is Planck’s constant and \( c \) is the velocity of light in a vacuum.

In figure 4.18 the diode was connected in reverse bias, making the dark current the reverse leakage current of the diode, which is small and relatively linear. The circuit was powered by a battery to avoid any feed-through of alternating current. This set-up should provide a current output linearly related to the input light intensity according to equation 4.18, with a constant offset due to the reverse leakage current.

2. **Current measurements.** The circuit was set up to take current, rather than voltage readings, because the voltage varies logarithmically with intensity, while the current response is linear. The ampere meter used was rated to detect currents in the range 1pA-1mA. The circuit was designed to have an output in the upper decades of this range, so as to avoid current noise problems when detecting low light intensities. For a saturated diode, i.e. when the diode is practically short-circuited, the maximum current can be seen from figure 4.18 to be approximately

\[ \frac{9V}{47K\Omega + 100K\Omega} \approx 60\mu A \]  

which corresponds well with actual readings.

Practical readings using this circuit proved to be stable down to a few nA. This provided a detection range of around four decades, or 40dB.
3. Zeroing potentiometer. There was a certain amount of current drift in the circuit due to the decrease in supply voltage with time, and due to the drift within the ampere meter. A zeroing potentiometer was included as shown to compensate for this drift, as well as the mismatch in components and leads. All measurements in this project were made with the initial current reading being adjusted to within ± 5 nA.

Calibration

Having set up the circuit as in figure 4.18, a recently calibrated light power meter was used to check the current readings of the ampere meter versus the intensity detected by the power meter. A beam splitter was inserted into the light beam just in front of the photodetector in figure 4.13, and the power meter was mounted to detect the reflection from the beam splitter. In this way, the readings from the two meters could be taken at the same instant, using neutral density filters in the light path to change the intensity. The results from the calibration readings are presented in figure 4.19, showing a highly linear response over several orders of magnitude. The standard error on the mean in figure 4.19 is 2.9% for 1.15μm and 4.6% for 1.523μm.
4.7 Waveguide Measurements

Two basic types of waveguide measurement are performed in this project. Firstly the mode profiles of the waveguides are plotted from the camera image using the video analyser and X-Y plotter shown in figure 4.13. In terms of the aim of the project these are the most important measurements, since they will show whether photoelastic waveguides can be made in bulk silicon and Si$_{1-x}$Ge$_x$/Si heterostructures, and whether they perform according to the modelling in chapters 2 and 3. Secondly, the propagation losses are found from insertion measurements. The loss measurements are important to determine whether this type of waveguide could be of practical use in optical circuitry.

4.7.1 Plotting Waveguide Mode Profiles

Using the equipment set-up in figure 4.13 the sample is mounted on the micro-positioning stage, as shown in figure 4.14, and the input and output objectives are adjusted to focus the waveguide output on the camera. The initial focussing is made with the red light for alignment. After switching to infrared light, the micropositioning controls at the focussing objectives, the sample and the mirror at E are repeatedly tuned to improve the image on the TV monitor.

The camera signal passes through a video analyser which generates a plot along any specified horizontal or vertical line drawn through the image. This intensity trace is output on the X-Y plotter. It is found practically that the intensity of the photoelastic waveguide modes is quite sensitive to the focussing conditions, while the modal profiles are not. The shape of individual intensity modes is therefore not a function of the system or focussing conditions. However, the size of the image seen by the camera which depends on the equipment configuration is regularly calibrated by focussing light through an electron microscope aperture of diameter 10±1/μm. This introduces an uncertainty of ±10% to the width and depth of the intensity plots. The same aperture was used to calibrate the system every time, so this should not introduce any relative uncertainty between different plots.

For the plots where the relative intensity between different modes is important, it has been attempted to initially focus on both or all modes and record their relative maximum intensity using the video analyser. Subsequently, it is focussed on the individual modes, and their relative intensities are plotted to best represent what is seen by the camera. There is nevertheless an uncertainty in the relative intensity of different modes, which cannot be quantified well.

4.7.2 Propagation Loss Measurements

As the light travels through the waveguide, the power $P(0)$ entering a waveguide at the facet will have reduced to a power $P(z)$ after travelling a distance $z$. The loss in dB/cm is found from

$$\frac{10 \log \left( \frac{P(z)}{P(0)} \right)}{z(\text{cm})} = \text{loss in dB/cm} \tag{4.19}$$

The losses are found from insertion measurements, where light is focussed through the sample and onto the camera in the same way as for the profile plots. The photodetector
at A in figure 4.13 is mounted on a micropositioning stage and is moved in front of the camera to record the intensity of light passing through the sample. Subsequently, the intensity is recorded with the sample removed, and the waveguide propagation losses are found from the ratio of the two readings, according to equation 4.19.

The insertion loss measurements involve a number of correction factors and system-related uncertainties, which determine the accuracy of these readings. The factors considered for the losses recorded here are explained below.

1. Since the losses depend on the difference between $P(z)$ and $P(0)$, they must be recorded under the same conditions. Therefore, after recording the output from the waveguide, the sample is removed, and only the output objective is used to focus onto the photodiode. This is done to avoid differences in the alignment of mirrors, input objective and the beam optics at B, C and D in figure 4.13, which can significantly affect the input power level.

2. The photodiode current readings relate linearly to the power incident on the diode, as shown in figure 4.19, so that the ratio of the currents recorded with and without the sample equals the corresponding power ratio. However, there is a standard error on the mean of the linear fit in figure 4.19 of 2.9% for 1.15μm and 4.6% for 1.523μm. For a three standard error accuracy on the readings both with and without the sample, the loss ratio $10\log\left(\frac{P(z)}{P(0)}\right)$ has an uncertainty of ±0.77dB at 1.15μm and ±1.21dB at 1.523μm.

3. The ampere meter readings for all the measurements taken here were stable over a period of several minutes to better than ±2% or ±0.09dB. This represents the power fluctuations of the lasers. For currents of less than 100nA, the reading accuracy becomes poorer. All measurements were therefore set up to give readings in the current range shown in figure 4.19. The fluctuations and drift shortly after switching on the equipment can be strong. Both the lasers and ampere meter are therefore switched on >30min before performing loss measurements. After recording the output from the sample, the corresponding measurement without the sample is recorded within 5-10 minutes, since the power output of the laser over periods >30min can vary more than ±2%. These fluctuations may also represent some of the spread of the photodiode linearity measurements in figure 4.19, which were performed over more than two hours.

4. Light focussed onto the waveguide facet will reflect back according to the Fresnel reflection equation (eq. 3.18), which assumes a normal incidence onto the facet. For 1.15μm and 1.523μm there will be losses of 1.67dB and 1.60dB, respectively, as calculated in section 3.6. According to section 4.4.1 the facet is polished at 90° to the direction of the waveguide, with a tolerance of ±1° in the vertical direction and ±0.5° in the horizontal direction. In the equipment set-up in figure 4.13 the mirror at E is mounted on a precision kinematic mount, which controls the light entering the input objective. As well as improving the focussing of the beam, this gives angular control of the light focussed onto the waveguide facet. For small changes in the facet angle, the light can still reach the facet at a normal angle. Therefore, when the light detected by the photodiode is at an optimum it will be assumed here that the light focussed onto the input facet is practically at normal incidence, and that the reflections are well described by equation 3.18. These Fresnel losses must be subtracted from the measured losses.
5. The length of the waveguide is required to find the propagation losses in dB/cm, according to equation 4.19. The length of each waveguide specimen is measured on a sliding microscope to within ±5μm. Since the shortest waveguides investigated here are approximately 3.5mm, the uncertainty due to the sample length is ±0.15% or less.

6. In addition to the Fresnel reflections, the measured losses must be corrected for the mode mismatch between the light focussed onto the waveguide facet and the guided modes, as calculated in figure 3.23. It was decided in section 4.6.2 to use a 10X lens with which the spot size can be focussed down to 4.2μm and 4.7μm with light of 1.15μm and 1.523μm, respectively, with corresponding losses of respectively 3.4dB and 3.7dB. There is also a tolerance in the horizontal and vertical movement of the micropositioning stage of 0.3μm, corresponding to an additional 0.05dB. The positioning tolerance can only increase the measured losses, and is therefore only a negative uncertainty.

7. In some waveguides there is poor separation between the edge modes and the substrate modes, making it difficult for the photodiode to detect only the edge mode without noise from the substrate. Nevertheless, it is often possible to determine the effect of the substrate noise to within a range by careful positioning of the photodiode. This has been done in figure 5.20, where the effect of substrate coupling is measured.

Formalised Measurement Procedure

Having prepared the waveguide specimens and equipment, and having measured and calculated the various correction factors and uncertainties, the measurement procedure is formalised as follows:

1. The overall uncorrected measurement losses are found from the photodetector current reading with the sample, $I(z)$, and without the sample, $I(0)$, as

   $\text{Uncorrected losses} = 10\log \left( \frac{I(z)}{I(0)} \right)$

2. Fresnel reflections and mode mismatch losses, representing what is not coupled into the waveguide, are subtracted. They amount to

   \[
   \begin{array}{ll}
   1.15\mu m & 1.523\mu m \\
   \text{Fresnel} & 1.67\text{dB} \quad 1.60\text{dB} \\
   \text{Modal mismatch} & 3.44\text{dB (TM)}, 3.55\text{dB (TE)} \quad 3.68\text{dB (TM)}, 3.78\text{dB (TE)}
   \end{array}
   \]

3. Measurement uncertainties are accounted for:

   \[
   \begin{array}{ll}
   1.15\mu m & 1.523\mu m \\
   \text{Diode linearity} & \pm0.77\text{dB} \quad \pm1.21\text{dB} \\
   \text{Power fluctuations} & \pm0.09\text{dB} \quad \pm0.09\text{dB}
   \end{array}
   \]
4. Losses with uncertainties are normalised to the sample length, to give losses in dB/cm. There is a small tolerance on the sample length measurement, giving an extra uncertainty to the losses. Finally, the positioning of the sample adds an uncertainty to the Fresnel reflections, which can only make the measurement poorer than the actual value.

<table>
<thead>
<tr>
<th>Sample length</th>
<th>1.15μm</th>
<th>1.523μm</th>
</tr>
</thead>
<tbody>
<tr>
<td>±0.0065 dB</td>
<td>±0.0065 dB</td>
<td></td>
</tr>
<tr>
<td>Sample positioning</td>
<td>-0.05dB -0.05dB</td>
<td></td>
</tr>
</tbody>
</table>

In addition to these corrections and uncertainties, the spread of the actual measurements are included in the results in chapter 5.

4.8 Summary

This chapter has discussed the fabrication of photoelastic waveguides, as well as characterisation of stressor films and waveguide profile and propagation loss measurements.

The waveguide fabrication, which includes plasma-deposition of SiNy onto bulk silicon or Si_{1-x}Ge_{x}/Si heterostructures, polishing of waveguide facets and definition of stressor stripes by photolithography and etching, was described in detail. The definition of stressor stripes all the way to the waveguide facets turned out to be the toughest challenge in the entire project, and no waveguide measurements could be made until the problem was solved. The problem arose due to the build-up of photoresist at the edges of the samples, so the stripes could not be well defined at the facets. A solution was eventually found by extending the waveguide surface with black wax, which is liquid when heated and runs into close contact with the specimen through the capillary effect, and becomes solid when at room temperature. This procedure may well become useful in other applications where photolithographic patterns must be defined close to facets.

An simple interferometer was set up to measure the curvature of samples, from which the edge force of stressor stripes can be calculated. The interferometer is useful in that it uses few components, and is used together with the attenuation measurement set-up, which can be turned into an interferometer in a matter of minutes. It also allows simple operation and accurate measurements. This set-up is useful for small-scale research, where it is preferable not to tie up space and equipment in dedicated measurement systems.

A detailed description was given of a waveguide measurement system, which allows propagation loss measurements and profile plots. It is also possible to save the waveguide output seen by an IR video camera as computer images. The reasons for the arrangement and the choice of components were presented, and measurement uncertainties were calculated for the set-up with due consideration of the uncertainties of the waveguides themselves.

From numerical aperture calculations it was concluded that high numerical aperture (N.A.≈0.6) objectives are not practical for coupling into photoelastic waveguides in bulk silicon, because the required stressor edge force would need to be impractically high. The measurements in this project are therefore taken using a 10X input objective with a numerical aperture of 0.17.
Chapter 5

Experimental Results

This chapter presents the experimental results of the characterisation of photoelastic waveguides in bulk silicon and Si$_{1-x}$Ge$_x$/Si heterostructures which were fabricated and measured as described in chapter 4. The results also include measurements of SiN$_y$ stressor films investigated by interferometry, as explained in section 4.3, showing the effect of film thickness and annealing temperature. Before assessing the measured results, it is useful to recap the aims of the experimental investigation, which include the main aims stated in chapter 1 as well as an evaluation of several of the modelling results from chapters 2 and 3, as presented below.

The main aims of the project were specified in chapter 1 as investigating whether photoelastic optical waveguides can be realised in bulk silicon and Si$_{1-x}$Ge$_x$/Si heterostructures, due to the compatibility of both the waveguide technology and the material systems with optoelectronic fabrication and integration. Of particular interest are the photoelastic waveguides in bulk silicon, since they will show whether optical channel waveguides can be realised using only photoelastic confinement, with no additional confinement from planar structures, which has not yet been demonstrated in any material. It will also be investigated whether the waveguides are useful for low-loss waveguiding, which is important if they are to be seen as a real alternative to other types of waveguide.

The modelling in chapters 2 and 3 revealed several characteristics of photoelastic waveguides in bulk silicon and Si$_{1-x}$Ge$_x$/Si heterostructures which it would be useful to investigate experimentally to find out whether the modelling accurately describes the waveguide behaviour. Some of these experimental results which are usefully compared with the modelling are

1. Differences in propagation losses at 1.15µm and 1.523µm. The phonon-assisted absorption at the energy band-edge is predicted to give an increase in propagation losses at 1.15µm above those at 1.523µm, amounting to 3.9dB/cm for bulk silicon and 4.9dB/cm for bulk Si$_{0.987}$Ge$_{0.013}$. In Si$_{0.987}$Ge$_{0.013}$/Si heterostructures there will be an additional 1.0dB/cm due to the strain-induced shift of the absorption band-edge, as predicted in figure 3.7. As well as being an important consideration for the waveguide propagation losses, the strain-induced shift of the absorption band-edge, which increases significantly with germanium content, is a good indication of whether the structure is strained or relaxed along the Si$_{1-x}$Ge$_x$/Si heterojunction.

2. The birefringence of the photoelastic waveguides on (100) substrates with stressor stripes oriented along the [100] crystallographic axes investigated here is predicted to be very weak, compared to waveguides oriented along
the [110] axes where both calculations and measurements demonstrate strong birefringence [60]. A comparison of the TE and TM waveguide modal patterns will also give a good indication of the correctness of the photoelastic constants calculated in chapter 2.

3. The relative intensity of the middle mode to the edge modes in photoelastic waveguides in Si$_{1-x}$Ge$_x$/Si heterostructures is predicted to increase as the stressor stripe width becomes narrower, giving three modes of equal peak intensity for stripe widths of about 4.5 μm. It is predicted that the relative mode intensity for photoelastic waveguides oriented along the [100] crystallographic axis be virtually identical for TE and TM modes.

The results presented in this chapter are arranged to first show how the optical mode profiles of photoelastic waveguides in bulk silicon and Si$_{1-x}$Ge$_x$/Si heterostructures correspond to the modelling in chapter 3 in terms of mode size and relative intensity, wavelength dependence and birefringence. Subsequently, the waveguide propagation losses are presented together with an investigation into their strain dependence.

5.1 Optical Mode Profiles in Photoelastic Waveguides in Bulk Silicon

Waveguide specimens were first produced by depositing a nominally 0.6 μm thick SiN$_y$ layer onto a bulk silicon substrate. Using the surface extension method described in section 4.5.3, stressor stripes of widths 2 μm to 9 μm were defined from the SiN$_y$ layer using standard photolithography and wet etching. Most of the waveguide samples did not produce any output correlating to the modelling in chapter 3, which is probably because the strain generated by the as-deposited stressor is too low. The results and discussion in this section and in section 5.2 refer to waveguides with measurable output using the as-deposited stressor films. A study of the stressor films and how to improve the photoelastic strains is presented later in the chapter.

5.1.1 Horizontal Intensity Profiles

For each stressor stripe two separate modes were found whose maxima were separated by slightly more than the stripe width, corresponding to the edge modes calculated in figure 3.14. The experimental TM intensity mode profiles for stressor stripes of width 2 μm and 6 μm are plotted in figure 5.1, showing strong lateral confinement. The edge modes are generally fairly symmetrical, but slightly inclined towards the stressor edge. Similar profiles were found for both TE and TM modes.

In figure 5.2 a number of edge mode widths, measured at half the maximum intensity, are presented together with the calculated widths from figure 3.19. The experimental mode widths are seen to be greater than predicted by modelling by around 20-30%, although they follow the predicted trend. By fitting second-order functions to the measured data, the TE and TM edge mode widths were found to increase with stressor stripe width and approach maxima of about 2.3 μm and 2.4 μm, respectively. Notice that the stressor stripe width refers to the width of the photomask used to define the stripes. In practice, some of the stripes were tapered by up to 0.5 μm towards the facet due to the photolithography and etching processes.
Figure 5.1 Horizontal TM intensity plots from photoelastic waveguides in bulk silicon with stressor stripes of respectively 2μm and 6μm measured at 1.523μm [116]. The plots show intensity peaks corresponding to the edge modes predicted in chapter 3 where the edge modes extend a few microns outside the stripe width. For each waveguide, the two edge modes were separately focussed and plotted. The edge modes are generally fairly symmetrical, but slightly inclined towards the stressor edge.

The discrepancy between the modelled and experimental mode widths reflects the discrete nature of the modelling in chapter 3 where the distance between the nodes in the finite difference calculations was 0.5μm and linear interpolation was used between the nodes. A more accurate value for the mode widths can be found by remodelling the waveguide with a finer mesh. However, since the modelling in chapter 3 chose to consider a significant portion of the waveguide structure, a finer mesh was impractical when using ANSYS or XMAPLE due to their high demand for computer power.

In addition to the measured data in figure 5.2, some mode widths in the range 3.1-3.7μm were obtained for stressor stripe widths of 3μm and 6μm. These data points are not included in figure 5.2. An example of such wide edge modes is given in figure 5.1 where the measured profiles for the 6μm wide stressor stripe are 3.2μm and 3.6μm wide. Apart from their width, these modes have the same characteristics as other edge modes. From the modelling in chapter 3 it is clear that a change in the edge force will not induce a change of edge mode width of this magnitude. All the waveguides investigated in this section were also taken from the same silicon wafer, and the SiNy stressor film thickness was measured by ellipsometry to be constant to within ±3.7% across the entire wafer, so the film can be expected to be uniform. There is therefore some guiding property of these waveguides making a small number of edge modes more than 1μm wider than predicted.
Figure 5.2 Edge mode widths from photoelastic waveguides in bulk silicon measured at 1.523\(\mu\)m compared to the calculated widths presented in figure 3.19. The widths are measured at half the maximum mode intensity. It is found that the TM modes are on average slightly wider than the TE modes, as predicted, but that the modes for both polarisations are wider than predicted. The error bars show a three standard deviation spread in the measured data. As mentioned in the text, there were also some readings of mode widths in the range 3.1-3.7\(\mu\)m, which have not been included here.

by the modelling, which cannot be explained by differences in the stressor film thickness or edge force.

A comparison was made of the edge mode output from both facets of each waveguide, which due to the symmetry of the structure should be the same. It was found that the edge modes were generally wider than predicted only at one end of the waveguide, while both edge modes at one facet would be comparable in width. The reason why some edge modes are wider than predicted is therefore probably that the stripe strains close to one facet are poorly defined, due to the adhesion between the stressor and the silicon or because the stripe is poorly etched, so that the light is poorly confined and spreads out close to the waveguide facet. This may also be some of the reason why the measured edge mode widths in figure 5.2 are wider than predicted.
Figure 5.3 Outline of one of the edge modes in a photoelastic waveguide in bulk silicon compared to the experimental vertical intensity profile of a TM edge mode. The drawing on the left shows the outline of an edge mode and the substrate modes for a typical waveguide. The substrate modes appear as a number of lines which become wider and less intense with depth into the substrate, although their exact shape and intensity depend on the coupling into the waveguide. A measured TM intensity plot from a photoelastic waveguide with a 6μm wide stressor stripe is shown on the right, showing that the edge mode is well defined at the waveguide surface, while there is a significant amount of substrate coupling. There is normally about 10μm between the edge mode and the substrate modes. The vertical edge mode profile and the substrate coupling are similar for TE and TM modes.

5.1.2 Vertical Intensity Profiles

In the finite difference modelling in chapter 3 substrate coupling was not considered, because only the top 12μm of the waveguide structure was included in the model. It is found from waveguide measurements that there is significant coupling into the substrate and that the substrate modes appear approximately 10μm below the edge modes. Figure 5.3 shows the vertical TM profile of the edge mode in a photoelastic waveguide in bulk silicon with a 6μm wide stressor stripe. While the edge mode seems well defined at the top of the waveguide, the confinement is not strong enough to prevent a significant amount of substrate coupling with the as-deposited stressor films. The strains induced by the stressor films will be investigated further in sections 5.4 and 5.6 in an attempt to improve the waveguide confinement.

The vertical intensity profiles of the TE and TM edge modes are similar for a photoelastic waveguide with a 6μm wide stressor stripe as shown in figure 5.4. It is noticeable how the mode cuts off abruptly at the silicon/air interface, while it decays more slowly...
Figure 5.4 Vertical intensity profiles plotted through an edge mode in a photoelastic waveguide in bulk silicon with a 6μm wide stressor stripe. The measured depth of the edge mode at half the maximum intensity is here about 1.6μm for the TM mode and 1.75μm for the TE mode. By comparing a number of vertical intensity plots from different samples, it could not be concluded that the TE and TM are generally different in shape, although the measured depth of the TE mode was generally 5-20% greater than for the TM mode. It is noticeable how the mode cuts off abruptly at the silicon/air interface, indicated with a thin dashed line, while it decays more slowly into the substrate. Notice that the location of the waveguide surface and the relative intensity of the two profiles in this figure are estimated from the measurements, although they are not exact.

into the substrate, corresponding to the finite difference calculations in chapter 3. The vertical profile does not change in character with increasing stripe width, although it becomes slightly deeper, as shown in figure 5.5. It is seen that the measured mode depth is around 0.4μm greater than predicted, which reflects the discrete nature of the waveguide modelling, while it may also indicate that the strain-induced confinement is reduced close to the waveguide facet.

5.1.3 Summary of Optical Mode Profiles in Photoelastic Waveguides in Bulk Silicon

In this section it has been shown that photoelastic waveguides can be made in bulk silicon, and also that waveguides can be made using only photoelastic confinement.

It was found that the optical intensity profiles measured here agree well with the model presented in chapter 3, but that the edge modes are generally wider and deeper than predicted. This discrepancy reflects the discrete nature of the waveguide model,
Figure 5.5 Edge mode depths from photoelastic waveguides in bulk silicon measured at 1.523 μm compared to the predicted widths presented in figure 3.18. The depths are measured at half the maximum mode intensity. It is found that the TE mode depths are on average slightly greater than for the TM modes, as predicted, but that the modes for both polarisations have a greater depth than predicted. The error bars represent a three standard deviation spread in the measured data.

in which the intensity was determined at discrete nodes, separated by 0.5 μm. A more accurate solution could be found by reducing the distance between the nodes.

It was found that some modes were as wide as 3.1-3.7 μm which is about twice as wide as predicted. These wide modes were generally only found at one facet of a waveguide, and are expected to be due to poor adhesion or definition of the stressor stripe close to the facet, reducing the waveguide confinement. This may also explain in part the discrepancy between the measured and predicted mode size. It would be therefore be useful to model the intensity profiles at the facet in detail, since the waveguide coupling losses depend on the relative size of the guided mode and the incident beam.

These measurements show a low degree of birefringence, as expected from the modelling. This confirms that the photoelastic constants are similar, as calculated in chapter 2. With the assumption that the edge forces act away from the centre of the stripe, as shown in figure 3.4, the appearance of two edge modes rather than one under the middle of the stripe confirm that the photoelastic constants are positive, as can be deduced from equations 3.11 and 3.12 and figure 3.3. For the edge forces to act towards the stripe centre there must either be a strong inherent stress at the SiN/Si interface or the SiN must
have a greater thermal expansion than silicon. It will be shown in section 5.4 that neither occurs here.

All the discussion in this section has been concerned with profiles at a wavelength of 1.523\(\mu\)m, showing only single mode behaviour in each edge waveguide. At 1.15\(\mu\)m there is a tendency for a second order mode to occur, and this will be considered in section 5.2.3 together with the photoelastic waveguides in Si\(_{1-x}\)Ge\(_x\)/Si heterostructures.

Although photoelastic waveguides can be fabricated in bulk silicon with well defined edge guiding regions, as demonstrated here, the results show a significant amount of substrate coupling. This indicates that the stressor layer does not produce a significant amount of strain. The waveguides with the as-deposited stressor films are therefore poorly confined and lossy. One way of improving the waveguide confinement is to increase the forces generated by the stressor by annealing, which will be investigated in section 5.4. Another method of reducing the substrate coupling is by defining the photoelastic waveguide within a Si\(_x\)Ge\(_{1-x}\)/Si heterostructure, which is investigated in section 5.2.

5.2 Optical Mode Profiles in Photoelastic Waveguides in Si\(_{1-x}\)Ge\(_x\)/Si Heterostructures

From the modelling in chapter 3 photoelastic waveguides in Si\(_{1-x}\)Ge\(_x\)/Si heterostructures are expected to be similar to the silicon waveguides in terms of the edge modes, but there will be an additional mode under the middle of the stressor stripe. The additional confinement due to the planar structure is also expected to virtually eliminate the substrate coupling from the edge modes. This section will investigate the middle mode and the substrate coupling, as well as the effect of wavelength on the mode profiles.

5.2.1 The Middle Mode

Waveguides were fabricated by depositing a 0.6\(\mu\)m thick SiNy layer onto a Si\(_{0.987}\)Ge\(_{0.013}\)/Si heterostructure, and defining the facets and stressor stripes as explained in chapter 4. The Si\(_{0.987}\)Ge\(_{0.013}\) layer thickness was 8\(\mu\)m. Apart from the introduction of the planar layer, the specimens were similar to the silicon waveguides investigated in section 5.1.

The measured horizontal profiles were similar to that of the silicon samples, with an additional mode between the edge modes for narrow stressor stripes, as predicted. Figure 5.6 shows the TM output of waveguides with 2\(\mu\)m and 6\(\mu\)m wide stressor stripes, corresponding to figure 5.1 for the silicon samples. The middle mode generally lies 1.5-2\(\mu\)m below the edge modes.

The relative mode intensity, defined here as the peak intensity of the middle mode divided by the peak intensity of the edge modes, was predicted in chapter 3 to increase with reducing stressor stripe width, and all modes would be of the same intensity for a stripe width of about 4.5\(\mu\)m. In figure 5.7, the predicted relative mode intensity has been calculated for an 8\(\mu\)m thick Si\(_{0.987}\)Ge\(_{0.013}\) layer on a silicon substrate, similar to the plot in figure 3.21. The calculated effect of optical wavelength and polarisation on the relative mode intensity is less than \(\pm 0.1\) for all stripe widths, and is not shown in figure 5.7. The experimental data show that the middle mode does increase as the stressor stripe becomes narrow, but that a relative mode intensity of unity is found for stripe widths of 2.5-3\(\mu\)m. For stripe widths of 6\(\mu\)m and 9\(\mu\)m no middle mode was observed, while for widths < 2.5\(\mu\)m the middle mode dominates and the edge modes decrease.
Figure 5.6 Horizontal TM intensity plots from photoelastic waveguides in Si$_{0.987}$Ge$_{0.013}$/Si heterostructures [117] with stressor stripe widths of respectively 2μm and 6μm measured at 1.523μm. The plots are similar those in figure 5.1, but for the 2μm stripe there is an additional mode under the middle of the stripe. The middle mode, shown here as a dashed line, is generally located 1.5-2μm below the edge modes.

The reason for the discrepancy between the predicted and experimental results is not clear. One possible explanation is that since all the modes were focussed and plotted separately, the coupling between the different guiding regions reduced the intensity of the middle mode relative to the edge modes. However, this cannot be determined from these measurements since all waveguide specimens studied here are of the same length, approximately 6mm. Since the introduction of a variable middle mode poses interesting possibilities for couplers and splitters, as is further discussed in chapter 6, the relative mode intensity is a convenient parameter for the design of devices. It would therefore be useful both to improve the waveguide model and to investigate experimentally the coupling between the guiding regions further.

The results generated by the finite difference model, such as those shown in figure 3.16, did indicate that two or more small maxima could occur between the edge modes. Though these higher-order modes are mathematical solutions to the waveguide intensity distribution, these effects were not seen in any of the waveguide specimens, possibly due to the high loss of these modes.
Figure 5.7 The relative intensity of the middle mode to the edge modes in photoelastic waveguides in Si$_{0.987}$Ge$_{0.013}$/Si heterostructures increases with a reduction in stressor stripe width. The measured data, presented here as stars, show that all modes have the same maximum intensity for a stripe width of 2.5-3 μm, while according to the modelling results, shown as a solid line, this should happen for a stripe width of approximately 4.5 μm. The experimental data include TE and TM measurements taken at 1.15 μm and 1.523 μm, although the data show no dependence on wavelength or polarization, which is consistent with the modelling.

5.2.2 Vertical Confinement and Substrate Coupling

The results presented in section 5.2.1 were from photoelastic waveguides defined in an 8 μm thick Si$_{0.987}$Ge$_{0.013}$ layer. Having seen that the substrate modes for the bulk silicon waveguides start approximately 10 μm below the edge mode, it was expected that this 8 μm thick planar layer would eliminate the substrate modes. However, as shown in figure 5.8, the vertical intensity profile changes significantly. While the width and depth of the edge mode profile do not change significantly, the Si$_{0.987}$Ge$_{0.013}$ layer is thick enough to allow one or two modes under the edge mode in the Si$_{0.987}$Ge$_{0.013}$ layer. This is also the case for the middle mode, whose maximum is generally 1.5-2 μm below the edge modes. The intensity of these additional modes vary strongly, and reflects that the strain induced by the stressor stripes varies between waveguides. A more appropriate thickness of the planar layer to avoid these additional modes would be 3-4 μm.

Since the middle mode according to chapter 3 requires the confinement from both the edge modes and the heterojunction, it is useful to see whether the middle mode can be supported in a thicker layer. Photoelastic waveguides were therefore fabricated as previously in a Si$_{0.987}$Ge$_{0.013}$/Si heterostructure where the planar layer was approximately 14 μm thick. While these structures support the edge modes, the middle mode was not
observed in any of them. However, with a thicker planar layer, the extra mode under the edge mode becomes less pronounced, as shown in figure 5.9. This comparison of photoelastic waveguides in Si$_{0.987}$Ge$_{0.013}$ layers of different thicknesses indicates that there is a limit to the thickness of the planar layer for the middle mode to be confined, and that this limit lies between 8µm and 14µm.
5.2.3 The Effect of Wavelength on Mode Profiles

According to the modelling in chapter 3, there should not be much difference between the intensity profiles measured at 1.15μm and 1.523μm. In practice there is often an indication of a small second order mode outside the main edge mode away from the stressor stripe for measurements taken at 1.15μm. This can be seen both in the bulk silicon and in the Si0.987Ge0.013 structures. Figure 5.10 presents horizontal TM profiles from photoelastic waveguides in Si0.987Ge0.013/Si heterostructures where the second order mode is clearly present. Although the second order mode is often not as evident as here, it clearly distinguishes these profiles from those taken at 1.523μm, which are generally single mode. The appearance of a second order mode makes the waveguides less useful for general waveguiding at 1.15μm than at 1.523μm, because the guided mode will be difficult to match to other waveguides and devices.
The reason why the second order mode was not predicted in chapter 3 is again probably the relatively coarse meshing of the waveguide model. The distance between nodes in the model was 0.5\(\mu\)m, which is seen to be quite large compared to the dip between the main edge mode and the second order mode in figure 5.10.

![Horizontal TM intensity plots from photoelastic waveguides in Si\(_{0.987}\)Ge\(_{0.013}\)/Si heterostructures at 1.15\(\mu\)m, for stressor stripes of respectively 2\(\mu\)m, 2.5\(\mu\)m and 9\(\mu\)m. The modes set up at 1.15\(\mu\)m tend to show a second order mode outside the edge mode, which is not seen at 1.523\(\mu\)m. It is seen that the middle mode, shown here as a dashed line, has roughly the same peak intensity as the edge modes for a stripe width of 2.5\(\mu\)m.](image)

5.2.4 Summary of Optical Mode Profiles in Photoelastic Waveguides in Si\(_{1-x}\)Ge\(_x\)/Si Heterostructures

It has been shown in this section that photoelastic waveguides can be made in Si\(_{1-x}\)Ge\(_x\)/Si heterostructures, and that they are similar to those made in bulk silicon in terms of the edge modes, while there is an additional middle mode under the stressor stripe, in accordance with the modelling. As the stressor stripe becomes narrower the intensity of the middle mode increases relative to the edge modes. According to measurements all modes have the same peak intensity for a stripe width of 2.5-3\(\mu\)m, while this was predicted by modelling to happen for stripe widths of approximately 4.5\(\mu\)m. The reason for this discrepancy is not clear from the modelling or measurements, although it may reflect the coupling between the middle and edge guiding regions. Since the introduction of a variable middle mode poses interesting possibilities for couplers and splitters, as discussed in chapter 6, the relative mode intensity is a convenient parameter for the design of devices.
It would therefore be useful both to improve the waveguide model and to investigate experimentally the coupling between the guiding regions further.

The relative peak intensity of the middle mode to the edge modes was not found to depend on light wavelength or polarisation, in accordance with the modelling. This also supports the conclusion from section 2 that the photoelastic constants $p_{11}$ and $p_{12}$ be similar in magnitude.

It was attempted to remove the substrate modes which in photoelastic waveguides in bulk silicon typically start $\sim 10\mu m$ below the edge modes by fabricating the waveguides in a $Si_{0.987}Ge_{0.013}/Si$ heterostructure with an $8\mu m$ thick $Si_{0.987}Ge_{0.013}$ layer. While this virtually eliminates the coupling into the silicon substrate, it introduces one or two additional modes within the planar layer, under the edge and middle modes. It is concluded that an appropriate planar layer thickness to avoid these additional modes would be $3-4\mu m$. An increase in the $Si_{0.987}Ge_{0.013}$ layer thickness to $14\mu m$ makes these additional modes less apparent, although the middle mode disappears. This shows that there is a maximum limit for the planar layer thickness of between $8\mu m$ and $14\mu m$ beyond which the middle mode will not be supported.

At $1.15\mu m$ a second order mode tends to appear outside the edge mode, while the edge modes are generally single mode at $1.523\mu m$. The appearance of a second order mode makes the waveguides less useful for general waveguiding at $1.15\mu m$ than at $1.523\mu m$, because the guided mode will be difficult to match to other waveguides and devices.

### 5.3 Losses

Sections 5.1 and 5.2 showed that photoelastic waveguides in bulk silicon and $Si_{1-x}Ge_x/Si$ heterostructures can be made and that their performance is fairly well described by the modelling in chapter 3. With these results, two of the main aims of this investigation have been covered. However, for the waveguides to be of practical use in optical circuits, they need to have low propagation losses. In chapter 1 results were presented for waveguides in both silicon and $Si_{1-x}Ge_x$ structures as well as for photoelastic waveguides in various structures with losses around $1dB/cm$ showing the loss levels which are achievable. Comparable loss levels should be achieved for the photoelastic waveguides investigated here, if they are to be considered for use in optical circuits.

It is not important here whether the materials chosen for these particular waveguides are lossy, since it has already been shown experimentally that both silicon and $Si_{1-x}Ge_x$ waveguides can be low-loss. What is important is the magnitude of the excess losses, which are the losses in excess of the material losses. It is therefore useful to measure the material losses separately from the excess losses of the photoelastic waveguides, which makes it easier to determine the various loss mechanisms.

#### 5.3.1 Material Losses in Bulk Silicon

The material losses are the intrinsic absorption losses of the materials, which do not depend on the waveguide structure. It depends on the free carrier concentration, giving losses of $0.022dB/cm$ and $0.039dB/cm$ at $1.15\mu m$ and $1.523\mu m$, respectively, as calculated in section 2.4. Due to the phonon-assisted absorption at the minimum energy bandgap, there will be additional losses at $1.15\mu m$, amounting to $3.9dB/cm$ for bulk silicon. There may also be absorption due to poor crystal quality or impurities, which is difficult to quantify without measurements.
The losses of bulk silicon are found here by focusing light through the substrate. This avoids problems associated with coupling into a small waveguide, numerical aperture, modal matching and scattering from sidewalls. It should therefore give a good measure of the material losses without most of the uncertainties.

Light was focused through the samples with a 10X objective with a numerical aperture of 0.17 with a beam expander lens as described in section 4.6.2. The width of the planar modes emerging from the waveguide output facet depends on the input focus. For wide outputs, a series of readings were taken by moving the photodiode along the transverse direction of the waveguide in steps of 1.3mm, the width of the diode, and adding the readings to give the total output. It was found that the total losses do not change with the width of the output. For the losses reported here, the output was made as narrow as possible.

The measured losses for the bulk silicon are given in figure 5.11(a). It is seen that the losses are of the order of 9-12dB/cm, which is much higher than expected, and which is probably due to impurities and poor crystal quality. It is useful to compare these losses to waveguide propagation losses reported in thermally regrown SOI structures, which had losses of 10-20dB/cm, while the same waveguides made in higher quality bond-and-etchback SOI had losses down to 1.5dB/cm [60], showing that the material quality can significantly affect the losses.

Figure 5.11 Material losses in (a) the bulk silicon samples and (b) in Si$_{0.987}$Ge$_{0.013}$/Si heterostructures with Si$_{0.987}$Ge$_{0.013}$ layer thicknesses of 8µm and 14µm. The three standard deviation spread in the measured data lies in the range ±1.5-2.7dB/cm for all points, but is not shown in figure (b) for the sake of clarity. There are also reading uncertainties of about ±1.4dB/cm at 1.15µm and ±2.2dB/cm at 1.523µm, which are applicable to all the measurements.
5.3.2 Material Losses in Si_{1-x}Ge_x/Si Heterostructures

Material losses were also recorded for the Si_{0.987}Ge_{0.013}/Si heterostructures, where light was focussed through the planar layers. Relatively thick Si_{0.987}Ge_{0.013} layers of 8\mu m and 14\mu m were used. This is much larger than the minimum spot size of the input beam, so that there is no difficulty involved in coupling into the waveguides. There are up to six planar modes in the planar waveguides, although all loss measurements were made by exciting only the fundamental mode. However, the losses are likely to be higher than for the bulk silicon, due to scattering at the Si_{0.987}Ge_{0.013}/Si interface.

The measured losses for the Si_{0.987}Ge_{0.013}/Si heterostructures are given in figure 5.11(b), and are seen to be even higher than for the bulk silicon. Other measurements were made on Si_{0.987}Ge_{0.013}/Si planar guides on the same measurement equipment with losses down to approximately 4dB/cm at 1.523\mu m, showing that the losses are not generated by the system. However, it is not important here that the materials are lossy, since the aim of the investigation is to find the excess losses of the photoelastic waveguides, and the waveguides can always be made from higher quality materials. The material losses are therefore only recorded as reference data for the further investigation.

In figure 3.7, the phonon-assisted absorption at 1.15\mu m was calculated to be 4.9dB/cm, which is higher than for bulk silicon. In addition, the Si_{0.987}Ge_{0.013} layers are expected to have losses of 1dB/cm due to the lattice mismatch strain. The measurement results show that the absorption at 1.15\mu m is always higher than at 1.523\mu m, as expected from the modelling. The measured difference is on average 4.35dB/cm for the 8\mu m thick planar layers and 3.16dB/cm for the 14\mu m thick planar layers. Since the difference is over 1dB/cm higher for the 8\mu m thick planar layers than for the 14\mu m ones, it is likely that the thicker layers are relaxed, and do not show a strain-induced shift of the absorption band-edge. It is also interesting that all the measured differences, including that of 1.45dB/cm for bulk silicon, are much lower than expected from the modelling in figure 3.7. While the measurement uncertainty is about ±1.4dB/cm at 1.15\mu m and ±2.2dB/cm at 1.523\mu m, which could account for the discrepancy, it is likely that the difference is overestimated by the calculations in chapter 2 and 3.

5.3.3 Excess Losses in Bulk Silicon Photoelastic Waveguides

The material absorption is important to the waveguide performance, since it affects the total propagation losses, while a more useful attribute to determine is the excess losses. Ideally, when both the material absorption, Fresnel reflections and modal mismatch are accounted for, the excess losses should drop to zero, unless the waveguide confinement is poor.

The excess losses of the photoelastic waveguides were found using the same equipment and procedure as for the planar and substrate measurements in section 5.3.1. For each measurement, the material losses were determined in the same layer close to the photoelastic waveguide and were subtracted from the total losses. Subtracting the material losses also accounts for the Fresnel reflections. The minimum spot sizes of the focussed laser beam are 4.2\mu m and 4.7\mu m for 1.15\mu m and 1.523\mu m, respectively, and both are greater than the edge mode width and depth. During the loss measurements the light will therefore be focussed to its minimum size, and the modal mismatch values subtracted from the readings correspond to the minimum spot sizes. However, since the measured edge mode profiles were found to be slightly larger than predicted, the mode mismatch will be slightly smaller than predicted in figure 3.23. For an increase in the edge mode
width and depth of 30%, the predicted mode mismatch losses lie 0.8dB below the values listed on page 89. This difference has been accounted for in the results presented here.

Figure 5.12 presents the excess losses for photoelastic waveguides in bulk silicon. These rather high losses of 10-15dB/cm are mainly due to the lack of photoelastic confinement, causing a significant amount of substrate coupling. With such high losses these waveguides are not useful for practical applications. One possible method for reducing the substrate coupling is by annealing the structure to increase the thermal mismatch between the stressor and the guiding layer, and so improve the photoelastic confinement, which is investigated in section 5.4. Another way of reducing the substrate coupling is by defining the photoelastic waveguide in a Si$_{0.987}$Ge$_{0.013}$/Si heterostructure, as investigated in section 5.3.4. In section 5.3.4 there is also a further discussion of excess losses which applies to photoelastic waveguides in both bulk silicon and Si$_{0.987}$Ge$_{0.013}$/Si heterostructures.

![Figure 5.12](image)  
Figure 5.12 Excess Losses of photoelastic waveguides in bulk silicon and Si$_{0.987}$Ge$_{0.013}$/Si heterostructures with planar layer thicknesses of respectively 8μm and 14μm. The stressor layers are made from as-deposited SiNy films of 0.6μm thickness. It is seen that the TE and TM losses for all the structures are similar, implying low birefringence. The higher losses found at 1.15μm reflect an error in calculating the overlap mismatch, because the second order mode, as seen in figure 5.10, was not considered in the modelling. It was found practically that the waveguides in the 8μm thick Si$_{0.987}$Ge$_{0.013}$ layers had relatively small second order modes, explaining why the difference in losses at 1.15μm and 1.523μm is relatively small for these structures.
5.3.4 Excess Losses in Photoelastic Waveguides in Si$_{0.987}$Ge$_{0.013}$/Si Heterostructures

The excess losses of the photoelastic waveguides in Si$_{0.987}$Ge$_{0.013}$/Si heterostructures were measured in the same way as the bulk silicon structures, by determining the material losses close to each photoelastic waveguide and subtracting them from the total losses. Losses were measured in photoelastic waveguides in Si$_{0.987}$Ge$_{0.013}$/Si heterostructures with planar layer thicknesses of both 8µm and 14µm. Figure 5.12 presents the results together with those from the bulk silicon structures, showing that the excess losses are much lower. These results refer only to the edge modes, since the possibility of coupling into more than one guiding region as well as the coupling between different guiding regions are difficult to quantify when measuring the middle modes, which makes it difficult to draw conclusions from the results. It is seen that the excess losses for the waveguides with an 8µm thick Si$_{0.987}$Ge$_{0.013}$ layer are practically zero, which shows the potential of these waveguides if produced in good quality materials. No correlation was found between the excess losses and stripe width.

The results in figure 5.12 have a measurement tolerance of approximately ±1.4dB/cm and ±2.2dB/cm at 1.15µm and 1.523µm, respectively. There is also a significant spread in the measured losses for each type of waveguide structure, which is of the order of ±3dB/cm for ±3σ. However, by repeating loss measurements on some waveguides on four to six independent occasions, it is found that the readings were consistent to better than ±1.2dB/cm on each waveguide. This indicates that the large spread in measured losses reflects a real difference in the waveguides, rather than poor measurement technique. From the profile measurements it is already clear that the quality of the stressor stripes varies significantly even on the same waveguide specimen. It is therefore likely that the spread in the measured losses reflects the difference in waveguide confinement due to the differing stressor quality.

The measured excess losses at 1.15µm are generally higher than the corresponding losses at 1.523µm. This difference is found to be greater for waveguides with a significant second order mode, as shown in figure 5.10. Since the calculated intensity profiles did not reveal any second order mode, as discussed in section 5.2.3, the calculated mode mismatch is underestimated, which increases the losses calculated from the measurements. The increase in excess losses at 1.15µm therefore reflects an error in correcting for the mode mismatch, and not a difference in propagation losses. For small second order modes, the corresponding error is small, while for significant second order modes, the measurements show that the error can be as large as 2.5-3dB before normalising for sample length.

While the excess losses for the Si$_{0.987}$Ge$_{0.013}$/Si heterostructure waveguides are low, they are still significant for the bulk silicon structures. This reflects that the photoelastic confinement in itself is not strong enough to prevent strong coupling into the substrate, as shown in figure 5.3. Notice also that figure 5.12 presents the losses of the best waveguides, and that in many of the waveguides the output was not detectable due to a lack of photoelastic confinement generated by the stressor stripe. The strength of confinement is therefore a problem which will be investigated further later in the chapter.

In the Si$_{0.987}$Ge$_{0.013}$/Si photoelastic waveguides there is also a problem with the lack of photoelastic confinement. However, due to the additional confinement from the planar structure, the light is not lost into the substrate, but appears as a mode within the planar layer underneath the edge mode, as shown in figure 5.9. Even though the amount of light underneath the edge mode varies strongly depending on the photoelastic confinement, the
measured losses are not affected as long as light is only coupled into the edge mode. This is because the light under edge mode is also detected by the photodiode. Although the planar layer could be made thinner to match the size of the edge mode and so eliminate the light under the edge mode, the photoelastic confinement is weak, which will generate excessive losses in bends. This will make the waveguides impractical for most optical circuitry.

These measurements show that photoelastic waveguides in bulk silicon and Si_{1-x}Ge_x/Si heterostructures can be low-loss if fabricated in good quality materials. However, the photoelastic confinement generated by the as-deposited stressor films is weak. The remainder of this chapter investigates the effects of annealing the stressor film in an attempt to improve the photoelastic confinement.

5.4 Annealing of Stressor Layers

According to section 3.2, the strains generated by the stressor film represent the difference in thermal expansion between the stressor and the guiding layer as the structure cools down from the deposition temperature to room temperature. The significant substrate coupling and high losses of the photoelastic waveguides in bulk silicon show that the strains generated by the as-deposited stressor films do not provide strong confinement of light. In this section the strains generated by the stressor films are investigated by interferometry as explained in section 4.3, and the effects of film thickness and annealing are evaluated in an attempt to improve the waveguide strains. The results will also reveal whether there is a significant intrinsic (non-thermal) stress at the stressor/guiding layer interface and whether the stressor film regrows at the annealing temperature.

A study was made of as-deposited SiNy films of nominal thickness 0.3μm, 0.6μm, and 0.9μm, deposited by PECVD onto bulk silicon. For each film thickness, three samples of approximately 15mm by 15mm were made from the same deposited wafer. The radius of curvature of each sample was measured by interferometry as described in section 4.3, and is presented in figure 5.13 (a). It is found that the radius of the samples varies by almost two orders of magnitude, and is not obviously related to the film thickness. The corresponding stressor force, calculated from equation 4.9, is presented in figure 5.13 (b). This lack of consistency between the data, even between samples from the same wafer, indicates that the adhesion between the SiNy and the silicon is poor, so that some parts of the film are highly stressed, while other parts are more or less relaxed. There is no evidence from these measurements of an intrinsic interface stress. The strong variation in the force generated by the stressor films seen in figure 5.13 (b) is consistent with the waveguide results where many of the samples did not give a detectable output, indicating a weak or poorly defined edge force.

It is investigated here whether the poor stressor adhesion can be improved with annealing. If the interface between the stressor and the silicon can be well defined at the annealing temperature, the forces set up represent the thermal mismatch given by equation 3.10 which increases with annealing temperature. However, this will only happen if the stressor film regrows at the interface at the annealing temperature.

Initially, a few test anneals were performed at 300-400°C to determine roughly the annealing times required. It was found that annealing times in the range 5-30 minutes normally causes the film to break up into clearly visible fragments. Annealing times of the order of one minute or less did not generate any visible damage to the films, although it would generally cause a colour change of the SiNy, indicating either a change of film...
thickness or a change of SiNy material properties. From these tests it was decided to anneal the samples for 10, 30 and 60 seconds.

Using an 8kW optical furnace with a computer based temperature control, the samples measured in figure 5.13 were annealed at temperatures of 300°C, 400°C, 500°C, 600°C, 700°C and 800°C. Each sample was annealed for 10s, 30s or 60s, cumulatively at all temperatures, and curvature measurements were performed after each anneal. In addition to the annealing time, there is a set linear temperature rise time of 10s, and a furnace cooling time which increases with annealing temperature. The results here refer only to the time at the annealing temperature.

Figure 5.14 presents the stressor force calculated from interferometry measurements after different annealing times and temperatures. The error bars include all the accuracies and tolerances discussed in section 4.3. These results give some useful information about the SiNy films:

1. In general, the force generated by the as-deposited films is poorly defined and can be both positive and negative, although it is normally relatively weak.

2. The stressor force increases with annealing temperature, showing not only that the stressor film adhesion is good, but also that the film regrows at the interface at the annealing temperature.

3. Most samples generate a maximum stressor force after a 500°C anneal. After a 600°C anneal the force generally drops off, indicating that the stressor force becomes excessive, such that structure relaxes at the stressor/silicon interface.

4. A further anneal at 700°C gives ambiguous results, with some films generating increased forces. However, the forces generated are not greater than after the 500°C
Figure 5.14 The forces generated by SiN$_y$ stressor films deposited onto bulk silicon substrates measured by interferometry after annealing the specimens for respectively 10, 30 and 60 seconds. Each sample was annealed at every temperature, but at only one annealing time. The error bars include all the accuracies and tolerances discussed in section 4.3. The measurements show no distinct difference between films of thickness 0.3$\mu$m (dashed line), 0.6$\mu$m (solid line) and 0.9$\mu$m (dot-dashed line), indicating that the relaxation of the stressor force seen for most samples after the 600°C anneal occurs at the actual stressor/silicon interface, and does not represent the overall strength of the stressor film.
anneal. This may indicate that the films do not regrow at 700°C, although some films may regrow at a lower temperature during the cooling of the furnace.

5. After an 800°C anneal, the force generated by some films was practically zero (bending radii >200m) while other films were visibly cracking up or peeling off. Only two samples retained a force of >0.1 \(10^6\) dyn/cm.

6. The maximum stressor force found here was approximately 2-3\(10^6\) dyn/cm, with the best results found here for the 30s annealing time. From this small number of specimens it cannot be concluded that one film thickness or annealing time is distinctly better than the others.

It is interesting to analyse these results further. From equation 4.9, the stressor force \(F\) is the product of the stress in the film, \(\sigma_{\text{film}}\), and the film thickness \(t\). A thick film therefore has a relatively lower stress than a thin film, and it could be expected that the thick film would reach a higher stressor force than the thin film before relaxing. This is not shown by these measurements, which indicates that the stress relaxation occurs at the interface between the stressor and the silicon, and does not reflect the overall mechanical strength of the film which increases with thickness.

Other PECVD SiNy films reported by Blaauw [70] deposited at 500°C onto (111) silicon did not show any stress relaxation after one hour anneals up to 700°C. However, the forces generated by those films, which were 0.75\(\mu\)m thick, were only of the order of 0.15 \(10^6\) dyn/cm, which is well below the maximum forces seen here. Kirkby et al [55], studying SiO\(_2\)/Si\(_3\)N\(_4\) films plasma-deposited on GaAs at 500°C, measured forces of up to 0.25 \(10^6\) dyn/cm in 0.25\(\mu\)m thick films, which is still only 10% of the maximum forces measured here. Therefore, while the as-deposited films studied here are very poorly defined, the forces generated after a 500°C anneal are relatively strong. However, it is important to notice that the deposition parameters of plasma-deposited SiNy films strongly influence the film properties [109]. It is also known that annealing above 500°C affects the film properties [118]. Changes in the deposition and annealing procedure are therefore likely to affect the generated forces.

The small number of measurements made here are not intended as a thorough study of SiNy films, since the film properties will change with deposition and annealing procedures, although they do show the level of stressor force which is achievable. In this project the results are useful because the measurements were made on the same films as used in the waveguides studied here. By following the same annealing sequence with waveguide samples, the edge forces generated by the stressor stripes can be expected to be similar to those in figure 5.14.

5.4.1 Calculating the Absolute Values of Strain and Refractive Index Change

In chapter 3 there were few references to absolute values of photoelastic strains and refractive index changes, because the SiNy film properties were based on measured data from other sources, which could be inappropriate for the films studied here. There is also the problem of stress relaxation at the stressor/waveguide interface, which was not modelled in ANSYS. Having now measured the forces generated by the stressor films, it is interesting to find the corresponding absolute values of strain and refractive index change.

Assuming a stressor edge force \(F\) after annealing of 2-\(10^6\) dyn/cm and a 2\(\mu\)m wide stressor stripe, the horizontal (X) and vertical (Y) strains are approximated from equations 3.6
Figure 5.15 Horizontal (X) strains in a photoelastic waveguide in bulk silicon calculated assuming a stressor force of $2 \times 10^6$ dyn/cm, corresponding to the stressor forces measured in several samples in figure 5.14 after annealing. The strains are calculated at depths of 1-4µm into the bulk silicon layer, assuming a stressor stripe width of 2µm. It is seen that strains of the order of -0.001 exist close to the stressor stripe.

Using equations 3.11 and 3.12, the refractive index changes corresponding to the strains in figures 5.15 and 5.16 have been calculated in figure 5.17, with contours shown for positive refractive index changes of 0.006, 0.01 and 0.05. Notice that the compressive strains induce positive refractive index changes, according to equations 3.11 and 3.12. It is seen that regions of depth >1.5µm and width >2µm exist outside the stripe edges, with refractive index changes of 0.005 and greater. This should cause a significant confinement, considering that the refractive index step in the Si$_{0.987}$Ge$_{0.013}$/Si planar structures studied here is about 0.01.

Most of the as-deposited films in figure 5.13 generate forces of about $2 \times 10^5$ dyn/cm or less, which is only 10% of the force generated after annealing at 500°C. Since the refractive index changes relate linearly to the edge force, the contours relating to a refractive index change of 0.005 in figure 5.17, will correspond to only 0.0005 for most of the as-deposited stressor films, providing rather poor confinement, while a refractive index change of 0.005 is only seen within the regions marked C, which are too small to use as practical waveguides.

These measurements and calculations imply that annealing of photoelastic waveguides will reduce the substrate coupling and the corresponding propagation losses. In section 5.6, waveguides are put through the same annealing sequence as the stressor films investigated here to see whether the rather high losses and strong substrate coupling found for the unannealed waveguides can be improved. However, before looking at the optical confine-
Figure 5.16 Vertical (Y) strains in a photelastic waveguide in bulk silicon calculated assuming a stressor force of $2 \times 10^6 \text{dyn/cm}$, corresponding to the stressor forces measured in several samples in figure 5.14 after annealing. The strains are calculated at depths of 1-4µm into the bulk silicon layer, assuming a stressor stripe width of 2µm. It is seen that strains of the order of $-0.001$ exist close to the stressor stripe.

Figure 5.17 Refractive index profiles in bulk silicon calculated for a stressor edge force of $2 \times 10^6 \text{dyn/cm}$ assuming a 2µm wide stressor stripe. The regions marked A, B and C refer to positive refractive index changes of 0.005, 0.01 and 0.05, respectively. The interferometry measurements indicate that as-deposited stressor films often generate forces of only $2 \times 10^5 \text{dyn/cm}$ or less, so that the corresponding refractive index change is also an order of magnitude lower than shown here, providing poor confinement.
ment, it is useful to compare the stressor film measurements and calculations to direct measurements of the strains under the stressor stripes in the photoelastic waveguides, to see whether the strains in the waveguides are well described by the measurements and calculations performed here. The strain measurements were performed by Professor Howard E. Jackson, using Raman spectroscopy, on some of the waveguides fabricated and studied here, and they are included as an important confirmation of the results given above.

5.5 Raman Measurements

One of the main problems with the photoelastic waveguides studied here has been the poorly defined stress generated by the as-deposited stressor layers. The interferometry results showed that the stress generated by stressor films can be significantly increased by annealing the structure. However, it is not certain whether annealing of a single stressor stripe will produce a similar increase in the stressor force, as shown in figure 5.14, with corresponding strains in the guiding layer focussed around the stripe edges, similar to those shown in figure 5.16.

A photoelastic waveguide fabricated in a Si$_{1-x}$Ge$_x$/Si heterostructure with a 0.6μm thick SiN$_y$ stressor stripe of width 6μm was investigated by Professor Howard E. Jackson,
using Raman spectroscopy. By scanning light across the waveguide in the region close to the stripe, information about the strain in the crystal could be gathered from the reflected Raman spectra. In figure 5.18, the shift in the measured Raman peak position has been plotted by scanning across the waveguide, first with the as-deposited stressor, and subsequently after a 600°C 30 second anneal. It is obvious how the shift in the Raman peak position, which reflects the strain underneath the stressor stripe, becomes both stronger and better defined with annealing. There is also a striking similarity to the calculated strain profiles, such as in figure 5.16, confirming the expected abrupt change from compressive to tensile strain in the region around each stripe edge.

The Raman results provide a useful confirmation of both the interferometry measurements and the strain modelling, showing that the stressor films can be improved by annealing, and that the strain under a stressor stripe improves accordingly. It can therefore be expected that photoelastic waveguides will generate a corresponding increase in photoelastic confinement after annealing.

### 5.6 Annealing of Photoelastic Waveguides

It was found that the excess losses of unannealed photoelastic waveguides in bulk silicon were as high as 9-10dB/cm at 1.523μm, while many samples did not produce an output. There was also strong substrate coupling which was clearly visible on the vertical intensity plots, as shown in figure 5.3, all of which indicate a poor photoelastic confinement. For the waveguides to be of use in optical circuits the confinement needs to be improved.

In section 5.4 it was found that the force generated by the stressor film can be significantly increased by annealing the sample. It is investigated here whether the annealing can be used to improve the photoelastic confinement through an enhancement in the edge force, as can be expected from the interferometry results. The measurements are performed on photoelastic waveguides in bulk silicon, because the light coupled into the substrate is clearly separate from the light confined in the waveguide so that any change in the confinement is easy to detect from loss measurements and the camera image. The results will also indicate whether low-loss waveguides can be made using only photoelastic confinement, which has so far never been reported.

For the photoelastic waveguides in the Si_{0.987}Ge_{0.013}/Si heterostructures, the confinement affects the losses in waveguide bends and is important when coupling and switching the light. However, the light which is not confined to the photoelastic waveguide region is still confined within the planar layer, as shown in figures 5.8 and 5.9, making it difficult to determine precisely the photoelastic confinement, since most or all of the light is still detected by the photodiode. The measurements are therefore performed only on silicon waveguides.

From the interferometry measurements in section 5.4 the annealing time in the range 10-60 seconds does not seem to be an important parameter in determining the stressor force. For this investigation, an annealing time of 30 seconds was chosen, which corresponds to the highest stressor forces in figure 5.14. A stressor film thickness of 0.6μm was chosen, corresponding to the waveguide measurements made previously in the chapter, although from the interferometry measurements the film thickness does also not seem to be an important parameter. The samples are made from the same wafer and with the same deposited films as investigated by interferometry in section 5.4.

The waveguide mode profiles presented earlier in this chapter were recorded as horizontal and vertical line plots, which are appropriate to determine the shape and size of
As Deposited  300°C  400°C  500°C  600°C  700°C

Figure 5.19 Waveguide output from a bulk silicon photoelastic waveguide with a 2μm wide stressor stripe, recorded for the 1.15μm TM images. The sequence of pictures shows how the substrate modes, clearly visible under the two edge modes, reduce after annealing the sample for 30 seconds at increasing temperatures. The substrate modes, which are significant with the as-deposited stressor film, are seen to be virtually eliminated after the 600°C anneal, while after a further anneal at 700°C the confinement weakens, which is in agreement with the interferometry measurements of the stressor films. Notice also that since two separate guiding regions are defined by one stressor stripe, and since the confinement improves with annealing, that confirms that they are generated by photoelastic confinement, and that the effect of strip-loading is negligible.

Figure 5.19 Waveguide output from a bulk silicon photoelastic waveguide with a 2μm wide stressor stripe, recorded for the 1.15μm TM images. The sequence of pictures shows how the substrate modes, clearly visible under the two edge modes, reduce after annealing the sample for 30 seconds at increasing temperatures. The substrate modes, which are significant with the as-deposited stressor film, are seen to be virtually eliminated after the 600°C anneal, while after a further anneal at 700°C the confinement weakens, which is in agreement with the interferometry measurements of the stressor films. Notice also that since two separate guiding regions are defined by one stressor stripe, and since the confinement improves with annealing, that confirms that they are generated by photoelastic confinement, and that the effect of strip-loading is negligible.

the confined modes. In this section it is more important to determine the amount of light coupled into the substrate, which has no well-defined size or shape. The results from this investigation are therefore presented as the actual camera images rather than as line plots, because they provide more complete information about the substrate coupling.

The waveguide output was recorded after each 30 second anneal from the camera image and is shown in figure 5.19 for 1.15μm TM polarized light, showing the two edge modes under a 2μm wide stressor stripe and also the changing substrate modes. The substrate coupling is similar for both polarisations and for 1.15μm and 1.523μm. In figure 5.19 both edge modes have been exited to show the substrate modes relative to the photoelastic guiding regions, although the relative amount of substrate coupling appears the same when focussing on only one edge mode.

It is noticeable how the amount of substrate coupling reduces with annealing temperature and reaches a minimum after the 600°C anneal. After a further anneal at 700°C the confinement becomes weaker. Figure 5.20 presents the measured excess losses, showing the same trend. Each edge mode was excited separately for the loss measurements. The initial losses in these waveguides, which were all on the same specimen, were relatively high, making it difficult to distinguish clearly between the edge modes and the substrate modes. An uncertainty value was estimated from the readings to account for this and has been included in the readings in figure 5.20. The average minimum losses at 1.523μm were as low as 4.3dB/cm and 6.2dB/cm for the TE and TM polarisations. At 1.15μm the characteristics were similar, with minimum losses of 6.35dB/cm and 7.43dB/cm for the TE and TM polarisations.
Figure 5.20 Excess losses measured at 1.523μm in photoelastic waveguides in bulk silicon, with 2μm wide stressor stripes, recorded after annealing the waveguides for 30 seconds at increasing temperatures, corresponding to figure 5.19. The losses are seen to drop to a minimum after the 600°C anneal, with minimum losses of 4.3dB/cm and 6.2dB/cm for TE (solid line) and TM (dashed line), respectively.

5.7 Summary

This chapter has reported the first experimental demonstrations of photoelastic waveguides in bulk silicon and Si$_{1-x}$Ge$_x$/Si heterostructures. The results show that these waveguide structures can be realised and that they are fairly well described by the modelling in chapter 3. However, the measured edge mode widths and depths are 20-30% greater than predicted, which probably reflects the discrete nature of the waveguide model, in which the intensity was determined at discrete nodes, separated by 0.5μm. A more accurate solution could be found by reducing the distance between the nodes.

The photoelastic waveguides in bulk silicon had one guiding region outside each edge of the stressor stripe. Photoelastic waveguides in 8μm thick Si$_{0.987}$Ge$_{0.013}$ planar layers grown on silicon, had an additional middle guiding region between the edge modes, as predicted by modelling. The relative intensity of the middle mode to the edge modes increases with a reduction in stressor stripe width. According to modelling the peak intensity of the middle mode and the edge modes should be equal for a stressor stripe width of approximately 4.5μm, while the measured results show this occurring for stripe widths of 2.5-3μm. The
reason for this discrepancy is not clear from the modelling or measurements, although it may reflect the coupling between the middle and edge guiding regions, reducing the relative intensity of the middle mode. An increase in the Si$_{0.987}$Ge$_{0.013}$ layer thickness to 14$\mu$m made the middle mode disappear. This shows that there is a maximum limit for the planar layer thickness of between 8$\mu$m and 14$\mu$m beyond which the middle mode will not be supported.

At 1.15$\mu$m a second order mode tends to appear outside the edge mode, while the edge modes are generally single mode at 1.523$\mu$m. The appearance of a second order mode makes the waveguides less useful for general waveguiding at 1.15$\mu$m than at 1.523$\mu$m, because the guided mode will be difficult to match to other waveguides and devices.

The waveguides show a low degree of birefringence. This confirms that the magnitude of the photoelastic constants are similar. The results also show that the photoelastic constants must be positive, which is consistent with the calculations in chapter 2. Previously reported photoelastic constants of silicon cannot describe the behaviour of the waveguides reported here.

Photoelastic waveguides were reported in bulk silicon with relatively high excess losses of 9-12dB/cm, showing that the photoelastic confinement generated by the as-deposited stressor layers is poor. By fabricating the photoelastic waveguides in Si$_{0.987}$Ge$_{0.013}$/Si heterostructures the substrate coupling was virtually eliminated, giving excess losses of close to zero at 1.523$\mu$m. However, despite the lower losses, the photoelastic confinement is low also in the Si$_{0.987}$Ge$_{0.013}$/Si photoelastic waveguides, which will create large losses in waveguide bends.

Interferometry studies were made of stressor films which were annealed at temperatures of up to 800°C for 10-60 seconds in an attempt to improve the photoelastic confinement generated by the stressor layers. The annealing generated a strong improvement in the stressor force, with maximum stressor forces of 2-3$\times$10$^6$ dyn/cm, which is higher than previously reported for stressor layers. Similar annealing of photoelastic waveguides in bulk silicon showed a strong reduction in the substrate coupling and a corresponding reduction in losses, with a minimum occurring after a 600°C anneal, in good agreement with the interferometry results. The average minimum losses at 1.523$\mu$m after annealing were as low as 4.3dB/cm and 6.2dB/cm for TE and TM, respectively.
Chapter 6

Discussion

The main aim of this project has been to investigate whether photoelastic waveguides could be fabricated in bulk silicon and Si$_{1-x}$Ge$_x$/Si heterostructures. Particular attention has been given to the bulk silicon structures, where waveguides are defined using only photoelastic confinement.

Experimental results have been presented showing that photoelastic waveguides can be fabricated in Si$_{1-x}$Ge$_x$/Si heterostructures and that the excess losses at 1.523 μm are practically zero. Similar waveguides were also made in bulk silicon, with excess losses down to 4.3 dB/cm, indicating that waveguides using only photoelastic confinement could become practical structures by further improving the stressor layer. These are the most important findings of the project and they give a positive conclusion to the investigation.

There are also several aspects of the investigation which in themselves are useful findings or which could be studied further to improve the performance of the waveguides. Some of these aspects are considered in this chapter together with a discussion of the usefulness of this type of waveguide in practical optical circuitry.

6.1 Modelling & Experimental Techniques

Most of the work in this project has been involved with the modelling and experimental study of the photoelastic strains induced by stressor layers and the corresponding refractive index changes and intensity profiles. The experimental work showed that well defined photoelastic strains can be difficult to generate, and that there are some differences between the modelled waveguide behaviour and the measured waveguide characterisation. This section presents some of the problems and useful techniques involved in defining the stressor layers and photoelastic strains. There will also be a discussion of the waveguide modelling, which can be improved to better explain the characteristics of photoelastic waveguides.

6.1.1 Fabrication and Investigation of Stressor Layers

The generation of photoelastic strains and strain-induced refractive index profiles depends on the quality of the stressor layer. Two separate issues relating to the stressor layer have been investigated in this project. The first issue is that of defining the stressor stripes close to the waveguide facets such that light is not lost on coupling into the facets. Secondly, the strain induced by the stressor layer must be sufficient to confine the light. Both these issues turned out to be significant challenges. The stressor films were eventually improved
enough to provide well confined photoelastic waveguides, although further work is needed on the stressor layers, as discussed below.

Defining Stressor Stripes at the Waveguide Facets Using Surface Extension

The greatest problem faced during the entire project was that of defining continuous narrow stressor stripes from the SiNy films such that they extend all the way to the facet. Since silicon turns out to be difficult to cleave to the optical quality required for the waveguide facets, the facets are mechanically polished using standard polishing equipment. The problem occurs during photolithography because the photoresist, which is spun onto the sample, builds up around the edges of the sample and prevents the photolithographic pattern from being defined across the entire sample. A number of possible solutions to this problem were investigated, as listed in section 4.5.3, but none were found to alleviate the problem of edge build-up.

It was found that the surface of the sample can be extended using a liquid medium, which runs into contact with the sample facet through capillary action, thus effectively removing the sample edge as seen by the photoresist, which practically eliminates the problem of edge build-up. A suitable medium for the surface extension is black wax, which is liquid at 200-300°C, while at 100°C, the temperature at which the photoresist is baked, it is sufficiently solid to support the sample. It also seemingly unaffected by buffered hydrofluoric acid, photoresist and photoresist developer, and the solvents acetone and isopropanol, allowing the sample to be further processed.

This technique is useful because it provides a smooth extension of the surface without solid mechanical contact with the facet. The inherent capillary effect of liquids also avoids the problem of careful alignment of the extending medium. It is therefore a technique which could usefully be applied to other processes, in particular where it is important to protect the end facets of specimens.

It should be noted that the edge build-up is a only problem because the facets cannot be polished with the stressor stripes already defined, as they will be torn off the sample close to the facet. In several other structures, such as indiffused waveguides or rib waveguides, the confinement does not rely on the effect of a stripe of a different material, such that polishing of the structure does not pose a problem. Even though the surface extension technique is appropriate for this type of waveguide fabrication, it does require time, and it would be useful to develop stressor films which are suitable for polishing.

Improving the Strain Generated by Stressor Layers

With respect to the strain generated by stressor layers it is interesting to consider work done on GaAs-based structures. Liu et al. [73] evaporated metal films onto the semiconductor surface and induced metal-semiconductor reactions by annealing the structure, generating stressor films such as Ni₃GaAs. The purpose of inducing this kind of reaction was to generate a well defined level of stress. It is not unlikely that films generated by chemical reactions with the semiconductor will be mechanically relatively strong, such that they can withstand polishing, which would be interesting for silicon waveguides. In terms of silicon-based materials, however, it may be difficult to generate stressor films by chemical reactions, because silicon is chemically a relatively stable material. A thermal oxide layer of 0.1μm thickness, for instance, would take around a 1000 minutes to grow on (100) silicon in dry oxygen at a temperature of 800-900°C [105]. It would still be useful
to investigate whether useful stressor layers could be generated from reactions with silicon by appropriate choice of surface reactant.

The method chosen here to improve the stressor forces was annealing of the stressor films, which was expected to increase the thermal mismatch between the guiding layer and the stressor layer. The results show a strong increase in the stressor force with annealing, with a maximum of around 2-3 \( \times 10^6 \) dyn/cm, which is about ten times higher than measured with most other films [70, 55, 71]. The highest stressor forces previously reported are by Liu et al. [71], who measured a maximum stressor force of \( 0.72 \times 10^6 \) dyn/cm by sputtering \( \text{Ni}_{0.05}\text{W}_{0.95} \) stressor layers, and Benson et al. [58] who generated \( 1.2 \times 10^6 \) dyn/cm using 2\( \mu \)m thick gold films, both on GaAs substrates. The forces generated here by annealing plasma-deposited \( \text{SiN}_y \) films are therefore comparatively high.

High stressor forces are useful in photoelastic waveguides in that they induce large strain-induced refractive index changes, so that the confinement becomes strong. It was shown here that it is possible to almost eliminate the substrate coupling and to bring the waveguide excess losses down to 4.3dB/cm using only photoelastic confinement, by appropriately annealing the stressor film. After further annealing at higher temperatures the confinement weakens, indicating a relaxation of the stressor force, which is consistent with the interferometry measurements of the stressor films. This suggests that the maximum stressor force has been reached.

Even though the interferometry measurements and the waveguide results show the stressor forces and photoelastic confinement which are possible, they do not show whether the stressor layers are stable after storage at room temperature for extended periods. It is also possible that the structures are unstable when the stressor force is at a maximum. However, the interferometry results imply that the reduction of the stressor force after reaching its maximum was due to relaxation along the stressor/silicon interface, and did not represent the overall strength of the stressor film. It may therefore be possible to generate even higher stressor forces if the adhesion at the stressor/silicon interface can be improved. A possible stressor layer which would be well defined and mechanically similar to silicon is \( \text{Si}_{1-x}\text{Ge}_x \), which can be grown onto the silicon with accurate thickness and alloy content, and it will be thermally stable.

This project has shown that is possible to produce photoelastic waveguides in silicon and \( \text{Si}_{1-x}\text{Ge}_x \), and that relatively high stressor forces and fairly strong photoelastic confinement can be achieved using plasma-deposited \( \text{SiN}_y \) films, although it is not clear from this study how stable the structures are. It is therefore important with further investigations to improve the stressor material and fabrication process.

6.1.2 Modelling of Photoelastic Waveguides

The modelling in this project gave a fairly good description of the measured behaviour of the waveguides. There are, however, three aspects of the modelling which could usefully be improved.

Firstly, the material losses are higher at 1.15\( \mu \)m than at 1.523\( \mu \)m, due to the phonon-assisted losses around the absorption band-edge. Calculated using experimental data from Braunstein et al. [80], this amounts to 3.9dB/cm for bulk silicon and even more for the \( \text{Si}_{1-x}\text{Ge}_x \) alloys, as shown in figure 3.7. The measured values, however, lie 1.5-2.5dB/cm below that predicted by calculations. Even though the measurement uncertainties of \( \pm 1.4dB/cm \) at 1.15\( \mu \)m and \( \pm 2.2dB/cm \) at 1.523\( \mu \)m could account for most of this discrepancy, it is likely that the calculated phonon-assisted absorption is overestimated. Al-
ternatively, the measurements could be wrong. It is peculiar, though, that a number of measurements can be made on three different structures, and that they are all on average significantly less absorbent than calculated. A comparison was therefore made with the data from the original paper by Macfarlane and Roberts [103] on absorption in silicon near the band-edge. At 290K they measured the square root of the absorption at 1.15μm to be approximately 0.7/cm^0.5, or around 2.1dB/cm, which is much closer to the experimental value for silicon of 1.45dB/cm.

The losses for the Si_{0.987}Ge_{0.013} if interpolated to the Macfarlane absorption value for silicon will reduce by nearly 1.3dB/cm, predicting losses of 3.64dB/cm and 4.64dB/cm for the unstrained and strained crystal, respectively. These loss levels are much closer to the measured values of 3.16dB/cm and 4.35dB/cm found for the 14μm and the 8μm thick Si_{0.987}Ge_{0.013} layers, respectively. From these measurements, it is likely that the 8μm thick Si_{0.987}Ge_{0.013} layer is strained, while the 14μm thick layer is relaxed. It is also quite likely from these measurements and calculations that the data by Braunstein et al. slightly overestimate the absorption at 1.15μm.

A second aspect of the modelling which could usefully be improved is the meshing density of the finite element and finite difference models. Solutions to the strain, refractive index and optical intensity profiles were calculated in both models at discrete nodes which were spaced 0.5μm apart close to the photoelastic waveguiding regions. It was found that the measured edge mode widths and depths were 20-30% greater than predicted, which is believed to be due to the rather large node spacing. Another discrepancy between the observed and predicted behaviour is that of the second-order mode often seen outside the main edge mode at 1.15μm, as shown in figure 5.10. The modelling, however, showed only single-mode behaviour of the edge modes for both 1.15μm and 1.523μm, which is probably also due to the relatively large spacing of 0.5μm between the nodes in the model. It can be seen that the excess losses of the photoelastic waveguides were consistently higher at 1.15μm than at 1.523μm, as shown in figure 5.12, which is believed to be a consequence of the second-order edge mode, which was not accounted for in subtracting the overlap mismatch.

In this investigation the finite element mesh in the vicinity of the stressor stripe was drawn up such that the entire structure, including the substrate, could be modelled without excessive use of computer power. The modelling of the substrate was useful here in showing that a significant amount of the mismatch strain energy is consumed by the substrate. However, since it represents a fairly constant background level of strain and is independent of the stripe strains, a model could be made with a finer mesh density around the guiding regions by considering only a small part of the structure around the stressor stripe, and representing the substrate strains as a constant. The finite difference analysis is similarly restricted by the demand for computer power, since it was chosen here to perform the finite difference calculations in a mathematical analysis computer package. By writing a dedicated program for these calculations, it would be possible to work with much larger files, such that a finer mesh density could be specified. These changes in the finite element and finite difference models will improve the accuracy of the calculations, and are expected to give edge mode dimensions closer to the measured values and also to show a second mode at 1.15μm.

A final aspect of the modelling relates to coupling strength and loss calculations, which have not been addressed in this investigation. The two or three guiding regions in the photoelastic waveguides are of interest for couplers and splitters, although it would be of great use for the design of such devices to be able calculate the coupling between
the guiding regions. It would also be useful to find the amount of light coupled into the substrate as a function of refractive index change. These calculations necessarily require the basic optical field patterns to be more accurate. It is seen as a natural extension to the work presented here to develop a more detailed model for the optical fields in photoelastic waveguides, which can precisely predict coupling lengths and substrate losses, since they are not given by the modelling in this investigation.

6.2 Photoelastic Waveguides in Optical Circuitry

Having shown that photoelastic waveguides can be made in bulk silicon and Si$_{1-x}$Ge$_x$/Si heterostructures, and that they are potentially low-loss, it is interesting to consider the potential uses of these waveguides in optical circuitry. In the following several possible applications for photoelastic waveguides are considered, drawing on the findings from this work as well as from other investigations.

6.2.1 Basic Photoelastic Waveguides

The work presented in this investigation has been concerned with straight waveguides on (100) substrates with stressor stripes oriented along the [100] crystallographic axis. Also, all the structures have had the stressor stripe under compressive strain, inducing positive refractive index changes outside the stripe edges. It is useful to look at how the sense of the stressor strain and the waveguide orientation can be used to control the waveguide properties.

The most useful properties of the photoelastic waveguides studied here are that they show little birefringence and that the excess losses measured at 1.523 μm are practically zero for the photoelastic waveguides made in 8 μm thick Si$_{0.987}$Ge$_{0.013}$ planar layers on silicon, showing that these structures can be low-loss if made in better quality crystals. Both the low degree of birefringence and the low losses are positive features for use with fibre-optic communications, which is the most likely application for optical waveguides at this wavelength.

It turns out that the photoelastic response of the Si$_{1-x}$Ge$_x$ crystals is highly anisotropic, and that similar waveguides oriented along the [110] axis on (100) silicon are highly birefringent, as shown experimentally by Yu et al. [60]. This anisotropy significantly restricts the design flexibility of photoelastic waveguides in Si$_{1-x}$Ge$_x$ alloys, since the birefringence will change with waveguide orientation. It is therefore important to investigate how much the direction of a waveguide is allowed to change without adversely affecting its guiding properties. On the other hand, it presents a tool for easy manipulation of the polarisation of light in devices, as discussed in section 6.2.3.

Another variable in the design of the waveguides is the direction of the stressor edge force. All the waveguides studied here had one guiding region outside each of the stripe edges because the stressor was under compressive strain such that the edge forces point outwards from the stressor stripe, as shown in figure 3.4. As explained in chapter 3, a change in sense of the edge forces would change the sense of all the refractive index changes, such that there would be one well defined refractive index maximum under the centre of the stressor stripe. This is easily illustrated in figure 3.8, with the positive refractive index changes represented by the thin lines, and the negative changes represented by the thick lines, i.e. the exact opposite of what has been studied here. Such a waveguide would be symmetrical in the horizontal direction, and its size would be variable depending on the
stripe width. In terms of losses and birefringence, it should behave in a similar way to the edge modes. For a single, symmetrical waveguide, this may turn out to be a useful structure which it will be interesting to investigate further.

It is useful here to consider the various aspects of photoelastic waveguiding in bulk silicon and $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ heterostructures, to see whether the waveguides studied here present a real alternative to other integrated optical waveguide technologies. Some of the most important aspects of basic waveguides are mentioned below.

**Propagation losses**

Integrated optical waveguides have been reported in both silicon [14, 15] and $\text{Si}_{1-x}\text{Ge}_x$-based structures [23, 48] with losses of $\leq 0.5\text{dB/cm}$, demonstrating their potential as low-loss optical materials. Although the materials used in this project were rather lossy, the results here show that the excess losses due to the photoelastic confinement can be practically zero when used in conjunction with a planar structure. It can therefore be concluded that the overall propagation losses at $1.523\mu\text{m}$ of photoelastic waveguides in $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ heterostructures can be as low as $0.5\text{dB/cm}$ or better when produced in good quality materials. With such low losses it is also clear that no other waveguide structure, whether photoelastic or otherwise, will be significantly better in terms of propagation losses.

It should be stressed that waveguides in $\text{Si}_{1-x}\text{Ge}_x$ alloys are only of practical use above the absorption band-edge, which lies at $1.1\mu\text{m}$ for silicon and in the region $1.1-1.8\mu\text{m}$ for $\text{Si}_{1-x}\text{Ge}_x$ alloys. $\text{Si}_{1-x}\text{Ge}_x$ waveguides can therefore usefully be employed with common optical fibres, which have propagation loss minima around $1.3\mu\text{m}$ and $1.55\mu\text{m}$, but they will not be useful for application in the visible spectrum.

One issue relating to propagation losses which has not been explicitly investigated here is that of losses in waveguide bends. With poor lateral confinement, light will be lost in the waveguide bends. For waveguides made by diffusion of germanium into silicon, bending losses of approximately $1.5\text{dB}$ for a $10\text{mm}$ bending radius have been reported [49]. In terms of the refractive index profile, these structures are similar to the photoelastic waveguides, and have a comparable refractive index change to that found with the maximum stressor force measured here. These values should give a rough indication of the bending losses which could be expected from well confined photoelastic waveguides in $\text{Si}_{1-x}\text{Ge}_x$ structures. However, in $\text{Si}_{1-x}\text{Ge}_x$ photodielectric waveguides the birefringence varies strongly with crystallographic direction, which may pose a problem for practical devices, and will need to be investigated.

**Mode size and profile**

Most of the edge modes recorded here have widths in the range $1.6-2.4\mu\text{m}$ and depths of $1.3-1.9\mu\text{m}$. They are also single mode at $1.523\mu\text{m}$ with a fairly constant mode profile, and they exhibit low birefringence along the [100] direction, as studied here. Being well confined, they are convenient to work with. However, for coupling into and out of components with a circular mode profile, such as optical fibres, the slight asymmetry of the edge modes will cause mode mismatch losses, which is a disadvantage. It may therefore often be advantageous to couple into the middle mode, which exists only in photoelastic

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1These measurements were actually made on S-bends comprising two separate $90^\circ$ bends, with total excess losses of the S-bend of approximately 3dB.
waveguides within planar layers, since it is more symmetrical. Alternatively, a reversal of the direction of the stressor edge force can be used to generate a single mode waveguide which is symmetrical in the horizontal direction, as mentioned above. As discussed later in section 6.2.3, the different guiding regions of photoelastic waveguides can all be usefully employed in optical circuits.

**Fabrication and integration**

One of the main objectives for investigating photoelastic waveguides was that they are easy to fabricate and integrate with electrical components. This investigation confirms that they can be made by patterning a dielectric film deposited onto a silicon substrate. In view of the findings from this investigation is useful to refer back to some of the arguments made in chapter 1 for studying photoelastic waveguides in Si$_{1-x}$Ge$_x$ alloys.

1. **Waveguide fabrication process** The photoelastic waveguides studied here were made using a single deposition of Si$_N_x$, one photolithography step and one etch. Etched ribs and indiffused waveguides need at least the same amount of processing, although some technologies require more processing steps [49]. Rib or strip-loaded waveguides also need a planar structure as a starting point, which may not be required in the silicon photoelastic waveguides if the photoelastic confinement is improved. The indiffused Si$_{1-x}$Ge$_x$ waveguides reported by Schmidtchen et al. [49], on the other hand, require long annealing times of around 65 hours at 1200°C, while 30-second anneals at 500-600°C were sufficient to significantly improve the performance of the photoelastic waveguides studied here. There is also the possibility of ion-implanted waveguides, which could in principle easily be integrated with VLSI fabrication and which could require only a few processing steps. However, even though some ion-implanted waveguides have been reported [44], the implantation energy needed to implant germanium just 1.5μm into silicon is more than 2MeV, which will probably make it an unattractive technology for integration with VLSI, where the implantation energies are normally much lower.

In comparison with other waveguide technologies, photoelastic waveguides are seen to be fast and easy to fabricate, and they rely on standard processing used for VLSI. It is probable that improvements will be made, particularly in terms of the stressor technology. Nevertheless, photoelastic waveguide fabrication is likely to remain a simple technology, where only surface stressor layers are required to define the waveguides, without doping or etching into the guiding layer. In terms of fabrication, photoelastic waveguides are therefore a simple alternative to other integrated optical waveguide technologies.

2. **Integration with other devices** Since strain engineering is becoming increasingly interesting for both electrical and optical devices, it is useful for the integration of optoelectronic circuitry with devices which do not require etching or relaxation of the guiding layer. In this respect, photoelastic and indiffused waveguides are appropriate for integration, although the long-term annealing at high temperatures required for the indiffused waveguides may complicate the fabrication of other devices on the same circuit.

It was known at the outset of this project that photoelastic waveguides can be fabricated in GaAs-based structures by depositing a stressor layer onto the guiding
layer. This investigation has confirmed that photoelastic waveguides can also be fabricated in bulk silicon and Si$_{0.987}$Ge$_{0.013}$ by simply straining the guiding layer.

From this comparison of waveguide technologies, the photoelastic waveguides promise to be a useful alternative to other waveguide technologies. Since they can be made in silicon and Si$_{1-x}$Ge$_x$ alloys, it should also be feasible to integrate them into silicon-based VLSI circuits.

6.2.2 Buried Structures

In this project much emphasis has been on the edge modes in bulk silicon photoelastic waveguides, as they depend only on the photoelastic confinement, so they could be used for optical waveguiding without the need for additional confinement from planar layers, doping or etched structures. The results indicate that such purely photoelastic waveguides are feasible, although the optical confinement should be further improved.

![Waveguide Diagram]

Figure 6.1 Buried planar waveguides with photoelastic horizontal confinement. The AlGaAs based structure, reported by Liu et al. [73], and the silicon based structure, reported by Yu et al. [60], both have planar waveguides buried some distance below the top surface, with photoelastic horizontal confinement generated by a stressor stripe, which may be either 'on-line' or 'off-line', as illustrated in figure 3.12. Both structures use W and Ni based stressor layers.

An interesting alternative application of photoelastic confinement is for lateral confinement within planar layers. Such planar photoelastic structures have been studied by Yu et al. [60] in silicon and Liu et al. [73] in AlGaAs. By defining stressor layers on top of buried planar layers of the type shown in figure 6.1, single mode waveguides are defined some distance below the specimen surface. Such waveguides are useful in that they have
a good vertical and horizontal symmetry, which can reduce mode mismatch losses when coupling into other components. In principle, other optical or electrical components could even be defined in the upper layer of the structure. The disadvantage with such buried structures is that the strain-induced refractive index change decays with distance from the stressor layer, so that the horizontal optical confinement is weaker for the buried guiding layers than it would be at the surface. The change in birefringence with crystal direction is also not removed with these structures, making it difficult to design waveguide bends.

The concept of using photoelastic confinement in buried layers may, however, be developed further. It is seen from figures 3.8 and 3.9 that below a depth of approximately 2μm the refractive index change is always negative under the centre of the stressor stripe. Assuming that the refractive index profiles calculated in figures 3.8 and 3.9 are precise, buried planar layers between, say, 2μm and 3μm below the surface, will see roughly the same photoelastic contribution for both TE and TM polarised light, whether the waveguide is oriented along the [100] or [110] axes. With a reversal of the stressor edge forces, such that they point inwards, there would be a positive refractive index change within the planar layer under the stressor stripe. Whether the photoelastic confinement at this depth is strong enough for a well-defined guiding region is not certain. However, if it does work, waveguides can be defined along both the [100] and the [110] axes with little birefringence, which would make it much easier to define practical optical circuits. This type of waveguide structure therefore poses an interesting challenge for further studies.

6.2.3 Couplers and Splitters

This project has only studied the basic waveguiding properties of photoelastic structures. The same technology would also be suitable for directional couplers and power splitters, although these structures have been given little attention. Figure 6.2 illustrates different guiding schemes which are possible in photoelastic waveguides. It is seen that one, two or three guiding regions can be defined using only one or two stressor stripes, allowing simple devices to be made based on the coupling between the different guiding regions. Notice that the stressor could also be defined as an off-line structure, as shown in figure 3.12, such that the required edge forces can be generated using the most appropriate stressor material.

The photoelastic directional coupler reported by Yu et al. [60] using two separate stressor stripes could be made more simply using only one stripe, as shown in figure 6.3, and their power splitter, fabricated as a Y-junction, could be made with two single stressor stripes, as shown in figure 6.4. Alternatively, the power splitter could be made with one single stressor stripe, if used in conjunction with a planar structure, as this would also define three guiding regions.

Although simple devices can be made with the stressor edges being parallel, changing the stressor width can be used to control the coupling strength between guiding regions. For waveguides with three guiding regions, of the type shown in figure 6.2(c), the stressor width will also control the relative intensity of the middle mode to the edge modes. Figures 6.5(a) and (b) suggest applications where the stressor width is used to control both the waveguide coupling and the relative positioning of the guiding regions, although some positioning of the guiding regions could be achieved with parallel stressor edges, as shown in figure 6.5(c).

The work by Yu et al. [60] indicates that silicon photoelastic waveguides oriented along the [110] axes on (100) substrates are highly birefringent, while along the [100] axes
Figure 6.2 Different possible guiding schemes in photoelastic waveguides. Depending on the direction of the stressor edge force, indicated here with arrows, there will be either one edge mode outside each of the stressor edges, as shown in (a), or one mode under the centre of the stripe, as shown in (b). If used in conjunction with a planar structure, there can even be three separate guiding regions, as shown in (c). Guiding schemes (a) and (c) have been investigated in this project. There is also the choice of using two or more stressor stripes to define multiple guiding regions, for instance as shown in (d) and (e). These guiding schemes are the same for TE and TM polarised light in silicon and Si$_{1-x}$Ge$_x$ photoelastic waveguides oriented along the [100] crystallographic axis on (100) substrates. Along other crystal directions the guiding regions may be different. Notice that these pictures do not intend to illustrate any precise optical profiles or relative distances within the waveguides.

they are nearly optically isotropic, as shown by this work. In some optical circuits it may therefore be difficult to include waveguide bends, and so it is important to assess the effect of waveguide orientation on the birefringence of the various photoelastic guiding schemes. The birefringent behaviour seen along the [110] axes may yet be employed purposefully in some optical devices, for instance as shown in figure 6.6, where on-line or off-line sections of waveguide along the [110] axes are inserted into waveguides along the [100] axes to define either TE or TM polarisers.

In GaAs it has been shown that a bias applied to metal stressor layers can change the propagation constant via the electro-optic effect [50] and has been used in a photoelastic directional couplers to switch light from one coupler channel to the other [57, 58]. This method of switching is not useful in Si$_{1-x}$Ge$_x$ alloys since there is no linear electro-optic effect. However, efficient silicon-based phase modulators have been realised using carrier injection to change the refractive index [30], which could also be usefully employed in photoelastic structures. With the guided modes of photoelastic waveguides being relatively small and close to the waveguide surface, it is likely that a relatively low level of carrier injection is needed to modulate the light, making this type of structure interesting.
Figure 6.3 **Photoelastic directional couplers** could be made as demonstrated by Yu et al. [72] with one stressor stripe per waveguide, as shown on the left. Alternatively, using the guiding scheme illustrated in figure 6.2(a), the coupler could be made using the two edge regions outside a single stressor stripe, as shown on the right.

Figure 6.4 **Power splitters** could be made as demonstrated by Yu et al. [72] with a Y-junction, as shown on the left. A similar device function can be performed with two straight stressor stripes, as shown in the middle, where light is be split into two or three beams by appropriate choice of coupling length. Using guiding scheme 6.2(c), light can be split into two beams using a single stressor stripe on top of a planar layer.
Figure 6.5 Making use of photoelastic waveguide bends. As determined in this project, the middle mode in the guiding scheme in figure 6.2(c) reduces with an increase in stressor stripe width. It should therefore be possible to couple into the middle mode, which subsequently reduces in strength as the stressor becomes wider, as shown on the left. Waveguide bends may also be used for simple beam positioning, as shown in the middle, although some positioning of the beam could be performed with coupler structures using straight stressor sections, for instance as shown on the right.

Figure 6.6 Photoelastic polarisers. Since silicon photoelastic waveguides along the [110] axes have been shown to be strongly birefringent [60], in contrast to waveguides along the [100] axes, which are nearly optically isotropic, it should be possible to make polarisers, as shown here, by insertion of a section of waveguide along a [110] axis. If the stressor edge forces in the [110] section point outwards, as shown on the left, it will become a TE polariser, and if the edge forces point inwards, as shown on the right, it will be a TM polariser. The guiding scheme indicated here along the [100] axis is that shown in figure 6.2(b).
for further investigation. Two possible concepts for Si$_{1-x}$Ge$_x$-based photoelastic switches and modulators are shown in figure 6.7, corresponding to the guiding schemes shown in figure 6.2(e) and (b) $^2$. Both concepts could be set up as diode-structures, by appropriate doping of the contact regions, which could be used to modulate the coupling length between the two guiding regions in figure 6.7(a), or to phase modulate the guided mode in figure 6.7(b). Alternatively, a third stripe contact could be added between the $V_1$ and $V_2$ contacts, to define a MESFET or MOSFET-like structure, as has been studied theoretically by Giguere et al. [119]. Although the exact form of such switches and modulators needs further investigation, their compact and simple design could make them attractive devices.

6.3 Summary

This chapter has discussed some of the problems and considerations faced during the modelling and experimental work performed during the project, as well as some potential applications of photoelastic structures. It is found that the practical potential for photoelastic structures is interesting, and that there are several issues which it would be useful to investigate further. Some of the issues discussed here are summed up below:

$^2$The stressor in this case is an off-line structure, making it equivalent to figure 6.2(d) with only the middle mode.
1. **Stressor films.** It was found that the forces generated by the SiN$_x$ films studied here are stronger than reported for other stressor layers, and they are sufficient to define photoelastic waveguides in silicon without the need for additional confinement from planar layers or from doping or etching of the guiding layer, although the lowest measured losses were still around 4.3dB/cm, indicating the need for even better photoelastic confinement. The results suggest that the relaxation of the stressor force under excessive strain occurs at the stressor/silicon interface, and does not represent the overall strength of the film. It may therefore be possible to generate even higher strains if the adhesion at the stressor/silicon interface can be improved. It is also important to investigate whether the stressor films are stable over time. Improving the stressor films is seen as one of the main tasks in the further development of photoelastic waveguides.

2. **Phonon-assisted absorption at the energy band-edge** There is supposed to be a difference in the material losses at 1.15µm and 1.523µm due to the phonon-assisted absorption at the energy band-edge. This difference was calculated to represent 3.9dB/cm in terms of propagation losses for bulk silicon, and 4.9dB/cm for Si$_{0.987}$Ge$_{0.013}$, based on measurements from Braunstein et al. [80]. In a Si$_{0.987}$Ge$_{0.013}$ planar layer on top of a silicon substrate, there should be an additional 1dB/cm due to the lattice mismatch strain. The losses measured here at 1.15µm and 1.523µm showed a difference of 1.5-2.5dB/cm below the expected value. By comparison with the data from the original paper by Macfarlane and Roberts [103] on absorption in silicon near the band-edge, the measured values were of the order of 0.5dB/cm lower than expected. It is likely from these measurements that the data by Braunstein et al. slightly overestimate the absorption at 1.15µm.

3. **Discrepancies between modelled and experimental mode profiles** The results from the waveguide modelling give a relatively good description of the waveguide behaviour, although it does not precisely determine the mode dimensions and it does not predict the small second-order mode seen outside the main edge modes when exited at 1.15µm. It is believed that these discrepancies between the modelled and experimental results reflect the discrete nature of the waveguide model, which used a relatively large spacing of 0.5µm between the nodes in the finite element and finite difference analysis. It is believed that the waveguides can be more precisely characterised by reducing the distance between the nodes in the model. For the further study of photoelastic structures, the model should also be improved to consider the coupling between waveguide modes and into the substrate.

4. **Evaluation of photoelastic waveguides** Photoelastic structures were evaluated in terms of their usefulness as basic waveguides. In comparison with other waveguide technologies it was concluded that they are relatively quick and easy to fabricate, and they are appropriate for integration since they do not require etching or doping of the guiding layer, and they use standard processing technology. When manufactured in Si$_{1-x}$Ge$_x$, they are also particularly attractive for integration with VLSI. In terms of propagation losses, no other technology will be significantly better. They are flexible in that they could be used without defining any planar layer, while they could also be used for guiding in buried layers. They are therefore not restrictive in terms of the design of other devices.
Their main drawbacks are that the edge modes are slightly asymmetrical, which can generate mode mismatch losses on coupling into other devices, and that their level of birefringence changes strongly with the crystallographic orientation of the waveguide, which can make it difficult to design waveguide bends. However, it is seen that the variable birefringence can be employed usefully in devices, and that the waveguide modes can also be made to be symmetrical, so that these issues pose only small restrictions on the practical integration of photoelastic waveguides in Si$_{1-x}$Ge$_x$. Overall, though, photoelastic waveguides in Si$_{1-x}$Ge$_x$ can be seen as a real alternative to other waveguide technologies.

5. Possible applications for photoelastic structures in optical circuitry A number of possible applications using photoelastic guiding were illustrated, showing that couplers, power splitters and polarisers can be made with simple structures using only photoelastic confinement. Diode- or transistor-like structures based on carrier-injection for switching or modulation of waveguides were also considered. Although the switches and modulators are likely to require some doping of the guiding layer in addition to the photoelastic confinement, they could become attractive devices due to their compact and simple design.
Chapter 7

Conclusions and Further Work

7.1 Conclusions

An investigation of photoelastic waveguides in bulk silicon and Si$_{1-x}$Ge$_x$/Si heterostructures, including theoretical and computer modelling as well as experimental studies of the structures, has been presented. The main aim of the investigation has been to determine whether these structures are realisable. Particular attention has been given to photoelastic waveguides in bulk silicon, as these waveguides are defined using only photoelastic confinement, which has not previously been reported in any material.

Three photoelastic waveguides structures were studied experimentally in this project. All comprise a stripe of Si$_N$ defined along the [100] axis on a (100) silicon substrate or a Si$_{0.87}Ge_{0.13}$/Si heterostructure. Both the modelling and experimental work show that there is one guiding region outside each edge of the Si$_N$ stripe, close to the waveguide surface. In the Si$_{0.87}Ge_{0.13}$/Si heterostructures, the additional optical confinement from the planar structure supports an additional mode under the middle of the Si$_N$ stripe. This additional middle mode was demonstrated here in the 8μm thick Si$_{0.87}Ge_{0.13}$ layers, while it was not seen in the 14μm thick layers, indicating that there is a maximum limit to the thickness of the planar layer for the middle mode to be confined, and that this limit lies between 8μm and 14μm. The size of the guided modes indicate that a more appropriate planar layer thickness would be 3-4μm. Both modelling and experimental results show a nearly optically isotropic behaviour in all guiding regions, while reports from silicon based photoelectric waveguides oriented along the [110] direction show strong birefringence. While the change in birefringence with crystal direction can complicate the design of some devices where waveguide bends are needed, it also presents a tool for simple control of light polarisation.

The experimental results presented here are useful in that they show that the photoelectric effect in silicon and Si$_{0.87}Ge_{0.13}$ is strong enough to define channel waveguides. The results from the photoelectric waveguides in bulk silicon are particularly interesting, since they prove that waveguides can be defined using only photoelectric confinement. At 1.523μm, excess propagation losses of down to 4.3dB/cm were measured in the silicon photoelectric waveguides. Although lower waveguide losses are desirable, these results indicate the potential of purely photoelectric waveguides, defined by simply depositing a stressor layer onto the surface of the structure. These waveguides would not require damaging or doping of the guiding layer, and they leave the material surface intact. Overall, they set few restrictions for the design of other components on the same substrate, and pose an interesting technology for optoelectronic integrated circuits.
The modelling of refractive index profiles and the optical mode patterns presented here depend strongly on the photoelastic constants, which give the change in refractive index with strain. The photoelastic constants were determined here from the strain-induced shifts in the energy band structure of silicon and germanium and the corresponding changes in the extinction coefficient, which gives the refractive index according to the Kramers-Krönig relationship. A good correspondence was found between the experimental study and the modelling of the waveguides, confirming that both the sign and the relative size of the photoelastic constants are correct. Previously published photoelastic constants are very different from the ones calculated here, and were used to describe photoelastic silicon-based waveguides with stressor stripes oriented along the [110] axes, however, they do not explain the experimental results presented here.

SiNx stressor films were studied by interferometry to determine the stresses generated between the film and the guiding layer. It was found that the stresses of the as-deposited films are poorly defined and generally quite low, so that many of the photoelastic waveguides did not produce any output. However, after annealing at 500-600°C, stresses of up to 2-3·10^6 dyn/cm can be generated, which is significantly higher than reported for other stressor films. Similar annealing of photoelastic waveguides showed a corresponding increase in the photoelastic confinement. After further annealing at higher temperatures the confinement weakens, indicating a relaxation of the stressor force, which is consistent with the interferometry measurements of the stressor films. This suggests that the maximum stressor force has been reached, although it may be possible to generate higher stresses by improving the stressor technology, and so increase the photoelastic confinement even further.

The greatest experimental problem faced during the project was that of defining continuous narrow stressor stripes from the SiNy films such that they extend all the way to the facet. The problem occurs during photolithography because the photoresist, which is spun onto the sample, builds up around the edges of the sample and prevents the photolithographic pattern from being defined across the entire sample. It was found that the surface of the sample can be extended using a liquid black wax, which runs into contact with the sample facet through capillary action, thus effectively removing the sample edge as seen by the photoresist, which practically eliminates the problem of edge build-up. This technique is useful because it provides a smooth extension of the surface without solid mechanical contact with the facet. The inherent capillary effect of liquids also avoids the problem of careful alignment of the extending medium. It is therefore a technique which could usefully be applied to other processes, in particular where it is important to protect the end facets of specimens.

The waveguide technology investigated in this project is unique in that a two- or three-arm coupler can be defined by depositing one single stressor stripe. In a three-arm coupler, the relative intensities of the guided modes are controlled by the width of the stressor stripe, which also determines the distance between the modes. This technology therefore allows a very simple and compact way of fabricating couplers. The waveguides used to study the effect of annealing in figure 5.19 illustrate how a two-arm coupler could be defined with the guiding regions only 2μm apart using a single stressor stripe. Alternatively, a single guiding region can be defined by the same technology.

The finite element model in chapter 3 included a large section of the substrate, which has previously been assumed to be rigid. The modelling results show that around one third of the strain energy is taken up by the substrate, rather than by the Si1-xGe_x guiding layer. Due to the strain in the guiding layer, there will be an increase in propagation
losses around 1.15µm, as calculated in figure 3.7. The measurement results show that the losses at 1.15µm are higher than at 1.523µm, which is attributed to the absorption band edge at approximately 1.1µm. It is also found that the losses in 8µm thick Si$_{1-x}$Ge$_x$ guiding layers grown on silicon are over 1dB/cm higher than those in 14µm thick guiding layers, suggesting that the 8µm thick layers are strained, with correspondingly higher losses. There are also small second-order modes seen in the waveguides when exited at 1.15µm, while at 1.523µm all guiding regions are single mode. For applications where it is preferable with low losses and single mode behaviour, the photoelastic waveguides studied here are therefore less appropriate at 1.15µm than around 1.523µm, which is also the wavelength region of interest for optical communications.

A number of results, problems and possibilities of photoelastic waveguides in bulk silicon and Si$_{1-x}$Ge$_x$/Si heterostructures have been presented in chapters 5, 6 and in this section. However, the most useful findings from this work can be summed up in a few points:

- It is possible to fabricate waveguides with well-defined guiding regions using only photoelastic confinement, where there is no additional confinement from planar structures or from doping or etching of the guiding layer.

- Photoelastic waveguides can be fabricated in bulk silicon and in Si$_{1-x}$Ge$_x$/Si heterostructures. At 1.523µm, waveguide excess propagation losses of down to 4.3dB/cm were measured in silicon, while in Si$_{1-x}$Ge$_x$/Si heterostructures, the excess losses were practically zero.

- Photoelastic waveguides in silicon and in Si$_{1-x}$Ge$_x$/Si heterostructures are nearly optically isotropic when oriented along the [100] crystallographic axis on a (100) substrate, in contrast to the highly birefringent silicon photoelastic waveguides reported previously along the [110] axis. This behaviour corresponds to the modelling presented here, but cannot be predicted with previously published values of photoelastic constants.

- In photoelastic waveguides in Si$_{1-x}$Ge$_x$/Si heterostructures a two- or three-arm coupler can be defined by depositing one single stressor stripe. In a three-arm coupler, the relative intensities of the guided modes are controlled by the width of the stressor stripe, which also determines the distance between the modes. This technology therefore allows a very simple and compact way of fabricating couplers.

In addition to these findings, there are several issues which should be further investigated, either to improve the results in this project or to exploit possible applications for photoelastic structures in optoelectronic circuitry. Some of these issues are outlined below.

### 7.2 Further Work

The work performed in this project could be studied in further detail, either to better describe the waveguide behaviour or to improve their performance. There are also a number of possible applications for these waveguides, as described in chapter 6. The issues which are regarded here as most interesting for further investigation in this field are listed below.
1. Studies of Stressor Films

(a) Stability of the stressor films

The measurements recorded here were performed over a relatively short period of time. If photoelastic waveguides are to be applied in optical circuits, it is important that the stressor films be stable over time. Several interesting options exist for defining stressor layers, including films generated by chemical reactions and growing crystalline Si$_{1-x}$Ge$_x$ layers onto silicon. Nevertheless, one of the main issues for further investigation of photoelastic waveguides is to generate stable stressor layers.

(b) Maximum strain

The maximum strain measured for the stressor layers studied here was $2-3 \times 10^6$ dyn/cm, which is higher than that recorded for other stressor materials. The results indicate that excess stresses cause a relaxation along the stressor/silicon interface. It would be interesting to investigate whether even higher stresses could be generated by improving the stressor adhesion.

2. Photoelastic Waveguide Modelling

(a) Profile accuracy

There were some discrepancies between the modelled and experimental results in this project: The mode sizes were slightly underestimated, the second mode seen when edge modes were exited at 1.15μm was not predicted, and the stressor stripe width at which all the maximum mode intensities are equal was overestimated by 1.5-2μm. It is expected that these discrepancies reflect the discrete nature of the waveguide model, which had 0.5μm between each node at which the solution was calculated. It would therefore be useful to define a model with higher resolution. These discrepancies may also reflect a poor photoelastic confinement at the end of waveguides or coupling between the guiding regions, and the significance of these effects should be investigated.

(b) Coupling Between Adjacent Waveguides

The model used in this investigation did not assess the coupling between guiding regions or the coupling into the substrate. For further studies of devices based on waveguide coupling, it would be useful to generate good quantitative estimates of coupling lengths and the effect of different waveguide variables. It would also be useful to estimate the substrate losses of waveguides using purely photoelastic confinement.

(c) Singularities

The waveguide modelling performed here considers only a two-dimensional section through a quasi-infinite straight waveguide. Close to the waveguide facets, the strain profiles change. Such changes will also occur at waveguide bends and at the end of stressor stripes, for instance as shown in figure 6.5(c). It would be useful to develop the waveguide model to incorporate these changes in the strain profiles.

(d) Birefringence

The results here, with stressor layers along the [100] axes, show a low birefringence, while a strong birefringence has been reported with stressor stripes...
along the [110] axes. However, previously reported photoelastic constants cannot explain this difference. It would be interesting to investigate why these previous reports are different, and to perform a theoretical and experimental study of the photoelastic effect along different crystallographic axes. As well as being a useful study of the crystals themselves, this is important for a thorough understanding of photoelastic waveguide bends.

3. Improving Waveguide Characteristics

(a) Change the sense of the stressor force

All the waveguides studied in this project had the stressor layer under compression. It was predicted that a reversal of the stressor force would set up a single well-defined waveguide which would be symmetrical in the horizontal plane. This reversal of the stressor force could be performed either by defining an off-line structure, as shown in figure 3.12, or by finding a stressor stripe which would be under tension. It is expected that this type of waveguide will be convenient for coupling into optical fibres, since the mode profile could be easily controlled.

(b) Planar layers

The planar Si_{1-x}Ge_x layers used in this project were 8\mu m and 14\mu m, respectively, while it is expected from the optical mode profile measurements that a planar layer of 3-4\mu m would be more appropriate. It will be useful to confirm experimentally that this is an appropriate planar layer thickness, and to determine its effect on the optical mode profiles.

(c) Buried photoelastic structures

It was predicted in section 6.2.2 that below a depth of approximately 2\mu m, the photoelastic contribution to both TE and TM polarised light would be roughly the same along the [100] and [110] axes in Si_{1-x}Ge_x alloys. Photoelastic waveguides in buried layers could therefore be optically isotropic along different directions. It would be useful to investigate whether this type of non-birefringent behaviour can be achieved. One major consideration is whether significant photoelastic strain can practically be induced so far into the structure.

4. Photoelastic Waveguide Devices

With the various guiding schemes which are possible in photoelastic waveguides, these structures lend themselves particularly well to couplers and power splitters. As shown in figures 6.3 and 6.4, several coupler structures can be defined without the use of waveguide bends. The concepts for photoelastic optical devices shown in figures 6.3 through 6.7, such as polarisers and switches, pose interesting research targets for photoelastic structures, which could become effective, and particularly simple and cheap optical devices.

Although this project has shown the feasibility of photoelastic waveguides in bulk silicon and Si_{1-x}Ge_x/Si heterostructures, which is an important development for silicon-based integrated optical circuits, it is clear that there are many improvements to be made and possibilities which should be investigated as a natural extension to the work performed here. The investigation into these waveguide structures has therefore by no means come to an end.
Appendix A

Materials Data

A.1 Silicon

Young's Modulus & Poisson’s Ratio

A value of Young’s Modulus of 1.3·10^{12} \text{ dyn/cm}^2 [120] and a Poisson’s ratio of 0.279 [120], both measured along the [100] direction, are used for all calculations in this project, since the physical waveguide structure and the corresponding calculations are set up such that the major stresses and strains are along the [100] directions.

Thermal Expansion Coefficient

Okada and Tokumaru[121], performed a least squares fit to 19 references, giving a temperature dependence of

\[
\alpha(t) = (3.725[1 - e^{(-5.88·10^{-3} \cdot (t-124))}] + 5.548·10^{-4} \cdot t) \cdot 10^{-6} K^{-1} \quad (A.1)
\]

Integrating with respect to temperature, equation A.1 becomes:

\[
\int \alpha(t) \, dt = (3.725[t + \frac{1}{5.88·10^{-3}} e^{(-5.88·10^{-3} \cdot (t-124))}] + \frac{5.548·10^{-4}}{2} \cdot t^2) \cdot 10^{-6} K^{-1} \quad (A.2)
\]

Integrating from room temperature to 300°C gives

\[
\int_{293 K}^{373 K} \alpha(t) \, dt = 0.921 \cdot 10^{-3} \quad (A.3)
\]

giving an average value of \( \alpha \) of 3.29 \cdot 10^{-6} K^{-1}. Values of the expansion coefficient for other temperatures are calculated similarly.

A.2 Germanium

Young's Modulus & Poisson’s Ratio

The elastic moduli of germanium according to McSkimin and Andreatch [122] are \( s_{11} = 9.7866·10^{-13} \text{ cm}^2/\text{dyn} \) and \( s_{12} = -2.6715·10^{-13} \text{ cm}^2/\text{dyn} \), giving a Young’s Modulus of \( 1/s_{11} = 1.022·10^{12} \text{ dyn/cm}^2 \), and a Poisson’s ratio of \( -s_{12}/s_{11} = 0.273 \).
Table A.1 Mechanical data used for stress and strain calculations of the photoelastic waveguides. A linear interpolation is used for all data for Si_{1-x}Ge_x alloys. The thermal expansion coefficients for silicon and germanium refer to the temperature interval from 300°C to 20°C. For other temperatures the thermal expansion is slightly different, and is found from equation A.2.

Thermal Expansion Coefficient

The expansion coefficient of germanium is \(5.75/2.33\) times that of silicon at 300K \([123]\). It will be assumed that it increases in this constant proportion to the expansion coefficient of silicon for all temperatures.

A.3 Silicon Nitride

Young’s Modulus & Poisson’s Ratio

A value of \(E/(1-\nu)\) of \(1.1\cdot10^{12}\) dyn/cm\(^2\) was measured by Retajczyk and Sinha \([124]\) on plasma-deposited SiN CVD films, where \(E\) is Young’s Modulus and \(\nu\) is Poisson’s ratio, and will be used for the SiN\(_y\) films deposited in this project.

A Poisson’s ratio of 0.17 will be used, assuming that it is similar to that of SiO\(^2\) films \([120]\). This gives a Young’s Modulus of \(0.913\cdot10^{12}\) dyn/cm\(^2\).

Thermal Expansion Coefficient

A value of \(1.5\cdot10^{-6}K^{-1}\), measured by Retajczyk and Sinha \([124]\) will be used as the thermal expansion coefficient of SiN\(_y\) films.
## Appendix B

### List of Physical Constants

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Symbol</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Velocity of light in a vacuum</td>
<td>$c$</td>
<td>$2.998 \cdot 10^{10}$</td>
<td>cm/s</td>
</tr>
<tr>
<td>Permittivity in a vacuum</td>
<td>$\varepsilon_0$</td>
<td>$8.85418 \cdot 10^{-14}$</td>
<td>F/cm</td>
</tr>
<tr>
<td>Planck's constant</td>
<td>$\hbar$</td>
<td>$6.62617 \cdot 10^{-34}$</td>
<td>J-s</td>
</tr>
<tr>
<td>Boltzmann's constant</td>
<td>$\kappa$</td>
<td>$8.62 \cdot 10^{-15}$</td>
<td>eV/K</td>
</tr>
<tr>
<td>Electron charge</td>
<td>$q$</td>
<td>$1.602 \cdot 10^{-19}$</td>
<td>Coulomb</td>
</tr>
<tr>
<td>Hole mobility (Si)</td>
<td>$\mu_{Si}$</td>
<td>450</td>
<td>cm$^2$/V-s</td>
</tr>
<tr>
<td>Hole mobility (Ge)</td>
<td>$\mu_{Ge}$</td>
<td>1900</td>
<td>cm$^2$/V-s</td>
</tr>
<tr>
<td>Electron rest mass</td>
<td>$m_0$</td>
<td>0.91095</td>
<td>$10^{-30}$ kg</td>
</tr>
</tbody>
</table>

All values are taken from Sze [125].
Appendix C

Tracer.c

A short C++ routine, named Tracer, was written to digitise hard-copies of profile plots. Having scanned the plots and saved them as a standard .pbm file, Tracer extracts the line data from the .pbm file and writes them into a new file as a list of X-Y data, which can easily be included in any presentation program. The source code of Tracer is listed below.

```c
#define COLUMN 876
#define ROW 624
#include <iostream.h>

void main()
{
    int row;
    int column = 1;
    int endofline;
    char c = 'O';

    while ( column < COLUMN )
    {
        row = 1;
        endofline = 0;

        while ( row < ROW + 1 )
        {
            cin.get(c);

            if ( c == 'O' )
                row++;

            if ( c == '1' )
            {
                if ( endofline == 0 )
                {
                    cout << column << "\t" << row << endl;
                    endofline++;
                }
            }
        }
    }
}
```

row++;
}
}
column++;
}

When compiled, the routine can be used with normal UNIX redirectioning commands: `Tracer.out < infile.pbm > outfile.lst`, where `Tracer.out` is the compiled C++ file, `infile.pbm` is the scanned picture saved in ASCII .pbm format, and `outfile.lst` is the resulting tabular data.
Bibliography


