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UV Raman studies of channel stress in transistors with embedded SiGe source and drain

by

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Summary

Channel strain engineering is important for improving the performance of metal-oxide-semiconductor (MOS) devices today. UV Raman spectroscopy is commonly used for stress measurements in microelectronics applications, but its use in channel stress studies of advanced transistors in sub-100nm nodes is relatively unexplored. This thesis presents a low-cost method for rapid characterization of channel stress of 45nm-node transistors with embedded SiGe source and drain, using UV Raman spectroscopy. Results of using a micro-meter sized laser beam to study the channel stress of repeating transistors are presented and discussed. The effects of changing the gate pitch as well as the impact of implantation and annealing on the channel stress are investigated. Simulation results are also included to provide insight into the interaction of light with the structures studied. The measurement approach presented in this thesis can be an attractive alternative to other approaches that require more time and resources to carry out.

1. Introduction

1.1 *Introductory words*

The metal-oxide-semiconductor field-effect transistor (MOSFET) plays a key role in modern integrated circuits. For the past three decades, the scaling of MOSFETs in accordance to Moore's Law saw to the birth of a new technology generation every two to three years. Each new generation comes with doubled device density in the integrated circuits, decreased cost per transistor, and improved device performance for the same cost [1-2]. However, as MOSFETs were being aggressively scaled into the deep sub-micrometer regime, many challenges began to appear. These include velocity saturation and high leakage current. To keep up with the scaling trend while continuing to improve device performances, new technology solutions were being proposed and implemented. Among them, strain engineering has become popular and important for boosting device performance [3-6].

Strain engineering is essentially about straining the MOSFET inversion channel. The inversion channel connects the source and drain electrodes and is a passage for electrons or holes to flow when the MOSFET is in the "on" state. Strain engineering improves device performance by increasing the mobility of the electrons or holes in the channel, thereby increasing the drive current. Different strain engineering techniques bring about different performance gains, as do varying the layout or changing the process flow parameters for each technique. To understand such gains, it is necessary to quantify the strain or stress in the channel.

This is the subject of study of this thesis. Specifically, UV Raman spectroscopy is used for stress studies of 45 nm node transistors with embedded silicon-germanium (SiGe) source and drain. For this strain

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engineering technique, SiGe, which is epitaxially grown in the source and drain regions, acts as a stressor to induce a compressive strain in the channel. By varying the Ge concentration, it is possible to increase or decrease the amount of strain. Ever since the first report of this strain technology appeared in the International Electron Devices Meeting in 2002 [3], it has rapidly gained popularity and has become the main method for inducing compressive strain in p-type MOSFETs in production nowadays.

1.2 Overview of this thesis

We begin with a literature review in Chapter 2. This chapter is divided into two main sections. The first section briefly reviews the field of MOSFETs with strained silicon channels. This section includes a description of the main physical mechanisms behind the improvement in carrier mobility when silicon is appropriately strained. It also provides information on the methods commonly used to strain the transistor channels. This section then moves on to describe the available methods that are used to quantify channel strain. Both simulation and experimental methods will be covered. A discussion of the strengths and limitations of current experimental methods, as well as the lack in studies in certain areas is then given. The second section of this chapter reviews the theory underlying the Raman scattering of semiconductors. Also included is the theory addressing the change in the Raman characteristics of silicon when a uniaxial stress is applied to it.

Next, the materials, instrumentation, and methods used for the work in this thesis are given in Chapter 3. The process flow for the devices used is briefly described under the *Materials* section. For the *Instrumentation and Methods* section, details of the hardware and operation of our Raman spectroscopy system are provided. Relevant concepts such as spatial and spectral resolution are explained. Also described in this section are the finite-

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difference time-domain (FDTD) method and the software program used for such work in the thesis.

Chapters 4 to 6 cover the main projects undertaken for this thesis. Chapter 4 lays the foundation that Chapters 5 and 6 build upon. The sample preparation method, approach for channel stress measurements, and data analysis and interpretation are given in Chapter 4. Chapter 5 extends the research to study the effect of implantation and annealing on the channel stress. Chapter 6 includes FDTD simulations to provide insight into the distribution of the Raman excitation light in the structures studied in Chapters 4 and 5. Implications of using Raman excitation light of different polarizations are discussed. Chapter 7 then follows. This brief chapter contains some results of near-field Raman mapping for high spatial resolution work.

Finally, Chapter 8 highlights the main conclusions of the work in this thesis and provides suggestions for further work.

Note: Unless otherwise stated, the sample preparation, data acquisition, data analysis, and data interpretation in Chapters 4 to 7 were carried out by me.

2. Literature review

2.1 Strained transistors for improving device performance

2.1.1 How straining the channels improves carrier mobility

To understand why straining the channel of the MOSFET can improve carrier mobility, we need to have some understanding of the silicon reciprocal lattice structure, its electronic band structure, and its transport behavior. We will confine our discussion to Si as the strained material and give a brief overview of the effect of strain on Si carrier mobility.

Fig. 2.1 (a): Reciprocal lattice, in k -space, of silicon. The first Brillouin zone is shown. Special high-symmetry points and the high-symmetry lines joining the points are depicted. The Γ point lies at the center of the Brillouin zone. (Figure from Ref. [7]) (b): Electronic band structure of silicon. (Figure adapted from Ref. [8])

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Silicon is an indirect band gap semiconductor whose valence band maximum and the conduction band minimum are not located at the same $\mathbf{k}$ value. From the electronic band structure of unstrained silicon, we can see the valence band maximum is at the Γ point and the heavy hole (HH) and the light hole (LH) bands are degenerate at this point. (Note: The hole mass is inversely proportional to the slope of the band. Close to the Γ point, we see the HH band and LH bands have different slopes and hence different hole masses.) The minimum of the lowest conduction band is located close to the X point, in the $[100]$ direction from the Γ point. It is called the Δ_1 valley. From the first Brillouin zone shown in Fig. 2.1 (a), we see that there are six equivalent faces each bearing the point equivalent to the X point. Therefore, although the conduction band minimum is non-degenerate for a particular $\mathbf{k}$ value (see band structure in Fig. 2.1 (b)), the conduction band minimum is six-fold degenerate as a result of degeneracy in reciprocal space. Hence, there are six equivalent Δ valleys. Figure 2.2 below shows ellipsoids which represent surfaces with equal energy at the vicinity of each of the six conduction band minima. The absolute band minima will correspond to the exact centers of these ellipsoids.

Fig. 2.2: The first Brillouin zone of unstrained silicon, with the six equivalent Δ valleys along the three principal axes. The ellipsoids are surfaces with equal energy at the vicinity of the conduction band minimum. The long axis of each

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ellipsoid corresponds to m_l , the longitudinal mass ($m_l = 0.916 m_0$) while the short axis corresponds to m_t , the transverse mass ($m_t = 0.19 m_0$), where m_0 refers to the free electron mass. (Figure adapted from Ref. [9])

For n-type devices whose carriers are electrons, we are concerned about the effect of strain on the conduction band of silicon. Let us understand what will happen to the conduction band of bulk silicon first. An applied stress will shift and split the six-fold degenerate valleys in accordance to the deformation potential theory developed by Bardeen and Shockley [10] which is later generalized by Herring and Vogt [11]. The theory relates the shift in energy of the bands to small deformations of the crystal as:

$$\Delta E = \sum_{ij} \Xi_{ij} \varepsilon_{ij} \quad (2.1)$$

where Ξ_{ij} is the deformation potential tensor and ε_{ij} is the strain tensor. It can be shown that there are three different deformation potentials for silicon and the number is reduced to two potentials, Ξ_u and Ξ_d , for the conduction Δ valleys in the $\langle 100 \rangle$ directions [7]. The linear shift for any one of the Δ valleys ($i = 1, 2, \dots, 6$) can be written as [9, 11]:

$$\Delta E_c^{(i)} = \Xi_d (\text{Tr}\{\varepsilon\}) + \Xi_u (\mathbf{k} \cdot \varepsilon \cdot \mathbf{k}) \quad (2.2)$$

where $\text{Tr}\{\varepsilon\}$ is the trace of the strain tensor ε , and $\mathbf{k}$ is a unit vector along the direction of the conduction valley i . This equation shows us that the energy shifts for the different valleys can be different for different stress conditions. For example, applying $[110]$ uniaxial tensile strain will cause the energy of the two out-of-plane conduction valleys labeled “3” in Fig. 2.2 to move down and the four in-plane valleys labeled “1” and “2” to move up [5, 12]. This will cause the electrons to preferentially repopulate from the in-plane valleys to the

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out-of-plane valleys. As now for in-plane conduction, we have more electrons with the lighter effective mass m_t , we have a smaller *average* conductivity effective mass resulting from the repopulation. (Note: applying stress in this particular direction will also cause band warping because of the presence of shear deformation [13]. This causes the values of both m_l and m_t to actually change with the shear stress values. Further details are found in Chapter 9 of Ref [9]. If there is no shear deformation like in the case of [100] uniaxial stress or in-plane biaxial stress, valley splitting but no band warping occurs. The values of m_l and m_t remain the same and valley splitting and electron repopulation alone can explain the change in electron mobility.) The lifting of the degeneracy of the valleys also alters the scattering of the electrons with phonons. Electrons are scattered by the phonons from one valley to another (intervalley scattering), and this is reduced by the splitting of the valleys [12]. There are other kinds of scattering mechanisms [7] but reduction of this kind of scattering is one of the main useful outcomes of applying appropriate strain.

It can be seen from the expression for the carrier mobility, $\mu = q\tau_{ave}/m^*$ [7, 12], that a change in the effective conductivity mass, m^* , and a change in the average scattering time, τ_{ave} , will change the carrier mobility. (The average scattering time refers to the average time between scattering events. Scattering will randomize the momentum of the carrier and will therefore reduce the average velocity vector of the carrier.) Therefore, from the discussion in the previous paragraphs, strain will change the electron mobility in bulk silicon.

The difference between bulk silicon and actual MOSFET devices need to be mentioned here. The channel of the MOSFET is a two-dimensional electron system. The carriers move in the surface inversion layer. They are free to move in the xy plane. However, in the z direction, their motions are constrained by a potential well at the gate oxide because a vertical electric field is applied to the gate. In brief, the effect of this confinement is to lift the

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degeneracy of the in-plane and out-of-plane valleys. Details can be found in the review paper by Ando et al [14]. Therefore even for unstrained MOSFETs, the in-plane valleys have an energy different from that of the out-of-plane valleys. Hence we need to consider whether the effects of the confinement and the band-splitting due to strain are additive or not. With a MOSFET device, yet another effect to consider is the surface roughness scattering, which we shall just mention here without elaborating.

For p-type devices whose carriers are holes, we are concerned with the heavy and light hole bands. The physics of strain-induced changes in hole mobility is rather complex because of the complexity of the valence band. In brief, we need to consider both band splitting and warping. Warping, with its associated effective mass change, is a very important factor to consider for strain effects on hole mobility. One needs to add a perturbative strain-dependent Hamiltonian to obtain the total Hamiltonian, and calculate the splitting and warping of the band within the degenerate version of the **k.p** framework. (The **k.p** method is one that is based on perturbation theory and is used to calculate band structures with or without strain.) More information can be found in Refs [9], [12], and [15]. Here, we simply show some results from Ref. [9] in Fig. 2.3 for applying the technologically important uniaxial compressive [110] stress to bulk silicon. This particular stress has been theoretically and experimentally shown to be more beneficial for hole mobility than are other stresses [16]. Similarly for actual MOSFET devices, one also needs to consider confinement arising from applying the vertical electric field, as well as the various types of scattering.

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Fig. 2.3: Energy dispersions of the heavy hole, light hole and split-off bands along the [110] and [100] directions. A compressive stress of 1 GPa is applied in the [110] direction. Band splitting and warping are observed. (Fig. from Ref. [9]) The split-off band arises from spin-orbit interaction in the valence band.

2.1.2 Methods for straining the channels

Techniques for straining the channels can be broadly classified into global strain methods and local strain methods. For the global strain methods, stress is introduced to the whole wafer; for the local strain methods, stress is introduced to separate transistors on the wafer independently.

A global strain technique is the use of the “virtual substrate”[17]. Multiple SiGe layers, whose Ge composition gradually increases from bottom up, are grown on the bulk Si wafer. A final relaxed SiGe layer with a constant Ge composition is grown on the graded SiGe film stack. A Si film, which will contain the channel eventually, is then epitaxially grown on this relaxed SiGe layer. There is lattice mismatch between the SiGe layer and the Si layer, hence

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the Si layer will experience an in-plane biaxial tensile strain. Another type of global strain method involves the growth of a thin, strained Si film on SiGe-on-insulator (SGOI) [18]. Yet another method eliminates the SiGe layer completely. It involves the use of the strained-silicon-directly-on-insulator (SSDOI) technology [19]. Details are found in the respective references. Figure 2.4 below shows the schematics of these globally strained wafers.

Fig. 2.4: Global strained wafers: bulk with graded and relaxed SiGe, SGOI, and SSDOI.

Global strain techniques are only able to induce one type of strain to the whole wafer. However, there is a need to strain the NMOS and PMOS differently – for example, biaxial tensile strain induced by a global strain technique is advantageous for NMOS but disadvantageous for PMOS. Hence, local strain techniques are necessary. The following section briefly describes some well-known local strain techniques.

One way of inducing uniaxial compressive strain in the p-channel is to fill the source and drain regions with $\text{Si}_{1-x}\text{Ge}_x$. This integration scheme was first proposed in Ref. [20] (though not for the purpose of straining the channel) and its strain effect on the drive current was first demonstrated by Ref. [3]. The source and drain regions are etched out to form recesses and SiGe is then

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grown in these areas by selective epitaxy. Single crystalline growth only takes place on bare silicon and not on dielectric films such as silicon dioxide or nitride. The resulting SiGe structures are embedded in the source and drain; hence they are often referred to as e-SiGe, or embedded SiGe.

For this straining technique, the strain is induced by the lattice mismatch between Si and $\text{Si}_{1-x}\text{Ge}_x$ ($a_{\text{Si}} = 5.43 \text{ \AA}$, $a_{\text{Ge}} = 5.66 \text{ \AA}$, and $a_{\text{Si}_{1-x}\text{Ge}_x} = (1-x)a_{\text{Si}} + xa_{\text{Ge}}$ by Vegard's Law, where a refers to the natural lattice constant of the corresponding material at 300 K [21]). At the edge of the channel, the Si lattice experiences a vertical tension because of the lattice mismatch. This results in a horizontal compressive strain which extends from the channel edge to the channel center [22]. This approach for inducing uniaxial compressive strain in the PMOS channel is already widely used in production and is technologically important. (*Note: This kind of device is the subject of study for this thesis.*) It is also possible to fill the source and drain with $\text{Si}_{1-x}\text{C}_x$, with a small mole fraction x , to induce a uniaxial tensile strain in the channel [23]. $\text{Si}_{1-x}\text{C}_x$ has a smaller lattice constant than Si. Epitaxially grown on Si, it will be stretched horizontally and compressed vertically. At the channel edge, the Si lattice interacts with the $\text{Si}_{1-x}\text{C}_x$ lattice and the Si lattice experiences a lateral tension [24]. Though not yet in mass production, it seems highly manufacturable and promising for this. The review paper (Ref. [24]) and references therein provide further information on transistors with embedded $\text{Si}_{1-x}\text{Ge}_x$ or $\text{Si}_{1-x}\text{C}_x$ source and drain as stressors, as well as advanced stress techniques that are related to these.

Another way of inducing uniaxial strain in the channel is by using stress transferred from a permanently stressed layer deposited on top of a transistor. It is possible to separately deposit a compressive nitride film over a PMOS and a tensile nitride film over an NMOS [25]. This approach is known as the dual stress liner (DSL) approach. Silicon nitride film can be made to be either tensile or compressive, depending on the growth conditions.

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Disposable films are used to induce a channel strain in the stress memorization (SMT) technique [26]. The usual high temperature, short duration anneal for dopant activation is applied after the deposition of a tensile stressor layer. This stressor layer is then removed before the salicidation process. The channel becomes strained because the stress that is imparted from the stressor layer gets “memorized” during the annealing process, where recrystallization of the gate, source and drain materials take place.

Shallow trench isolation (STI) structures can also stress the transistor channels [27-28]. Nevertheless, device performance gains are generally modest compared to other strain techniques.

Figure 2.5 below show some of the stressors used in the semiconductor industry.

Fig. 2.5: Stressors used in the semiconductor industry. Shallow trench isolation, highly stressed compressive and tensile nitride films, and embedded SiGe source and drain are used. Figure from Ref. [9].

An advanced local stressing technique related to the high- κ dielectric/metal gate technology should be mentioned here. In the gate-last approach, the dummy poly gate is removed and later substituted by a metal gate. The removal of the dummy gate releases the repulsive force due to the gate on the channel, thereby increasing the compressive stress from the

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embedded SiGe source and drain [6, 29]. This will be beneficial for PMOS performance. As this phenomenon is related to the work in this thesis, more information and discussion will be given in Chapter 4.

2.1.3 Quantifying channel strain: simulations and experimental methods

2.1.3.1 Simulations

There are many different types of simulations for semiconductor devices. We shall limit our discussion here to the simulation of strain or stress in strain-engineered MOSFET devices. This kind of simulation can be done using Technology Computer-Aided Design (TCAD) applications. TCAD applications are specifically meant for the semiconductor industry. Examples include Sentaurus from Synopsys, the TCAD tools from SILVACO, as well as those from Crosslight. It is also possible to simulate strain using non-TCAD finite-element method (FEM) applications. Examples of such applications include Abaqus FEA from SIMULIA, COMSOL Multiphysics from COMSOL, and the various tools from ANSYS.

The earliest simulation work done on strain-engineered MOSFET devices appears to be that of Yeo et al [22], which was reported at the April 2004 Materials Research Society Symposium. Here, they used ABAQUS (now known as Abaqus FEA), which is a non-TCAD application based on the finite element method. Their journal publication followed this work shortly after [30]. They performed a theoretical evaluation of the strain field of a p-channel transistor with embedded SiGe source and drain. Elastic isotropy approximation was used. The lattice mismatch was simulated in the framework of thermoelasticity. This means that a pseudo thermal strain represented the lattice mismatch strain – they let the thermal expansion coefficient be equal to the value of the lattice mismatch strain between SiGe and Si, and then raised the temperature of SiGe by 1 K [22, 31-32]. The finite element simulation followed the Newton method of numerical iteration to

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solve some specific equations described in Refs. [22] and [32]. They found that the strain field in the channel consists of a *lateral compressive* component and a *vertical tensile* component, and that the magnitudes of the components depend on the Ge mole fraction as well as the spacing between the source and the drain. The lateral strain component is larger than the vertical. An interesting insight they provided is that the SiGe lattice in the source and drain is not fully strained – in fact they have to be so, in order that the Si lattice be strained [30]. Yeo also extended their FEM simulation work to that of an n-channel transistor with embedded Si:C source and drain subsequently [24].

Other early simulation works are those carried out by workers from Synopsys [33-34]. In these works, TCAD process tools were used to simulate the strain. However, likely due to the emphasis on the engineering aspects of their work, no information was provided on the kind of physical models or framework used for their TCAD strain simulations. Nevertheless, these works paved the way for using TCAD tools (notably from Synopsys) for simulating strains and the resulting electrical behavior in strain-engineered MOSFETs [35-43] – after simulating the strained structures from the TCAD *process* tool, one will then input the results into the TCAD *device* tool to simulate the electrical behavior of the devices. (Note: TCAD *process* simulation tools model the fabrication steps of semiconductor devices. These include diffusion, implantation, oxidation, etching, deposition, and silicidation steps. One will typically input process conditions such as ambient chemical composition, temperature, and pressure for each of the step. TCAD *device* simulation tools, on the other hand, simulate the electrical characteristics of devices [44-46].) So far, devices with embedded SiGe or Si:C source and drain with or without stress liner films have been simulated. Some devices are built on bulk Si substrate while others are built on SOI substrates.

A rather recent piece of work that seems particularly striking is that cited in Ref. [38]. In their second figure, they showed that the lateral stress in

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their device simulated using Sentaurus Process Tool [45] corresponds very closely to experimental stress data obtained from TEM-based techniques from other research groups. The figure is reproduced below:

Fig. 2.6 a) Distribution of the lateral stress components in a transistor structure with Si:C S/D stressors. Experimental data is shown for comparison. b) Distribution of the lateral stress components in a transistor structure with SiGe S/D stressors. Experimental data is shown for comparison. (Figure from Ref. [38])

Another highly noteworthy piece of work is that of Ref. [47], published in *Nature Letters* in 2008. The emphasis of their work is on the experimental determination of strain in embedded SiGe PMOS devices using the holographic interferometry technique that they invented. Strain simulation was done using FEM in COMSOL Multiphysics. Details of the physical models used for simulation can be found in the appendix of their publication. Similar to Yeo et al [22, 30], they treated the strain as arising from thermal expansion. Excellent agreement is achieved between their experimental and simulated results (see Fig. 2.7 below).

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Fig. 2.7: Experimental results are on the left and simulated results are on the right. The color scale gives the percentage change with respect to the silicon for substrate deformation, ε_{ij} , and degrees for rotation, ω_{xz} . (Figure from Ref. [47].)

These two examples illustrate the importance of both simulations and experiments for quantifying device strain – they serve to mutually confirm and validate each other and to provide workers in this field more confidence in their data. With an accurate knowledge of the strain present in the device, workers can then predict, develop and optimize their devices more effectively. Having introduced simulations in this section, we will next look into experimental approaches for strain determination in the next section.

2.1.3.2 Experimental methods

Different experimental techniques have been used to study transistor channel strain. Among them, those based on transmission electron microscopy (TEM) are the most common. Another technique, one that is based on X-ray diffraction (XRD), has also been reported in the literature in at least one publication. This section will review the relevant works, discuss the strengths and limitations of these techniques, and point out the lack of studies in

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particular areas. This section will also discuss works published prior to our own that are related to the use of UV Raman spectroscopy for channel strain studies.

Techniques based on TEM

- *Convergent-beam Electron Diffraction (CBED)*: This technique is used in the works in Refs. [48-55] to study strain in MOSFETs. CBED uses a converging electron beam with a large angle of convergence to generate enlarged diffraction spots in the form of disks. The central disk contains higher-order Laue zone (HOLZ) lines that arise from satisfying the Bragg condition for some high-order reflections. These lines are very sensitive to small changes in the crystal lattice [56]. One will analyze the strain by obtaining the best fit between the HOLZ line intersections in the experimental and simulated patterns. Commercial simulation software packages for this purpose are available. Strains of the order of 10^{-4} can be detected by HOLZ line shifts [50-51, 53-55, 57-58]. For silicon, strain of this order of magnitude corresponds to a stress magnitude of 10^1 MPa.

Strain is measured in a point-by-point manner. The spatial resolution is related to the electron spot size and the interaction volume between the electron beam and the specimen. It is possible to have a converged electron beam with a spot size of 1 nm [57]. However, the actual spatial resolution is limited by the angle of tilt away from the [110] axis, where no HOLZ lines are produced. (Many specimens with semiconductor devices have specimen planes normal to this direction.) According to Armigliato *et al* [59], the spatial resolution will be 7 nm for the [340] axis and 10 nm for the [240] axis for a specimen thickness of 200 nm and a zero-diameter spot size. Strain relaxation due to specimen thinning is a valid concern. However according to Zhang *et al* [51], as long as sharp CBED patterns are collected, lattice plane rotation arising from strain relaxation must be negligible. Zhang also reasoned that

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because the predominant and characteristic strain of the MOSFET is in the source to drain direction where the sample is not thinned, there should be negligible strain relaxation along this direction of interest.

For the works cited in Refs. [48-55], some performed measurements closer to the actual transistor channel, some further away into the silicon substrate. The closest regions are around 10 nm and the furthest is around 150 nm, taking the vertical distance from the centre of the gate oxide interface. The closer it is, the more desirable it is – this is because the *channel* strain is the strain of interest. It is less meaningful to study regions deeper into the substrate. The actual channel is only around 2nm deep into silicon, from the gate oxide interface.

- *Nano-beam Diffraction (NBD) [or Nano-beam Electron Diffraction (NBED)]*: The works cited in Refs. [58, 60-62] make use of NBED to study MOSFET strain. Like CBED, NBED is a TEM diffraction technique. However, instead of using a converging electron beam, it uses an almost parallel beam. The beam is nanometer-sized. Sharp diffraction *spots* can be obtained. The advantage of this technique is that it can be used for strain analysis along the [110] zone axis [63], thereby avoiding lateral resolution degradation. Strain quantification is carried out by comparing the diffraction spots from strained regions with a single chosen unstrained region in the substrate. At least one commercial software package (*FEI True Crystal Strain* software) is available for this purpose. Similar to CBED, strain is measured in a point-to-point manner. Spatial resolution is dependent on the spot size of the electron beam. The spot size can be down to 10 nm or less – 10 nm for Ref. [64], 6 nm for Ref. [62], and 2.7 nm for Ref. [65]. Slightly different degrees of strain sensitivity of this technique have been reported – 1×10^{-3} for Refs. [58, 61] and 6×10^{-4} for Refs. [62, 65].

Similar to CBED, a valid concern for this technique is its accuracy being affected by strain relaxation. According to Beche et al [65], if one looks

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at the measured strain values directly without taking into account strain relaxation or the probe shape, an accuracy (i.e. error) of 5% can be realized. (Note: they studied blanket Si/SiGe/Si wafers rather than MOSFET structures.) However, Favia et al [58] reported there is no effect of possible relaxation in their samples for the studied thickness range and device structure. Favia reasoned this is because the strain values for specimens of three different thicknesses are rather similar, within the strain sensitivity of the technique which they determined to be 1×10^{-3} .

- *Electron Diffraction Contrast Imaging (EDCI)*: This technique is used by Li *et al* in the work cited in Ref. [66] to study stress in a MOSFET structure. So far, it appears to be the only paper published on the use of this technique for this purpose. It is a 2D mapping technique. In this work, the authors acquired their EDC image by TEM imaging of their specimen under the (400) two-beam condition and compared their experimental EDC image to a simulated EDC image. (They performed FEM simulation before simulating the EDC image. They then used a special program to extract the relevant parameters from the FEM simulation to create the simulated EDC image, using the relevant TEM conditions.) If the experimental and simulated EDC images did not match well, they would change the FEM conditions until they did. They reported that their technique has a spatial resolution of 10 nm and a stress sensitivity of tens of MPa, and that the stress in the source to drain direction in their specimen is relaxed by 5% compared to that before specimen preparation.

- *High Resolution Transmission Microscopy (HRTEM) with Fast Fourier Transform (FFT) Diffraction Analysis*: This technique is used by Ang *et al* to study strain in a MOSFET [67]. So far, it appears to be the only published paper that uses this particular TEM technique for this purpose. First, they obtained a high magnification HRTEM image of the studied device. Then, they selected discrete 3 nm by 3 nm regions within the image for FFT to

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obtain the reciprocal space diffractograms for those regions. The (002) and (220) reflections of the diffractograms would give information on the vertical atomic spacing (in the [001] direction) and the lateral atomic spacing (in the [110] direction), respectively. As discrete 3 nm by 3 nm regions were selected for FFT diffractogram analysis, this technique is considered to be a point-to-point technique. Though strain characterization issues such as spatial resolution, sensitivity, and possible strain relaxation affecting accuracy were not discussed in this work, the work is nonetheless significant *because it appears to be the first published work that provides direct experimental measurements of MOSFET channel strain*. The data points were acquired from regions as close as 2.5 nm from the gate oxide interface – this can be taken as the depth where the actual channel resides.

- *High Resolution Transmission Microscopy (HRTEM) with Geometric Phase Analysis (GPA)*: This technique is used by He *et al* [68] and Chung *et al* [69] to study MOSFET strain. The GPA method is based on the original work by Htch *et al* [70]. This method is based on centering a small aperture around a strong reflection in the Fourier transform of an HRTEM lattice image and carrying out an inverse Fourier transform. The resulting complex image has a phase component that gives information about local displacements of atomic planes. GPA always measures strain relative to a region that is presumably unstrained. Commercial software packages are available for performing the strain analysis. Rather than isolated points, 2D strain images are obtained with this technique. This technique has a strain sensitivity of 0.001 and a spatial resolution better than 5 nm. Both He *et al* and Chung *et al* reported the significant modification for the strain component in the direction of sample thinning. Strain relaxation in the other two directions is not significant.
- *Dark-Field Off-Axis Holography (Holography Interferometry)*: The works cited in Refs. [47, 62, 71] used this technique to study MOSFET strain.

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A patent has been filed for this technique. Specially designed equipment and uniform specimen thickness are required. Two diffracted beams, one from the strained lattice of the specimen, and the other from the unstrained, are interfered using an electrostatic biprism. Their phase difference will encode the strain information. Two-dimensional strain images can be obtained. This technique enables thicker samples to be used and larger fields of views (1 μm or more) compared to those based on HRTEM GPA (100 nm). Strain sensitivity is as high as 2×10^{-4} and spatial resolution is 4 nm.

- *Dark Field Inline Holography*: Koch *et al* [72] developed this imaging technique and used it to study MOSFET strain. So far, it appears they are the only group working on this technique. In brief, this technique derives strain information from variations in the intensity of dark-field TEM images with defocus. It requires a much smaller electron dose than do strain mapping techniques based on HRTEM. It also can be done using conventional TEM setups without the need for special hardware; hence it is poised to be more accessible than techniques that do. The field of view is several micrometers, the precision is better than 1×10^{-4} , and the spatial resolution is better than 1 nm.

Methods based on XRD

- *X-ray Microbeam Diffraction*: This technique was used by Murray *et al* [73] to study MOSFET strain. It is a synchrotron-based method. The measurements were carried out at The Advanced Photon Source (APS) at the U.S. Department of Energy's Argonne National Laboratory. Murray *et al* took advantage of the fact that the crystallographic orientations of the SOI layer containing the channel and the underlying bulk silicon substrate are offset by approximately 0.24° - this enabled them to resolve the information coming from these two regions. (Had the MOSFET been built on bulk wafer rather than SOI wafer, this method would not have been feasible.)

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DISCUSSION

All in all, it seems TEM-based techniques are powerful tools for studying MOSFET channel strain. Some advanced TEM techniques can provide large fields of views plus high spatial resolution and sensitivity. It is also possible to extract different strain components using those techniques. With regard to the issue of strain relaxation caused by sample thinning, I think it is not a very big problem as various authors have shown that the strain component of interest, which is in the source-to-drain direction, is not significantly modified. Only the strain component normal to the specimen plane suffers from significant modification. Nonetheless, there is a need to prepare TEM specimens for all these techniques. TEM specimen preparation requires a rather big input in terms of time, skill, and resources. There is also a need for access to the specific equipment (e.g. FIB) for sample preparation. In the real life scenario, TEM specimen preparation facilities are often overwhelmed with job requests. Furthermore, the advanced TEM techniques require special hardware or software or both, limiting their accessibility. TEM-based techniques are therefore less suitable for a worker who is less concerned about the technique itself than how the strain measurement results can possibly help him or her (quickly!) to improve on the process flow and device performance. On the same note, X-ray microbeam diffraction requires a synchrotron light source – this is often not readily accessible.

Hence, there is a strong need to develop other methods that are less experimentally complex and more accessible, and which require just simple sample preparation. These will make it much easier to study *numerous* samples with different process parameters at one go, which is desirable for workers seeking to improve process flows and device performance. Indeed, for the works reviewed here, few studied MOSFETs batch-wise, i.e., vary process or layout parameters and systematically study how they affect channel strain. Most would study just one or two specimens. Likely this is also due to the

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emphasis on the technique itself rather than on practical applications. In any case, it highlights a general lack in the literature on experimental studies of how MOSFET channel strain varies with certain process or layout parameters.

The work in the thesis aims to bridge these gaps using UV Raman spectroscopy. I will review and discuss some related works in the subsequent few paragraphs.

Raman Spectroscopy

Raman spectroscopy is a very popular tool in the area of semiconductor characterization [74-75]. It is a rapid characterization method that requires little or no sample preparation. Generally, it is also non-destructive to the sample. Raman spectroscopy has long been used to study the stress in microelectronics structures such biaxial strained Si blanket films on technologically relevant substrates [76-79], shallow trench isolations (STIs) [80-84], silicon regions surrounding through-silicon vias (TSVs) [85-86], as well as at the edges of technologically important thin films [87]. *UV laser is used as the Raman excitation source in situations where surface sensitivity is required* – it has a penetration depth of less than 10 nm in silicon, therefore it can avoid signals from the substrate that can obscure the strain signals coming from just a thin layer on the top. The figure below shows the optical penetration depths for light of different energies for bulk Si (and also for $\text{Si}_x\text{Ge}_{1-x}$, for $x = 0.22$.)

Fig. 2.8: Optical penetration depths in bulk Si and in Si_{0.78}Ge_{0.22} for light of different energies. (Figure obtained from Ref. [88].) Here, the authors of Ref. [88] have defined the optical penetration depth to be $d_{\text{opt}} = 1/(2\alpha)$, where α refers to the absorption coefficient of silicon. For this thesis, we use the definition $d_{\text{opt}} = 1/\alpha$. UV light with a wavelength of 325 nm has an energy of 3.82 eV – we can see the shallow optical penetration depth for this wavelength.

Prior to our own work presented in this thesis, there have been some publications that use Raman spectroscopy for channel stress studies [89-91]. Mayuzumi et al [89] and Yamakawa et al [90] studied gate-last pMOSFETs fabricated using the damascene process. After removing the polysilicon dummy gate, they used UV Raman spectroscopy to study the stress in the exposed channels. Different gate lengths and gate widths were investigated. The smallest gate length that they studied is 0.26 μm . They performed point-

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by-point Raman line scans and 2D mappings. Some of the results from Mayuzumi et al [89] are shown in Fig. 2.9 below:

Fig. 7 Raman peak shift dependence on gate position along L_{gate} for damascene gate pFETs with 40-nm c-Si and 80-nm eSiGe at (a) $L_{\text{gate}} = 10 \mu\text{m}$, (b) $1 \mu\text{m}$ and (c) $0.26 \mu\text{m}$. The devices after dummy gate removal are used.

Fig. 2.9: UV Raman spectroscopy being used to study channel stress in gate-last PMOSFETs. The dummy gates are removed, exposing the channels. (Figure from Ref. [89])

Kosemura et al [91] used UV Raman spectroscopy to study channel stress induced by SiN films. The transistors had a gate length of $2 \mu\text{m}$. Similar to Refs. [89-90], a point-to-point scanning approach was used. Some of their results are shown in Fig. 2.10 below:

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Fig. 5. (Color online) Strain-line profile in dummy-gate sample with compressive stress (-1.0 GPa) film.

Fig. 11. (Color online) Strain-line profiles for dummy-gate samples with tensile stress (1.0 GPa) film and a recess of 30 or 15 nm.

Fig. 2.10: UV Raman spectroscopy being used to study dummy MOSFETs with dummy gates transparent to UV light. (Figure from Ref. [91]) Allowing the UV light to pass through the gates and reach the channels is important for probing the channels.

We can see from the above discussion that UV Raman spectroscopy, being surface sensitive, is useful for studying channel stress. It is necessary to have either transparent dummy gates or to remove the gates to expose the channels for this technique. It appears that the smallest gate length studied prior to our own work using UV Raman spectroscopy is $0.26\text{ }\mu\text{m}$. It is desirable to study much smaller gate lengths, which would be more technologically relevant today. Sub-100 nm gate lengths appear to be relatively unexplored.

In this thesis, I will show how it is possible to use a micrometer-sized laser spot to study transistors from the 45 nm technology node. Useful information can be obtained rapidly under such conditions, as can be seen from Chapters 4 and 5. Ideally, it would also be desirable to combine the high surface sensitivity that comes with the use of UV light with high spatial resolution using near-field techniques so that individual structures might be

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resolved spatially. Chapter 7 shows the results of some preliminary efforts in this area.

In the next two sections, I will review the theory of Raman scattering and describe what will happen to the Raman spectrum of silicon when a stress is applied to it.

2.2 Raman spectroscopy for strain characterization of silicon

2.2.1 Raman scattering of semiconductors

General Theory

The theory of Raman scattering relevant to solid state crystalline semiconductors has been well reviewed in many works. Some of these works are cited in Refs. [7, 74-75, 92-93].

Raman scattering occurs as a result of light interacting with the lattice vibrations (phonons) in a crystal. Atomic vibrations in a lattice, which are present at any finite temperature, will modify the electric susceptibility of a crystal. Hence, the expression for the electric susceptibility will look different from the case where we do not consider the local atomic vibration at all. Specifically, we will have extra terms for its expression. Since electric polarization (which arises as a response of the crystal to an external E-field) is dependent on the electric susceptibility, the extra terms for the susceptibility will give rise to extra terms for the polarization. The radiation arising from the “extra polarization” is the Raman-shifted light. Hence, the presence of the phonons in a crystal give rise to Raman-shifted (or scattered) light when an E-field from an electromagnetic wave (i.e. light) is incident upon the crystal. The following discussion using equations expresses this phenomenon more explicitly.

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First, consider monochromatic light incident on a crystal. Its E-field is given by:

$$\mathbf{E}(\mathbf{r}, t) = \mathbf{E}_i(\mathbf{k}_i, \omega_i) \cos(\mathbf{k}_i \cdot \mathbf{r} - \omega_i t) \quad (2.3)$$

The light wavevector is denoted by $\mathbf{k}_i$ and the light frequency is denoted by ω_i . The polarization induced in the crystal in response to this E-field is given by

$$\mathbf{P}(\mathbf{r}, t) = \mathbf{P}(\mathbf{k}_i, \omega_i) \cos(\mathbf{k}_i \cdot \mathbf{r} - \omega_i t) \quad (2.4)$$

It has the same wavevector and frequency as the incident light and its amplitude is given by

$$\mathbf{P}(\mathbf{k}_i, \omega_i) = \chi(\mathbf{k}_i, \omega_i) \mathbf{E}_i(\mathbf{k}_i, \omega_i) \quad (2.5)$$

where χ denotes the susceptibility.

Now, consider the atomic displacements associated with a phonon. They are given by

$$\mathbf{Q}(\mathbf{r}, t) = \mathbf{Q}(\mathbf{q}, \omega_0) \cos(\mathbf{q} \cdot \mathbf{r} - \omega_0 t) \quad (2.6)$$

The phonon wavevector is denoted by $\mathbf{q}$ and the phonon frequency is denoted by ω_0 .

As said, these atomic vibrations will modify the susceptibility. The susceptibility will be a function of $\mathbf{Q}$. $\mathbf{Q}$ is small, and it is possible to express χ as a Taylor expansion series in $\mathbf{Q}(r, t)$:

$$\chi(\mathbf{k}_i, \omega_i, \mathbf{Q}) = \chi_0(\mathbf{k}_i, \omega_i) + (\partial \chi / \partial \mathbf{Q})_0 \mathbf{Q}(r, t) + \dots \quad (2.7)$$

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χ_0 here denotes the susceptibility in the absence of phonons.

If we replace the χ in Equation (2.5) with the expression for χ given by Equation (2.7), we will see that the polarization in the presence of phonons is given by

$$\mathbf{P}(\mathbf{r}, t, \mathbf{Q}) = \mathbf{P}_0(\mathbf{r}, t) + \mathbf{P}_{ind}(\mathbf{r}, t, \mathbf{Q}) \quad (2.8)$$

where

$$\mathbf{P}_0(\mathbf{r}, t) = \chi_0(\mathbf{k}_i, \omega_i) \mathbf{E}_i(\mathbf{k}_i, \omega_i) \cos(\mathbf{k}_i \cdot \mathbf{r} - \omega_i t) \quad (2.9)$$

and

$$\mathbf{P}_{ind}(\mathbf{r}, t, \mathbf{Q}) = (\partial\chi / \partial\mathbf{Q})_0 \mathbf{Q}(\mathbf{r}, t) \mathbf{E}_i(\mathbf{k}_i, \omega_i) \cos(\mathbf{k}_i \cdot \mathbf{r} - \omega_i t) \quad (2.10)$$

Equation (2.9) is that of a polarization vibrating in phase with the incident radiation and Equation (2.10) is that of *a polarization induced by the phonon*.

Using the trigonometry relation $2\cos A \cos B = \cos(A + B) + \cos(A - B)$, we can re-write Equation (2.10) as

$$\begin{aligned} \mathbf{P}_{ind}(\mathbf{r}, t, \mathbf{Q}) &= (\partial\chi / \partial\mathbf{Q})_0 \mathbf{Q}(\mathbf{q}, \omega_0) \cos(\mathbf{q} \cdot \mathbf{r} - \omega_0 t) \mathbf{E}_i(\mathbf{k}_i, \omega_i) \cos(\mathbf{k}_i \cdot \mathbf{r} - \omega_i t) \\ &= \frac{1}{2} (\partial\chi / \partial\mathbf{Q})_0 \mathbf{Q}(\mathbf{q}, \omega_0) E_i(k_i, \omega_i t) \{ \cos[(k_i + q) \cdot r - (\omega_i + \omega_0) t] + \cos[(k_i - q) \cdot r - (\omega_i - \omega_0) t] \} \end{aligned} \quad (2.11)$$

The radiation corresponding to the first cosine term in Equation (2.11) is an *anti-Stokes* shifted (or scattered) light, with wavevector $\mathbf{k}_{AS} = (\mathbf{k}_i + \mathbf{q})$ and frequency $\omega_{AS} = (\omega_i + \omega_0)$. It is more energetic than the incident light. The radiation corresponding to the second cosine term is a *Stokes* shifted (or scattered) light, with wavevector $\mathbf{k}_S = (\mathbf{k}_i - \mathbf{q})$ and frequency $\omega_S = (\omega_i - \omega_0)$. It

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is less energetic than the incident light. The difference in the frequency between the incident light and the scattered light corresponds to the phonon frequency. This is the *Raman frequency* or *Raman shift*. These two terms involve only one phonon each. (Equation (2.11) can actually be expanded to give higher order terms where more than one phonon is involved.) We also see from Equation (2.9) that there will be radiation with the same frequency as that of the incident light. This corresponds to elastically scattered light, or *Rayleigh* scattered light.

The theory of Raman scattering can also be explained using quantum mechanical concepts. Readers who are interested may refer to Refs. [7, 92-93] for more information.

Conservation of wavevector: implication

According to fundamental laws in physics, energy and momentum are conserved in inelastic Raman scattering. This implies frequency and wavevector are conserved. Using Stokes scattering to illustrate, we have

$$\hbar\omega_s = \hbar\omega_i - \hbar\omega_0 \quad (2.12)$$

which is already noted in the discussion following Equation (2.11), and

$$\hbar\mathbf{k}_s = \hbar\mathbf{k}_i - \hbar\mathbf{q} \quad (2.13)$$

Since most semiconductors are opaque to visible light, the backscattering geometry is adopted. In this geometry, the wavevectors of the incident light and scattered light are in antiparallel directions. Hence we have

$$q = k_i + k_s \quad . \quad (2.14)$$

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And since the frequency of the incident radiation is usually in a range where there is little dispersion, i.e., the relative difference between ω_i and ω_s is small, $|\mathbf{k}_s| \approx |\mathbf{k}_i|$, hence we have

$$q = k_i + k_s \approx 2k = 2\omega_i n(\omega_i) / c \quad (2.15)$$

where $n(\omega_i)$ refers to the refractive index of the medium for ω_i . Assuming visible light is used for Raman scattering for a medium with a refractive index of 3, q is around 10^6 cm^{-1} . This corresponds to 1/100 of the size of the Brillouin zone in a semiconductor. ***Therefore, only phonons at the center of the Brillouin zone, namely, at the Γ point, are probed in one-phonon Raman scattering.***

Raman Tensor and Polarization Selection Rules

From Equation (2.11), we can see that we will be able to observe one-phonon (or first order) Raman scattering for $(\partial\chi/\partial Q)_0 \neq 0$. For non-zero values, $(\partial\chi/\partial Q)_0$ will affect how strong the Raman scattered intensity will be. Here we introduce a concept known the *Raman tensor*, which is proportional to $(\partial\chi/\partial Q)_0$. Raman tensors are second-rank tensors and are derived from group theory considerations. The Raman scattered intensity depends on the Raman tensors and on the *polarization* vector of the incident ($\mathbf{e}_i$) and scattered ($\mathbf{e}_s$) light, and is given by

$$I_s \propto |\mathbf{e}_i \cdot \mathbf{R} \cdot \mathbf{e}_s|^2 \quad (2.16)$$

Interested readers may refer to works such as Ref. [93] for derivation of Raman tensors for crystals with different point groups. Here, we simply state the Raman tensors for diamond-type crystals with the point group O_h . We are interested in this because the work in this thesis focuses on Si and also, to a

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less extent, $\text{Si}_x\text{Ge}_{1-x}$. For the crystal coordinate system where $x = [100]$, $y = [010]$, and $z = [001]$, we have

$$R_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & d \\ 0 & d & 0 \end{pmatrix} \quad \text{along the } [100] \text{ direction} \quad (2.17)$$

$$R_y = \begin{pmatrix} 0 & 0 & d \\ 0 & 0 & 0 \\ d & 0 & 0 \end{pmatrix} \quad \text{along the } [010] \text{ direction} \quad (2.18)$$

$$R_z = \begin{pmatrix} 0 & d & 0 \\ d & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \text{along the } [001] \text{ direction} \quad (2.19)$$

The (001) surface of silicon is the technologically relevant one. For backscattering from a (001) surface, $\mathbf{k}_i$ is along [001], and $\mathbf{k}_s$ is along [00-1]. By wavevector conservation, $\mathbf{q}$ has to be in the same direction as $\mathbf{k}_i$, namely, in the [001] direction. The phonon whose vibrating atoms have displacements parallel to $\mathbf{q}$ is the longitudinal optical (LO) phonon, and is described by the R_z in Equation (2.19). The phonons whose vibrating atoms have displacements perpendicular to $\mathbf{q}$ are the transverse optical (TO) phonons, and are described by R_x and R_y in Equations (2.17) and (2.18) respectively. For backscattering from this (001) surface, $\mathbf{e}_i$ and $\mathbf{e}_s$ must take the form $[\alpha\beta 0]$, for arbitrary α and β . Substitute this into Equation (2.16), we realize only R_z will give rise to a non-zero Raman scattered intensity value. ***Therefore we can only observe the LO mode for backscattering from the (001) plane.***

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2.2.2 How straining silicon affects its Raman characteristics

To understand how straining silicon will affect its Raman characteristics, let us first have some basic understanding of how its phonon dispersion looks like. Figure 2.11 below shows its phonon dispersion curves along high symmetry directions of unstrained silicon. Recall from Section 2.2.1 that first order Raman scattering for crystalline semiconductors only involves the phonons at the center of the Brillouin zone, that is, the Γ point. If we look at the red arrows in the figure, we can see that at this point, the LO branch and the two TO branches merge – in other words, they are degenerate at a particular energy. This is a result of symmetry considerations for the O_h point group of silicon. The effect of applying a stress on silicon would be to distort the crystal lattice and shift the phonon branches, lifting the degeneracy. The phonon modes will have different energies and hence different Raman shifts compared to the situation without strain. For this thesis, we are interested in backscattering from the (001) plane and uniaxial stress applied in the [110] direction. The subsequent discussion will explain what will occur and be observed under these conditions and why.

Fig. 2.11: (Left) Reciprocal lattice of silicon with its first Brillouin zone. High symmetry points and directions are labeled. (Right) Phonon dispersion curves

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of silicon. The different phonon branches along these directions in the first Brillouin zone are as labeled: LO and TO refer to the longitudinal and transverse optical phonons respectively; LA and TA refer to the longitudinal and transverse acoustic phonons respectively.[Figures adapted from Ref. [7].]

Pioneering works on the theory of the effect of a uniaxial stress on the Raman spectrum of a diamond-type crystal include those cited in Refs. [94-97]. When such a crystal is strained, the dynamical equation for the $\mathbf{q} \approx 0$ optical phonons (i.e., at the Γ point) to terms linear in strain has the following form:

$$\overline{m}\ddot{u}_i = -\sum_k K_{ik}u_k = -\left(K_{ii}^{(0)}u_i + \sum_{klm} \frac{\partial K_{ik}}{\partial \varepsilon_{lm}} \varepsilon_{lm}u_k \right) \quad (2.20)$$

where u_i is the i th component of the relative displacement of the two atoms in the unit cell, $\overline{m}$ is the reduced mass of the two atoms, $K_{ii}^{(0)} = \overline{m}\omega_0^2$ is the effective spring constant of the F_{2g} modes (see Ref. [93] for phonon mode notation and meaning) in the absence of strain. The first equality sign reminds us of the familiar Newton's second law and Hooke's law. The second equality sign simply means we are expressing the right hand side as a Taylor's expansion of the left hand side, ignoring terms non-linear in strain. *Note that this equation implies that spring "constant" is not really a constant – it is actually a function of strain.* And we have

$$\frac{\partial K_{ik}}{\partial \varepsilon_{lm}} \varepsilon_{lm} = K_{iklm}^{(1)} \varepsilon_{lm} = K_{ikml}^{(1)} \varepsilon_{ml} \quad (2.21)$$

for the change in spring constant due to an applied strain ε_{lm} ; and i, k, l , and m refer to x or y or z , the crystallographic axes. From symmetry considerations

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for a cubic crystal, it can be shown that there are only three independent components of the tensor $K^{(1)}$:

$$\begin{aligned} K_{1111}^{(1)} &= K_{2222}^{(1)} = K_{3333}^{(1)} = \overline{mp}, \\ K_{1122}^{(1)} &= K_{2233}^{(1)} = K_{1133}^{(1)} = \overline{mq}, \\ K_{1212}^{(1)} &= K_{2323}^{(1)} = K_{1313}^{(1)} = \overline{mr}. \end{aligned} \quad (2.22)$$

Here, p , q , and r are the *phonon deformation potentials* (PDPs). The greater the value of the PDP, the greater the change in the spring constant per unit strain. The PDPs are material constants.

By combining Equation (2.20) and the equations in (2.22), one obtains the following well-known secular equation:

$$\begin{vmatrix} p\varepsilon_{xx} + q(\varepsilon_{yy} + \varepsilon_{zz}) - \lambda & 2r\varepsilon_{xy} & 2r\varepsilon_{xz} \\ 2r\varepsilon_{xy} & p\varepsilon_{yy} + q(\varepsilon_{zz} + \varepsilon_{xx}) - \lambda & 2r\varepsilon_{yz} \\ 2r\varepsilon_{xz} & 2r\varepsilon_{yz} & p\varepsilon_{zz} + q(\varepsilon_{xx} + \varepsilon_{yy}) - \lambda \end{vmatrix} = 0 \quad (2.23)$$

where λ refers to the eigenvalue of the problem. There are three different eigenvalues, λ_j ($j = 1, 2, 3$):

$$\lambda_j \equiv \omega_j^2 - \omega_0^2 = (\omega_0 + \Delta\omega_j)^2 - \omega_0^2 \approx 2\omega_0(\omega_j - \omega_0) \quad (2.24)$$

where ω_0 refers to the triply-degenerate optical phonon frequency in the absence of strain, and ω_j refers to the optical phonon frequency for the j th optical phonon in the presence of strain. The change in the Raman shifts, $\Delta\omega_j$, is given by:

$$\Delta\omega_j = \omega_j - \omega_0 \approx \frac{\lambda_j}{2\omega_0} \quad j = 1, 2, 3 \quad (2.25)$$

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For uniaxial stress applied in the $[110]$ direction that is relevant to the work in the thesis, the specific eigenvalues have been worked out in Refs. [97-99]. They all give the same results. A coordinate transformation is required to transform the stress in the $x'//[110]$, $y'//[-110]$, $z'//[001]$ coordinate system to the $x//[001]$, $y//[010]$, $z//[001]$ crystal coordinate system. It will yield the following stress matrix in the crystal coordinate system:

$$\sigma_{ij} = \begin{bmatrix} 0.5\sigma_{[110]} & 0.5\sigma_{[110]} & 0 \\ 0.5\sigma_{[110]} & 0.5\sigma_{[110]} & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad (2.26)$$

To obtain the strain matrix, we need to use Hooke's law in the compliance form for cubic crystals like silicon:

$$\begin{bmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ 2\varepsilon_{xy} \\ 2\varepsilon_{yz} \\ 2\varepsilon_{zx} \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} & S_{12} & 0 & 0 & 0 \\ S_{12} & S_{11} & S_{12} & 0 & 0 & 0 \\ S_{12} & S_{12} & S_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & S_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & S_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & S_{44} \end{bmatrix} \begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{xy} \\ \sigma_{yz} \\ \sigma_{zx} \end{bmatrix} \quad (2.27)$$

where S_{11} , S_{12} , and S_{44} are the elastic compliance constants of silicon, ε_{ij} are the strain tensor components, and σ_{ij} are the stress tensor components. (Note: $\varepsilon_{ij} = \varepsilon_{ji}$ and $\sigma_{ij} = \sigma_{ji}$.) So, using Equations (2.26) and (2.27), we obtain the following strain matrix in the crystal coordinates:

$$\varepsilon_{ij} = \begin{bmatrix} \frac{(S_{11} + S_{12})}{2} \sigma_{[110]} & \frac{S_{44}}{2} \sigma_{[110]} & 0 \\ \frac{S_{44}}{2} \sigma_{[110]} & \frac{(S_{11} + S_{12})}{2} \sigma_{[110]} & 0 \\ 0 & 0 & S_{12} \sigma_{[110]} \end{bmatrix} \quad (2.28)$$

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Using the ε_{ij} components in Equation (2.28), the solutions to Equation (2.23) for λ will be

$$\begin{aligned}\lambda_1 &= \frac{1}{2} [p\sigma_{[110]}(S_{11} + S_{12}) + q\sigma_{[110]}(S_{11} + 3S_{12}) + 2r\sigma_{[110]}S_{44}] \\ \lambda_2 &= \frac{1}{2} [p\sigma_{[110]}(S_{11} + S_{12}) + q\sigma_{[110]}(S_{11} + 3S_{12}) - 2r\sigma_{[110]}S_{44}] \\ \lambda_3 &= [q(S_{11} + S_{12}) + pS_{12}]\sigma_{[110]}\end{aligned}\tag{2.29}$$

corresponding to the eigenvectors $[1,0,0]$, $[0,1,0]$ and $[0,0,1]$ respectively. For backscattering from the (001) plane, only λ_3 corresponding to ω_3 is observed. (Also see Chapter 6, pages 125 and 126 for this.) Therefore from Equations (2.25) and (2.29), the change in the Raman shift is given by

$$\Delta\omega = \frac{\lambda_3}{2\omega_0} = \frac{q(S_{11} + S_{12}) + pS_{12}}{2\omega_0} \sigma_{[110]}\tag{2.30}$$

From the above discussion, we can see that an applied stress will result in a shift in the Raman peak position of silicon. The amount of shift is proportional to the applied stress. The constant of proportionality is determined by the elastic compliance constants, the phonon deformation potentials, and the triply-degenerate optical phonon frequency of silicon in the absence of strain. These are constants that are characteristic of the material and have been well studied a long time ago for silicon. Knowing these constants, we can work out the magnitude of the stress from the amount of shift in the peak position.

3. Materials, instrumentation, and methods

3.1 Materials

The subject of study of this thesis is 45 nm node transistors with embedded silicon-germanium (e-SiGe) source and drain. The following process flow steps are those common to the transistors used for the projects described in Chapters 4 and 5. GLOBALFOUNDRIES Singapore Pte. Ltd. had kindly supplied me these wafers for the work in this thesis. Further sample preparation steps unique to each project, which I carried out in the university myself or with assistance from others, will be described in Chapters 4 and 5.

Fig. 3.1: Process flow steps for the devices used in this work.

3.2 *Instrumentation and methods*

The main characterization tool used for the work in this thesis is Raman spectroscopy. Section 3.2.1 will describe the details of the hardware and operation of our Raman spectroscopy system. Relevant concepts such as spatial and spectral resolution are also explained. Simulation work is also carried out. Section 3.2.2 will describe the simulation method and software used.

3.2.1 **Raman spectroscopy**

3.2.1.1 *Components of the Raman spectroscopy system*

Our lab is equipped with a *Renishaw inVia* Raman spectroscopy system. Our Renishaw inVia Raman setup is typical of what one finds for a Raman spectroscopy setup. This setup is used for the main work of this thesis. As can be seen from the photos of our setup (Figs. 3.2 to 3.5), it consists of the following main components:

- **Lasers** as sources of monochromatic light (Raman excitation source). We have three lasers to cover the optical spectrum from the UV to the NIR range. At any one time, only one laser out of these three is used for Raman spectroscopy. All three are continuous-wave (cw) lasers, and are classified as Class 3B. They are a He-Cd gas laser for 325 nm light (*IK5751I-G, Kimmon Koha*), a frequency-doubled Nd:YAG solid state laser for 532 nm light (*MSL532, Changchun New Industries*), and a solid state diode laser for 785 nm light (*LIPNIR785, Renishaw plc*). Motorized neutral density filters are used with these lasers so that 16 different powers are possible – from 0.00005% to 100% of the laser power emitting from the respective laser heads. As the focus of this work is UV Raman spectroscopy, the characteristics of the UV laser light and the focused UV laser spot will be elaborated on later.
- A **microscope** to direct laser light onto the sample and to collect scattered light. Here, an adapted research-grade *Leica* microscope

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(*Leica DM 2500 M*) is integrated into our system (see Fig. 3.2). It comes fitted with various *Leica* objective lenses (5x, 20x, 50x, and 100x). Objective lenses of other brands can easily be used with the microscope as long as suitable thread mount adaptors are used. A 40x UV objective lens (*OFR LMU-40×-NUV, Thorlabs*) with a numerical aperture (N.A.) of 0.5 is used for UV Raman spectroscopy. A color video camera and a white light source (*Philips*) are integrated into the microscope so that we can view the white light optical image of the sample under the objective lens, using reflected light illumination. This allows us to choose the region of the sample that we wish to acquire Raman spectra from. Viewing of the sample can also be done using the eyepieces. The microscope is fitted with an XYZ motorized mapping stage (*Renishaw MS 20 Encoded Stage*) with trackball and software control. The minimum step size of the stage is 100 nm in the XY directions and 1 μm in the Z direction. Having a motorized mapping stage with controls is necessary for precise positioning of the sample and for performing mappings.

- **Rayleigh rejection filters** to suppress most of the Rayleigh scattered light and to allow the Raman scattered light to pass. Our system uses magnetically-attached dielectric edge filters that are interchangeable. These filters suppress most of the very intense Rayleigh scattering, which will otherwise pose a problem manifesting as intense background due to scattering of stray light. The filters allow the Stokes-scattered light to pass. For the 325 nm, 532 nm, and 785 nm filters, measurements of the Raman spectrum down to 200 cm^{-1} , 80 cm^{-1} and 100 cm^{-1} from the laser lines are allowed, respectively.
- A **diffraction grating** for separating out the various wavelengths of the collected Raman scattered light so that a spectrum can be created. We can choose between two diffraction gratings for performing our

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Raman experiments – the 1200 grooves/mm grating, or the 2400 grooves/mm grating. Their positions are interchangeable. The groove density of the grating will affect the spectral range and spectral resolution of the spectrum obtained. Spectral resolution will be discussed later.

- A **charged-coupled device (CCD) detector** for detecting and quantifying (in arbitrary units) the intensity of the light at the various wavelengths of the spectrum. Our CCD is Peltier-cooled to -70°C . No water or liquid nitrogen is required for cooling. It is an array detector that consists of 576×384 pixels.
- A **computer** to control the instrument and motors and to analyze and store the data. Our computer runs on the Windows XP Professional operating system. WiRE Raman software version 3.1 is installed on the computer. The software is for system control and configuration as well as for analysis and processing of acquired data.

References for this section can be found in Refs. [100-101].

Fig. 3.2: Components of the Renishaw inVia Raman microscope system visible from the front.

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Fig. 3.3: Components of the Renishaw inVia Raman microscope system visible from the back. The wavelengths of the respective lasers are as labeled.

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Neutral density filter. Behind this filter are a few other neutral density filters of different optical densities. They can be used in various combinations to allow different intensities of light to go into the system unit. Here, all filters are stacked in place for the smallest light intensity setting. Behind this stack of filters is a shutter that can block light or allow light to go into the system unit.

Fig. 3.4: View inside the enclosure behind the system unit. The casing of the enclosure has been removed for this photo. Under normal circumstances, the casing is always in place as a safety precaution as well as to keep dust out of the components.

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Fig. 3.5: View of the interior of the system unit. The components are labeled as shown.

More information on the components used for UV Raman spectroscopy

The main emphasis of this thesis is UV Raman spectroscopy. Hence, the components of our system specific to this type of work are important and require a more in-depth account. The following is a list of specifications for the UV laser [102]:

- brand and model: Kimmon Koha, IK5751I-G
- type: helium-cadmium gas laser
- wavelength: 325 nm
- output power: 30 mW *
- mode: TEM₀₀ (i.e. beam profile is Gaussian)
- polarization: linear
- polarization ratio: better than 500:1
- 1/e² beam diameter: 1.2 mm
- beam divergence: 0.2 mrad

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- pointing stability: $\pm 25 \mu\text{rad}$
- power stability at 25°C over 4 h: $\pm 2\%$
- warm-up time to 90% of maximum power: 20 min
- coherence length: 30 cm
- spectral bandwidth: 1 GHz

(*Note: Even without using any neutral density filters to attenuate the UV laser beam, the laser power reaching the sample eventually is around 10% of the laser output power. This is because most of the light is absorbed or scattered along the way by the optical components. There are probably losses due to imperfect alignment as well.)

Special optics need to be used for UV light. This is because UV light is highly energetic and the photons have energy greater than the band gap of many materials. Therefore, absorption of UV light by optical components is a serious issue. There are not many materials that allow for high transmission of UV light and which are practical enough for actual UV applications. The few commonly used materials are fused silica, calcium fluoride (CaF_2), magnesium fluoride (MgF_2) and sapphire [103]. Our UV microscope objective lens (*Thorlabs*, OFR LMU-40 $\times$ -NUV, see Ref. [104]) has lens elements made of excimer grade UV fused silica and CaF_2 . It also comes with an anti-reflective coating. The purpose of the coating is to reduce surface reflections, which can result in “ghost” images and reduce the overall transmission through the optics. The overall transmission for 325 nm light is approximately 85% through the lens. Here are other features of this lens:

- magnification: 40 $\times$
- numerical aperture: 0.50
- working distance: 1 mm
- effective focal length: 5 mm
- entrance aperture: 5 mm

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- theoretical focal spot size*, assuming entrance aperture is filled and beam profile is Gaussian: 1 μm

(* Note: the actual UV laser spot size was measured to be 1.6 μm . More information will be given in Section 3.2.1.6 when discussing spatial resolution.)

The UV pre-slit lens, post-slit lens, and CCD lens inside the system unit are also made of materials that allow for high transmission of UV light. They are air-spaced achromatic doublets that consist of a flint material and a crown material. The two materials work together to counterbalance the chromatic aberration of each other. The flint material is fused silica and the crown material is CaF_2 [105].

3.2.1.2 Light path inside the system

The schematics on the next page show the path that the light follows after it enters the system unit.

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Fig. 3.6: Renishaw Raman inVia spectroscopy system: light path

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3.2.1.3 Typical operating procedures

In a typical Raman spectroscopy experiment using this system, the sequence of steps executed are as follows:

- Turn on the desired laser. For the UV laser, a warm-up time of approximately 30 min is required.
- Start the WiRE 3.1 software program. Select the appropriate laser light wavelength from a drop-down list in the program. The motorized laser shutter for the chosen wavelength will then allow the chosen laser light to pass into the light path enclosure behind the system unit. The other two laser shutters will remain blocking the other two laser light beams. (Hence, even if the other two lasers are turned on, their light beams will not go into the enclosure and interfere with the operation of the system.) Now, although the desired laser beam can travel along the light path enclosure, it is stopped from entering the system unit by the system unit laser shutter. The system unit laser shutter is shut under normal circumstances when no Raman spectrum acquisition is taking place. This is a safety feature. Without this feature, the laser light will travel all the way - into the system unit and out through the microscope objective and onto the sample stage. This is potentially harmful to the eyes of the unprepared experimenter and may also cause accidental sample damage. Ideally the laser light should be shining on the sample only during the actual acquisition of the Raman spectrum.
- Select the appropriate diffraction grating from the appropriate drop-down list. The motorized grating mount will then rotate so that the correct grating is facing the prism mirror planes.
- The program will prompt us to change the pre-slit, post-slit, and pre-CCD lenses to the ones appropriate for the wavelength and work (i.e. Raman or photoluminescence) chosen. Open the door of the system unit to do this.

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- Shut the door of the system unit.
- Calibrating the system for the Raman peak position is very important and has to be done before performing runs for actual samples. Place a piece of silicon wafer on the sample stage under the objective lens. Open the shutter of the microscope white light lamp by clicking on the appropriate icon on the program. Focus and locate a clean region on the silicon piece for performing Raman spectroscopy. The exact spot should be at the center of the cross hairs. This is because the system has been aligned to allow laser light to fall onto that position.
- Set appropriate values for the laser intensity, Raman spectral range, exposure time, and confocality. Start the Raman acquisition. Now, the system unit laser shutter will open and allow the laser beam to travel into the unit and out through the microscope objective lens and onto the sample. The CCD shutter will open for the duration of acquisition. After acquisition, the CCD shutter will shut. The system unit laser shutter may or may not be shut after that, depending on whether we set it to be. It is better that we do, to prevent sample damage.
- Do curve-fitting (see Section 3.2.1.4) to determine the position of the silicon Raman peak. The position should be within plus or minus 1 cm^{-1} of 520 cm^{-1} . If not, set an appropriate value for the offset calibration feature of the program, re-take the spectrum and re-check the position.
- Now we can perform runs on actual samples. Additional experimental details specific to each of the main projects will be described in Chapters 4 and 5 respectively.

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Fig. 3.7: Screen shot of the WiRE 3.1 workspace. The video camera capture (left panel) and a Raman spectrum of silicon acquired using 325 nm excitation (right panel) are shown.

3.2.1.4 Data analysis

Curve-fitting of the acquired Raman spectra must be carried out to determine the peak parameters – the position, intensity, and full-width at half-maximum (FWHM). The peak position and intensity is not simply determined by looking at the coordinates of the experimental data point with the highest intensity value. The importance of curve-fitting is illustrated by the figure below:

Fig. 3.8: The first-order Raman peak of silicon, acquired using our setup with the 325 nm excitation source. The experimental data and the fitted curve are shown.

From the figure, we can see that the experimental data point with the greatest CCD count does not coincide exactly with the center of the fitted curve. The data point has a position of 520.07 cm^{-1} while the fitted curve has a position of 520.31 cm^{-1} . Note also that their intensity values do not coincide as well. Therefore, curve-fitting using a profile (e.g. Lorentzian or others) that suitably describes the physics of the sample under study is needed to correctly determine the peak parameters.

We also note that our experimental data point spacing, which is very much influenced by the pixel density of the CCD, is more than 3 cm^{-1} . However, with careful curve-fitting, it is possible to discern peak shifts much smaller than the data point spacing. This is an important point that must be emphasized for this thesis. For our existing UV Raman spectroscopy

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configuration, the experimental data point spacing may be big; but with curve-fitting of many repeated measurements and performing analysis of these repeated measurements, our approach can discern significant peak shifts of down to 0.1 cm^{-1} . This is important for the work presented in this thesis because we are looking at smaller relative peak shifts. Further details will be given in Chapters 4 and 5.

A brief digression here – the sensitivity of our measurements is a concept separate from that of the spectral resolution of our system. In the context of this thesis, the sensitivity of our measurements is related to how well we can discern small shifts in a particular Raman peak when we are comparing sample A with sample B. A sensitivity of 0.1 cm^{-1} is possible, using the approach described in the previous paragraph. Spectral resolution, on the other hand, is related to how well we can distinguish two closely spaced peaks in the same spectrum. This issue will be covered in Section 3.2.1.5 and in Chapter 4.

Back to the issue of curve-fitting – the spectrum shown in Fig. 3.8 is fitted using a Lorentzian profile. This kind of profile, or model, is most commonly used for fitting the Raman peaks of single-crystalline, defect-free, semiconductors without doping. The profile takes the form of the following equation:

$$I(x) = I_{\max} \frac{\left(\frac{1}{2}w\right)^2}{(x - x_0)^2 + \left(\frac{1}{2}w\right)^2} \quad (3.1)$$

where $I(x)$ refers to the intensity I at any x -axis value, $I_{\max}$ refers to the maximum intensity, w refers to the full-width at half-maximum (FWHM) value, and x_0 refers to the position of the inflexion point of the profile. We can see that when $x = x_0$, I goes to $I_{\max}$. The shape of the profile is symmetrical.

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Curve-fitting for all the spectra in this thesis was done using the curve-fitting function of the WiRE 3.1 software. For this function, the method of least squares is applied [100]. The program minimises the sum of the squared deviations of the curve fit model from the experimental data using an iterative process – hence we must specify some initial values for the peak position, intensity, and width. The initial values can be set easily by adding the fitting curve into the spectrum window and adjusting its parameters to roughly match those of the experimental peak by clicking and dragging with the mouse. The program expresses the chi-squared value as a measure of the goodness of fit.

3.2.1.5 Spectral resolution

The spectral resolution of a Raman spectroscopy system is the ability of the system to separate adjacent peaks [106]. It is often studied by analyzing the spectrum of CCl_4 – the higher the resolution, the deeper the troughs between the bands [107]. The following figure illustrates this concept:

Fig. 3.9: Spectra of CCl_4 taken with standard and high resolution inVia Renishaw Raman microscope (figure from Ref. [107])

Performance is normally quantified by the ratio of trough-to-baseline to peak-to-baseline. It is also possible to directly measure the spectral

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resolution of a spectrometer by measuring the width of a very narrow atomic emission line from a gas emission lamp, such as that of neon. There are many factors that affect the spectral resolution of a spectrometer. The factors include (and are not limited to) the following [106]:

- Diffraction grating groove density
- Spectrometer slit width
- Detector pixel size
- Spectrometer focal length (distance between grating and detector)

The concept of spectral resolution is pertinent to the work in this thesis because we need to separate the strained Si peak from the adjacent strained Si-Si of SiGe peak. For UV Raman work, our system is configured to use only the 2400 grooves/mm grating. The spectrometer slit width is changeable though. By specifying whether we want a “standard” or “high” confocality setting*, we can set the slit size to be 65 μm or 20 μm respectively. A narrower slit gives narrower Raman peaks. This is useful for spectrally resolving the two closely spaced peaks. More information will be given in Chapter 4. Using the smaller slit size will result in a FWHM of single crystalline silicon of around 6 cm^{-1} , for our system configuration for UV work. Here, we can also see that although our data point spacing of more than 3 cm^{-1} is rather big, we will not be “skipping” or “missing” any peaks because the FWHM of the narrowest possible peak for our kind of materials is much larger than the data point spacing.

(* Note: the slit, together with the CCD area, acts like the pinhole that is characteristic of a confocal microscope. They work together as a “virtual pinhole” [105]. Because of the presence of the “virtual pinhole”, our setup is always operating in the confocal mode. The smaller the pinhole, the higher the confocality. See Ref. [108] for information on confocal optical systems.)

3.2.1.6 Spatial resolution

When we discuss spatial resolution, we are concerned with how well an optical system is able to separate two points inside, or on the surface of the sample. The higher the spatial resolution, the better we can discern two closely spaced points. Spatial resolution considers the depth resolution as well as the lateral resolution. For confocal systems, to quantify the resolution, one needs to work out the FWHM of a quantity known as the point spread function (PSF) behind the pinhole. The PSF is basically the light intensity distribution in the image space. For confocal systems, the PSF behind the pinhole is a function of the PSF of the illuminating beam path and the PSF of the detection beam path. A smaller pinhole gives a tighter PSF for the detection beam path and hence a tighter overall PSF, giving a higher spatial resolution, especially depth resolution. See Ref. [108] for the details.

For the work in this thesis, little additional benefit to our understanding of our transistors is achieved by having a better depth resolution. A better depth resolution that comes along with using the smaller slit width simply manifests as the need to be more careful when adjusting the height of the sample stage so that we are indeed optimizing the z-focusing. Small deviations from the optimal z-positioning will give a lower signal-to-noise ratio for the Raman spectrum acquired. Nevertheless, whether the sample is positioned at exactly the focal plane or slightly off by a few micrometers, we are getting the Raman signals from ~8 nm deep into the sample (see Chapter 4 for explanation). (Note: the numerical aperture of the lens also affects depth resolution. In our case, we only have one UV microscope objective lens with an N. A. of 0.5.)

Lateral resolution is much more important for our work. For any single spectrum, the sampling area of our sample is dependent on the spot size of our laser. (Note: Changing the confocality setting will have no effect on the incident laser spot size.) Therefore, quantifying the size of the focused laser

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spot is very important for the work in this thesis. The approach for measuring the beam is following that of Veshapidze et al [109], using a scanning edge method. Performing a line scan across a sample with a step-profile for its cross-section gave the experimental data shown in Fig. 3.10. The intensity in this figure is that of the Si Raman peak. As the laser spot approached the step, the Si Raman peak intensity dropped as its signal was blocked by the SiGe layer.

Fig. 3.10: Line scan intensity versus position on sample. The line scan was done for a sample whose cross section is shown in the inset.

Each experimental data point was obtained by curve fitting the silicon peak of each spectrum along the profile to find its peak intensity. The experiment data were fitted to the equation:

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$$I(x) = \frac{I_0}{2} \left\{ 1 - \operatorname{erf} \left[\frac{\sqrt{2}(x - x_0)}{w} \right] \right\} \quad (3.2)$$

where $I(x)$ refers to the intensity at point x (μm) along the profile on the sample, x_0 refers to the inflexion point of the equation, and w refers to the $1/e^2$ half width of the Gaussian beam. The FWHM of the Gaussian beam is related to the $1/e^2$ half width via the following equation:

$$FWHM = w\sqrt{2 \ln 2} \quad (3.3)$$

Figure 3.11 below shows the relationship between w and the FWHM pictorially:

Fig. 3.11: The Gaussian beam profile

After fitting to find w and using the second equation to find the FWHM from w , a value of $1.6 \mu\text{m}$ is obtained for the FWHM of our focused UV laser spot.

3.2.2 Finite-Difference Time-Domain (FDTD)

The finite-difference time-domain (FDTD) method is used in the work in this thesis to simulate the light distribution in the structures studied. More information will be given in Chapter 6. This section will briefly introduce this simulation method and the application software used.

Finite-difference time-domain is a computational numerical modeling method that is commonly used for providing insights into problems in photonics, optics, and electromagnetics. It looks at how electromagnetic waves interact with physical structures. Basically, it solves Maxwell's equations in the time domain. This means that the electric field and the magnetic field are obtained as functions of time. By performing Fourier transformations, it is also possible to obtain the fields as functions of frequency. Details of this method can be found in Refs. [110-112].

Let us look at the differential forms of Maxwell's equations:

$$\frac{\partial \mathbf{D}}{\partial t} = \nabla \times \mathbf{H} \quad (3.4)$$

$$\frac{\partial \mathbf{H}}{\partial t} = -\frac{1}{\mu_0} \nabla \times \mathbf{E} \quad (3.5)$$

Here, $\mathbf{H}$ and $\mathbf{E}$ are the respectively the magnetic and electric fields, μ_0 is the permeability of free space, and $\mathbf{D}$ is the displacement field inside a medium, given by

$$\mathbf{D}(\omega) = \epsilon_0 \epsilon_r(\omega) \mathbf{E}(\omega) \quad (3.6)$$

where ϵ_0 is the permittivity of free space, and $\epsilon_r(\omega)$ is the complex relative dielectric constant. By examining the above equations, we can see that a change in the electric field with respect to time (the time derivative) is related to a change in the magnetic field across a small piece of space (the curl).

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Conversely, a change in the magnetic field with respect to time is related to a change in the electric field across a small piece of space. Therefore, a time-stepping approach for finding the updated electric or magnetic field is possible for a particular point – the updated electric field at each time step can be found from the old electric field at that point and the change in magnetic field around that point; and the updated magnetic field at each time step can be found from the old magnetic field at that point and the change in electric field around that point.

To run FDTD, a computational region must be set up. The entire computational region must be gridded in a mesh. The electric and magnetic fields are obtained for every point in space for that mesh. The mesh is made up of so-called Yee cells. A Yee cell is shown in Fig. 3.12 below.

Fig. 3.12: A Yee cell (left) used for FDTD. The electric and magnetic field vectors are distributed as shown. Many repeating Yee cells make up a three-dimensional mesh (right) that is the computational region. Figure from Ref. [113].

The structures of interest are drawn inside the computational region and their real and imaginary parts of the refractive index must be specified. The materials are commonly air, metal, or dielectric. The source of electromagnetic waves also needs to be defined within the computational

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region. The source may be a plane wave, a point source radiator, a Gaussian beam, or others, depending on the actual application.

The computational region is finite, hence has boundaries. Care must be taken to set up the appropriate boundary conditions. To simulate an infinite computational region, most FDTD applications use a “perfectly matched layer” (PML) boundary condition. This PML is actually a highly absorbing region that can minimize errors arising from unwanted reflections at the boundary.

The FDTD application software used for the work in this thesis is *FDTD Solutions* from Lumerical Solutions, Inc. It uses a graphical user interface (GUI) for users to set up their simulations. The screenshot below shows the various tools and windows of this application.

Fig. 3.13: Screenshot of *FDTD Solutions* application software in use. Here, the user has set up a simulation involving photonic crystal cavities. Screenshot from [113].

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Reference [113] contains many more details on using the tools, setting up the simulations, running the simulations, and analyzing the simulation data. Details of the algorithms, scripts, and the physics involved are given in Ref. [114].

4. Channel stress measurements of 45 nm node transistors with embedded SiGe source and drain

4.1 *Introduction*

Often, we do not need to spatially resolve individual structures whose spacings are smaller than the probing size of the characterization tool, or perform a point-by-point analysis across the channel. Collection of information over large arrays of repeating structures can prove insightful. Our work is different from those based on TEM techniques in the sense that we are using a micrometer-sized laser beam to study the *average* channel stress of repeating transistors rather than using a point-by-point approach. Studying the average channel stress is also valuable as one is interested in the overall behavior of the carriers across the whole channel. In this chapter, I present our work done on 45 nm node transistors with embedded silicon-germanium (e-SiGe) source and drain using UV-Raman spectroscopy. The motivation for our work has been described in Section 2.1.3.2 on pages 22 to 26. The effect of varying the pitch of the polycrystalline silicon gates (poly-pitch) is investigated, keeping all other parameters constant. The main results and analysis for the work in this chapter are published in the journal paper cited in Ref. [115].

4.2 *Experimental details*

Sample fabrication

PMOS transistors with SiGe source and drain regions were fabricated on Si (001) wafer by Si recess etch using reactive-ion etching, followed by

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cleaning and epitaxial SiGe selective growth using low-pressure chemical vapor deposition. The Ge concentration was 17%, from inline measurements done in GLOBALFOUNDRIES Singapore Pte Ltd using ellipsometry. The channels were oriented in the $[110]$ direction. The schematics for the process flow for this fabrication have been shown in Section 3.1, on page 38. Dense transistors with different poly pitches were patterned in discrete $50\ \mu\text{m}$ by $50\ \mu\text{m}$ pads for each pitch. The pitches ranged from 140 nm to 280 nm, in steps of 20 nm. The layout and appearance of the structures can be understood from the bright field optical microscopy images in Fig. 4.1, the plan view SEM images in Fig. 4.2, and the cross-sectional TEM image in Fig. 4.3. (Acknowledgement: GLOBALFOUNDRIES Singapore Pte Ltd for providing these wafers.)

Fig. 4.1: Bright field optical microscope image of as-received sample. Within each square pad is an array of periodically repeating transistors. The label below each square pad denotes the corresponding pitch. For example, UPC280 will mean a poly pitch length of 280 nm for that pad. The pitches range from 140 nm to 280 nm. Those from 200 nm onwards are shown in this image. Within each pad, the poly lines run in the direction perpendicular to the channel orientation.

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Fig. 4.2: Plan-view SEM image of transistors within pad UPC280. The poly pitch is 280 nm. The polycrystalline silicon (polysilicon) gates appear as bright lines in this image. The dark areas are the SiGe source and drain regions.

Fig. 4.3: Cross-sectional TEM image of the transistors located within the square pad UPC280. The SiGe growth thickness is 82 nm. (Acknowledgement: Failure Analysis (FA) team in GLOBALFOUNDRIES Singapore Pte Ltd for this TEM image.)

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I then removed the gates so that the UV laser used in our Raman experiments can probe the strained Si channels directly. The gates were hand-polished away using a cotton swab whose tip had been dipped in de-ionized water. The cotton swab used is a commonly available one, as shown in Fig. 4.4. This method of gate removal is advantageous as it is practically cost free and requires no additional steps in the device process flow. (An alternative method of gate removal, which uses chemical rather than mechanical means, will be introduced later.) The plan view SEM image in Fig. 4.5 and the cross-sectional TEM image in Fig. 4.6 show the appearance of the gate-less structures after polishing. The exposed Si channels appear as dark lines in the SEM image.

Fig. 4.4: Cheap and commonly available cotton swabs of this kind are used for mechanical polishing by hand to remove the gates.

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Fig. 4.5: Plan view SEM image of transistors with a poly pitch of 280nm *after gate removal*. The exposed channels appear as dark lines. Compare this image with that shown in Fig. 4.2.

Fig. 4.6: Cross-sectional TEM image of transistors with a poly pitch of 280nm *after gate removal*. An important observation that the thickness of the SiGe source and drain material remains the same as before. (Acknowledgement: Failure Analysis (FA) team in GLOBALFOUNDRIES Singapore Pte Ltd for this TEM image.)

By comparing Fig. 4.3 with Fig. 4.6, we can see that the SiGe source and drain material remains completely intact. This is possible because using a cotton swab to polish will mechanically separate the gates from substrate at

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the gate oxide – i.e. they are being mechanically stripped off the substrate. The adhesion of the gate to the substrate via the gate oxide should be very much weaker compared to the strong, extensive covalent forces that are present throughout the single crystalline S/D material. Also, the gates are protruding while the S/D regions are relatively flat. Therefore it should be much easier to mechanically remove the gates by stripping than to remove the S/D material by disturbing the extensive covalent lattice of the SiGe material. Figure 4.7 illustrates how the gates get removed.

Fig. 4.7: Illustration of how mechanical polishing using the above described method removes the polysilicon gates. The single crystalline material remains intact.

UV Raman Spectroscopy

For Raman measurements, a Raman microscope setup coupled with a He-Cd 325 nm UV laser was used in the backscattering configuration. The incident light was focused onto the (001) surface of the sample by a 40x microscope objective lens with a numerical aperture (N.A.) of 0.5. The laser spot size was measured to be 1.6 μm using the scanning edge method [109]. The details of the instrumentation and the spot size measurement have been

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covered in Section 3.2.1. Figure 4.8 illustrates the lateral size relationship between the laser spot and the gate-less structures probed:

Fig. 4.8: Lateral size relationship between the laser spot and the gate-less structures. A poly pitch of 280 nm is shown as an example. For the smaller pitches, more channels will be probed by the laser spot.

Here, we see that the laser spot is relatively huge compared to the structures probed. It is therefore not possible to *spatially resolve* the individual structures. Nevertheless, we show that it is still possible to obtain useful information from probing several transistors at one go, provided we can *spectrally resolve* the strained Si-Si Raman peak of SiGe from the strained Si Raman peak of the channels. More information will be provided in a later part of this chapter. Indeed, the highlight of the work in this thesis is obtaining useful information in a rapid and simple way without having to spatially resolve structures point by point.

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The wavelength of the laser used (325 nm) allows us to probe only the top strained layer and avoid the underlying bulk substrate signals that would obscure the strained signals. The following discussion explains why.

The intensity of light in a medium decreases exponentially with depth z according to the following relation:

$$I(z) = I(z_0)e^{-\alpha z} \quad (4.1)$$

where $I(z_0)$ refers to the intensity of light on the surface of the medium and α refers to the absorption coefficient of the medium. The absorption coefficient is given by

$$\alpha = \frac{4\pi k}{\lambda_0} \quad (4.2)$$

where k refers to the imaginary part of the refractive index which is also known as the extinction coefficient, and λ_0 refers to the wavelength of the light in vacuum. At a depth z inside the medium where the intensity falls to $1/e$ of the original value,

$$\begin{aligned} I(z) &= \frac{1}{e} I(z_0) \\ \alpha z &= 1 \quad \text{and} \\ z &= \frac{1}{\alpha} \end{aligned} \quad (4.3)$$

Here, the quantity $1/\alpha$ is known as the optical penetration depth. For silicon, $k = 3.211$ for $\lambda_0 = 325$ nm [116], hence the optical penetration depth works out to be 8 nm, to one significant figure. For $\text{Si}_{0.83}\text{Ge}_{0.17}$, $k = 3.33$ for this wavelength [117-118], hence the optical penetration depth is also 8 nm, to one significant figure.

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Therefore, Raman signals come from very similar depths in the SiGe S/D regions and in the Si channel regions for our sample. At depths deeper than 8 nm, the intensity of light is very weak and should give rise to very weak Raman signals. Therefore using this wavelength, we only probe the top strained layer.

The following discussion covers the details of the Raman data acquisition. Each spectrum was acquired over a duration of 30 s. The power of the laser on the sample was measured to be 3.5 mW. Sample heating was negligible at this laser power. This was checked by reducing the power to half – no significant difference could be discerned in the peak position. Hence we do not have the issue of heat-induced red-shifts in the Raman peak position that can confuse with peak position differences arising from stress differences. The incident laser power over the entire course of the experimental session was taken to be acceptably consistent given that the power stability of the laser was $\pm 2\%$ over 4 h at 25°C (given by manufacturer's specs sheet). The confocality setting was set to "high" – this gave a smaller slit width which in turn gave narrower Raman peaks than the "standard" confocality setting would. Narrow Raman peaks are desirable for our work as it would be easier to separate adjacent peaks, which are closely spaced for our kind of sample. In other words, we have better spectral resolution. The incident laser polarization was in the [110] direction, i.e. along the channel direction from source to drain for all the pads studied.

The data acquisition strategy was to take multiple spectra from each pad from random locations and to later work out the average and standard deviation of the peak positions for each pad. We also took multiple spectra from bulk unstrained Si wafer. The amount of shift in the peak relative to the unstrained case would be indicative of the stress present. Taking multiple spectra is very important as we are looking at small relative shifts and we want to ensure that our conclusions are statistically sound. The spectra were

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acquired in this sequence (read across each row and read one row after another):

280-1, 260-1, 240-1, 220-1, 200-1, 180-1, 160-1, 140-1, Si-1,
 280-2, 260-2, 240-2, 220-2, 200-2, 180-2, 160-2, 140-2, Si-2,
 280-3, ... , Si-3
 :
 :
 280-10, ... , Si-10

For example, 280-1 refers to the first spectrum acquired from the gate-less pad with a poly pitch of 280 nm (UPC280), and Si-1 refers to the first spectrum acquired from the reference bulk unstrained silicon wafer. As we can see, ten spectra were acquired from each gate-less pad and from the reference Si wafer. Within each pad, the ten spectra were taken from ten different locations randomly chosen. This sequence was adopted for the data acquisition because it can monitor any possible measurement drift of the Raman spectroscopy system. After each set of eight spectra acquired from UPC140 to UPC280, we were able to monitor the calibration and stability of the Raman system by looking at the position of the reference Si bulk wafer. Imagine we were to adopt a different sequence such as this, instead:

280-1, 280-2, ... , 280-10,
 260-1, ... , 260-10,
 :
 :
 140-1, ... , 140-10,
 Si-1, ... , Si-10.

There would be no way for us to monitor the Raman system for measurement fluctuation and drift at the earlier stages when the spectra from the gate-less pads were being acquired. We would not know whether the difference in the

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peak positions between any two pads is due to differences in strain alone, or due to measurement drift as well.

Lorentzian functions were fitted to all spectra. The equation describing this function and the procedure for the curve fitting have been described in Section 3.2.1.4.

For comparison, we also took spectra from UPC280 before gate removal. We also acquired spectra using a 532 nm green laser as the excitation source for this pad before and after gate removal, to illustrate the importance of the choice of Raman excitation wavelength.

4.3 Results, analysis and discussion

Figure 4.9 below shows the Si Raman peak positions for the 10 spectra (Si-1, Si-2, ... , Si-10) acquired from the bulk unstrained Si wafer.

Fig. 4.9: Si peak positions from bulk unstrained Si wafer, from 10 spectra. These spectra were taken over an entire course of around 4 h. Each spectrum took 30 s to acquire.

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By examining Fig. 4.9, the Raman spectroscopy system appeared to exhibit random fluctuations in calibration over the entire experimental session lasting for around 4 h. No significant systematic drift can be discerned. This is fortunate given that the entire experimental session was quite long and if significant changes in room temperature had occurred, changes in the Raman spectrometer would be induced and the stability of the Raman system would be significantly affected. System stability for our kind of experiments is a very important consideration as we are looking at small relative shifts in the Raman peak positions. Undesirably large standard deviations and hence large error bars would be obtained with large random fluctuations. And if a systematic drift had occurred, it would not be possible to obtain meaningful conclusions on the peak positions of the UPC pads. De Wolf et al [82, 118] also discussed the influence of the room temperature and changes in the temperature of their nitrogen-cooled detector on the interpretation of their data. Similar to our work, they also looked at small relative shifts in Si Raman peak positions due to stress. Hence it is important to monitor system stability for our kind of work. Srikar et al [99] also performed such monitoring for related work.

By mere observation, we see from Fig. 4.9 that the second spectrum (Si-2) has a peak position that is rather different from those of the other spectra. Checking with Chauvenet's criterion [119], the rejection of this data point is statistically justified. For the remaining nine spectra, it is possible to analyze the experimental data using a simple statistical approach of finding the mean and standard deviation of the Raman peak positions of the bulk unstrained Si wafer. A normal distribution is implicitly assumed in doing this. For the bulk unstrained Si wafer, the mean of the Si Raman peak position is 520.67 cm^{-1} and its standard deviation is 0.04 cm^{-1} . The spread in our data is comparable to those of De Wolf et al [82], who obtained a spread of 0.05 cm^{-1} after taking into account the measurement drift induced by changes in temperature of their detector. Srikar et al [99] had a better stability at 0.02 cm^{-1} .

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¹. Our results, together with De Wolf's and Srikar's, are indicative of the typical precision for such measurements. Because of this, we will express all our experimental means of the Raman peak positions and their respective errors to the second decimal place.

We see that although the pixel density of our CCD is not especially high (giving a data point spacing of more than 3 cm^{-1} – see Section 3.2.1.4), the repeatability of the spectra of our reference unstrained Si wafer is very good. Therefore, the sensitivity of our system to peak shifts is definitely much better than the data point spacing. To exactly quantify the system for sensitivity to peak differences between two samples, we will need to carry out statistical testing and see whether their peak positions are statistically different, given the particular mean and the standard deviation for each sample. This concept will be elaborated on in Chapter 5, wherein it has a greater importance.

Figure 4.10 below illustrates the necessity of removing the polysilicon gates for the measurement of channel stress by UV Raman spectroscopy.

Fig 4.10: Raman spectrum obtained using UV laser as the excitation source for bulk unstrained Si and structures with a poly pitch of 280 nm. The strained Si signal can only be obtained when the gates are removed.

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The top spectrum in Fig. 4.10 shows the UV Raman data collected from pad UPC280, after gate removal, averaged from 10 spectra. The experimental data are shown as dots and the individual fitted peaks and overall fitted profiles are shown as broken and solid lines, respectively. Two strong peaks, one on the left arising from the Si-Si vibration of strained SiGe and the other on the right arising from the exposed strained Si are seen. The bottom spectrum shows the unstrained Si peak position from the bulk unstrained Si wafer, averaged from 10 spectra. *The strained Si peak of the channel in the top spectrum is blue-shifted with respect to the bulk unstrained Si peak in the bottom spectrum, indicating a compressive stress (see later paragraphs for explanation).* The Si-Si peak of SiGe and the strained peak of the channel are spectrally well resolved, minimizing error in determination of peak positions. [If we have severely overlapping peaks, the uncertainty involved for trying to fit for each peak will be significant. Quoting Ref. [120], for successful separation of overlapping peaks and reliable estimation of their positions though mathematical analysis, the peaks have to be separated by at least four-tenths of the full width at half maximum (FWHM).] The respective Raman shifts of these two peaks, averaged from the 10 spectra acquired from this pad, are 512.60 cm^{-1} (standard deviation = 0.15 cm^{-1}) and 523.87 cm^{-1} (standard deviation = 0.15 cm^{-1}). For bulk unstrained Si, the Raman shift and its standard deviation are 520.67 cm^{-1} and 0.04 cm^{-1} respectively, as already mentioned.

From the middle spectrum in Fig. 4.10, it is clear that no strained Si signals can be obtained with the gates intact, since UV light has a shallow penetration depth in silicon and could not penetrate through the overlying gates to reach the channels. The peaks shown arise from polycrystalline silicon (broad peak at $\sim 497 \text{ cm}^{-1}$ [Ref. [121]], and at $\sim 521 \text{ cm}^{-1}$) and from SiGe ($\sim 513 \text{ cm}^{-1}$).

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Figure 4.11 below illustrates the importance of the choice of Raman excitation wavelength. Using 532 nm visible light whose penetration depth in silicon is close to 1 μm , no strained Si peak can be resolved with or without gates as it is severely obscured by the polycrystalline silicon and/or substrate bulk Si signals at $\sim 521 \text{ cm}^{-1}$.

Fig. 4.11: Raman spectra collected using 532 nm laser, for comparison. No strained Si signals can be resolved.

For Fig. 4.10, the amount of stress in the exposed channels can be analyzed by studying the shift in its strained Si peak (top spectrum) relative to the unstrained peak (bottom spectrum). Here, we are assuming uniaxial stress because it is predominantly uniaxial [30]. (Note: the relationship between the Raman shift and complex stress states is less straightforward. See for example, Refs. [120, 122-124].)

As already covered in Section 2.2.3 in Equation 2.30, the uniaxial stress in silicon can be evaluated using the following relation:

$$\Delta\omega \approx \frac{\lambda_3}{2\omega_0} = \frac{q(S_{11} + S_{12}) + pS_{12}}{2\omega_0} \sigma_{[110]} \quad (4.4)$$

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where S_{11} and S_{12} are two of the three elastic compliance constants of silicon defined in Equation (2.27) of Section 2.2.3, and p and q are two of the three the phonon deformation potentials defined in Equation (2.22) in Section 2.2.3. Note that an accurate stress and peak shift relationship is dependent on using accurate values for the elastic compliance constants and the phonon deformation potentials. The values for the elastic compliance constants for silicon are well established [125] and are given in Table 4.1 below. These values are confirmed by other independent studies to be accurate.

Elastic compliance constant	Value
S_{11}	$7.68 \times 10^{-12} \text{ Pa}^{-1}$
S_{12}	$-2.14 \times 10^{-12} \text{ Pa}^{-1}$
S_{44}	$12.6 \times 10^{-12} \text{ Pa}^{-1}$

Table 4.1: Elastic compliance constants of silicon, from Ref. [125].

As for the phonon deformation potentials, p , q , and r , there have been different values reported by different studies:

Phonon Deformation Potential	Anastassakis et al [95]	Chandrasekhar et al [126]	Anastassakis et al [127]
p	$-1.25 \omega_0^2$	$-1.49 \omega_0^2$	$-1.85 \omega_0^2$
q	$-1.87 \omega_0^2$	$-1.97 \omega_0^2$	$-2.31 \omega_0^2$
r	$-0.66 \omega_0^2$	$-0.61 \omega_0^2$	$-0.71 \omega_0^2$

Table 4.2: Phonon deformation potentials of silicon, from Refs. [95, 126-127].

ω_0 refers to the unstrained phonon frequency of silicon.

We can see that the values from one study differ from another by an average of roughly 20%. Among these three sets of values, we chose to use the most recent values obtained by Anastassakis et al [127]. Srikar et al [99] obtained a better match with simulations for their experimental data using values from

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Anastassakis et al [127] than they did using values from Chandrasekhar et al [126].

Substituting the values for the elastic compliance constants and the chosen values for the phonon deformation potentials into Equation (4.4), and using the generally accepted true unstrained value of Si at $\sim 521 \text{ cm}^{-1}$, we obtain

$$\sigma_{[110]}(\text{MPa}) \cong -434(\text{cm})(\text{MPa})\Delta\omega(\text{cm}^{-1}) \quad (4.5)$$

In other words, for every 1 cm^{-1} shift in the Raman peak with respect to the unstrained, a stress magnitude of 434 MPa is present. The negative sign in the equation means that a blue shift (i.e. positive $\Delta\omega$) indicates a negative σ , which is a compressive stress. This relation is also used by Srikar et al [99], De Wolf [82], and Nouri et al [35].

Using Equation (4.5), we obtain an average compressive stress of -1.4 GPa in the Si channels for the pad with a poly pitch of 280 nm. Similarly, the average stress probed in the SiGe S/D regions for this pad can be evaluated under the assumption of uniaxial stress in the [110] direction. Because SiGe has the same crystal symmetry as Si [128], we take Equation (4.4) to be applicable to the Si-Si optical mode of SiGe as well. We need to use the appropriate phonon deformation potential values and elastic compliance constant values for the optical mode of Si-Si in our SiGe material, for our particular alloying ratio (17% Ge). We also need to know the unstrained Si-Si optical frequency of our SiGe material. The values for the phonon deformation potentials were estimated by reading off the graphs published in the work by Reparaz et al [129]:

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FIG. 2. Dependence on Ge concentration of the phonon deformation potentials $\tilde{K}_{11}$ and $\tilde{K}_{12}$ of the Ge-Ge, Si-Ge, and Si-Si optical modes for the SiGe material system. Solid lines are guides for the eyes.

Fig 4.12: Data used for the estimation of the phonon deformation potentials of the Si-Si optical mode (bottom graph) for Ge content $x = 0.17$. These graphs are from Reparaz et al [129]. Here, $\tilde{K}_{11}$ and $\tilde{K}_{12}$ refer to p/ω_0^2 and q/ω_0^2 , respectively, for the different optical modes of SiGe.

And from reading off the graphs in the above figure, we have:

Phonon Deformation Potential	Reparaz et al [129]
p	$-1.4 \omega_0^2$
q	$-2.1 \omega_0^2$
r	Unavailable and not required for our analysis

Table 4.3: Phonon deformation potential values for SiGe for Si-Si optical mode, at $x = 0.17$. Here, ω_0 refers to the unstrained phonon frequency of Si-Si vibration at this Ge composition.

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As for the elastic compliance constants for SiGe, they are worked out from the elastic stiffness constants:

Elastic stiffness constant	Value from Schaffler [128]
C_{11}	$165.8 - 37.3x$ GPa
C_{12}	$63.9 - 15.6x$ GPa
C_{44}	$79.6 - 12.8x$ GPa

Table 4.4: Elastic stiffness constants of SiGe, at a temperature of 300 K.

For cubic crystals, the stiffness constants are related to the compliance constants via the following relations [130]:

$$\begin{aligned}
 S_{11} &= \frac{C_{11} + C_{12}}{(C_{11} - C_{12})(C_{11} + 2C_{12})} \\
 S_{12} &= \frac{-C_{12}}{(C_{11} - C_{12})(C_{11} + 2C_{12})} \\
 S_{44} &= \frac{1}{C_{44}}
 \end{aligned} \tag{4.6}$$

Using Table 4.4 and Equations (4.6), we get:

Elastic compliance constant	Value
S_{11}	$7.97 \times 10^{-12} \text{ Pa}^{-1}$
S_{12}	$-2.21 \times 10^{-12} \text{ Pa}^{-1}$
S_{44}	$1.29 \times 10^{-11} \text{ Pa}^{-1}$

Table 4.5: Elastic compliance constants for SiGe, for $x = 0.17$.

For SiGe, there are three Raman peaks arising from Si-Si, Si-Ge, and Ge-Ge vibrations [131-132]. Their peak positions are dependent on both the Ge composition and the strain present. For our analysis, we need to work out the unstrained peak position for the Si-Si vibration for our SiGe material for the

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given Ge composition. Pezzoli et al [132] performed experimental studies and reported the values of the *unstrained* positions, as a function of x , to be:

$$\begin{aligned}\omega_{\text{Si-Si}} &= 520.7 - 66.9x \\ \omega_{\text{Si-Ge}} &= 400.1 + 24.5x - 4.5x^2 - 33.5x^3 \\ \omega_{\text{Ge-Ge}} &= 280.3 + 19.4x\end{aligned}\tag{4.7}$$

Care must be taken when looking at Equations (4.7), as the first term of each equation is actually dependent on the calibration of their Raman instrument used in their study. The first equation gives us an unstrained Si-Si peak position of 509.3 cm^{-1} . In any case the actual number after the decimal place does not make a significant difference to the stress-shift relation worked out later. It is generally accepted that the true unstrained Si position is $\sim 521 \text{ cm}^{-1}$ – and the first term in the first equation is close to this.

Using the unstrained Si-Si peak position of 509.3 cm^{-1} , and the values in Tables 4.3 and 4.5, we obtain from Equation (4.4) the stress-shift relation for the Si-Si mode of SiGe for this Ge composition:

$$\sigma_{[110]}(\text{MPa}) \cong -436(\text{cm})(\text{MPa})\Delta\omega(\text{cm}^{-1})\tag{4.8}$$

To the best of my knowledge, such a stress-shift relation for uniaxial stress in SiGe for a particular Ge composition is not available in the literature prior to our own study so I am unable to do a comparison of our relation with established ones. However Equation (4.8) should be reasonable because it is close to the stress-shift relation for pure silicon – and this should be the case because the Ge composition here is not high, meaning that the Si-Si vibration in SiGe should respond to stress in a way similar to the Si-Si vibration in pure silicon. Using this relation for our experimental peak position of Si-Si of SiGe averaged from the 10 spectra for the pad with a pitch of 280 nm (see Fig. 4.10), we get a stress of -1.4 GPa in our SiGe S/D regions probed for this pad.

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This is interesting because the uniaxial stress in the SiGe S/D regions probed works out to be the same as that in the Si channels, to two significant figures. Also, like the stress in the channel, it is also compressive. Further discussion will be given later.

We also analyzed the Raman spectra of each of the other pads. Figure 4.13 presents the Raman spectra for pitch lengths from 140 nm to 280 nm. Each displayed spectrum was obtained from averaging the 10 spectra acquired for that pad. The spectra have been offset along the vertical axis direction for clarity. The experimental data points are shown as dots while the individual fitted peaks and overall fitted profiles are shown as broken and solid lines respectively. The blue lines (guides for the eyes) illustrate the increase in compressive stress in both the S/D regions and in the channels with poly pitch length. Figure 4.14 plots the channel stress and the SiGe S/D stress versus the poly pitch length, using the respective stress-strain relations worked out earlier. The error bars give the spread in the experimental readings. The increase in the channel stress with pitch is in agreement with other findings in the literature – from simulation results for 45nm node PMOS, a larger poly pitch for dense transistor layouts should give rise to a larger stress [43] (see Fig. 4.15). This is due to the larger volume of SiGe present in the S/D regions. Larger strains were also observed from NBD measurements of isolated transistors with larger S/D regions [61].

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Fig. 4.13: Raman spectra for different poly pitch lengths.

Fig. 4.14: Compressive stress values for the Si channel versus the pitch length.

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Simulation of stress in the center of the channel as a function of poly-to-poly distance for dense transistor structures

Fig. 4.15: Simulation data from Eneman et al [43], showing how stress in the center of the channel varies with pitch for different S/D recesses. They used 20% Ge in the SiGe S/D regions and a gate length of 100 nm. The gate length used in our own work is ~ 37 nm. Reading off this graph for a recess depth of 70 nm which is the closest to our recess depth of 62 nm, their simulated stress values for pitches of < 300 nm are smaller than what we obtained experimentally. The difference in the gate length used in their work and our work is probably the main reason for this difference.

Figure 4.14 shows that the stress magnitude in the SiGe S/D regions is rather close to that in the Si channels. The largest difference in their average stresses is within 200 MPa and the smallest difference is 50 MPa. Like the Si channels, the SiGe S/D regions probed by UV Raman spectroscopy are compressively stressed. Figure 4.16 illustrates our explanation for this:

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Fig: 4.16: Conceptual schematic of the balance of forces. The green arrows show the force exerted by the Si channel regions on the SiGe S/D regions; the purple arrows show the force exerted by the SiGe S/D regions on the Si channel regions.

We will picture the scenario in intuitive macroscopic terms and attempt to comprehend things as a whole. Here, we have the two SiGe regions exerting forces on the Si channel in the directions indicated by the purple arrows. This results in the Si channel being compressively stressed. Similarly, two neighboring Si channels will exert forces on the SiGe region between them in the directions indicated by the green arrows. This results in the SiGe regions being compressively stressed as well. For any vertical SiGe/Si boundary, these two kinds of forces must be of the same magnitude and in opposite directions for equilibrium (otherwise the boundary will move). Therefore, we get similar stresses experimentally for the SiGe and the Si regions probed, and both stresses are compressive. (It may be helpful to think of a scenario in real life that is analogous to this – imagine there is a row of seats meant for slim people to sit on. However instead of having slim persons taking all of those seats, we have an overweight person and a slim person on alternating seats. All persons, whether they are overweight or slim, will feel compressively stressed with shoulders pressing against their neighbors'. Person A will feel as great a force

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exerted on her by Person B as Person B does, by Person A. The overweight persons are analogous to the SiGe regions, which are “forced” to take sites smaller than their natural lattice constants.) This is a macroscopic description of the overall effect on the SiGe and Si regions. To understand the scenario microscopically and to evaluate the sign and magnitude of each tensor component of the strain or stress point-by-point, one can perform simulation studies (discussed in Section 2.1.3.1). Simulations such as those from Yeo et al [30] suggest that although the strains in the SiGe and Si regions are not purely uniaxial, they are predominantly so, in the source-to-drain direction. Therefore, we view the scenario macroscopically with uniaxial forces as described. Note however that the stress or strain in the SiGe regions is not likely to be predominantly uniaxial for very large poly pitches where $L_{\text{SiGe}} \gg L_{\text{Si}}$. Under such a scenario, it will take on an overall character that is similar to blanket SiGe films grown on Si substrates, which are under *biaxial* compressive stress.

Our understanding of the forces is supported by simulation results from other groups. The simulated stress image from Eneman et al [43] is shown in Fig. 4.17 below as an example. They used repeating structures similar to ours. Notice that the grayscale coloration is continuous from the channel region to the S/D region across the vertical Si/SiGe boundary and that the stress is compressive.

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Fig. 4.17: Simulated image from Eneman et al [43] for repeating transistors, showing the stress component in the source-to-drain direction (MPa). The negative MPa values indicate compressive stresses.

On a separate note, simulations displaying variations in strain rather than stress will not exhibit continuity of strain across the boundary. (See Yeo et al [30], for example.) This is because while stress is directly related to force (being force per unit area), strain is dependent on the elastic constants for the material. Hence, for the same force and stress acting on Si and SiGe over the same area, they will be strained differently because they have different elastic constants.

The implications of removing the gate on the channel stress should be mentioned. Enhancement of channel stress by removal of the polycrystalline silicon gate was previously reported – etching away the dummy gate in a damascene process for gate-last fabrication released the repulsive force due the dummy gate on the channel, thereby increasing the compressive force on the channel [6, 133]. Simulation results from Wang et al [133] are shown in Fig. 4.18 below:

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Fig. 4.18: Simulation results from Wang et al [133]. A recess depth of 80 nm and a Ge concentration of 18% was used for their work.

Notice that the channel stress increases from around -500 MPa to around -800 MPa with gate removal, and that the channel stress remains very much the same after the fabrication of the final gate as compared to the gate-less case. As for Auth et al [6], the channel stress increased from around -800 MPa to around -1200 MPa. The actual amount of stress increase should be dependent on the geometry of the device and the process conditions used. We propose that our method for stress measurement here is useful for understanding gate-last devices that take advantage of the increase in channel stress with dummy gate removal. We can assume the channel stress with the final gate will be very similar to the gate-less case, based on simulation results from Wang et al [133] shown above.

4.4 An alternative way to remove gates

In this section, an alternative way to remove the gates using chemical rather than mechanical means is presented. Chemical means of gate removal are desirable because it will be more practical if one needs to prepare many samples. One can prepare numerous samples at one go using this approach. This is unlike using the method described in the previous sections, where one can only work on one piece of sample at a time. Chemical means of gate

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removal will also avoid the issue of unintentionally scratching the sample surface.

Note that the gate material is polycrystalline Si and the S/D material is SiGe. If we want to etch away the gates chemically, there has to be good chemical selectivity between polycrystalline Si and single crystalline SiGe for the chosen chemistry. Unfortunately, chemicals that attack the Si-Si bonds in polycrystalline Si will also attack the Si-Si bonds in SiGe.

We can get some ideas from the gate-last (damascene) technology for gate removal via chemical means. In the gate-last process flow used by the semiconductor industry, a polycrystalline Si dummy gate is fabricated first. It is then etched away, and the final functional gate will eventually take its place. The dummy gate acts like a placeholder for the final gate. The process was developed by Intel in their 45 nm technology node as an integration strategy for the high k/metal gate technology [134]. In the process flow, an interlayer dielectric (ILD) film is deposited over the entire transistor after the S/D formation and silicidation steps. A “poly opening” step is then carried out using polishing – this serves to expose the top of the polycrystalline silicon. The polycrystalline silicon gate is then etched away chemically while the surrounding ILD protects the SiGe S/D regions. Figure 4.19 below illustrates the main idea:

Fig. 4.19: A chemical approach to remove the polycrystalline silicon gate and preserve the SiGe S/D regions, borrowing concepts from the gate-last process flow.

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It is possible to have an adaptation of this approach for our own work using chemicals to etch away some thickness of the ILD rather than using polishing to accomplish this. The end point for the ILD etch process must be well determined beforehand.

A chemical approach that is rather different from the one introduced above was actually used instead. This approach is simpler than the above and does not require the deposition of another film. The strategy was to delaminate the gates by undercutting the gate oxide using HF etch. Fig. 4.20 below describes this method.

Fig. 4.20: Method to remove gates chemically.

For this chemical etching work, a wafer with different patterning was used. The process parameters for this wafer are similar to those for the previous wafer. There are also UPC pads with repeating transistor structures on this wafer. The gate length and spacers are also the same as those of the previous wafer.

The etch chemicals and etch conditions were decided using Refs. [135-136] as guides. To etch away the nitride spacer, phosphoric acid (H_3PO_4) was

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used without further diluting the commercially prepared solution, which had a concentration of 85% by weight. A reflux bath was used as recommended by the references consulted, in order to create a constant temperature (160°C) and acid concentration. For stoichiometric silicon nitride (Si_3N_4), the etch rate is 4.5 nm/min [136]. An etch duration of 6 min was used to ensure an over-etch. It is very important to ensure the complete removal of the nitride – otherwise the second step would not work as the hydrofluoric (HF) acid would not be in contact with the gate oxide. At these conditions, the etch rates of polycrystalline silicon and single crystalline are very low [136] and can be neglected. Therefore, we do not need to worry about them being etched away.

Dilute HF acid was prepared for the second step by mixing 10 parts water to one part HF (50%). An etch duration of 1 h at room temperature was used to delaminate the gates. The etch duration was determined by trial-and-error. It was found that this duration enabled the pads to be partially stripped of their gates. Similarly, the etch rates of polycrystalline Si and single crystalline SiGe are negligibly low at these conditions. After the HF etch, the sample was rinsed by immersing it in a vessel containing de-ionized water.

Figure 4.21 shows the appearance of the sample after these etching steps. As can be seen in this figure, it was easy to tell whether gates have been delaminated or not simply by looking at the sample under a conventional bright field optical microscope.

Figure 4.22 shows the appearance of the sample under SEM. As can be seen from the annotation, the line structures measure 38.6 nm across. This indicates that the nitride has been etched away – we can tell this by comparing with the dimensions of the gate and spacer in Fig. 4.3. With the spacer, the line should measure approximately 60 nm across. 38.6 nm should be close to the actual dimension of the polycrystalline silicon material itself.

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Fig. 4.21: Bright-field optical microscopy image of sample after the two-step etch process. A 50x objective lens was used for this image. The letters “UPC-126” mean that the poly pitch for this pad is 126 nm.

Fig. 4.22: SEM images of this pad at different magnifications.

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Raman spectroscopy then was done for pad UPC126 (i.e. pitch = 126 nm) and pad UPC252 (i.e. pitch = 252 nm). The respective measured stresses were -0.63 GPa and -1.2 GPa respectively. Comparing these values with those in the graph in Fig. 4.14, the stresses obtained using samples with gates chemically removed are similar to those with gates removed mechanically.

4.5 Summary and conclusions

In this chapter, I have provided a means to measure the channel stress in 45nm node PMOS transistors with SiGe source and drain using UV Raman spectroscopy. The gates were removed in a simple and cost-free step using polishing to allow direct probing of the stress in the exposed channel. Well-resolved Raman peaks enabled the analysis of stress in the Si channel as well as in the SiGe source and drain. Using appropriate values for the phonon deformation potentials and the elastic constants for these two materials, the stress-shift relationship was worked out for each. Both stresses are compressive and increase with poly pitch length. For each pitch, the stress in the SiGe source and drain is similar in magnitude to that in the Si channel. This is under the assumption of uniaxial stress in both these regions and within the limits of the poly pitches used for our work. An alternative method of removing the gates, which is more practical for preparation of numerous samples, was also presented in this chapter. This work provides a convenient and low cost way for rapid characterization of stress in 45nm node transistors and beyond.

5. Impact of implantation and annealing on channel stress

5.1 Introduction

This chapter will present our investigations on the impact of implantation and annealing on 45 nm node transistors with embedded SiGe source and drain, using UV Raman spectroscopy. This work studies the relaxation of channel stress with implantation and the recovery of channel stress with different annealing schemes. The main results and conclusions for this work are published in the journal paper cited in Ref [137].

5.2 Background and motivation

The general motivation for our work has been addressed in Section 2.1.3.2. In that section, I pointed out the general lack of experimental studies in the literature in the area of understanding how the channel strain (or stress) of strained-engineered transistors varies with different process parameters or process steps. An important example of this would be the investigation of how the channel strain changes with implantation and annealing. In the next few paragraphs, I will provide further information on the specific background and motivation for our work described in this chapter which aims to address this area of concern.

Implantation and annealing are crucial steps in device integration. However, they are known to lead to significant channel strain relaxation [61]. Channel strain relaxation is undesirable because device performance is intricately linked to the level of strain in the channel [4]. Therefore it is important to study how channel strain changes with implantation and

annealing and to implement steps to retain channel strain. However, studies that analyze the channel strain (or stress) directly to do this are not common. Most related studies present data collected from implanted and annealed blanket SiGe films, in which one will indirectly infer a channel strain relaxation from the relaxation of the SiGe blanket films [138-140]. As for studying the effect of implantation and annealing by direct channel strain measurements, the work by Liu et al [61] seems to be one of the very rare papers published in this area prior to our study, if not the only one. (Note: Liu is one of the co-authors for our paper [137].) Liu et al [61] used nano-beam diffraction (NBD) to analyze the combined effect of implantation and a single-step anneal using rapid thermal anneal on 65 nm node transistors.

The work in this chapter studies the separate effects of implantation and annealing on channel stress of 45 nm node transistors using UV Raman spectroscopy. Here, halo implantation and S/D extension implantation were carried out as we believe these have a significant effect on the channel stress because of their proximity to the channel. Annealing was carried out by furnace anneal or rapid thermal anneal, or by a two-step anneal where furnace anneal precedes rapid thermal anneal.

It has been reported in some works [141-142] that such a two-step thermal treatment can be beneficial for junction characteristics for Si implanted with BF_2^+ ions. The low-temperature, long-duration anneal can recrystallize the Si substrate damaged by ion implantation, before an indispensable high-temperature, short-duration annealing step is applied for dopant activation. Performing furnace annealing before rapid thermal annealing is also important for annealing out point defects via recombination of the interstitials and vacancies during solid phase epitaxial growth (SPEG) of the amorphous layer [143]. This results in reduced transient enhanced diffusion (TED) during the subsequent rapid thermal annealing step, and leads to shallower junctions than if the annealing steps were reversed [141]. A

smaller junction leakage current can also be achieved using this sequence [142]. Other than junction characteristics, it would be important to elucidate the effects of these thermal treatments on the channel strain of transistors with embedded SiGe, since strain is the primary concern for such technology.

5.3 Experimental details

Sample preparation

PMOS transistors with SiGe source and drain regions were fabricated on Si (001) wafer by Si recess etch using reactive-ion etching, followed by cleaning and epitaxial SiGe selective growth using low-pressure chemical vapor deposition. Undoped SiGe was used. The channels were oriented in the [110] direction. A dense transistor layout with a polycrystalline silicon pitch of 252 nm was adopted. The schematics for the process flow for this fabrication are shown in Section 3.1, on page 38. For our study, we have picked a Ge concentration of 17% (typical concentrations of Ge used in the S/D regions for such technology range from 15% to 25%). Following SiGe growth, halo and S/D extension implantations were carried out using arsenic (As^+) ions and molecular boron difluoride (BF_2^+) ions respectively, at typical implantation conditions. GLOBALFOUNDRIES Singapore Pte Ltd had kindly supplied me with these implanted wafers.

One die from this wafer was subjected to thermal treatment using a low temperature furnace anneal at 650°C for 10 minutes, and another die was treated with a high temperature rapid thermal anneal at 1000°C for 3 seconds in nitrogen gas. A separate die underwent a two-step anneal involving a furnace anneal prior to rapid thermal anneal at the same conditions. Figure 5.1 below shows the schematics of the transistors used as well as the process flows involved.

Fig. 5.1 (a) Schematics of transistors used. Halo and S/D extension implantations were carried out followed by annealing by furnace anneal (FA) or rapid thermal anneal (RTA), or by a two-step anneal involving FA before RTA. (b) Prior to performing UV Raman spectroscopy, the gates were removed to expose the strained channels.

Next, the gates were removed using the hand-polishing method described in Chapter 4. The reason for removing the gates, as already described in Chapter 4, was so that the UV laser used in our Raman experiments can probe the channels directly. The appearance of the sample before and after gate removal is shown in Fig. 5.2 below, using the as-grown sample as an example.

Fig. 5.2: Bright field optical microscopy images of sample before hand-polishing (a) and after hand-polishing (b), taken using a 50x objective lens. Regions inside the pad where the gates had been stripped off appear lighter in color than those with gates still intact. This is the as-grown sample. Later when taking Raman spectra from this pad, I avoided locations with the obvious scratches. The spots where the spectra were taken from should be all right because of the reasonably small error bars involved for the channel stress (see results in later section).

Figure 5.3 below shows the cross-sectional transmission electron microscopy (XTEM) images of the implanted sample before and after gate removal. As with the samples with as-grown SiGe in our previous work described in Chapter 4, the S/D material of the implanted sample here remains intact after hand-polishing. This shows that although there may be the concern that implantation may weaken the topmost portion of the SiGe regions mechanically (thereby making it easy to get polished away), the topmost portion is still mechanically strong enough to withstand the mechanical polishing. We can deduce that the SiGe regions for all the other samples would also be intact because they should mechanically be even stronger than those of the implanted sample.

Fig. 5.3 (a) and (b) XTEM images of implanted sample before gate removal, at different magnifications. (c) and (d) XTEM images of implanted sample after gate removal. The images show that the S/D material remains intact after hand polishing. (Acknowledgement: Failure Analysis (FA) team in GLOBALFOUNDRIES Singapore Pte Ltd for the XTEM work.)

UV Raman spectroscopy

For UV Raman studies, the conditions used for acquiring the Raman spectra were the same as those described in Chapter 4. The incident laser polarization was in the [110] direction, i.e. along the channel direction from source to drain for all pads studied. Ten spectra were acquired from each sample and the bulk unstrained Si reference wafer using an alternating sequence. Using the as-grown sample as an example, the spectra acquisition sequence was: Si-1, AG-1, Si-2, AG-2, ... , Si-10, AG-10, where Si-1 refers to the first spectrum acquired from the reference Si wafer and AG-1 refers to the first spectrum acquired from the as-grown sample, and so on. As discussed in Chapter 4, the alternating sequence was used to monitor the system stability throughout the entire experimental session. Spectra from the different samples

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were taken over separate experimental sessions on different days. During each experimental session, the alternating sequence was adopted for that particular sample and the reference wafer. All spectra were taken from randomly chosen locations. Although the calibration of the system was (very) slightly different on different days, it would not affect our data analysis and interpretation because we are eventually interested in the relative Raman shifts of the strained channel with respect to the unstrained Si wafer rather than the absolute Raman shifts. All other settings on the Raman spectroscopy system were kept the same for the different experimental sessions. Lorentzian profiles were then fitted to the spectra.

5.4 Results, analysis, and discussion

The results for the fitted peak positions (mean and standard deviation) are tabulated below:

Sample	Si peak from channels (cm ⁻¹)	Si-Si peak of SiGe from S/D regions (cm ⁻¹)	Si peak from bulk unstrained reference wafer, taken during the same experimental session as that sample (cm ⁻¹)
As-grown	523.51 ± 0.08	512.93 ± 0.14	520.40 ± 0.07
Implanted	522.75 ± 0.20	511.08 ± 0.60	520.37 ± 0.07
Implanted/FA	523.33 ± 0.17	511.92 ± 0.48	520.32 ± 0.06
Implanted/RTA	522.89 ± 0.22	508.96 ± 0.42	520.32 ± 0.04
Implanted/FA+RTA	523.10 ± 0.22	509.56 ± 0.76	520.34 ± 0.04

Table 5.1: Means and standard deviations of the fitted peak positions

For the purpose of clarity in displaying the spectra of the different samples together, a standard peak position of 520.35 cm⁻¹ was used for the peak position of the bulk reference unstrained wafer. Appropriate offsets were applied to each of the peak positions given in the table. For example, this means that for the as-grown sample, the mean Si peak position from the

channel would be given as $523.51 + (520.35 - 520.40) = 523.46 \text{ cm}^{-1}$. Note that applying this offset does not change the relative peak shift of the strained channel with respect to the reference wafer, which is equal to 3.11 cm^{-1} with or without offset. Figure 5.4 shows the averaged spectra for each sample and their fittings.

Fig. 5.4 (a) Raman spectra of as-grown and implanted samples. The spectrum for bulk unstrained silicon is also shown for comparison. The blue vertical lines are drawn as guides for the eyes through the centers of the individual fitted peaks of the as-grown sample. (b) Comparison of Raman spectra for implanted samples after annealing at various conditions. The blue vertical lines are drawn through the centers of the individual fitted peaks of the implanted sample with furnace annealing (FA). The spectra have been offset in the vertical direction for clarity.

For each of the spectra (other than that of the bulk Si), the peak on the left arises from the Si-Si vibration of strained SiGe and that on the right arises from the exposed strained Si. Their peak positions are labeled as shown. Referring to Fig. 5.4 (a), there is a clear blue-shift in the Si peak of the as-grown sample with respect to the bulk unstrained Si. This indicates a compressive strain in the channel [82]. Comparing the spectrum of the implanted sample with that of the as-grown sample, there is a distinctive strain relaxation in the Si channels of the implanted sample, which can be seen from the red shift of the Si peak of the implanted sample with respect to that of the as-grown sample. Such channel strain relaxation is attributed to the damage in the crystalline structure of SiGe by implantation. This damage results in a strain relaxation in SiGe, which debilitates effective stress transfer from SiGe to the channel. Indeed, for embedded SiGe which experiences a compressive strain [30], a red shift in the Si-Si peak of SiGe which indicates a strain relaxation of SiGe can be observed after implantation. Significant defect formation in SiGe is also implied by the decrease in relative intensity and the broadening of this peak. Illgen et al [36] have reported that S/D extension implantation using BF_2^+ ions at an energy of 2.3 keV and dose of $1.2 \times 10^{15} \text{ cm}^{-2}$ causes amorphization of the top layer of the embedded SiGe. On a separate note, we see how the method of characterization employed here enables useful information to be acquired simultaneously for the embedded SiGe regions as well as for the Si channels.

Figure 5.4 (b) compares the averaged Raman spectra from the implanted samples after undergoing different thermal treatments. Upon close examination of the relative positions of the strained Si peaks, we see that furnace annealing results in a greater strain in the Si channel regions compared to what rapid thermal annealing does. Very importantly, we also note that the two-step annealing scheme results in a greater strain in the channels compared to what rapid thermal annealing alone does. Our results suggest that when a

high temperature anneal is required for fabricating transistors – as is almost always the case for dopant activation – a two-step anneal involving a low-temperature, long-duration furnace anneal prior to a high-temperature, short-duration rapid thermal anneal can be beneficial for recovering channel strain. It is reasonable to ask whether the difference in the positions of the strained Si peak between these two samples is significant or not. Later in this chapter, I will include a further discussion on this issue using a statistical approach.

Care needs to be exercised when interpreting the positions of the Si-Si peaks of SiGe in Fig. 5.4 (b), as the S/D regions are expected to have high concentrations of activated dopants after implantation and annealing. High concentrations of activated dopants ($\sim 6 \times 10^{19} \text{ cm}^{-3}$ and above) are known to cause discernible red-shifts and broadening in the Raman peaks of Si [144] and Ge [145]. Similarly, we expect the Si-Si peak positions of SiGe here to be dependent on the concentration of free carriers, in addition to the well known parameters [131] of Ge concentration and strain in SiGe. Here, the Si-Si peak position of SiGe should be dependent on all three parameters. However, if we assume comparable amounts of free carriers and negligible out-diffusion of Ge atoms [146] for both the rapid thermal annealed sample and the two-step annealed sample, we observe qualitatively that the latter has a greater SiGe strain than the former. We believe this is because furnace annealing has annealed out most of the implantation-induced defects in the SiGe S/D material, thereby suppressing the nucleation and propagation of misfit dislocations in the subsequent rapid thermal annealing step.

Another observation is that the Si-Si peak position of SiGe for the rapid thermal annealed sample and the two-step annealed sample are both red-shifted compared to that of the furnace annealed sample. We attribute the main reason for this to the effective dopant activation of the rapid thermal annealing step, which produced sufficient free carriers to result in this red-shift. Figure 5.5 below is reproduced from Ref. [144] for readers to get a sense of how

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much the peak of p-type Si will shift with different carrier concentrations. Due to the lack of information in this area for the behavior of the Si-Si peak of SiGe, we assume here that it will behave similarly, for low concentrations of Ge.

Fano parameters of the optic phonon and ^{11}B local mode in Si for different exciting frequencies and carrier concentrations.

Carrier concentration (cm^{-3})	Exciting wavelength ($\text{\AA}$)	Optic Phonon			^{11}B local mode		
		q_p	Γ_p (cm^{-1})	$\omega_p + \Delta\omega_p$ (cm^{-1})	q_L	Γ_L (cm^{-1})	$\omega_L + \Delta\omega_L$ (cm^{-1})
$4 \times 10^{20\text{a}}$	4579	4.54	12.4 ± 0.5	512 ± 2	1.82	8.0 ± 1.5	615 ± 2
	5145	2.57	11.8 ± 0.5	511 ± 2	1.16	7.4 ± 1.5	614 ± 2
	6471	0.55	12.6 ± 0.5	509 ± 2	0.15	10.0 ± 1.5	613 ± 2
			average	average		average	average
			12.3 ± 0.5	510.7 ± 1.5		8.5 ± 1.8	614 ± 2
1.5×10^{20}	4880	6.0	9.2	516.7	2.7	7.3	614.8
	6471	1.8	8.5	514.8	0.93	6.4	614.2
			average	average		average	average
			8.85 ± 0.5	515.7		6.9 ± 0.6	614.6
6×10^{19}	4880	10	6.2	519.7	3.2	6.4	615.8
1.5×10^{19}	4880	44	3.1	520.2	8	6.0	617.1
	6471	20.0	2.65	520.2	5.8	5.9	617.3
			average	average		average	average
			2.88	520.2		5.95	617.2
5×10^{18}	4880	200	1.8	520	33	6.8 ± 1.0	618
Pure Si (10^{13})			1.5	520.0		5.5^b	620^b

Fig. 5.5: Shift in the Raman peak for p-type Si doped with boron, with different levels of free carrier concentrations. (Reproduced from Ref. [144]) The columns containing information of interest are boxed up. Notice that the amount of red-shift increases with increasing carrier concentration and that it is dependent on the excitation wavelength used.

For the Si channels which are the primary concern for this work, the carrier concentration level in the channel regions is not high enough to cause discernible red-shifts in the Si Raman peaks [144]. (See Fig. 5.5 above for reference.) This also applies for the piece of unstrained bulk Si used as our reference. Hall effect measurements indicate it only had a concentration of approximately $2 \times 10^{16} \text{ cm}^{-3}$ of p-type carriers. For the strained Si channels, by

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attributing the shift in the Si Raman peak position solely to the strain present, we are able to evaluate the level of stress in the channels quantitatively. A quantitative summary for the strained channels is given in Fig. 5.6, obtained using the relation $\sigma_{xx} = -434\Delta\omega$, where σ_{xx} is the uniaxial stress in the channel given in megapascals (MPa) and $\Delta\omega$ refers to the amount of shift from stress-free silicon given in wavenumbers (cm^{-1}) [82, 98-99]. (See also Chapter 4 for this.) Uniaxial stress in the [110] direction (from source to drain) in the Si channels is assumed.

Fig. 5.6: The $\Delta\omega$ and compressive stress values for the various samples. Stress relaxation with implantation and different degrees of stress recovery with the annealing can be seen from this figure.

From our results, approximately 23% of the original channel stress is lost after implantation. Furnace annealing alone is able to recover up to 97% of the original stress. Rapid thermal annealing alone, on the other hand, recovers only 83%. The two-step annealing scheme recovers 89% of the

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stress, giving an improvement of 6% compared to rapid thermal annealing alone.

It is necessary to do a statistical analysis to see if the channel stress arising from the two-step annealing scheme is significantly better than that of rapid thermal annealing alone. First, let us understand how the error bars (i.e. their standard deviations) are derived:

Strained Si peak of sample: $(A \pm \Delta A) \text{ cm}^{-1}$, where A is the mean and ΔA is the standard deviation of the ten spectra taken from that sample,

Si reference: $(B \pm \Delta B) \text{ cm}^{-1}$, where B is the mean and ΔB is the standard deviation of the ten spectra taken from the bulk unstrained Si wafer,

Relative Raman shift of strained peak for sample: $(A-B) \pm (\Delta A + \Delta B) \text{ cm}^{-1}$

Standard deviation of stress measurement for sample = $434 (\Delta A + \Delta B) \text{ MPa}$

We can do a hypothesis testing [147] to check whether the two-step annealing process gives significantly higher stress compared to the rapid thermal annealing process. A hypothesis is a statement that may or may not be true, concerning one or more populations. For hypothesis testing, the main steps involved are:

- 1) State the null hypothesis (H_0)
- 2) State the alternative hypothesis (H_1)
- 3) Choose the level of significance, α – the smaller the value of α , the more stringent the test
- 4) Establish the critical region for the t -distribution (See t -distribution table given in Appendix)
- 5) Compute the statistic from the sample
- 6) Conclusion: reject H_0 if the statistic has a value within the critical region, otherwise do not reject H_0 .

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We will use the independent t-test for our hypothesis testing. Our own situation is framed into the problem for hypothesis testing as stated below:

The average channel stress value for the two-step annealed sample is 1199.79 MPa, with a standard deviation of 112.64 MPa. (Keeping many significant figures for now.) The average channel stress value for the rapid thermal annealed sample is 1113.30 MPa, with a standard deviation of 113.69 MPa. The sampling size for each sample is 10. We need to test the claim that the mean stress for the two-step annealing process is statistically greater than that of the rapid thermal annealing process, using a level of significance of (a) 0.10 and (b) 0.05.

Working:

$H_0: \mu_1 - \mu_2 = 0$ (null hypothesis: the means of the channel stress are the same)

$H_1: \mu_1 - \mu_2 > 0$ (alternative hypothesis: the mean of the channel stress for the two-step annealing process is greater than that for the rapid thermal annealing process)

$$\bar{x}_1 = 1199.79$$

$$s_1 = 112.64$$

$$n_1 = 10$$

$$\bar{x}_2 = 1113.30$$

$$s_2 = 113.69$$

$$n_2 = 10$$

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$$s_p^2 = \frac{(n_1 - 1)s_1^2 + (n_2 - 1)s_2^2}{(n_1 - 1) + (n_2 - 1)}$$

$$t = \frac{(\bar{x}_1 - \bar{x}_2)}{\sqrt{s_p^2 \left(\frac{1}{n_1} + \frac{1}{n_2} \right)}} = 1.709$$

$$\nu = \text{degrees of freedom} = (10 - 1) + (10 - 1) = 18$$

(a) $\alpha = 0.10$

Critical region: $t > 1.330$, for a one-tailed test. (See t-distribution table in Appendix)

Our t value, being 1.709, lies within the critical region.

Therefore, we reject the null hypothesis and accept the alternative hypothesis.

We conclude at the significance level of 0.10 that the two-step annealing process gives higher stress in the channel compared to the rapid thermal annealing process. This significance level means that there is a probability of 10% or less that this phenomenon is due to chance alone. In other words, there is a probability of 10% or less that we are erroneously making this conclusion.

(b) $\alpha = 0.05$

Critical region: $t > 1.734$, for a one-tailed test. (See t-distribution table in Appendix)

Our t value, being 1.709, does not lie within the critical region.

Therefore, we do not reject the null hypothesis. We conclude that the two-step process does not give significantly higher channel stress compared to the rapid thermal annealing process, at the significance level of 0.05.

By testing at these two levels of significance, we conclude that the two-step annealing process gives higher channel stress compared to the rapid

thermal annealing process, and that the probability of erroneously making this conclusion is lower than 10% and approaches 5%. The results indicate that it should be worthwhile to put in efforts to further optimize the two-step annealing scheme. On a separate note, we can see that our approach can meaningfully discriminate a stress difference of 90 MPa in silicon uniaxially stressed in the [110] direction. This corresponds to a strain difference of 5×10^{-4} . This sensitivity is comparable to those of the TEM-based techniques reviewed in Section 2.1.3.2.

5.5 Summary and conclusions

In summary, we have investigated the impact of implantation and annealing on the channel strain of 45 nm node transistors with embedded SiGe source and drain, using UV Raman spectroscopy. We have found that a two-step anneal involving furnace anneal before rapid thermal anneal can be beneficial for recovering channel strain. We thus recommend the optimization and implementation of this scheme where a high-temperature annealing step is essential for dopant activation for fabricating strained transistors with embedded SiGe source and drain. We also found that our approach for stress measurements has a sensitivity of approximately 90 MPa.

6. Effect of incident laser polarization on gate-less structures

6.1 Introduction

This chapter studies the interaction of 325 nm laser light with the gate-less structures. Specifically, the distribution of light in these structures for different incident light polarizations is investigated using FDTD simulations, so that a better understanding can be achieved on the actual regions being probed for stress measurements. The implications of using different laser polarizations for the study of stress in such structures using Raman spectroscopy are then discussed.

6.2 Simulation conditions

The software used for the simulation work in this chapter is *FDTD Solutions* from Lumerical Solutions, Inc. It uses the Finite Domain Time Difference (FDTD) method to solve Maxwell's equations in complex geometries. Further information on the method and software has been given in Section 3.2.2. The following provides the details of the conditions used for the simulations in this chapter:

- Light source
 - Shape: plane wave
 - Wavelength: 325 nm
 - Geometry: x span = 6.109 μm
 - Direction of polarization: varied for different simulations
 - Direction of propagation: towards the structures and normal to the surface of the structures

- Material(s)

Geometry: varied for different simulations. Where the actual gateless structures are being simulated, the geometry mimics that shown in the cross-sectional TEM image in Chapter 4.

Refractive indices at 325 nm: $n = 5.052$, $k = 3.211$ for Si [116]; $n = 4.65$, $k = 3.33$ for $\text{Si}_{0.83}\text{Ge}_{0.17}$ [117-118].

Optical isotropy: materials are taken to be optically isotropic, i.e., have the same optical constants along different directions inside the material. This is valid for materials with the cubic structure where there is no stress [148]. The non-isotropy induced by stress [149-151] will also be discussed.

- FDTD simulation (2D)

Geometry: x span = $0.84\ \mu\text{m}$, y span = $0.3\ \mu\text{m}$. As the simulations are done in two-dimensions, the z direction is taken to be infinite.

Mesh size: $1.5\ \text{nm}$ (dx) by $1.5\ \text{nm}$ (dy)

Boundary conditions: x min and x max = periodic, y min and y max = PML (perfectly matched layer). The periodic boundary condition is used for x min and x max. This essentially simulates a wafer that is very large in the x direction. Using this boundary condition will also make the plane wave light source periodic in the x direction. The PML boundary condition is used for y min and y max because we want the electromagnetic (EM) energy to be absorbed completely at these two boundaries so that no light will be reflected back from these boundaries into the simulation region and interfere with the simulation.

Background refractive index: 1, i.e. the structures are surrounded by air.

Further information on simulation setup conditions can be found in Refs. [113-114].

6.3 *Simulation results and discussion*

First, we look at the simulation for light interacting with plain, featureless silicon wafer. Figure 6.1(a) below shows the simulation setup for light propagating in the direction depicted by the pink arrow. This is the wave-vector direction of the electromagnetic wave. The E field polarization direction of the light is indicated by the blue arrow (shown as a dot in this case), which is directed out of the plane of the page, along the z axis. The white horizontal line shows where the plane wave originates. The cross-section of the silicon wafer is drawn as a green rectangle in the xy plane. The inside of the orange box demarcates the FDTD simulation region. Text has been added to indicate the type of boundary condition (BC) used at each of the boundary of the FDTD simulation region. The yellow box around the simulation region demarcates the extent of an “analysis group”. The “analysis group” contains “monitors” to monitor quantities like the E field intensity and the H field intensity inside the simulation region. The simulation was then run and the results are shown in Fig. 6.1(b).

CHAPTER 6: EFFECT OF INCIDENT LASER POLARIZATION ON GATE-LESS STRUCTURES

(a)

(b)

Fig. 6.1: (a) Simulation setup for 325 nm light incident on smooth, featureless Si wafer. The E field polarization direction is out of the page, along the z axis. (b) Simulation results for the spatial profile of the E field intensity for this simulation setup.

From Fig. 6.1 (b), we can observe the distribution of the E field intensity ($|E^2|$) above the Si wafer surface and below it. Above the Si wafer surface, the region (air) takes on intensity values that saturate above the maximum value for the color bar. (Note: the injected E field intensity is $1 \text{ V}^2/\text{m}^2$.) The light in this region contains the injected light as well as that reflected off the surface of the Si wafer. Below the surface of the Si wafer, we observe a decrease in the E field intensity with increasing depth into the Si wafer. Upon close examination of this figure, the depth where the E field intensity drops to $1/e$ of $1 \text{ V}^2/\text{m}^2$ is approximately 8 nm from the surface of the wafer. This is congruent with what we understand about the optical penetration depth of 325 nm light in Si (See Chapter 4).

Now, we look at the E field intensity for the situation where the E field polarization direction of the light is along the x axis instead. Figures 6.2 (a) and (b) below show the simulation setup and results respectively. The results are exactly the same as the previous (Fig. 6.2 (b)). This is because silicon is a cubic crystal and cubic crystals are optically isotropic – they have the same refractive index in all directions [148]. This is unlike crystals with the trigonal, tetragonal, or hexagonal structure which exhibit two distinct indices of refraction; or crystals with the triclinic, monoclinic or orthorhombic structure which exhibit three distinct indices of refraction [148]. Therefore, if we take the x axis to be parallel to the [110] crystallographic direction of Si and the z axis to be parallel to the [1-10] crystallographic direction, the E intensity spatial profile will be the same whether the E field of the injected light is polarized along the [110] direction or along the [1-10] direction.

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(a)

(b)

Fig. 6.2: (a) Simulation setup for 325 nm light incident on smooth Si, with the E field polarization direction along the x axis. (b) Simulation results for the spatial profile of the E field intensity for this simulation setup.

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Next, we look at the simulation for the gate-less structures that have been the subject of study for Chapters 4 and 5. The simulation setup and results are shown in Figs. 6.3 and 6.4 below. Here, the cross-sectional geometry of the gate-less structures mimics the geometry shown in the cross-sectional transmission electron microscopy (XTEM) image shown in Chapter 4, in Fig. 4.6. The SiGe source and drain are slightly raised, as shown.

(a)

(b)

Fig. 6.3 (a): Simulation setup for 325 nm light incident on gate-less structures. Dimensions and geometry are as shown. E field polarization direction is out of the page, along the z axis. We define the x, y, and z axes of the simulation to be along the [110], [001], and [1-10] crystallographic directions. This is because the real structures are fabricated on (001) wafer and the source-to-drain direction is in the [110] direction. (b) Simulation results. The region above the structures (air) has been rendered black to show the outline of the structures clearly.

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(a)

(b)

Fig. 6.4 (a): Simulation setup for 325 nm light incident on gate-less structures with E field polarization direction along the x axis. (b) Simulation results.

From Fig. 6.3 (b) and Fig. 6.4 (b), we observe a rather distinct difference in the E field intensity distribution pattern inside the structures for the two different incident E field polarizations. (Note: the polarization direction shown in Fig. 6.4, i.e., along the [110] direction was used experimentally throughout both projects in Chapters 4 and 5.) The latter polarization direction gives relatively greater E field intensity at the channel regions than does the former. Also, for the latter polarization, light is distributed across the entire channel with slight concentration at the edges of the channel; while for the former, light is concentrated at the center of the channel and is almost absent close to the edges of the channel.

To explore the reasons for this difference in the E field intensity distribution pattern for the two different polarizations, the following simulations were carried out – first, the source-drain material was changed from SiGe to Si with the geometry remaining unchanged; second, the source-drain geometry was changed from raised to flat with the source-drain material remaining unchanged. Figures 6.5 and 6.6 show the first scenario for the two different polarizations, and Figures 6.7 and 6.8 show the second scenario for the two different polarizations.

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(a)

(b)

Fig. 6.5 (a): Simulation setup for 325 nm light incident on gate-less structures with E field polarization direction out of the page, along the z axis. The source-drain material has been changed from SiGe to Si. The geometry remains unchanged. (b) Simulation results.

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(a)

(b)

Fig. 6.6 (a): The same simulation setup as the previous (Fig. 6.5(a)), but with the E field polarization along the x axis instead. (b) Simulation results.

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(a)

(b)

Fig. 6.7 (a): Simulation setup for 325 nm light incident on gate-less structures with E field polarization direction out of the page, along the z axis. The source and drain geometry has been changed from raised to flat. The source and drain material remains unchanged (SiGe). (b) Simulation results.

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(a)

(b)

Fig. 6.8 (a): The same simulation setup as the previous (Fig. 6.7(a)), but with the E field polarization along the x axis instead. (b) Simulation results.

It can be seen from Figs. 6.5 to 6.8 that the geometry plays a much more significant role in causing the difference in the E field distribution pattern between the two different polarization directions than does the mismatch in the optical constants at the SiGe/Si interface. The source and drain must be raised above the channel level to result in this difference. The optical constants of Si_{0.83}Ge_{0.17} and Si are probably not distinct enough at 325 nm to create an obvious difference in the distribution pattern when the two different polarizations are used.

All of the above analysis is carried out ignoring the effects of stress. Although silicon is optically isotropic under normal conditions, birefringence will result when a uniaxial stress is applied to silicon [149-155]. Instead of having the same real refractive index value, n_0 , in all directions, Si will exhibit two different values, $n_{//}$ and $n_{\perp}$, in directions parallel and perpendicular to the direction of stress respectively. This phenomenon is known as photoelasticity.

Ideally, the corrected optical constants of Si and Si_{0.83}Ge_{0.17} under uniaxial compressive stress applied in the [110] for both materials should be used for the simulations. Information on the corrected n values need to be obtained for stress uniaxially applied in the [110] direction for a wavelength of 325 nm, and in the directions parallel and perpendicular to the direction of stress applied. The work containing information that comes closest to what is desired appears to be that of Adachi et al [151]. It gives the n values of Si for directions parallel and perpendicular to the 2 GPa uniaxial stress applied in the [100] direction, for wavelengths down to 367 nm. ($n_0 = 6.571$, $n_{//} - n_{\perp} \approx -0.76$) Owing to the lack of the desired information for our specific case, additional simulations were not carried out. Nevertheless, it can be reasoned that Si_{0.83}Ge_{0.17} will likely exhibit similar photoelastic behavior as Si because the Ge concentration is low and SiGe has the same cubic structure as Si; therefore the mismatch of the corrected optical constants at the SiGe/Si interface will be low again. Although the actual values of n of Si and SiGe for the [110]

direction and for the $[-110]$ direction will differ from what has been used in the simulations owing to photoelastic effects, the light distribution *patterns* for light polarized in the $[110]$ and $[-110]$ directions should look similar to the respective cases without stress.

Next, we examine the implications of using different polarizations for Raman studies of Si with uniaxial stress applied in the $[110]$ direction. Let us first consider uniformly distributed light in bulk Si that has been stressed in that manner, possibly using a mechanical clamp system similar to that used in Ref.[156]. We consider the two scenarios depicted in Fig. 6.9 below.

Fig. 6.9: Incident laser light with its E field polarized parallel to the uniaxial stress direction, and incident laser with its E field polarized perpendicular to the uniaxial stress direction. The crystallographic directions are as indicated.

As we have already seen in Chapter 2 Section 2.2.1, the Raman scattered intensity depends on the Raman tensors ($\mathbf{R}$) and on the polarization vector of the incident ($\mathbf{e}_i$) and scattered ($\mathbf{e}_s$) light, and is given by

$$I_s \propto |\mathbf{e}_i \cdot \mathbf{R} \cdot \mathbf{e}_s|^2 \quad (6.1)$$

and that the Raman tensors of Si are given by

$$R_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & d \\ 0 & d & 0 \end{pmatrix} \quad \text{along the [100] direction} \quad (6.2)$$

$$R_2 = \begin{pmatrix} 0 & 0 & d \\ 0 & 0 & 0 \\ d & 0 & 0 \end{pmatrix} \quad \text{along the [010] direction} \quad (6.3)$$

$$R_3 = \begin{pmatrix} 0 & d & 0 \\ d & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \text{along the [001] direction} \quad (6.4)$$

When a stress is applied, the Raman tensors will change. For the case of uniaxial stress applied in the [110] direction, it has been shown by Srikar et al [99] that the resulting Raman tensors will be

$$R_1^\sigma = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & d \\ 0 & 0 & d \\ d & d & 0 \end{pmatrix} \quad \text{along the [100] direction} \quad (6.5)$$

$$R_2^\sigma = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & d \\ 0 & 0 & -d \\ d & -d & 0 \end{pmatrix} \quad \text{along the [010] direction} \quad (6.6)$$

$$R_3^\sigma = \begin{pmatrix} 0 & d & 0 \\ d & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \text{along the [001] direction} \quad (6.7)$$

For backscattering of light from the (001) crystallographic plane, the polarization vectors, e_i and e_s , must take the form $[\alpha\beta 0]$, for arbitrary α and β . As with the case without stress, only the Raman tensor along the [001] direction will give rise to non-zero scattering efficiency when a [110] uniaxial stress is applied. And as with the case without stress, this means only the LO mode will be observed. The change in the Raman peak position for the LO mode has been discussed and presented in Section 2.2.2 as

$$\Delta\omega = \frac{\lambda_3}{2\omega_0} = \frac{q(S_{11} + S_{12}) + pS_{12}}{2\omega_0} \sigma_{[110]} \quad (6.8)$$

As we can see from the above discussion, whether e_i is [110] (in the direction of the applied stress) or [-110] (perpendicular to the direction of applied stress) makes no difference to Raman mode observed. In both cases, the Raman spectrum will only contain a single peak belonging to the LO mode – i.e. the same mode and only that mode is being observed with either polarization direction.

6.4 Conclusions

The analysis in the last two pages tell us that for uniform light falling on bulk smooth Si, one can perform Raman experiments with the laser polarization direction parallel to or perpendicular to the [110] uniaxial stress direction. For either polarization, one can observe the shift in the LO mode and from there, calculate the magnitude of the [110] uniaxial stress. However, simulation results tell us that the *light distribution pattern* in the gate-less structures is not the same for the two different polarizations. The main reason for this has been attributed to the geometry of the structures, specifically to the fact that the source and drain regions are raised higher than the channel regions. Since the light distribution is not the same, light with different

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polarizations do not probe the various locations within the channel with the same intensity. This implies that when performing Raman studies to study stress within structures, one needs to take into consideration the light distribution within the structures probed so as to get a sense of where exactly is being probed. This also implies that it is important to keep the polarization direction consistent when performing such studies, as was done for the projects in Chapters 4 and 5. Keeping the polarization direction consistent, we have seen that our approach for studying channel stress is especially useful for comparative studies (e.g. effect of varying pitches and effect of changing annealing conditions).

7. Some visible-light near-field Raman mapping results

7.1 Introduction

What we have seen so far in this thesis are Raman data acquired by a micrometer-sized laser beam and the light distribution inside the structures for this kind of incident light. It is also desirable to use a much smaller laser beam so that high spatial resolution could be achieved. This will make the study of individual transistors feasible. Some works in the literature, such as those of Kasim et al [157], Yoshikawa et al [158], Mai et al [159], and Zhu et al [160] provide information on ways to reduce the size of a laser beam to perform high spatial resolution work. A combination of high spatial resolution, high surface sensitivity, as well as reasonably strong Raman signals would be ideal.

To achieve high spatial resolution, working in the near-field is necessary to overcome the diffraction-limited spatial resolution in the far-field dictated by Rayleigh's criterion: $R = 0.61\lambda / \text{N.A}$ [148]. Here, λ refers to the wavelength of the light source used and N.A. refers to the numerical aperture of the lens. Kasim et al [157] have developed a near-field Raman imaging method with a spot size of ~ 80 nm, using a dielectric microsphere optically trapped by the excitation laser with a wavelength of 532 nm. (Note: Kasim was in our research group.) The setup is simple, performing the experiment is reasonably easy, results are highly reproducible, and the success rate is high.

The following figure briefly illustrates the principle of optical trapping. This phenomenon is observed by Ashkin in 1970 [161]. Many articles on optical trapping are available, including Ref. [162].

Figure 7.1: Illustration of the mechanisms behind optical trapping. (Figure adapted from Ref [163].) There are two components to the optical force of a focused laser beam. The effect of the radial *gradient force* component is to pull the colloidal particle towards the center of the beam waist, where the radial electric field gradient is the strongest. The effect of the *scattering force* component is to displace the particle in the light propagation direction. For stable 3D trapping, the gradient force pulling the particle towards the center of the beam waist must be stronger than the scattering force displacing it from that position. A strong gradient force requires a beam tightly focused by a high N.A. lens.

The work in this chapter is carried out following the method of Kasim et al [157], who showed that the spot size of the laser *after passing through the polystyrene sphere could be reduced to approximately 80nm*. The following sections provide the experimental details and my results.

7.2 Experimental details

The experimental setup used for the work in this chapter is the same as that of in Ref [157]. The figure below illustrates:

- ①water immersion lens ②water ③incident laser
④cover glass ⑤polystyrene sphere ⑥sample ⑦sample cell

Fig. 7.2: Experimental setup for near-field Raman mapping work. The Raman system used is a WITec CRM200 confocal Raman microscopy system with an Olympus microscope water immersion objective lens (60x, N.A. = 1.2). Figure from Ref. [157].

For this setup, the laser that is used for optical trapping is exactly the same laser used for acquiring the Raman data. The laser would grab hold of the polystyrene sphere while each Raman spectrum was being acquired for a particular mapping session. The mapping was enabled by moving the piezo-stage in specified step sizes. A polystyrene sphere with a diameter of 3 μm was used.

7.3 Results and discussion

The following figures show the sample used as well as my Raman mapping results.

Fig. 7.3: Sample used for near-field Raman mapping. The gate pitch is 280 nm.

Fig. 7.4: (Left) Near-field Raman image, acquired using the procedure and setup described above. The transistor lines can be clearly resolved. (Right) Far-field Raman image, acquired without the polystyrene sphere. The

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scanning step size is indicated. Images are constructed using the integrated intensity of the Si peak – the brighter regions depict regions where the Si peak is more intense, and vice versa. Images are displayed in “3D” – here, this means that the software assigned an arbitrary “height” value to the intensity value. Note that this “height” variation for either image has nothing to do with the actual physical height variation due to the surface topography.

From the above it is clear that the transistor lines could be well resolved spatially with this near-field technique. In the far-field, the lines could not be spatially resolved. This demonstrates the effectiveness of the near-field technique employed for this work for spatially resolving these structures. The following figure displays two Raman spectra from different locations of the near-field mapping:

Fig. 7.5: Near-field image, displayed in 2D here. Spectra from two different locations are also shown here.

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For Fig. 7.5, the more intense spectrum (top) corresponds to that acquired with the polystyrene sphere above the gate regions; while the less intense spectrum corresponds that acquired with the sphere above the source and drain regions. Despite numerous attempts in curve-fitting the spectra from this near-field mapping, it is not easy to separate the various contributions from the strained silicon region, the polysilicon gate, and the underlying bulk silicon substrate as they all appear as a single peak. The bulk substrate signal here is overwhelmingly strong.

It would be desirable to use UV light instead of 532 nm light for shallower penetration depth. UV light could be used with gate-less structures for near-field work. In such case, a much shallower penetration depth as well as high spatial resolution could be achieved. As a water immersion lens for the 325 nm light source in our lab was unavailable, this was not carried out. Suggestions for further work for near-field Raman mapping are given in the next chapter.

8. Conclusions and suggestions for further work

8.1 Conclusions

Several conclusions have been drawn from Chapters 4, 5, and 6. They are highlighted again in this section, as follows:

Often, we do not need to spatially resolve individual structures whose spacings are smaller than the probing size of the characterization tool, or perform a point-by-point analysis across the channel. Collection of averaged information over large arrays of repeating structures can prove useful. In our case, we used a UV laser with a spot size of 1.6 μm to study the channel stress of repeating transistors with pitches ranging from 140 nm to 280 nm. The gate length of these transistors is only ~ 37 nm. The Raman spectra consist of signals coming from the *several repeating* source and drain regions and the Si channel regions covered by the large laser spot. Although we do not have high spatial resolution that will enable us to *spatially* resolve *individual* transistors, we can nonetheless yield useful information because we can *spectrally* resolve the strained Si channel signals from the other signal, namely, that arising from the Si-Si vibration in the SiGe source and drain regions. In our case, we do not have the bulk signal from the Si substrate because using a 325 nm laser for the Raman work allowed for high surface sensitivity. This is due to the shallow penetration depth (~ 8 nm) of this wavelength in both regions. If the bulk signal were present (such as in the case of using a 532 nm laser), it would not have been possible to spectrally resolve the strained Si channel signal from the bulk signal. This demonstrates the importance of the choice of Raman excitation wavelength for such work.

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Our approach for Raman work requires the removal of the polycrystalline Si gates so that the UV laser can probe the exposed channels directly. A simple and cost-free method of polishing the structures manually was adopted for the gate removal.

Analysis of the Raman spectra acquired using the 325 nm UV laser shows that both the source and drain regions and the channel regions are under compressive stress and this compressive stress increases with the pitch length. Under the assumption of [110] uniaxial stress for both the SiGe and Si regions, we have found that the average stress in the SiGe source and drain is similar in magnitude to that in the Si channel for each pitch studied. This similarity in magnitude agrees well with the stress simulation results of another group for the stress component in the source-to-drain direction.

We then extended our method of channel stress measurements to study the impact of implantation and annealing on the channel stress. We have found that implantation is detrimental to channel stress. This is because implantation causes damage to the SiGe crystalline structure, reducing its ability to induce stress on the channel regions. We have also found that a two-step annealing scheme involving a long duration, low temperature furnace anneal before a short duration, high temperature rapid thermal anneal can be beneficial for channel stress recovery. We believe this is because the furnace annealing step anneals out most of the implantation-induced defects in the SiGe S/D material, thereby suppressing the nucleation and propagation of misfit dislocations in the subsequent rapid thermal annealing step. Therefore, we recommend the optimization and implementation of this two-step annealing scheme. Also, we have found that our stress measurement approach has the ability to discriminate a stress difference of around 90 MPa.

Simulations using the finite-difference time-domain (FDTD) method were also carried out to understand the light distribution in the gate-less structures. Different light polarizations result in different light distribution

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patterns inside the structures. This difference is attributed to the raised source and drain geometry. Therefore, it is important to keep the polarization of the laser consistent when performing comparative studies, as was done throughout the Raman experimental work in Chapters 4 and 5 respectively.

The measurement approach that has been presented in this thesis can be an attractive alternative to other approaches that require more time and resources to carry out. It is rapid and requires only simple sample preparation and is suitable for studying numerous samples at one go.

Ideally, it is also desirable to have high spatial resolution combined with high surface sensitivity. This expands our possibilities so that even individual structures might be spatially resolved and studied. Chapter 7 has provided the results of some efforts in this area.

To conclude, we believe that our work is timely and important for the semiconductor industry as well as for the academic field.

8.2 *Suggestions for further work*

From where the work ends off in this thesis, some further research directions are possible. They are described in the following paragraphs.

As mentioned in the last chapter, it would be desirable to combine UV light with gate-less structures for near-field work. The choice of wavelength would be 364 nm instead of 325 nm for the work in mind. This is because resonant Raman scattering can be achieved at 364 nm since silicon has a direct band gap of this energy at the Γ point. Resonant Raman scattering will enhance the scattering intensity. Another reason for the choice of this wavelength is a more practical one. An online search indicates that water immersion lenses for 325 nm lenses are currently unavailable in the market, while water immersion lenses usable with 364 nm are more readily available.

We need to take note that the Raman backscattering geometry that has been assumed and applied throughout the entire thesis may no longer hold for

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Raman data acquired using this kind of near-field light sources. This is because the scattered light collection angle is now much larger. Therefore, one may not necessarily only observe the LO Raman mode of (001) silicon. The collection of Raman signals and data interpretation may need different treatments.

Another research direction that can be possibly pursued is to use the approach described in the main chapters of this thesis to study transistors with embedded SiGe source and drain, comparing the effects of changing process flow parameters such as source and drain recess depths or Ge composition. Also, this approach can compare the effects of changing the substrate from bulk Si wafer to the more advanced SOI wafer. For such studies, as long as the light distribution in the channels of one sample is the same as that in another sample, comparisons should be meaningful. Again, FDTD simulations should be carried out to check this. Studies can be extended to such transistors from the more advanced technology nodes, such as those from the 32 nm node, using our approach.

The insights gained from Chapter 6 could also lead to some interesting further work. We have seen that different polarizations for the incident light can give us selectivity in terms of the actual regions probed. It is possible to explore this concept and carry out further experimental and simulation work using various interesting structures. These structures need not be limited to those relevant to the semiconductor industry; they can be relevant to the biomedical or pharmaceutical fields. An idea would be a structure with repeating recessed channels having widths in the nano-scale for transport of biomedical fluids. Using the appropriate incident polarization, one can choose to study the character of the recessed channels and minimize signal contribution from the non recessed regions. The possibilities for study are numerous.

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Appendix

PERCENTAGE POINTS OF THE t DISTRIBUTION

The table gives the value of $t_{\alpha; \nu}$ — the 100α percentage point of the t distribution for ν degrees of freedom.

The values of t are obtained by solution of the equation:—

$$\alpha = \Gamma\left\{\frac{1}{2}(\nu+1)\right\} \left\{\Gamma\left(\frac{1}{2}\nu\right)\right\}^{-1} (\nu\pi)^{-1/2} \int_t^{\infty} (1 + x^2/\nu)^{-(\nu+1)/2} dx$$

Note. The tabulation is for one tail only i.e. for positive values of t . For $|t|$ the column headings for α must be doubled.

$\alpha =$	0.10	0.05	0.025	0.01	0.005	0.001	0.0005
$\nu = 1$	3.078	6.314	12.706	31.821	63.657	318.31	638.62
2	1.886	2.920	4.303	6.965	9.925	22.326	31.598
3	1.638	2.353	3.182	4.541	5.841	10.213	12.924
4	1.533	2.132	2.776	3.747	4.604	7.173	8.610
5	1.476	2.015	2.571	3.365	4.032	5.893	6.869
6	1.440	1.943	2.447	3.143	3.707	5.208	5.959
7	1.415	1.895	2.365	2.998	3.499	4.785	5.408
8	1.397	1.860	2.306	2.896	3.355	4.501	5.041
9	1.383	1.833	2.262	2.821	3.250	4.297	4.781
10	1.372	1.812	2.228	2.764	3.169	4.144	4.587
11	1.363	1.796	2.201	2.718	3.106	4.025	4.437
12	1.356	1.782	2.179	2.681	3.055	3.930	4.318
13	1.350	1.771	2.160	2.650	3.012	3.852	4.221
14	1.345	1.761	2.145	2.624	2.977	3.787	4.140
15	1.341	1.753	2.131	2.602	2.947	3.733	4.073
16	1.337	1.746	2.120	2.583	2.921	3.686	4.015
17	1.333	1.740	2.110	2.567	2.898	3.646	3.965
18	1.330	1.734	2.101	2.552	2.878	3.610	3.922
19	1.328	1.729	2.093	2.539	2.861	3.579	3.883
20	1.325	1.725	2.086	2.528	2.845	3.552	3.850
21	1.323	1.721	2.080	2.518	2.831	3.527	3.819
22	1.321	1.717	2.074	2.508	2.819	3.505	3.792
23	1.319	1.714	2.069	2.500	2.807	3.485	3.767
24	1.318	1.711	2.064	2.492	2.797	3.467	3.745
25	1.316	1.708	2.060	2.485	2.787	3.450	3.725
26	1.315	1.706	2.056	2.479	2.779	3.435	3.707
27	1.314	1.703	2.052	2.473	2.771	3.421	3.690
28	1.313	1.701	2.048	2.467	2.763	3.408	3.674
29	1.311	1.699	2.045	2.462	2.756	3.396	3.658
30	1.310	1.697	2.042	2.457	2.750	3.385	3.646
40	1.303	1.684	2.021	2.423	2.704	3.307	3.551
60	1.296	1.671	2.000	2.390	2.660	3.232	3.460
120	1.289	1.658	1.980	2.358	2.617	3.160	3.373
∞	1.282	1.645	1.960	2.326	2.576	3.090	3.291