Study of surface-micromachined poly-silicon-germanium cantilevers

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Abstract

Monolithically integrated MicroElectroMechanical Systems (MEMS) on Complementary Metal-Oxide Semiconductor (CMOS) substrates are expected to be very successful. To avoid damage of the CMOS substrate poly-SiGe is a promising structural MEMS material having the required material properties when deposited at CMOS-compatible temperatures. But not all material properties of this poly-SiGe are known yet.

In this thesis the influence of heating on the deflection profile of surface micromachined poly-SiGe cantilevers is studied. The difference in deflection before and after heating was analyzed. The difference in thermal expansion coefficient between different layers cannot be used to explain the deflection behaviour. Other effects, like a densification of the layer during heating, seem to dominate.

In a second experiment, the stress profile in a 4 µm thick poly-SiGe layer is determined by measuring the tip deflection of cantilevers at various film thicknesses. From the tip deflection the linear stress gradient can be determined. A polynomial fit of the values for the linear stress gradient can be used to calculate the stress profile through the layer. A model from Molfese et al. was adjusted and used for this purpose. The acquired stress profile is correct in the measured region, but for smaller layer thicknesses it is no longer valid. A method to achieve thinner layers is proposed.

The last topic of research in this thesis is the transverse curvature of cantilevers. From measurements of this curvature it is theoretically possible to obtain a value for the poisson ratio. It is found that the biaxial stress state is mainly responsible for the transverse deflection. The clamping and underetching also play an important role in this phenomenon.
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1 Introduction and technology assessment

"Citius, altius, fortius" is the Olympic motto. Freely translated into English this means: "Faster, higher, stronger". The microelectronic industry is more or less forced by economical reasons to use a similar motto: "Smaller, faster, cheaper!" This means that new developed devices have to meet up to high expectations. They have to work faster than their precursors, have smaller dimensions (more implemented devices at the same volume) and these devices must be as cheap as possible.

To achieve smaller dimensions, MicroElectroMechanical Systems (MEMS) were developed. These are batch-fabricated micro-scaled devices that can operate as a sensor or an actuator. The sensors will convert an input signal from chemical or physical origin (light, pressure, magnetism, ...) into an electrical signal. This signal is then electronically processed. The output signal can be used to steer an actuator. Because of the small dimensions of these devices, they can be used in places where ordinary sensors and actuators are too large to be placed.

MEMS and their driving and signal processing electronics are nowadays normally combined in a hybrid system. To improve the performance, a monolithic integration (instead of wires) can be used to connect the two systems. This monolithic integration requires the fabrication of MEMS on top of a Complementary Metal-Oxide Semiconductor (CMOS) substrate. However, the CMOS substrates cannot withstand the high deposition temperatures (more than 800°C) required to deposit the standard polysilicon MEMS. Therefore, a new material with appropriate properties is introduced in the MEMS industry: poly-SiGe (an alloy of silicon and germanium).

Poly-SiGe is nowadays widely used in the MEMS research, but still many properties of this material are unknown. To study the behaviour and material properties of MEMS, various structures are under development. One of these structures is a cantilever. This is a single-sided clamped beam. With this structure, it is possible to study a wide variety of material properties. Due to the mean stress and stress gradient of the layer, the cantilever will be subjected to a bending moment and this will result in a deflection of the cantilever.

The surface-micromachined poly-SiGe cantilever is the main subject of this thesis. In chapter 2 the general basics of surface micromachining are introduced. Chapter 3 presents the different measurement techniques used to measure the cantilever deflection profile or tip deflection. The origin of stresses in thin films is explained in chapter 4 together with the effect of stress on microfabricated structures. Chapter 5 discusses the use of cantilevers to determine material properties together with models found in literature that describe the cantilever deflection at temperature. A general model for the cantilever deflection is derived together with a model to determine the stress profile of the layer by measuring the tip deflection at different layer thickness. Also, an overview of the anticlastic curvature of cantilevers is given together with some results found in literature. Chapter 6 presents and discusses the experimental results. First the influence of heating on the cantilever deflection is studied. Then the stress profile of a 4 µm thin poly-SiGe layer is determined and finally the transversal deflection is studied using properly designed cantilever structures and finite element modeling simulations.
2 Surface micromachining

One of the techniques used to create microelectromechanical systems is surface micromachining. In surface micromachining the structures are build layer by layer on top of a substrate. The structural layers, which will form the actual microcomponents, are deposited onto a sacrificial layer. This sacrificial layer can be etched away in a final process step without affecting the structural layer to become a freestanding structure.

There are three basic processing steps for a surface micromachined device. There is the layer deposition (sacrificial or structural), the formation of a mask on the layer by photolithographic imaging and the subsequent etching of the layer using the mask. After removal of the mask, the next layer can be deposited. A surface micromachining process flow is depicted in Figure 2.1. This chapter first gives a small overview of the different surface micromachining processing steps. Then for the samples used in this work the layer composition and layout will be shown. A more detailed overview of all surface micromachining processes can be found in [1]. The different process steps used to create samples for this thesis are accurately described by Van Barel [2].

![Figure 2.1: Example of a surface micromachining process steps [2]](image)

2.1 Deposition techniques

Many techniques exist to deposit layers onto substrates. The two main techniques, chemical vapour deposition (CVD) and physical vapour deposition (PVD), are briefly discussed in this section.

2.1.1 Chemical vapour deposition (CVD)

During CVD, the constituents of a vapour phase, often diluted with an inert carrier gas, react at a hot surface (typically higher than 300°C) to deposit a solid film. In CVD, the diffusive convective transport to the substrate involves intermolecular collisions.

In the reaction chamber, the reactants are adsorbed on the heated substrate surface, and the adatoms undergo migration and film-forming reactions. Gaseous by-products are desorbed and removed from the reaction chamber. The reactions forming a solid material do not always occur on or close to the heated substrate (heterogeneous reactions) but can also occur in the gas phase (homogeneous reactions). As homogeneous reactions led to gas phase cluster
deposition and result in poor adhesion, low density, and high-defect film, heterogeneous reactions are preferred.

The slowest of any CVD steps mentioned, the gas phase or surface process determines the rate of deposition. The sample surface chemistry, its temperature, and thermodynamics determine the compounds deposited. The most favorable end product of the physical and chemical interactions on the substrate surface is a stoichiometric-correct film with the correct mechanical, electrical and other properties. Several activation barriers need to be surmounted to arrive at this end product. Some energy source, such as a thermal, photon, or ion bombardment, is required to achieve this.

The CVD method is very versatile and works at low or atmospheric pressure and at relatively low temperatures. Amorphous, polycrystalline, epitaxial and uniaxially oriented polycrystalline layers can be deposited with a high degree of purity, and control.

The most widely used CVD process is the plasma-enhanced chemical vapour deposition (PECVD). This process uses a plasma as an energy source to achieve the required end products. The advantages of the PECVD process are the lower substrate temperatures, a good adhesion and the high deposition rate. A disadvantage is the particle contamination that can occur.

Another type of CVD used is the low pressure chemical vapour deposition (LPCVD). Working at a lower pressure results in a large diffusion coefficient, which leads to a growth limited by the rate of surface reactions rather than by the rate of mass transfer to the substrate. LPCVD results in uniform layers with excellent purity. A disadvantage is the high operating temperature and the low deposition rate.

2.1.2 Physical vapour deposition (PVD)
PVD covers a number of deposition technologies in which the base material is released from a source and transferred to the substrate without a chemical reaction. The two most important technologies are evaporation and sputtering.

2.1.2.1 Evaporation
In evaporation the substrate is placed inside a vacuum chamber, in which a piece (source) of the material to be deposited is also located. The source material is then heated to the point where it starts to boil and evaporate. The vacuum is required to allow the molecules to evaporate freely in the chamber. These molecules subsequently condense on all surfaces. This principle is the same for all evaporation techniques; only the method used to heat the source material differs.

There are two popular evaporation technologies, namely e-beam evaporation and resistive evaporation in which the name refers to the heating method. In e-beam evaporation, an electron beam is aimed at the source material causing local heating and evaporation. In resistive evaporation, a tungsten boat containing the source material is heated electrically with a high current to make the material evaporate. Many materials are restrictive in terms what evaporation method can be used, which typically relates to the phase transition properties (the temperature at which the material starts to evaporate) of that material.

2.1.2.2 Sputtering
Sputtering is a technology in which the material is released from the source at a much lower temperature than in the evaporation method. The substrate is placed in a vacuum chamber with the source material, named a target, and an inert gas is introduced at low pressure. A gas plasma is formed using an RF or DC power source, causing the gas to become ionized. The ions are accelerated towards the surface of the target, causing atoms of the source material to
break off from the target in vapour form and condense on all surfaces including the substrate. As for evaporation, the basic principal of sputtering is the same for all sputtering technologies. The differences typically relate to the manner in which the ion bombardment of the target is realized.

2.2 Lithography
The most widely used form of lithography is photolithography. This process involves different major steps: the deposition of a photosensitive film (resist), the alignment of the mask and wafer, the illumination and the development of the patterns.

First a photosensitive film (resist) has to be deposited onto the wafer by spincoating. Following the spincoating of the resist a pre-exposure baking step can be incorporated to evaporate the solvent from the resist and to improve the adhesion of the resist onto the wafer. In the next step the wafer is aligned with the mask. Then the mask-wafer combination is exposed to UV radiation to transfer the mask pattern into the resist. Exposure changes the photoresist solubility, which enables selective removal of the resist during the development step. For positive resists, the exposed regions become more soluble and are thus easily removed during development.

The pattern that is formed in the positive resist is an exact copy of the pattern on the mask. For negative resists, the exposed regions become less soluble, and the patterns formed in the resist are the opposite of the mask patterns. After the development step again a postbaking step may be used to increase the adhesion of the resist to the substrate and to improve the resistance during the etching process. In the next phase of the photolithography the resist pattern is used as an etch mask. Once the desired patterns are transferred onto the substrate, the remaining resist can be removed from the surface and the wafer is ready for the next step in the fabrication process.

2.3 Etching
Etching is a very important step in surface micromachining. It is used to create patterns with the masks created by lithography (anisotropic etching) or it is used to etch away sacrificial layers to achieve freestanding structures (isotropic etching). There are two types of etching: wet and dry etching. Both types are briefly discussed in this section.

2.3.1 Wet etching
During wet etching the sample is immersed into the etching fluid (Figure 2.2). A diffusion of the reactants towards the substrate is needed for the reaction to occur. Afterwards, the reaction products need to be transported away from the substrate. The etching rate is determined by the diffusion rates of the reactants and by the reaction time of these reactants with the substrate. HF is used for the removal of SiO₂.
2.3.2 Dry etching

There exist many dry etching techniques, but only one will be discussed because it was used to thin the poly-SiGe layers for the study of the stress profile: the reactive ion etching with inductive coupled plasma (RIE-ICP). An Oxford Plasmalab System 100 was used for this purpose. A schematic representation of this device is shown in Figure 2.3.

The RIE-ICP process is a plasma process in which there is a gas mixture containing radicals that react with the surface, producing volatile and easily removable substances. This kind of process normally exerts also a considerable physical ablation on the sample. The reaction chamber is planar with the samples on top of a three inch dummy wafer which rests on an electrode connected to a RF supply, which accelerates the ions. These are also accelerated by a magnetic field produced by a winding around the pipe, which introduces the gas mixture in the reaction chamber. The gas pressure is usually some mTorr.

There are two mechanisms for material removal: the chemical and the physical (atomic peening) etching. Using the RIE-ICP etcher with a very low RF power, and a rather low inductive power, it is possible to obtain a low damage etching process in which the physical effect is practically avoided and where there is almost only chemical etching. In the chamber SF$_6$ and O$_2$ are introduced which dissociate after electron impact forming radicals, which react with SiGe and permit etching:

$$SF_6 + e^- \rightarrow S + F_2 + F^* + e^-$$  \hspace{1cm} (Eq. 2.1)

Etching under these conditions results in an etch rate of poly-SiGe of 40 nm/min. It is important to underline the fact that this etching is not completely selective with respect to the SiO$_2$. The etch rate of the SiO$_2$ was determined to be about 4nm/min. In order to measure the thickness of the poly-SiGe layer after etching, a part of the sample has to be covered during etching and afterwards the step has to be measured between this part and the etched part.
2.4 Sample layer composition

A thick p-doped (with boron) poly-SiGe layer can be grown at low temperature (450°C) with plasma (PECVD) or without plasma (CVD). The CVD deposition has as disadvantage the very low deposition rate. The PECVD deposition in contrary has a higher deposition rate but the obtained films have high stresses and bad electric characteristics (high resistivity). A way to decrease these disadvantages is the combination of these two deposition processes in a multilayer process.

The layer build-up used in this thesis is depicted in Figure 2.4. At the bottom of the picture the (1 0 0) Si wafer is visible. Deposited onto the wafer is a 250 nm thick PECVD SiO₂ layer. This layer will serve as the sacrificial layer. On top of the SiO₂ layer a small PECVD SiGe seedlayer (94nm) is visible. This layer serves as nucleation layer for the second SiGe layer which is CVD deposited. This second layer (370nm) helps crystallizing the subsequent PECVD layer. This layer is grown until the required layer thickness is reached. All the SiGe layers are deposited using a gas mixture of silane (SiH₄), germane (GeH₄), diborane (B₂H₆) and hydrogen (H₂). The CVD layer contains about 62% of Ge while the PECVD SiGe layer contains about 65% of Ge. The deposition rate is 74 nm/min for a 4 µm thick SiGe layer.

![Figure 2.4: Cross section of a PECVD poly-SiGe layer [33]](image)

2.5 Sample layout

To study the difference in deflection at elevated temperatures and the stress profile samples having a thickness of 4 µm were made with the M&M maskset [3]. From this mask only the cantilevers with a length of 1 mm and a width of 100 µm were used.
To study the plate effect, a new mask was designed containing cantilevers of different length and width (Figure 2.6). The lengths were 50, 100, 150 and 300 µm. For each of these lengths the width varied from 30 to 100 µm in steps of 10 µm, from 100 to 1000 µm in steps of 50 µm, from 1000 to 2000 µm in steps of 100 µm and from 2000 to 5000 µm in steps of 1000 µm.
3 Characterisation techniques

In this thesis the deflection profile of cantilevers is used to study the stress in thin layers. To determine the mean stress in thin films the wafer curvature method is used. To have an idea of the stress gradient in the layer, the deflection profile of a cantilever is important. To determine this profile different instruments have been used throughout this thesis. Laser profilometry, optical interference profilometry and surface profilometry are commonly used to study the deflection profile. These techniques, together with the necessary equipment, are briefly introduced. Electron microscopy was never before used for the determination of the deflection profile. The scanning electron microscope is discussed in more detail because a large amount of time was spend to develop a measuring technique for determining the deflection profile of the cantilever.

3.1 Wafer curvature device

One common measurement easily performed on films attached to substrates is the residual film stress measurement. The curvature of the substrate is measured before and after film deposition. Curvature can be measured in a number of ways. The most common technique is to use a laser which scans the surface and detects the angle of the reflected signal. Assuming that the film is thin compared to the substrate, the average residual stress in the film, $\sigma_f$, is given by Stoney’s equation [4]:

$$\sigma_f = \frac{1}{6} \frac{E_f}{(1-\nu_f) t_f} \left( \frac{1}{R_1} - \frac{1}{R_2} \right)$$  \hspace{1cm} (Eq. 3.1)

where the subscripts $f$ and $s$ refer to the film and substrate, respectively; $t$ is the thickness, $E$ is Young’s modulus, $\nu$ is Poisson’s ratio and $R$ is the radius of curvature before ($R_1$) and after ($R_2$) film deposition. This measurement will reveal the average residual stress of the film.

3.2 UBM laser profilometer

A laser profilometer uses a point light source and detector pinhole to determine depth. The laser beam emitted from the point light source is focused on a specimen through an objective lens that moves rapidly up and down. The maximum light intensity occurs when the specimen lies within the focal plane of the objective. As the objective moves closer to or further from the specimen, the reflected light reaching the pinhole is defocused and does not pass through it. As a result, the quantity of light received by a detector behind the pinhole decreases rapidly. A detector signal is only generated when the maximum of light goes through the pinhole. A precise height measurement of the illuminated point is achieved by continuously scanning along the z-axis. The spot size of the laser beam that is used is 2 µm. The maximal vertical resolution is 0.1 µm. The lateral resolution can vary from 0.08 to 13.1 µm [5].

3.3 Veeco WYKO NT3300 optical interference profilometer

Interferometry is a technique known for more than one hundred years. It consists of viewing the optical path difference between a sample beam and a reference beam; the beams undergo constructive and destructive interference and this results in a pattern of bright and dark fringes. Illumination from a white light beam passes through a filter, then through a microscope objective lens to the sample surface. The light reflecting back from the surface recombines with the reference beam and interference fringes are formed. The pattern of these fringes is captured on a CCD camera array. If the sample is a perfectly flat mirror but tilted, and the illumination is done by monochromatic light then the resulting interference pattern
will be a series of fringes. The distance between the maximum of the dark or light fringes is proportional to the wavelength of light used and the tilt of the mirror. Each band in the interference pattern represents a contour height difference of half the wavelength of light used in the measurement. The contour bands are purely sinusoidal and the phase of the interference fringe pattern can be measured with very high accuracy. The maximal vertical resolution that can be achieved is 0.1 nm [6].

3.4 Dektak\textsuperscript{3}ST surface profilometer
The Dektak [7] is a surface profile measuring system, which can accurately determine step heights or trench depths on a surface. It uses a surface contact measurement technique where a very low force stylus (1-40 mg) is dragged across the surface. Vertical features ranging in height from 131 µm to 10 nm can be observed on a wide variety of substrates. The vertical resolution can go to ~0.1 nm. The lateral resolution can be changed from 0.4 to 40 points per µm. The scan length can be varied from 50 µm to 50 mm. A video camera allows a manual placement of the stylus. After the measurement the determined profile is displayed and the desired dimensions can be directly determined on-screen or the data can be saved onto a disk for further analysis.

3.5 Zeiss Axiotron2 Optical microscope
With the optical microscope it is possible to look at the state of the samples. It is also possible to determine the height difference between the beginning and the end of a cantilever in an accurate way. Van der Donck et al. concluded in his work that the optical microscope measurements are in good agreement with laser profilometry measurements [8].

3.6 Philips XL30 Scanning Electron Microscope
The scanning electron microscope (SEM) is an apparatus that makes it possible to create images of specimens by sending an electron beam onto the surface and looking at the emitted products. When an electron beam is irradiated on a specimen surface, interactions between the electron beam and the atoms composing the specimen produce various kinds of information. This information can be in the form of emitted electrons or even X-rays. Figure 3.1 shows the regions from where this information is produced.

![Figure 3.1: Regions were information is produced during electron-specimen interaction.](image)

In this section the working principle of SEM will briefly be presented. A more detailed overview can be found in [9, 10, 11, 12 and 13].
The electron beam of the electron microscope is generated by an electron gun. The most widespread system uses thermionic emission from a heated tungsten filament (Figure 3.2). At temperatures in excess of 2700 K a tungsten wire emits an abundance of both light and electrons. In a light bulb only the light is used, but in an electron gun the electrons can be accelerated across a potential difference of tens or hundreds of kilovolts to generate a beam of electrons of known energy (and hence of known velocity and wavelength). A piece of tungsten, usually a wire bent into a hairpin, acts as a cathode. This filament is heated by the passage of a current to about 2800 K while being held at a high negative potential with respect to an anode and the rest of the microscope.

Electrons emitted from the filament are accelerated rapidly towards the anode and a beam of high-energy electrons is emitted through a hole at the centre of the anode into the microscope column. The addition of a Wehnelt cap, which is held at a voltage slightly more negative than the filament, controls the diameter of the area at the end of the filament, which emits electrons. The most important feature of the gun is that the paths of the electrons leaving the anode usually cross at one point in space and hence the gun is acting as a lens. The diameter of the beam at the crossover is dependent on the area of the filament that is emitting electrons and hence can be controlled by the difference in potential between the filament and the Wehnelt cap. This crossover diameter is effectively the size of the electron source, and is of great importance in calculations concerning the resolution of electron microscopes.

The composition of a standard SEM column is presented in Figure 3.3. To control the size of the beam and to achieve a good focus, electromagnetic lenses are used. These lenses have the same effect as glass lenses for light. A coil consisting of a large number of turns of wire is wound on a soft iron core, which has only a very small accurately machined air gap across which the field is produced. By varying the current passing through the coil the magnetic field strength and hence the focal length of the lens can be varied at will. The lenses (A and B in Figure 3.3) are condenser lenses and are used to control the size of the beam or the amount of electrons travelling down the column. The final lens (C in Figure 3.3) is called an objective lens or a final probe-forming lens. This lens projects the diminished image of the electron crossover as a spot focused on the surface of the specimen. A diaphragm immediately following the lens defines the solid angle of the focused beam. The bore of the final lens also contains the stigmator, necessary to ensure that the scanning spot is truly circular, and the deflection system responsible for scanning the electron probe. Pairs of beam deflection coils
are supplied with current from the scan generator, an oscillator which proves separate frequencies for the line scan (x-deflection) and the frame scan (y-deflection).

As mentioned above, the interaction between the electron beam and the specimen surface results in the emission of electrons and X-rays (Figure 3.1). This means that there are different modes of operation for the SEM. Different kind of signals can be obtained that carry different types of information and can be used for different purposes. For example, the secondary electrons give information about the topography of the surface and X-rays give information about the composition of the specimen. Each mode of operation uses a different setting and mostly a different kind of detector.

Figure 3.4 shows the energy distribution of backward scattering electrons that are generated when the specimen is illuminated with an electron beam. On the ordinate is plotted the number (N) of electrons generated, and on the abscissa is plotted the ratio of the energy of the generated electrons (E) to the energy of incident electrons (E₀). Region A is a low-energy region ranging from 0 to several tens of eV, and the electrons in this region are generally called secondary electrons. Region B is a high-energy region, and the electrons in this region are called backscattered electrons.

For this work only the most frequently used technique is used, namely secondary electron imaging. Secondary electrons are produced by inelastic interactions of high-energy electrons with valence electrons of atoms in the specimen, which cause the ejection of the electrons.
from the atoms. After undergoing additional scattering events while travelling through the specimen, some of these ejected electrons emerge from the surface of the specimen.

A secondary electron detector (Figure 3.5) collects the secondary electrons emitted from the specimen surface. It collects secondary electrons (SE) easily by means of a positively biased collector grid placed on one side of the specimen thanks to their low exit energy of a few electronvolts. Behind the collector grid, the SE are accelerated onto a scintillator biased at +10kV and the light quanta generated are recorded by a photomultiplier.

![Figure 3.5: Schematic design of a secondary electron detector [13].](image)

The image formation process is depicted in Figure 3.6. The beam in the SEM is moved over the sample in a raster pattern in synchronization with the beam in the cathode ray tube (CRT). Thus, for each point on the specimen there is a conjugate point on the CRT. The video amplifier modulates the intensity of the beam in the CRT so that the intensity of the spot on the CRT is proportional to the signal detected from its conjugate point on the specimen.

![Figure 3.6: Image formation in the SEM [14].](image)

The magnification is simply the ratio of the length of the scan C on the CRT to the length of the scan x on the specimen (Figure 3.6). Changing magnification does not involve a change in the setting of lenses.

One of the great advantages of SEM images is the unusually great depth of focus they exhibit. This makes it possible to examine surfaces much rougher, and at much higher magnifications, than is possible with light microscopes. The reason for this great depth of focus arises from the geometry of the beam optics (Figure 3.7).
The final lens of the SEM focuses the electron beam to a ‘crossover’ at the plane of best focus. The beam diameter increases as the beam converges and diverges above and below this plane. At some distance $D/2$ above and below the focus plane the diameter of the beam becomes twice the pixel diameter for the magnification being used, whereupon the signals from adjacent pixels overlap enough to cause the image to appear blurred. Over the distance $D$ between these limits, however, the image will appear to be in acceptably sharp focus, and so this distance is called “the depth of field” or “the depth of focus”. According to Bigelow [14] the depth of field $D$ can be simply expressed in terms of the aperture diameter $A$, the magnification $m$ and the distance between the objective lens an the object in focus (called the free working distance) $W$:

$$D = \frac{4 \times 10^5 W}{A \cdot m} \quad \text{(Eq. 3.2)}$$

These operational variables can be altered during operation to adapt the depth of field. (Eq. 3.2) is not adequate enough to define the depth of field. Therefore a better prediction of the depth of field in function of operational variables was searched. Goodhew [11] introduced a different expression for the depth of field:

$$D = \frac{\lambda}{\mu \sin^2 \alpha} + \frac{1}{7m \sin \alpha} \quad \text{(Eq. 3.3)}$$

where $\lambda$ is the wavelength of the electrons, $\mu$ is the refractive index of the medium between the object and the objective lens, $m$ is the magnification and $\alpha$ is the half-aperture angle.

(Eq. 3.4) gives the expression for the wavelength of an electron as a function of the acceleration voltage [11]. From this it can be seen that the depth of field is inverse proportional to the acceleration voltage.

$$\lambda = \frac{h}{\sqrt{2m_e eV}} \quad \text{(Eq. 3.4)}$$

with $h$ Planck’s constant, $V$ the acceleration voltage, $m_e$ the electron mass and $e$ the electron charge.

The quality of the image produced in an SEM depends basically on the signal-to-noise (S/N) ratio. Noise involves the statistically random fluctuations in the signal that are inherent in the processes that produce the signal electrons, plus similar fluctuations introduced by amplification, and is analogues in character and effect to ‘snow’ in a weak TV image. Signal...
generation is a random process that follows Poisson statistics. High quality images require a high S/N ratio. Operationally this can be achieved in two ways: by using a high beam current (high spot size), and by using a slow scan rate so that the beam spends a longer time on each pixel.
4 Origin of stress in thin films

Ideally, thin films are free of stress. They have been grown epitaxially to perfect single crystals onto substrates with identical lattice parameters, hopefully at the temperature of their future application. So far, however, such films only have virtual existence in the dreams of the manufacturers. In reality film growth by no means proceeds in thermodynamical equilibrium, most of the growth processes are predominantly kinetically controlled. Therefore thin films in general contain many defects of different types, which constitute departures from the ideal crystal structure and thus may act as sources of stress. In this section the most common stress contributions are discussed and classified according to their range of action — either within the films or at the film/substrate and film/vacuum interfaces.

This chapter treats stresses in thin films. These stresses can lead to crack formation, film delamination and void formation [1]. The vast majority of thin films are subjected to residual stresses due to a mismatch in thermal expansion coefficient, nonuniform plastic deformation, lattice mismatch, substitutional or interstitial impurities and growth processes. The stress-causing factors can be categorized as either intrinsic or extrinsic. A detailed overview of all stresses in thin films can be found in [15 and 16].

4.1 Extrinsic stresses

Extrinsic stress has an external cause, for example a thermal mismatch (different thermal expansion coefficients) between the film and the substrate leads to extrinsic stress. These thermal stresses are well understood and can be easily calculated if the coefficients of thermal expansion are known. The packaging of the created thin film device can also create an extra contribution to the extrinsic stress.

4.1.1 Thermal stress

From all the possible extrinsic stresses the thermal stress is the one that is best understood. When a coated substrate (Figure 4.1) is at a temperature that is different from its temperature during deposition, a thermal strain \( \varepsilon_{th} \) will be present as a result of the differences in the film and substrate thermal expansion coefficients, respectively noted as \( \alpha_f \) and \( \alpha_s \) [17]. This thermal strain induces a thermal stress \( \sigma_{th} \):

\[
\sigma_{th} = \frac{E_f}{1-v_f} \varepsilon_{th} = \frac{E_f}{1-v_f} \int_{T_0}^{T_1} (\alpha_f - \alpha_s) dT
\]  

(Eq. 4.1)

with \( T_0 \), \( T_1 \) the deposition temperature, \( T_1 \) the temperature after cooling down, \( E_f \) the Young’s modulus of the film and \( v_f \) the Poisson ratio of the film. Keep in mind that (Eq. 4.1) is only valid in the elastic regions and can therefore only be calculated over a limited temperature range. When the thermal strains exceed the elastic limit of the film, they are relaxed by various mechanisms such as dislocation glide or grain boundary diffusion creep [17]. These relaxation mechanisms are accompanied by changes of the film morphology and are often detrimental for the stability and performance of thin-film devices.
4.1.2 Other origins of extrinsic stress

Another type of extrinsic stress originates when various molecules can penetrate open voids or pores present in not fully dense films. These molecules adsorb on pore walls thereby interaction forces between adsorbed species, in particular, between polar species such as water molecules can act to modify residual stresses [18].

A non-uniform plastic deformation can also cause stress [1]. Finally the packaging of micromachined structures is also accompanied by a temperature step, which can also induce an extra stress contribution.

4.2 Intrinsic stresses

The intrinsic stress can be defined as that component of the total measured stress that cannot be attributed to thermal stress or external loading. The intrinsic stresses find their origin in interactions within the film, at the film/substrate interface or at the surface of the film.

4.2.1 Stress contributions within the film

In this section the different effects that cause stresses within the film are briefly discussed.

4.2.1.1 Small-angle grain boundaries

Polycrystalline films, in particular those growing by columnar grains, naturally exhibit a high concentration of small-angle grain boundaries [15], which separate the randomly oriented grains. A schematic illustration is shown in Figure 4.2a, where the boundaries between the three crystallites are easily recognized as regions of reduced density. Grain boundaries have been presumed from very early on to be a possible source of intrinsic stress. According to Hoffman ‘... the interatomic forces at the boundaries tend to close any existing gap, with the result that the neighbouring crystallites are strained in tension’ [19].

Notice however, that not all grain boundaries necessarily have to be strained. For example, the interatomic forces at equilibrium grain boundaries cancel out. In real films nucleation of the later grains and in particular their positions relative to each other are controlled by the substrate. Usually, when grains grow together, they are not located in the correct position to form equilibrium grain boundaries. Thus the small-angle grain boundaries on average produce a tensile stress contribution in the films.
4.2 Intrinsic stresses

4.2.1.2 Domain walls
In the case of epitaxial growth, when epitaxially oriented islands coalesce, a special type of grain boundary may be formed. Due to the strong film/substrate interaction no stress component due to the misfit between different lattice parameters of film and substrate is generated. Isolated islands therefore grow free from stress with the lattice parameter appropriate for the film material. However, since they have nucleated at positions determined by the substrate, the lattices of the coalescing islands may be improperly spaced either along one or along two dimensions as illustrated in Figure 4.2b.

The boundaries between different islands can be regarded also as domain walls, because they separate epitaxial film domains. Respective stress investigations so far have revealed that on average compressive stress develops at domain walls, a result that is in contrast to the tensile stress of small-angle grain boundaries. Atoms that arrive at the domain walls and close the gap between formerly isolated islands can form a larger number of energetically favourable nearest-neighbour bonds by immersing in the respective deepest layer (Figure 4.2c) and thereby generating compressive strain in both epitaxial islands.

4.2.1.3 Recrystallization processes
If the self-diffusion of the deposited film material is high enough, the films may recrystallize actually during the film deposition and also after the completion of the deposition. In the course of such processes defects are annealed and the average grain size of the polycrystalline films is increased. By eliminating all kinds of defect (grain boundaries, voids, point defects, etc.), recrystallization processes usually lead to a densification of the films and therefore should give rise to a tensile stress contribution.

4.2.1.4 The lattice expansion mechanism
Strain can be introduced into a growing film if the film grows with an epitaxial relationship to the substrate and a mismatch between the lattice spacings of the two materials exist. As the thickness of the epitaxial layer increases, the strain energy in the film increases until it becomes more energetically favourable for a series of misfit dislocations to form at the interface. A critical thickness thus exists, below which the coherent strained film is stable and above which an array of misfit dislocations forms to accommodate the lattice mismatch.
4.2.1.5 Impurities
The growth of thin films can never occur in perfect conditions. There will always be an unwanted contamination of the film with ambient atoms. An example where these impurities are deliberately used is doping [20]. Strange atoms or impurities are put into the lattice to achieve better material properties. The size of the doping atom in comparison with the original lattice atom will determine the sign of the intrinsic stress. When boron is used in poly-Si, a tensile stress is expected due to the fact that the boron atom has a smaller radius than the Si atom. Phosphor has a larger radius than Si and introduces a compressive stress. Strange enough, the logic used here is not always true. Some studies reported a compressive stress when using boron as a dopant in poly-Si. The reason for this unexpected phenomenon has not yet been revealed.

4.2.1.6 Phase transformation
Due to the high temperatures that are needed to grow the thin films some materials can reach the point where they undergo a phase transformation. This normally goes together with a volume change and results in an additional stress in the thin film.

4.2.1.7 Conic crystal growth
The columnar coarse-grain structure arises from a process of grain growth competition among the small grains, during which those grains preferentially oriented for fast vertical growth survive at the expense of misoriented, slowly growing grains [Figure 4.3]. The growth competition between the grains can induce stresses and result in a stress gradient through the layer.

Figure 4.3: Example of conic crystal growth.

4.2.2 Stress contributions in the film/substrate interface
The deposition of a thin film on a substrate always goes together with an interaction between the film and the substrate at their interface. This interaction can result into an intrinsic stress. Two types of these stresses are mentioned in this section.

4.2.2.1 Misfit stress
In the case of epitaxial film growth the lattices of film and substrate are usually not identical but differ at least with respect to the magnitude of the lattice constants in certain crystallographic directions. For a film deposited onto thick substrates the misfit \( f \) (along a crystallographic direction) is conveniently defined as:

\[
f = \frac{a_i^0 - a_f^0}{a_i^0}
\]  
(Eq. 4.2)

with \( a_i^0 \) and \( a_f^0 \) being the stress free lattice constants of film and substrate, respectively. If the misfit does not exceed a critical value \( f_{\text{crit}} \), which is usually of the order of several per cent, at least the first film layers may grow pseudomorphically, i.e. with perfect registry between film and substrate atoms. In this growth stage the misfit is completely accommodated by
elastically straining the films, which means that simultaneously a respective misfit stress contribution should be observed. The misfit stress is huge compared to the contributions of other stress mechanisms [15]. As growth proceeds eventually a critical film thickness is reached where it becomes energetically more favourable to introduce misfit dislocations for total or partial strain relief.

4.2.2.2 Solid state reactions and/or interdiffusion
When two solid phases – in our case the substrate S and a film F – are brought together, they may undergo a chemical reaction, by means of which a new compound $F_pS_q$ is formed at the interface. The respective phase diagrams provide useful information on possible chemical reactions. Frequently solid-state reactions are accompanied by considerable stress generation. The magnitude and sign of the stresses cannot simply be derived from comparing the volumes of the educts ($pF+qS$) and products ($F_pS_q$) of the chemical reaction. Once a continuous layer of $F_pS_q$ has formed, which separates the two solid phases F and S, the rate of reaction is additionally determined by the diffusion of the species F and S in the intermediate layer. If one species is more mobile than the other, the new phase will predominantly grow at the interface lying opposite to the faster component. Therefore only the volume of the less mobile phase has to be considered. The overall stress behaviour is mostly more complex, as the reaction stress is superimposed by relaxation effects. A further stress contribution may arise from mobile species, which are incorporated into the substrate and diffuse into the growing film.

4.2.3 Stress contributions in the film/vacuum interface: surface stress
Due to the reduced number of bonds at surfaces, the equilibrium interatomic distances of isolated surface layers are usually different from that of the bulk. Consequently, if the surface layers are arranged coherently with the crystal planes beneath, they experience stress, more specific surface stress.

4.2.4 Effect of stress and gradient stress on microfabricated structures
A stressed film on top of a substrate will bend this substrate by a measurable degree. A tensile stress will bend and render the surface concave; a compressive stress renders the surface convex. A microfabricated structure will undergo a deformation when being subjected to residual stresses. This is illustrated for a double-sided clamped beam in Figure 4.4. A compressive stress can cause a double-sided clamped beam to buckle. A tensile stress can even result in cracking of a double-sided clamped beam.
Figure 4.4: Influence of stress on a double-sided clamped beam (adapted from [2]).

For structures fabricated from thin deposited films, the stress gradient can be just as important as the stress itself. Dardalhon et al. [21] have simulated the influence of a stress gradient on micromachined structures (bridge and Guckel structure). As can be seen in Figure 4.5, the sides of a bridge structure curl up under influence of a stress gradient. This means that the dimensions of the structure change.

Figure 4.5: The sides of a bridge structure seem to curl up due to a stress gradient. This causes a decrease in width [21].

Figure 4.6 shows a simulation of the influence of a stress gradient on a Guckel ring structure. A Guckel ring structure is used to measure tensile stresses. Tensile forces on the anchors will be converted by the structure into compressive stresses, which will cause the central beam to buckle at a certain critical stress (dependent on the size of the beam). The device is designed to be completely planar; however, stress gradients in the film cause the structure to bend out of the plane.

Figure 4.6: Effect of a stress gradient on the behaviour of a Guckel ring [21].
5 Theoretical background and modeling

Different structures have been designed to study material properties of MEMS. A complete overview of these structures has been made by Van Barel [22]. The structure that is used in this thesis is the cantilever. This structure can be used to determine various material properties like the modulus of Young and the thermal expansion coefficient. Due to an internal mean and gradient stress (see chapter 4), the cantilever will be subjected to a bending moment and will have an out-of-plane deflection. The deflection profile can be used to study the stresses in the layer. In this chapter a general model for the cantilever deflection will be introduced together with an improved model to determine the stress profile of the layer by measuring the tip deflection of cantilevers with different layer thickness. This adapted model is compared with its precursor. Finally the anticlastic curvature of the cantilever is explained together with some measurements found in literature. These are briefly analyzed and discussed.

5.1 Cantilever model

In this section some general relations for the cantilever deflection profile are derived. Also some models found in literature to determine stresses and thermal expansion coefficients from the deflection profile are briefly presented.

5.1.1 General model

All procedures to derive the deflection of a beam are based on the deflection curve and the associated relationships like the equilibrium of the acting forces and moments [23]. From Figure 5.1 the following expression for the curvature can be deduced.

\[
\kappa = \frac{1}{\rho} \quad \text{(Eq. 5.1)}
\]

with \( \rho \cdot d\theta = ds \) so

\[
\kappa = \frac{1}{\rho} = \frac{d\theta}{ds} \quad \text{(Eq. 5.2)}
\]

Here \( \kappa \) represents the flexure of the beam and \( \rho \) the radius of curvature. (Eq. 5.2) is valid for all flexures. \( \theta \) represents the angle of rotation with \( O \) the centre of rotation (\( ds \), \( dv \) and \( dx \) are presented in Figure 5.1).
The following relations result from Figure 5.1 and (Eq. 5.2):

\[
\frac{dv}{dx} = \tan \theta \Rightarrow \theta = bg \tan \frac{dv}{dx} \tag{Eq. 5.3}
\]

\[
\cos \theta = \frac{dx}{ds} \tag{Eq. 5.4}
\]

\[
\sin \theta = \frac{dv}{ds} \tag{Eq. 5.5}
\]

The exact solution gives:

\[
\kappa = \frac{1}{\rho} = \frac{d\theta}{ds} = \frac{d(bg \tan v')}{dx} \cdot \frac{dx}{ds} \tag{Eq. 5.6}
\]

with \(ds^2 = dx^2 + dv^2 \rightarrow ds = \sqrt{dx^2 + dv^2} \) (Pythagoras)

A small conversion leads to:

\[
\frac{ds}{dx} = \sqrt{1 + \left(\frac{dv}{dx}\right)^2} = \sqrt{1 + (v')^2} \rightarrow \frac{dx}{ds} = \frac{1}{\sqrt{1 + (v')^2}} \tag{Eq. 5.7}
\]

From goniometry/analysis:

\[
\frac{d(bg \tan v')}{dx} = \frac{v''}{1 + (v')^2} \tag{Eq. 5.8}
\]

Combining (Eq. 5.6), (Eq. 5.7) and (Eq. 5.8) gives the exact solution:

\[
\kappa = \frac{1}{\rho} = \frac{v''}{\left[1 + (v')^2\right]^{3/2}} \tag{Eq. 5.9}
\]

Now the equation for small rotations will be derived (\(ds \sim dx\)):

\[
\kappa = \frac{1}{\rho} = \frac{d\theta}{dx} \tag{Eq. 5.10}
\]
Since $\theta$ is small, (Eq. 5.3) can be written as:

$$\theta = \tan \theta = \frac{dv}{dx}$$  \hspace{1cm} (Eq. 5.11)

Combining (Eq. 5.10) and (Eq. 5.11) results in an approximation for the curvature of a cantilever with small deflection:

$$\kappa = \frac{1}{\rho} = \frac{d^2v}{dx^2}$$  \hspace{1cm} (Eq. 5.12)

### 5.1.2 Longitudinal elasticity in the cantilever

The flexure and the associated deformations were analysed. For this purpose a section $ab$ is taken from the beam. This piece is assumed to be in pure bending with positive bending moments. A sketch of the situation is depicted in Figure 5.2.

![Figure 5.2: Deformation of a cantilever in pure bending](image)

Pure bending means that the bending is induced by a constant bending moment $M$. This means that pure bending only occurs at places where the shear forces are zero ($F = dM/dx$ with $F$ the shear force). In contrast to this is the non-uniform bending where the bending moment changes along the axis of the cantilever.

The dotted line $ss$ in Figure 5.2 is the neutral axis ($y = 0$ at this axis). The lines above are in compression while the lines underneath are in tension. From (Eq. 5.2) follows:

$$d\theta = \frac{ds}{\rho}$$  \hspace{1cm} (Eq. 5.13)

For the longitudinal line $ef$, the length $L_1$ can be calculated as:

$$L_1 = (\rho - y) \cdot d\theta = ds - \frac{y}{\rho}ds$$  \hspace{1cm} (Eq. 5.14)

The original length of the line $ef$ was $ds$. This means that the change in length (shortening) is equal to $L_1 - ds$. To get the longitudinal strain, this change in length needs to be divided by the initial length $ds$. This results in:

$$\varepsilon_x = -\frac{y}{\rho} = -\kappa y$$  \hspace{1cm} (Eq. 5.15)

(Eq. 5.15) is in general valid for all rotations.
5.1.3 Normal stresses in cantilevers

For linear elastic materials Hooke’s law is valid:

\[ \sigma_x = E \varepsilon_x = -\frac{E y}{\rho} = -E \kappa y \]  \hspace{1cm} \text{(Eq. 5.16)}

The forces and moments that appear with pure bending are in equilibrium and satisfy the static equations:

\[ \sum F_x = 0 \]
\[ \sum M_x = M \]  \hspace{1cm} \text{(Eq. 5.17)}

From the first static equation from (Eq. 5.17) the location of the neutral axis can be determined:

\[ \int_A \sigma_x dA = -\int_A E \kappa y dA = 0 \]  \hspace{1cm} \text{(Eq. 5.18)}

Since the flexure \( \kappa \) and Young’s modulus \( E \) are not zero at any cross section of the curved beam, (Eq. 5.18) can be reduced to:

\[ \int_A y dA = 0 \]  \hspace{1cm} \text{(Eq. 5.19)}

The second static equation gives the moment-flexure relationship.

\[ dM = -\sigma_x y dA \]  \hspace{1cm} \text{(Eq. 5.20)}

\[ M = -\int_A \sigma_x y dA = \int_A \kappa E y^2 dA \]  \hspace{1cm} \text{(Eq. 5.21)}

\[ M = \kappa EI \]  \hspace{1cm} \text{(Eq. 5.22)}

with

\[ I = \int_A y^2 dA \]  \hspace{1cm} \text{(Eq. 5.23)}

This results in the moment-flexure equation (Eq. 5.24) with \( EI \) the bending stiffness and \( I \) the moment of inertia.

\[ \kappa = \frac{1}{\rho} = \frac{M}{EI} \]  \hspace{1cm} \text{(Eq. 5.24)}

For rectangular beams the moment of inertia is given by:

\[ I = \frac{w \cdot b^3}{12} \]  \hspace{1cm} \text{(Eq. 5.25)}

where \( w \) and \( b \) represent the width and height, respectively. According to (Eq. 5.24) the flexure is determined by the bending moment and the bending stiffness. Pure bending results in a constant curvature (circle), while a non-uniform bending moment leads to a varying flexure.

Finally the normal stresses can be expressed in function of the bending moment when the neutral axis and the moment-flexure relation is known. Combining Hooke’s law (Eq. 5.16) and (Eq. 5.24) leads to Navier’s formula for bending stresses.
5.1 Cantilever model

\[ \sigma_x = -\frac{My}{I} \]  
(Eq. 5.26)

5.1.4 Determining residual stresses in thin films using cantilevers

Fang et al. introduced a model to retrieve the mean and gradient residual stresses in thin films using micromachined cantilevers [24]. They started from the assumption that the uniaxial residual stress field in a thin film can be approximated by a mean stress \( \sigma_0 \) and a gradient stress \( \sigma_1 \) (Figure 5.3). After release of the cantilever beam the structure becomes free to deform out-of-plane following relief of the internal stress.

In Figure 5.4 the deformation of a cantilever beam under influence of mean and residual stress is depicted according to Fang et al. The curvature in the top of the picture is caused by the stress gradient \( \sigma_1 \). The tilt of the cantilever beam, which is depicted at the bottom of the picture, is caused by both the mean stress \( \sigma_0 \) and the gradient stress \( \sigma_1 \). The bottom of the cantilever is attached to the substrate, but the top is free to move under influence of the stress. This causes the tilt with a total angle \( \theta \), which is the sum of two angles. \( \theta_0 \) is caused by the mean stress and \( \theta_1 \) is the result of the stress gradient.

Using finite element modelling Fang et al. acquired an empirical model to determine the mean and gradient stress from the cantilever profile by measuring the curvature \( R \) of the beam and the tilt deflection \( \theta \) of SiO\(_2\) beams.

\[ \theta_0 = \frac{\sigma_0}{E} \left(1.33 + 0.45\nu\right)(-0.014h+1.022) \]  
(Eq. 5.27)

\[ \theta_1 = \frac{\sigma_1}{E} \left(0.0086h^2 - 0.047h + 0.81\right) \]  
(Eq. 5.28)

\[ \sigma_1 = \frac{Eh}{2R} \]  
(Eq. 5.29)
with $h$ the thickness of the layer and $\nu$ the poisson ratio. These equations are evaluated for $0.1 \leq \nu \leq 0.4$, $0.5 \mu m \leq h \leq 3 \mu m$ $10^{-4} < \sigma / E < 10^{-1}$ and $10^{-4} < \sigma / E < 10^{-1}$ and appear to represent $\theta_0$ and $\theta_1$ well within these parameter ranges. The equations can be used to analyse the deflection profiles at different temperatures. These are the only available formulas stated in literature to analyse the stress-induced curvature of cantilevers.

### 5.1.5 Determining thermal expansion coefficient using cantilevers

There exist many techniques to determine the thermal expansion coefficient of materials. James et al. [25] give a review of most of the existing techniques together with their accuracy and the temperature range in which the techniques can be used. There exist only few techniques that use a cantilever to determine the thermal expansion coefficient of materials.

A simple method to determine the linear thermal expansion coefficient (LTEC) of thin films independent of material properties was presented by Pan [26]. In this method the thermally induced displacements of micromachined structures are measured to determine the LTECs of thin films. The displacements can be measured directly under an optical microscope with the specimen placed in a heating stage. In this method it is not necessary to know the Young's modulus, the Poisson's ratio and the thickness of the thin film, and furthermore, the method is absolutely independent of the underlying substrate.

The used microstructure consists of a pair of cantilever beams with different lengths connected by a short tip beam (Figure 5.5). Two cantilever beams are designed as test beams, and the tip beam acts as an indicator. As the temperature increases or decreases, the difference between the two test beams with respect to elongation or contraction causes the deflection of the two beams, thereby magnifying the lateral displacement of the tip.

The elongation or contraction is due to thermally induced strain. Since the displacement of the tip beam is sufficiently large, direct observations under an optical microscope can be used to collect reasonable accurate data. A Vernier gauge located at the free end of the indicator beam can be used to quantify the displacement, but this is optional. An analytical expression is then derived to relate the displacement to the LTEC of the thin film.

The influence of the stress gradient in the cantilever has not been taken into account. This means that the reading of the lateral displacement of the tip beam is not very accurate in the case that there is a stress gradient present.

![Figure 5.5: Schematic diagrams (top and side views) of the microstructure for the LTEC determination of thin films [26].](image-url)
temperature changes by a heating stage. The vertical deflection is determined using optical interferometric techniques on the heat-deformed microcantilevers. They developed a model for single-layer microcantilevers and one for bi-layer microcantilevers, both these models are dependent on material properties. First the single-layer microcantilever method will be described.

As shown in Figure 5.6a, the boundary of the single layer microcantilever is fixed to the substrate on only one surface. When the temperature is increased, the points A and B indicated in the figure will move as a result of the in plane expansion of the thin film and the substrate. The moving distance of points A and B will be different if the LTEC between the substrate and the thin film is different.

Thus the microcantilever is supported by a deformed boundary A'B' after thermal expansion, as shown in Figure 5.6b, and then experiences an angular deflection. The two-dimensional stress state and deformation of the single layer microcantilever was analysed with a finite element model. From the finite element analysis a relationship between the angular deflection \( \theta \) and the LTEC \( \alpha \) was determined in an empirical representation of \( \theta \):

\[
\theta = \frac{3.86 \times 10^{-4} \Delta T \Delta \alpha (0.92 + 0.1 r - 0.02 r^2)(0.95 + 0.35 \nu)}{(2.98 \times 10^{-4} - 1.32 \times 10^{-16} \Delta E)}
\]  
(Eq. 5.30)

where \( t \) and \( \nu \) are the thickness and Poisson’s ratio, respectively, between the substrate and the thin film. \( \Delta T \) is the rising temperature. \( \Delta E \) and \( \Delta \alpha \) are the differences in values for the Young’s modulus and the LTEC, respectively, between the substrate and the thin film.

(Eq. 5.30) has been evaluated for \( 0.2 \mu m \leq t \leq 2 \mu m \), \( 50 \text{GPa} \leq \Delta E \leq 180 \text{GPa} \), and \( -30 \times 10^{-6}/^\circ C \leq \Delta \alpha \leq 30 \times 10^{-6}/^\circ C \) and appears to represent \( \theta \) well within this parameter range.

In literature a description can be found on the behaviour of a bilayer microcantilever. The cantilever will bent with a radius of curvature \( \rho \) after experiencing a temperature change if the thermal strains of the two films (from which the bilayer cantilever exists) are different. In this case, the thermal strains are introduced by the temperature change \( \Delta T \) and the difference in LTEC between the films \( \Delta \alpha_f \). According to Timoshenko [28], through standard stress analyses, the relationship between the curvature \( 1/\rho \) of the bilayer beam and the difference in LTEC \( \Delta \alpha_f \) between the films becomes:
5.2 Determination of a thin layer stress profile

From previous sections, it is known that the average residual stress can be determined with the wafer curvature method and the average linear stress gradient can be obtained from the deflection of a cantilever after etching away the sacrificial layer. For the determination of the exact stress profile in the layers, a differential technique can be used. Samples are processed similarly and are then thinned to obtain layers with different thickness. Using this method it is possible to obtain values of the average linear stress gradient for different thickness. The problem is reduced to rebuilding the stress profile from the obtained stress gradient values. This has been done using different methods. These were proposed by Yang et al. [30], Van Der Donck [31] and Furtsh [32]. Molfese compared these methods and concluded that there were too many restrictions on the existing methods [33]. Therefore an improved model was proposed that is explained in the following section.

5.2.1 Molfese's model

In order to rebuild the stress profile from the measurements in an improved way, Molfese et al. proposed a different method. The experiments they used started from linear stress gradient $\Gamma(t)$ measurements instead of stress $\sigma(t)$ measurements. At first, the best approximation of this function has to be found. Then the stress profile can be deduced from this approximation. In order to do this operation, an analytical relation between $\Gamma(t)$ and $\sigma(t)$ is needed. The first order expression for the stress $\sigma(t)$ in a beam is given as a combination of a constant stress $\sigma_0$ (stress at zero thickness) and a linear contribution:

$$\sigma(t) = \sigma_0 + \Gamma \cdot t$$  \hspace{1cm} (Eq. 5.32)

where $\Gamma$ is the linear stress gradient (see Figure 5.7).
5.2 Determination of a thin layer stress profile

As a result of a linear stress variation with thickness, a bending moment $M$ is produced. Assuming uniform elastic constants over the thickness of the beam, the neutral axis can be taken in the center of the beam ($t = T/2$) as the average stress is zero for a released beam.

It is known that the bending moment has the following expression (with the hypothesis that the neutral axis is in the middle):

$$M = \int_a^b \left( \sigma(z) \left( z - \frac{T}{2} \right) \right) dA$$  \hspace{1cm} (Eq. 5.33)

The insertion of (Eq. 5.32) gives:

$$M = \int_a^b \left( \sigma_0 \left( z - \frac{T}{2} \right) + \Gamma \left( z - \frac{T}{2} \right) \right) dA$$
\hspace{1cm} (Eq. 5.34)

$$= w \Gamma \int_0^T \left( z - \frac{T}{2} \right) dz = \Gamma \frac{wT^3}{12}$$

$$M(t) = \frac{\Gamma(t) \cdot w \cdot T^3}{12} = w \cdot \int_0^t \sigma(y) \left( y - \frac{t}{2} \right) dy$$  \hspace{1cm} (Eq. 5.35)

With a derivation of this relation, the following relation is obtained:

$$\frac{dM(t)}{dt} = \frac{d}{dt} \left( \frac{\Gamma(t) \cdot t^3}{12} \right) = \sigma(t) \cdot t - \frac{t}{2} \cdot \sigma(t) - \frac{1}{2} \int_0^t \sigma(y) dy = \frac{t}{2} \cdot \sigma(t) - \frac{1}{2} \int_0^t \sigma(y) dy$$  \hspace{1cm} (Eq. 5.36)

A second derivation gives:

$$\frac{1}{w} \frac{d^2 M(t)}{dt^2} = \frac{d^2}{dt^2} \left( \frac{\Gamma(t) \cdot t^3}{12} \right) = \frac{\sigma(t)}{2} + \frac{t}{2} \frac{d \sigma(t)}{dt} - \frac{\sigma(t)}{2} = \frac{t}{2} \frac{d \sigma(t)}{dt}$$  \hspace{1cm} (Eq. 5.37)

In this way a differential equation is obtained that links $\sigma(t)$ and $\Gamma(t)$:

$$\frac{d \sigma(t)}{dt} = \frac{2 \frac{d^2}{dt^2} \left( \frac{\Gamma(t) \cdot t^3}{12} \right)}{t \frac{d \Gamma(t)}{dt}}$$  \hspace{1cm} (Eq. 5.38)

Integrating (Eq. 5.38) leads to:
\[ \int_0^\gamma \frac{d\sigma(t)}{dt} \, dt = \int_0^\gamma \frac{2}{t} \frac{d^2}{dt^2} \left( \Gamma(t) \cdot t^3 \right) \, dy \]  
(Eq. 5.39)

This results in a relation that makes it possible to deduce the relative stress profile from a good approximation of the function \( \Gamma(t) \):

\[ \Delta \sigma(y) = \sigma(y) - \sigma(0) = \int_0^\gamma \frac{2}{t} \frac{d^2}{dt^2} \left( \Gamma(t) \cdot t^3 \right) \, dy \]  
(Eq. 5.40)

Finally it is possible to obtain \( \sigma(0) \) from the relative stress profile and residual stress in the following way:

\[ \sigma(0) = \sigma_\text{nr} - \frac{1}{T} \int_0^T \Delta \sigma(t) \cdot dt \]  
(Eq. 5.41)

With this approach the problem of determining the stress profile has been transformed in finding the best approximation of \( \Gamma(t) \). Several methods can be used to approximate this function; the only precaution to take into account is that the function must be \( C^2(0,T) \) (continuous with first and second continuous derivatives in the measurement interval). In his work Molfese compared a polynomial and an exponential fit for \( \Gamma(t) \) and concluded that the polynomial fit gives the best results.

\[ \Gamma(t) = \sum_{k=0}^n a_k \cdot t^k \]  
(Eq. 5.42)

With the polynomial fit for \( \Gamma(t) \), after the application of the formula, (Eq. 5.43) is obtained:

\[ \Delta \sigma(t) = a_0 \cdot t + a_1 \cdot t^2 + \frac{10}{9} \cdot a_2 \cdot t^3 + \frac{5}{4} \cdot a_3 \cdot t^4 + \frac{7}{5} \cdot a_4 \cdot t^5 + \frac{14}{9} \cdot a_5 \cdot t^6 + \frac{12}{7} \cdot a_6 \cdot t^7 + \ldots \]  
(Eq. 5.43)

To calculate the stress gradient starting from the tip deflection of a cantilever, Molfese related the deflection of the cantilever \( v(x) \) and the bending moment \( M \) for beams with small width/thickness ratio and small deflections ((Eq. 5.12) and (Eq. 5.24)) to acquire the following differential equation:

\[ \frac{d^2 v(x)}{dx^2} = \frac{M}{EI} \]  
(Eq. 5.44)

where \( E \) is the Young’s modulus and \( I \) is the moment of inertia of the section (= \( wT^3 / 12 \)). Solving this differential equation with the boundary conditions \( x = 0 \Rightarrow v = 0 \) and \( x = 0 \Rightarrow dv/dx = 0 \) leads to the following relation:

\[ v(x) = \frac{Mx^2}{2EI} = \frac{\Gamma}{2E} x^2 \]  
(Eq. 5.45)

After measuring the deflection \( \delta \) of the free end of a cantilever of length \( L \), the linear stress gradient can be calculated from:

\[ \Gamma = E \frac{2\delta}{L^2} \]  
(Eq. 5.46)
Measuring the stress gradient using cantilevers of different thickness results in a fitting function for $\Gamma(\tau)$ from which the stress profile can be deduced.

### 5.2.2 The neutral axis

In Molfese's method it is assumed that the neutral axis is always in the middle of the cantilever (for a homogenous material). In this section it will be explained why this assertion is true.

When the neutral axis (surface) is defined as the axis, in which there is no deformation, i.e. where the sum of forces is zero, it can be expected that the neutral axis is in the middle for a linear stress profile, but not necessarily for other types of stress profiles.

In Figure 5.8(a) a particular stress profile is shown. The value of stress is zero for a large part of the thickness of the cantilever and is positive in a small part near the surface. In this situation it seems that the neutral axis is not in the middle because the sum of the force and moments is not zero there. However, this approach is false because it does not take into account that the cantilever is released. In fact, the stress profile can always be split in a stress profile being the sum of two parts: one with the neutral axis in the middle (as from previous definition) and one constant (Figure 5.8(b)). The constant part is not important when the cantilever is released, so it can be concluded that the neutral axis is always in the middle for a homogeneous material (constant Young's modulus).

![Figure 5.8](image)

(a) An example of a stress profile in a cantilever; (b) splitting of the stress profile into two parts.

### 5.2.3 Improvement of Molfese's model

Molfese used (Eq. 5.12) to determine the stress gradient from the cantilever tip deflection. This equation is only valid for small deflections of cantilevers. In Molfese's work the largest deflection that was measured was 591 µm for a cantilever of 1mm length. This cannot be considered as a small deflection. In the model proposed by Molfese there is an overestimation of the stress gradient for large deflections of cantilevers. Therefore an adaptation is proposed to improve the calculation of the stress gradient from the cantilever tip deflection.

To deduce a better approximation for the stress gradient the exact expression for the flexure, (Eq. 5.9), is used. The deflection profile of a cantilever beam can be considered as a circle. Making use of the equation for a circle with center $(0, r)$ and radius $r$ and applying, the exact formula for flexure, gives:

\[ x^2 + (v-r)^2 = r^2 \]  \hspace{1cm} (Eq. 5.47)

\[ v = r - \sqrt{r^2 - x^2} \]  \hspace{1cm} (Eq. 5.48)
\[ v' = \frac{x}{\sqrt{r^2 - x^2}} \]  
(Eq. 5.49)

\[ v' = \frac{r^2}{(r^2 - x^2)^{3/2}} \]  
(Eq. 5.50)

\[ \kappa = \frac{1}{\rho} = \frac{v'}{1 + (v')^2} = \frac{r^2}{(r^2 - x^2)^{3/2}} \]  
(Eq. 5.51)

Combining (Eq. 5.48), (Eq. 5.51) and (Eq. 5.24) leads to an exact expression for the deflection of the cantilever:

\[ v(x) = \frac{EI}{M} - \sqrt{\frac{EI}{M}^2 - x^2} \]  
(Eq. 5.52)

Since \( \Gamma = M / I \) the expression for the end deflection \( \delta_x \) for a cantilever of length L is:

\[ \delta_x = \frac{E}{\Gamma} \sqrt{\left(\frac{E}{\Gamma}\right)^2 - L^2} \]  
(Eq. 5.53)

Now the stress gradient can be written as a function of the cantilever tip deflection:

\[ \Gamma = \frac{2\delta_x E}{L^2 + \delta_x^2} \]  
(Eq. 5.54)

For small deflections \( (\delta_x \ll L) \) this formula goes to (Eq. 5.46).

### 5.2.4 Comparison of the models

The data published by Molfese [33] is reviewed with the adjusted expression for the stress gradient from (Eq. 5.54). The stress profile was determined for a 10 \( \mu \text{m} \) thick layer by thinning the layer and measuring the cantilever tip deflection. The experimental values for the layer thickness and the cantilever tip deflection are shown in Table 5.1 together with the calculated values for the stress gradient with (Eq. 5.46) and (Eq. 5.54). The difference between the values is also given. The correction is below 1\% for thickness values over 4 \( \mu \text{m} \). For the thinnest layer thickness (0.95 \( \mu \text{m} \)) however the correction is 35\%. This means that Molfese overestimates the linear stress gradient for a small layer thickness. In Figure 5.9 Molfese’s calculated values for the stress gradient are plotted together with the recalculated values. It can be seen that there is no large difference for a large layer thickness. In Figure 5.10 the stress profiles are determined from the linear stress gradient values from Figure 5.9. A polynomial fit of the seventh order was used to calculate the profile. The profiles only differ in the part of the layer thinner than 4 \( \mu \text{m} \). This is evident, because only in this part of the layer the values of the linear stress gradient differ significantly.
Table 5.1: Experimental values for the layer thickness and the cantilever tip deflection together with the calculated stress gradient values and their difference

<table>
<thead>
<tr>
<th>Layer thickness (µm)</th>
<th>Deflection (µm)</th>
<th>Old gradient (MPa/µm)</th>
<th>New gradient (MPa/µm)</th>
<th>Difference (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>22.60</td>
<td>6.64</td>
<td>6.64</td>
<td>0.05</td>
</tr>
<tr>
<td>9.5</td>
<td>28.50</td>
<td>8.38</td>
<td>8.37</td>
<td>0.08</td>
</tr>
<tr>
<td>8.4</td>
<td>33.80</td>
<td>9.94</td>
<td>9.93</td>
<td>0.11</td>
</tr>
<tr>
<td>7.6</td>
<td>37.90</td>
<td>11.14</td>
<td>11.13</td>
<td>0.14</td>
</tr>
<tr>
<td>7.2</td>
<td>42.40</td>
<td>12.47</td>
<td>12.44</td>
<td>0.18</td>
</tr>
<tr>
<td>6.6</td>
<td>44.90</td>
<td>13.20</td>
<td>13.17</td>
<td>0.20</td>
</tr>
<tr>
<td>6.5</td>
<td>47.00</td>
<td>13.82</td>
<td>13.79</td>
<td>0.22</td>
</tr>
<tr>
<td>5.45</td>
<td>64.60</td>
<td>18.99</td>
<td>18.91</td>
<td>0.42</td>
</tr>
<tr>
<td>5.3</td>
<td>75.20</td>
<td>22.11</td>
<td>21.98</td>
<td>0.57</td>
</tr>
<tr>
<td>4</td>
<td>113.8</td>
<td>33.46</td>
<td>33.03</td>
<td>1.30</td>
</tr>
<tr>
<td>3.9</td>
<td>119</td>
<td>34.99</td>
<td>34.50</td>
<td>1.42</td>
</tr>
<tr>
<td>1.6</td>
<td>469.40</td>
<td>138.00</td>
<td>113.09</td>
<td>22.03</td>
</tr>
<tr>
<td>0.95</td>
<td>591.00</td>
<td>173.75</td>
<td>128.78</td>
<td>34.93</td>
</tr>
</tbody>
</table>

Molfese's data

Recalculated data

Figure 5.9: Comparison of the calculated stress gradients

Molfese concluded that the calculated profile is valid for the entire layer. He stated that the fluctuations in area II in Figure 5.10 are due to the polynomial fit that was used. In this region the stress is more or less constant and equals the mean stress determined by the wafer curvature method at 72 MPa. From area I, he concluded that the profile projects the influence of the amorphous seedlayer and the LPCVD layer, which are compressive layers. As can be seen later in this thesis (section 6.3), this conclusion is not valid.
5.3 Cantilever tranverse curvature

In the previous sections where the longitudinal strain and normal stresses were determined, the rectangular cross-section of the beam is assumed to remain plane and Hooke’s law is assumed to apply. Timoshenko already stated that these two underlying assumptions made to achieve (Eq. 5.22) and (Eq. 5.26) can lead to an overestimation of the bending moment [34].

In order to be within Hooke’s law the maximum stress must not exceed the elastic limit of the material. This restriction is usually satisfied. The assumption of a plane cross-section means that the radius of curvature must be large compared to the height of the cross-section. The curvature itself may not be large, but in that case the height of the cross-section must be extremely small.

However, it is well known that an elongation $\varepsilon$ in one direction causes a contraction in perpendicular directions equal to $\nu \varepsilon$, where $\nu$ is Poisson’s ratio. Thus on the convex side with respect to the elastic line the cross-section will be subject to lateral contraction and on the concave side, where the longitudinal fibers are under compression, there will be lateral dilatation in the plane of the cross-section. This is called anticlastic curvature (Figure 5.11). The transverse curvature has the opposite sign of the principal curvature.
5.3 Cantilever transverse curvature

As a consequence of the anticlastic curvature, the cross-section distorts; therefore the neutral axis cannot remain straight and it is easy to see that its curvature will be $\rho_s/v$. As long as the width $b$ of the cross-section is of the same order as the height $h$ and $h/\rho$ is a small quantity, the additional deflection due to this curvature will be a small quantity of second order, which can be neglected. In this way the fact of the bending of the neutral axis will not interfere with the assumption that the cross-sections remain plane.

Searle [35] states and shows experimentally that for wider beams this anticlastic bending is neutralized due to forces that act radially inward toward the center of curvature of a bent sample. As the width reaches a certain size, this radial force becomes large enough to reduce the anticlastic curvature and causes a plane strain condition along the sample width. Poisson contraction and expansion are prevented in regions above and below the specimen's neutral axis.

Since in the bending of a thin, wide strip, the cross-sections (with a negligible distortion at the corners) remain substantially as before it is evident that (Eq. 5.22) and (Eq. 5.26) should be modified [34].

Timoshenko determined the bending moment of a wide curved beam in which the neutralizing radial force (presented by Searle) is incorporated:

$$M = \frac{EI}{\rho} \cdot \frac{1}{1-v^2}$$  \hspace{1cm} (Eq. 5.55)

This is the formula that should be used in the case of bending thin, wide strips according to Timoshenko's approach [34]. This neutralizing effect for wide beams is called the plate effect.

Now (Eq. 5.22) and (Eq. 5.55) furnish solutions for the problem of bending in two extreme cases. For intermediate cases more detailed consideration of the distortion of the cross-section is necessary. Timoshenko stated that in the case of a strip acted upon at its terminal cross-sections by equal and opposite (uniaxial) bending moments, a different equation than (Eq. 5.22) and (Eq. 5.55) is obtained:

$$M = \frac{EI}{\rho} \cdot \frac{1-kv^2}{1-v^2}$$  \hspace{1cm} (Eq. 5.56)
in which the quantity \( k \) is a function of the radius \( \rho \), the thickness \( h \), and the width \( b \) of the strip. A number of values of \( k \) are given in Table 5.2 where:

\[
\beta b = b\sqrt{\frac{3(1-v^2)}{v^2\rho^2 h^2}} = 1.286 \frac{b}{\sqrt{\rho h}} \quad \text{(Eq. 5.57)}
\]

<table>
<thead>
<tr>
<th>( \beta b )</th>
<th>0.5</th>
<th>1.0</th>
<th>1.5</th>
<th>2.0</th>
<th>2.5</th>
<th>3.0</th>
<th>4.0</th>
<th>5.0</th>
<th>&gt;5.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>( K )</td>
<td>0.999</td>
<td>0.995</td>
<td>0.975</td>
<td>0.877</td>
<td>0.818</td>
<td>0.725</td>
<td>0.534</td>
<td>0.420</td>
<td>2/(( \beta b ))</td>
</tr>
</tbody>
</table>

**Table 5.2: Values for \( k \) according to Timoshenko [34]**

Roark and Young [36] recognize the same problem and introduce a correction factor \( K \) in (Eq. 5.24):

\[
\frac{1}{\rho} = \frac{M}{KEI} \quad \text{(Eq. 5.58)}
\]

For a rectangular beam of width \( b \) and depth \( h \) bent to a radius of curvature \( \rho \) by a bending moment \( M \), Table 5.3 shows the value of \( K \) for several values of Poisson’s ratio and the quantity \( b^2/\rho h \) as given by Roark and Young. This correction factor \( K \) is similar to the correction factor proposed by Timoshenko.

<table>
<thead>
<tr>
<th>Value of ( \nu )</th>
<th>0.25</th>
<th>1.00</th>
<th>4.00</th>
<th>16.0</th>
<th>50.0</th>
<th>200.</th>
<th>800.</th>
</tr>
</thead>
<tbody>
<tr>
<td>( b^2/\rho h )</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.1000</td>
<td>1.0000</td>
<td>1.0003</td>
<td>1.0033</td>
<td>1.0073</td>
<td>1.0085</td>
<td>1.0093</td>
<td>1.0097</td>
</tr>
<tr>
<td>0.2000</td>
<td>1.0001</td>
<td>1.0013</td>
<td>1.0135</td>
<td>1.0300</td>
<td>1.0349</td>
<td>1.0383</td>
<td>1.0400</td>
</tr>
<tr>
<td>0.3000</td>
<td>1.0002</td>
<td>1.0029</td>
<td>1.0311</td>
<td>1.0710</td>
<td>1.0826</td>
<td>1.0907</td>
<td>1.0948</td>
</tr>
<tr>
<td>0.3333</td>
<td>1.0002</td>
<td>1.0036</td>
<td>1.0387</td>
<td>1.0895</td>
<td>1.1042</td>
<td>1.1146</td>
<td>1.1198</td>
</tr>
<tr>
<td>0.4000</td>
<td>1.0003</td>
<td>1.0052</td>
<td>1.0569</td>
<td>1.1357</td>
<td>1.1584</td>
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<td>1.1825</td>
</tr>
<tr>
<td>0.5000</td>
<td>1.0005</td>
<td>1.0081</td>
<td>1.0923</td>
<td>1.2351</td>
<td>1.2755</td>
<td>1.3045</td>
<td>1.3180</td>
</tr>
</tbody>
</table>

**Table 5.3: Correction factor \( K \) for rectangular beams from Roark and Young [36]**

Ashwell derived a formula for the distortion of the cross-section of a curved rectangular beam [37]. He started from the Euler-Bernouilli beam equation to retrieve a formula for the transverse beam deflection.

\[
y / d = B \cosh \alpha b (x / b) \cos \alpha b (x / b) + C \sinh \alpha b (x / b) \sin \alpha b (x / b) \quad \text{(Eq. 5.59)}
\]

where

\[
B = \frac{v}{\sqrt{3(1-v^2)}} \frac{\sinh(\alpha b/2) \cos(\alpha b/2) - \cosh(\alpha b/2) \sin(\alpha b/2)}{\sinh \alpha b + \sin \alpha b}
\]

\[
C = \frac{v}{\sqrt{3(1-v^2)}} \frac{\sinh(\alpha b/2) \cos(\alpha b/2) + \cosh(\alpha b/2) \sin(\alpha b/2)}{\sinh \alpha b + \sin \alpha b}
\]

\[
\alpha = \sqrt{\frac{3(1-v^2)}{d^2 \rho^2}}
\]

\[
\text{where}
\]

\[
y / d = B \cosh \alpha b (x / b) \cos \alpha b (x / b) + C \sinh \alpha b (x / b) \sin \alpha b (x / b)
\]

\[
B = \frac{v}{\sqrt{3(1-v^2)}} \frac{\sinh(\alpha b/2) \cos(\alpha b/2) - \cosh(\alpha b/2) \sin(\alpha b/2)}{\sinh \alpha b + \sin \alpha b}
\]

\[
C = \frac{v}{\sqrt{3(1-v^2)}} \frac{\sinh(\alpha b/2) \cos(\alpha b/2) + \cosh(\alpha b/2) \sin(\alpha b/2)}{\sinh \alpha b + \sin \alpha b}
\]

\[
\alpha = \sqrt{\frac{3(1-v^2)}{d^2 \rho^2}}
\]
Here $\nu$ is the Poisson ratio, $b$ is the width of the beam, $d$ is the thickness of the beam and $\rho$ is the longitudinal radius of curvature. (Eq. 5.59) describes different modes of distortion of the cross-section for different values of width, thickness and curvature. To get a better understanding of these formulas stated by Ashwell, the beam distortion is plotted in Figure 5.12 for different widths ($x/b$ represents the reduced width, $y/b$ is the vertical deflection divided by the thickness). The simulated thickness was 4 µm, the radius of curvature 6000 µm and the poisson ratio was 0.3. It can be seen that as the width increases, the middle surface remains plane and the edge shows a distortion. This is the plate effect.

![Distortion of the cross-section](image)

**Figure 5.12:** Distortion of the cross-section with different width and constant thickness, poisson ratio and curvature

Creating a sample from which the transverse deflection profile can be measured, in theory gives the possibility to determine the poisson ratio of the material since the width, thickness and curvature are known or can be determined. The influence of the poisson ratio on the distortion is plotted in Figure 5.13. For this plot, the thickness was held at 4 µm, the curvature is equal to 6000 µm and the width is equal to 1000 µm. By comparing the measured deflection profile with the calculated profiles, the poisson ratio can be estimated.
A recent study by Hou et al. [38] showed the transverse deflection of surface-micromachined bilayer cantilevers. The bilayer cantilevers all have a constant length of 30 µm and consist of a 200 nm thick chromium layer on top of a 2 µm thick polysilicon layer. A measured transverse profile in this study is depicted in Figure 5.14. This distortion profile resembles the prediction of Ashwell for a beam with large width. But the longitudinal deflection of the cantilever was concave (bending upwards). So the predicted deflection by Ashwell should be convex. This means that the transverse deflection is determined by a biaxial stress situation while Ashwell's calculations start from an uniaxial bending moment.

In the same study performed by Hou et al. with micromachined bilayer cantilevers, it was concluded that the effect of the width on the stress distribution in cantilevers cannot be neglected. In their study, the tip deflection of a bilayer cantilever gradually increases as the width increases until the width-to-length ratio reaches a critical value, in which the micromachined cantilever can be regarded as an infinitely wide cantilever, and any cross
section along the length is in plane strain state. In Figure 5.15 the tip deflection is shown versus the width-to-length ratio according to the experiments performed by Hou et al. [38].

![Figure 5.15: Measured tip deflection versus width-to-length ratio of surface micromachined bilayer cantilevers with constant length and different width from Hou et al. [38].](image)

The opposite result for the tip deflection in function of the width to length ratio has been found with simulations done by Watts et al. [39] and by Iannotti et al. [40]. The result from Watts et al. can be seen in Figure 5.16. The geometry of their cantilever beam can be seen in Figure 5.17(b). The following parameters are used: \( l = 40 \text{ mm}, \ t_s = 400 \mu\text{m}, \ t_f = 72 \text{ nm}, \ E_s = 68 \text{ GPa}, \ Y_f = 218 \text{ GPa}, \ \nu_s = 0.22, \ \nu_f = 0.28 \) and the width is variable.

Looking at the profile of the curve in Figure 5.16, three regions can be observed. For \( w/l \) going to 0 the deflection is 202 nm. For \( w/l \) around 1, the deflection remains constant at 157 nm. These values can be related to the poisson ratio \( \nu_s \). Looking at the thickness of both layers, the 400 \( \mu\text{m} \) will have the largest influence on the deflection. Multiplying 202 nm with \( (1-\nu_s) \) gives 157.56 nm and a multiplication with \( (1-\nu_s^2) \) gives 192.22 nm. This indicates that these three different cases for the deflection of cantilever, which depend on the width to length ratio, can be explained by a different poisson effect.

The beam goes from a uniaxial stress state (with \( E_{\text{eff}} = E \)) to a biaxial stress state (\( E_{\text{eff}} = E/(1-\nu_s) \)) when the width to length ratio increases. In between these two states a region exists where a plate-like effect plays a role (possibly due to clamping instead of due to the effects explained earlier in this chapter) and \( E_{\text{eff}} \sim E/(1-\nu_s^2) \). This should be clear from the transverse deflection. In the uniaxial stress state the anticlastic (convex) curvature dominates, while in the biaxial stress state the curvature will be concave. In between there is a transition area where the cross-section is free from distortion. This effect can be used in a new method to determine the poisson ratio of materials. Creating cantilevers with the same length, but different width and measuring the tip deflection will result in a figure like Figure 5.16. From the deflection at \( w/l = 0.01, 1 \) and 10, the poisson ratio can be simply deduced. The same relations and transition (uniaxial to biaxial stress state) could not be calculated for Figure 5.15.
The difference in width to length behaviour in the studies of Hou et al. [38] and Watts et al. [39] indicates that the clamping of the cantilever beam also plays an important role in this process. Figure 5.17 shows the different geometries used in these studies. It can be seen that the cantilever used in [38] makes an angle when released from the surface. This probably causes the difference in deflection behaviour in the two studies.

Figure 5.17: Geometry of the cantilevers used to study the influence of the width on the deflection of the cantilever; a) geometry used by Hou [38], b) geometry used by Watts [39].
6 Experimental results and discussion

The experimental work in this thesis can be divided into three parts. The first part is the study of the deflection profile at elevated temperatures using scanning electron microscopy. A completely new technique was developed for this purpose. In the second part the stress profile of a thin layer was determined by thinning the layer using a low power etching plasma. In the last part the transverse deflection of cantilevers is studied as function of the cantilever width.

6.1 Measuring cantilever deflection profile with scanning electron microscopy

The determination of the deflection of cantilevers usually occurs with laser profilometry or with optical surface profilometry. Scanning electron microscopy (SEM) has never been used for this purpose. It is only used to check the design of the structures. The use of SEM to determine the deflection profile can be interesting because it is possible to build in a heating stage into the microscope. This makes it possible to look at the deflection profile at different temperatures and to study properties like the thermal expansion coefficient.

When the profile of a cantilever is studied with SEM, the profile can be determined from one image, simply by tilting the sample and viewing it from the side. With the samples used in this study tilting was not possible due to the surrounding structures, which are blocking the view. Dicing the samples was too risky. Therefore a new technique was developed to determine the deflection profile of cantilevers by looking on top of the cantilevers with SEM. The difference in free working distance between two measured points will be very important to determine the profile. The measurement error will be determined by different parameters. The influence of the different parameters on the measurement error will be discussed in this section.

6.1.1 Measurement process

Figure 6.1 shows the cantilevers from which the deflection profile has to be determined. The profile has to be determined by looking at the cantilever from the top because other structures are blocking the side-view. The idea behind the measurement is as follows. After focusing on one position of the cantilever the free working distance can be read out. Focusing on a second position on the cantilever gives a different value of the free working distance. The difference between these two values of the free working distance is the difference in height between the two positions. By measuring over the length of the complete cantilever a deflection profile can be determined.
The SEM can be controlled using a program created in LabVIEW. To achieve an automated measuring process, an adapted software program was written to measure the deflection profile of a cantilever. The points that will be used during the measurement are shown in Figure 6.2. When the program is started a window will appear where the user can insert the number of points that have to be measured on the cantilever and the number of times the profile has to be measured together with the magnification. The profile has to be measured a certain number of times to reduce the measurement error by taking the average of all measurements. After this, the program will ask the user to move the microscope to point 1 which is situated 30 µm before the freestanding part of the cantilever. At this point the cantilever is still attached to the underlying layer. Then the user has to make sure that the microscope is in focus at point 1. After the confirmation that these actions have been performed, the program saves the position of the microscope and the value of the free working distance.

In the next step, the program will ask the user to go to point two, which is at the end of the cantilever, and to focus on that position. After confirmation, the program will again save the coordinates of this position together with its value of free working distance. Then the coordinates of the intermediate points between point 1 and 2 are calculated together with an estimation of the free working distance at these points. This estimation uses a circular deflection profile between point 1 and 2 to calculate the free working distance of the intermediate points. There is also an extra point added which is called the reference point. This point is like point 1 positioned at a place that is still connected to the underlying layer. The height difference between point 1 and the reference point can be used to correct the measured values if the substrate is not lying perfectly horizontal.
Now the program starts the measurement. It will move the microscope to every position and will use the saved value of the free working distance to be very close to the point where the sample is in focus. Because the contrast and brightness between the lowest (point 1) and highest point (point 2) can differ, an autocontrast function was inserted. This means that the microscope determines the best contrast/brightness settings for every point. Then the program uses the autofocus function, where the microscope adjusts the position of objective lens to get the sample in focus. When this is done, the new value of the free working distance is saved and the microscope moves to the next position. This will be done for every point requested by the user.

Figure 6.3 shows the profile determined after measuring each point one time. It can be seen that there exists a height difference between point 1 and the reference point. This means that the sample was not lying perfectly horizontal and that a correction of the measured values is needed. The profile of the cantilever in Figure 6.3 is not very smooth. To achieve a smoother profile the number of measurements can be increased and the average values can be used. Every new measurement uses the value of the free working distance of the previous measurement. After every measurement of the profile the data are saved.
6.1.2 Problems and possible solutions
The large depth of field is a disadvantage in this case. By using the autofocus function of the microscope the measurement error is mainly determined by the depth of field. The depth of field determines the part of the free working distance in which the sample is reasonably good in focus. When the depth of field is large, there exists a 'large' area in which the sample will be in good focus. Thus there is a large area in which the autofocus function can decide that the sample is in focus. This means that there is a large error on the measurement of the profile. The only solution is to decrease the depth of field. Changing some operational parameters like the magnification and even the acceleration voltage can result in a diminution of the depth of field.

Another problem can be a drift of the sample when it is heated. This is caused by a difference in thermal expansion coefficient between adjacent layers of the sample (see Figure 2.4). Thermal stresses are introduced and this will lead to an expansion of the layers. The structure will try to relax most of the stress, but will undergo a shift. The only solution to overcome this problem is waiting until the stresses have relaxed. This can take up to 8 hours.

6.1.3 Adjusting measurement settings
On top of the figures presented in the following section the settings used for the measurement can be found. For example in Figure 6.4 the measurements were executed with an acceleration voltage of 10 kV, spot size 3 and a magnification of 5000 times. The figure at the left of Figure 6.4 is the average deflection determined with 4 measurements. The right side shows the average deflection determined after 16 measurements. It can be seen that the deflection profile from 4 measurements is not that smooth. The average of 16 measurements on the other hand leads to a much smoother profile.
6.1 Measuring cantilever deflection profile with scanning electron microscopy

Figure 6.4: Measured cantilever deflection at 10 kV, spot size 3 and magnification 5000 after 4 (left side) and 16 measurements (right side).

In Figure 6.5 the measurements of Figure 6.4 are repeated at a higher magnification (20000x). In this case, the profile determined after 4 measurements has improved, but is still not as smooth as the average after 16 measurements.

Figure 6.5: Measured cantilever deflection at 10 kV, spot size 3 and magnification 20000 after 4 (left side) and 16 measurements (right side).

The average standard deviation of the measurement with a magnification of 5000 times is 9.4 µm (after 16 measurements). This standard deviation decreases to an average of 6.1 µm working at a magnification of 20000 times. This result was expected since the depth of field is proportional to the inverse of the magnification ((Eq. 3.2)). The difference in standard deviation for different magnifications is clearly visible in Figure 6.6.
6 Experimental results and discussion

Figure 6.6: Comparison of the standard deviation with different magnifications at 10 kV, spot size 3 and 16 measurements.

The same conclusion can be made from Figure 6.7. This figure shows the standard deviations (after 16 measurements) for different magnifications used with an acceleration voltage of 5kV and spot size 3. On average, the standard deviation drops from 6.6 µm at 5000 times, to 6.4 µm at 10000 times and 6.2 µm at 20000 times.

Figure 6.7: Influence of magnification on the standard deviation at 5 kV with spot size 3 and after 16 measurements

The influence of the acceleration voltage on the standard deviation was also studied. Measurements were performed with an acceleration voltage of 5, 10 and 20kV. The magnification was 20000 times, spot size 3 and the average was calculated from 16 measurements. The average standard deviation was 6.2 µm with an acceleration voltage of 5kV. This reduces to 6.1 µm using a 10kV acceleration voltage. The smallest standard deviation that was achieved was 5 µm with an acceleration voltage of 20kV. These results are confirmed by (Eq. 3.3) in which the depth of field in inverse proportional to the acceleration voltage. From now on all further experiments will be done with an acceleration voltage of 20kV.

Because 16 measurements of the cantilever profile take a long time, an effort was made to reduce the number of measurements to 8. The result is presented in Figure 6.8. The average standard deviation of this measurement is 6.6 µm. The measured profile does not show bumps or holes. It can be concluded that lowering the number of measurements to 8 does not lead to a large increase of the standard deviation and gives a good indication of the profile.
6.1 Measuring cantilever deflection profile with scanning electron microscopy

Figure 6.8: Measured deflection profile with an acceleration voltage of 5kV and a magnification of 20000 times (average of 8 measurements).

Figure 6.9 shows the standard deviations for different spot sizes. The profiles were measured with an acceleration voltage of 20kV, a magnification of 20000 times and with 16 measurements. The average standard deviation is 6 µm with spot size 4. Spot size 5 gives an average standard deviation of 4.9 µm. Spot size 6 gives the best result with an average standard deviation of 2.5 µm. The higher spot size increases the signal to noise ratio which will result in a better autocontrast and autofocus of the SEM. This causes the decrease of the standard deviation.

Figure 6.9: Comparison of standard deviations with different spot sizes with an acceleration voltage of 20kV, magnification 20000x and after 16 measurements.

To check the reliability of a SEM measurement, a comparison is made with a UBM laser profilometer measurement. The SEM measurement was done with an acceleration voltage of 20 kV, a magnification of 20000 times and a spot size of 4. The result is shown in the left of Figure 6.10. The average standard deviation was 5 µm. In the same figure a second order polynomial fit is visible. This fit is again plotted in the right of Figure 6.10 together with the UBM measurement. It can be seen that both measurements agree with each other.
From the results of the experiments performed in this section it can be concluded that the scanning electron microscope can be used to determine the deflection profile of cantilevers. Although there is a standard deviation on the determined height, a polynomial fit of the second order corresponds very well to the deflection profile determined by the UBM laser profilometer.

6.2 Measuring the deflection profile at different temperatures

Now that the standard deviation of the measuring process has been decreased under 3 µm and the fit of the measurement agrees with the laser profilometer measurement, experiments can be done at elevated temperatures. The sample used for this experiment has unknown processing and preparation conditions for the SiGe layer but the Ge concentration will correspond more or less to the values mentioned earlier in section 2.4. This sample is used because there were no other samples available at that time. It has a thickness of 2 µm. With this thickness a large deflection is expected as the stress gradient normally decreases with increasing thickness. The main purpose of the experiment on this sample is to demonstrate the effect of heating on the cantilever deflection.

The results of the first temperature experiments are shown in the left of Figure 6.11. The average standard deviation for the profile determined at 40 °C is 3.4 µm. For the profile determined at 250°C the average standard deviation is 1.4 µm. This difference in standard deviation can indicate a better signal to noise ratio at 250°C than at 40°C. This has an influence on the contrast and brightness of the image on the SEM, which in its turn has an influence on the accuracy of the autocontrast and autofocus mode of the SEM. It could also mean that the sample morphology changes during the heating process.

On the left side of Figure 6.11 the difference in deflection can be seen. The difference in deflection seems to increase linearly which indicates a tilt of the cantilever beam due to a mismatch in thermal expansion coefficient between the cantilever and the underlying substrate. The change in deflection at the tip of the cantilever beam is over 30 µm. Calculating the change in deflection from the predicted angular deflection from (Eq. 5.30) results in a predicted tip deflection of 0.45µm using the following parameters: $v_{SiGe} = 0.23$, $a_{SiGe} = 4.3 \text{ e-6 } /\text{K}$, $a_{Si} = 2.6 \text{ e-6 }/\text{K}$, $E_{SiGe} = 147$ GPa and $E_{Si} = 169$ GPa. The thickness of the cantilever beam used in this experiment is 2 µm, which means that the use of the equation should be valid for this case (see section 5.1.5). The measured change in tip deflection is a lot higher. Clearly temperature effects alone cannot predict this behaviour.
6.2 Measuring the deflection profile at different temperatures

Now that the effect has been demonstrated, the same experiment is done with a sample with known composition (P050135D03-18). The thickness of the sample is 4 µm and the stack build-up of the SiGe is as mentioned in section 2.4. The sample was heated to a temperature of 300°C. This temperature is higher than in the previous experiment because the expected deflection is a lot smaller with a cantilever of this thickness. In the left side of Figure 6.12 the fits of the deflection profile at 300°C and at room temperature are depicted. The average standard deviation of the measurement at room temperature was 3.7 µm. At 300°C the average standard deviation was 1.9 µm. In the right of Figure 6.12 the difference in deflection is presented. The trend of this curve indicates a stress gradient effect combined with a mean stress effect.

Now the difference in deflection is decomposed into a linear and a gradient contribution. The linear part can be observed in the left of Figure 6.13. At the right side of the same figure the gradient deflection is presented. The origin of the linear deflection is expected to be due to the difference in thermal expansion coefficient between the substrate and the cantilever layer. In contrary to the upwards deflection, this thermal stress would cause the cantilever to tilt downwards as SiGe becomes more compressive as the temperature increases.

The origin of the gradient deflection is not clear. It is known that the Ge% at the top of the layer is larger than at the bottom. This would mean that the layer could be regarded as a bilayer with two layers having a different thermal expansion coefficient. But the top of the
layer has the largest thermal expansion coefficient (due to the larger Ge% [41]) and thus again the deflection is expected towards the substrate. Other effects can cause the cantilever to bend upwards. A densification of the top layer can result in a tensile stress causing the upwards curvature. The outgassing of H-atoms, which were built in during processing, can also cause a tensile stress at the top of the layer. A detailed study of the morphology of the samples before and after the heating process is needed to find out whether the layer composition has changed or not.

![Figure 6.13: Linear (left side) and gradient contribution (right) to the deflection profile of a 4 µm thick layer.](image)

Now an attempt will be made to calculate the changes in mean and gradient stress from the formulas proposed by Fang et al. [24] (Eq. 5.27), (Eq. 5.28) and (Eq. 5.29)). The radius of curvature from the gradient deflection can be used to calculate the stress gradient. The radius of curvature is determined at 216741 µm and this results in a linear stress gradient $\sigma_1/h$ of 1.356 MPa. With this stress gradient the angular deflection caused by the stress gradient can be calculated: $\theta_1 = 0.007\, \text{mrad}$. From the linear deflection profile the total angle $\theta$ is calculated at 3.03 mrad. This means that $\theta_0 = 3.023\, \text{mrad}$ and $\sigma_0 = 314\, \text{MPa}$. The values for the mean and gradient stress are plausible. The mean stress is expected to consist mainly of thermal stress. The (uniaxial) thermal stress is calculated to be 69 MPa with parameters: $\nu_{\text{SiGe}} = 0.23$, $\alpha_{\text{SiGe}} = 4.3 \times 10^{-6}/K$, $\alpha_{\text{Si}} = 2.6 \times 10^{-6}/K$, $E_{\text{SiGe}} = 147$ GPa. The increase in mean stress cannot be explained by thermal stress. This indicates that other effects play a role in the generation of stress. Similar as explained for the stress gradient, film densification at high temperature can result in a tensile stress and thus a positive deflection. It should be kept in mind that the proposed model was only valid for a layer thickness below 3 µm. An empirical model should be derived using finite element modelling simulations that can be used for this case like was done by Fang et al. [27].

The resulting difference in deflection due to heating of the cantilever cannot be explained by general thermal effects. Existing models are not able to predict the behaviour that is observed. A detailed study of the sample morphology, before and after the heating process, is needed. This can give a better indication of what processes dominate the behaviour at higher temperatures. When these dominating processes are known, new models can be created to predict the behaviour.

### 6.3 Determination of the stress profile for a 4 µm SiGe-layer

The purpose of this experiment was to check the reproducibility of the measurements of Molfese et al. [33] and the correctness of the adapted model. For this purpose samples of the M&M mask with a layer thickness of 4 µm were thinned using the Oxford Plasmalab System 100 as described earlier in section 2.3.2. The lowest layer thickness that could be achieved by thinning was 0.92 µm. There were samples with a smaller thickness, but the cantilevers on
these samples did not survive the release-process, which made it impossible to determine their tip deflection. The layer thickness was determined using the Dektak. The thickness was determined before and after the etching process. A small square sample was put on top of the sample during the etching. By measuring the step in the thickness (due to the small square sample) the final thickness could be determined. The tip deflections were measured using an optical microscope. All the tip deflections of 1mm long cantilevers with a width of 100 µm were determined, except for the thinnest layer. In this case only a cantilever of 100 µm length and 50 µm width was available on the sample. This means that the error on the stress gradient for this thickness is larger. The mean stress of the wafer was determined to be 37.55 MPa using the wafer curvature method.

Table 6.1 shows the measured layer thickness together with the cantilever tip deflection. The right column of the table shows the calculated stress gradient determined with (Eq. 5.54) using a Young's modulus of 147GPa for SiGe. In Figure 6.14 the calculated stress gradients are depicted for each layer thickness. In the same picture polynomial fits of different orders are plotted. The behaviour of these fits is more or less the same in the region where there are measurement points available (central area). The higher the order of the fit, the better the function goes through the data points. In the lower and higher part of the layer the fits all have their own behaviour.

<table>
<thead>
<tr>
<th>Layer thickness (µm)</th>
<th>Deflection (µm)</th>
<th>Gradient (MPa/µm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.02</td>
<td>86</td>
<td>25.1</td>
</tr>
<tr>
<td>3.9</td>
<td>93</td>
<td>27.1</td>
</tr>
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<td>3.43</td>
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<td>110</td>
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<td>1.43</td>
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<tr>
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<td>545</td>
<td>123</td>
</tr>
<tr>
<td>0.92</td>
<td>6</td>
<td>175</td>
</tr>
</tbody>
</table>

Table 6.1: Experimental values for the layer thickness and the cantilever tip deflection together with the calculated stress gradient
Experimental results and discussion

Figure 6.14: Linear stress gradient in function of the layer thickness determined from the tip deflection together with polynomial fits of different orders.

Figure 6.15 shows the calculated stress profiles with the different polynomial fits from Figure 6.14 using (Eq. 5.40), (Eq. 5.41) and (Eq. 5.43). Again the conclusion can be drawn that the stress profile is well defined in region II where there are measurement points. The stress profile is more or less constant and equal to the mean stress of 37.55 MPa determined by the wafer curvature method. To reduce the fluctuation of the profile in the 1 to 4 µm region a larger amount of measurement points is needed. From region I no conclusions can be drawn for the stress profile. The profile in this region is determined by the behaviour of the fit that was used. The only way to get more insight into the behaviour of the stress profile at a smaller layer thickness is to actually achieve these thicknesses and to determine the cantilever deflection. This is very difficult due to the fact that the cantilevers are very fragile for these small layer thicknesses.

For these thin layers a different approach is required. A possible solution is to deposit the layer until the required thickness is achieved. This method makes the etching process superfluous. This approach can be successful because the values for the linear stress gradient obtained in this work come very close to those obtained in Molfese’s work [33] and in Van der Donck’s work [8]. The stress at a certain depth in the layer originates during the growth and is barely influenced during the deposition of the rest of the layer. This method requires less processing steps for the samples and reduces the risk of damaging the samples. The chance for the cantilevers to stay free of damage will be higher. To ensure that the deposition process of top layers does not change the stress in lower lying layers, data points for a certain thickness can be obtained by the two methods (after deposition and after thinning down) and the results can be compared.
To get a better idea of the influence of measurement points for small layer thicknesses the proposed method to achieve these thicknesses is assumed to be true. After the deposition of a 250 nm layer SiGe layer the cantilever was found bending towards the substrate indicating a negative stress gradient. The length of the cantilever was 5000 µm and the deflection was 500 µm. The calculated stress gradient was \(-5.88\) MPa/µm. Figure 6.16 shows the calculated stress profile for different orders of polynomial fits. The stress profile in the 1 to 4 µm region is more or less constant and almost equals the mean stress of 37.55 MPa determined by the wafer curvature method. In the upper part of the layer (above 1 µm) the stress is tensile. The profile has the largest change in the 0.25 to 1 µm region. This is logic because the lowest part of the layer (PECVD seedlayer and CVD layer (see section 2.4)) is expected to have the largest stress contribution. These layers are also expected to be compressive which explains the negative (compressive) stress profile for the smaller layer thickness. Again no conclusions can be drawn from region I due to the lack of measurement points.
6.4 Study of transverse deflection of cantilevers

To study the transversal deflection of cantilevers a mask was designed containing cantilevers of different width and length (see section 2.5). The layer composition is the same as already mentioned in section 2.4. They were released by immersion in a HF-IPA 1:1 solution for 50 minutes. Only the samples with a length of 50 and 100 µm were fully released. This indicates an etch length between 100 and 150 µm. This also means that the samples with a length of 50 µm are highly underetched. This is shown in Figure 6.17. This underetching (yellow lines in the picture) will influence the longitudinal deflection and the transverse deflection profile of the cantilever. The clamping is therefore not at the position where it was expected to be. A vertical cross-section is shown in Figure 6.18. The underetching effect is clearly visible.
Figure 6.17: Measured cantilever surface by optical interference profilometer with indicated underetching (top view)

Figure 6.18: Vertical cross-section of Figure 6.17 showing underetching

Figure 6.19 shows the transverse deflection profile of a 50 µm wide cantilever beam for different widths. The cross-section distortion shows a strange behaviour. There is a concave transverse curvature for the smaller beam which goes to a convex curvature for a wider beam. The underetching and clamping effects probably causes this phenomenon as can be seen in Figure 6.18. These effects are more pronounced for short beam than for long beams.
Figure 6.19: Measured transversal deflection profile for a 50 µm long cantilever
width different width

Figure 6.20 shows the measured cross-section deflection of a 100 µm long cantilever for
different widths determined with the WYKO NT3300 optical profilometer. Again a concave
curvature is observed. This indicates that the transversal deflection is the result of the biaxial
stress state. It also seems that the transverse deflection shows a plate-like behaviour which
might be caused by the clamping.

To check whether the stress state really is the cause for the transversal curvature some FEM
simulations were evaluated. The deflection of a cantilever with a width and length of 1mm
was simulated using the stress profile that was determined by Molfese [33]. The thickness of
the cantilever was 4 µm. A uniaxial and a biaxial stress situation were simulated for a poisson
ratio of 0.23 and 0.3. In Figure 6.21 the resulting transversal deflection is depicted for the case
of a uniaxial stress in the longitudinal direction. Anticlastic (convex) curvature can be
observed in the picture (the longitudinal curvature is concave). The center tip deflection for a poisson ratio of 0.23 is 107.7 µm while the center tip deflection for a poisson ratio of 0.3 is 106.9 µm. This indicates that the beam is stiffer for a higher poisson coefficient and thus the deflection is lower.

![Figure 6.21: FEM simulation of transverse curvature of a 1000 by 1000 cantilever with a poisson ratio of 0.23 (left) and 0.3 (right) using a uniaxial stress](image)

Figure 6.21: FEM simulation of transverse curvature of a 1000 by 1000 cantilever with a poisson ratio of 0.23 (left) and 0.3 (right) using a uniaxial stress

Figure 6.22 shows the simulation of the cantilever deflection for a biaxial stress state with different poisson coefficients. Using a biaxial stress state obviously results in a different transverse deflection profile. The anticlastic curvature has disappeared. The maximal cantilever deflection is lower for the biaxial stress state than for the uniaxial stress state. Again the tip deflection is higher for a decreasing poisson ratio.

![Figure 6.22: FEM simulations of transverse curvature of a 1000 by 1000 cantilever with a poisson ratio of 0.23 (left) and 0.3 (right) using a biaxial stress](image)

Figure 6.22: FEM simulations of transverse curvature of a 1000 by 1000 cantilever with a poisson ratio of 0.23 (left) and 0.3 (right) using a biaxial stress

Figure 6.23 and Figure 6.24 show the simulated transverse deflection profile for a 1000 µm and 50 µm long cantilever, respectively, with different widths and a poisson coefficient of 0.3. In both cases the plate-like effect is clearly visible. For the 50 µm cantilever the central section remains plane for large widths. Although the length of the cantilevers is not the same, there is a good correspondence between Figure 6.20 and Figure 6.23.
The influence of the poisson ratio on the transverse deflection profile of a 50 µm long and 5000 µm wide cantilever using a biaxial stress state is depicted in Figure 6.25. This confirms the possibility to determine the poisson coefficient from the transverse deflection profile of a cantilever even if the transverse deflection is determined by the biaxial stress instead of by the poisson effect.
In this section it was pointed out that the clamping and underetching effects cannot be neglected when evaluating the transverse deflection profile of cantilevers. The transverse deflection is caused by the biaxial stress state. Even induced by a biaxial stress there is a plate-like effect visible. More experiments should be performed with properly designed samples which reduce the effects of clamping and underetching.
7 Conclusions and future work

Poly-SiGe is the most promising material to be used in a monolithic integration with CMOS substrates. Still a lot of material properties are unknown. Also the behaviour of the material has to be studied under various circumstances. In this thesis the surface micromachined poly-SiGe cantilevers play a central role to study some of these unknown properties.

In a first experiment, the effect of thermal heating on the deflection profile of cantilevers was studied. For this purpose a new technique was developed using a scanning electron microscope to determine the deflection profile. The deflection difference due to heating cannot be explained by plain thermal stresses. There are other phenomena that cause a change of the stress situation in the cantilever. One of the possibilities is a densification of the top of the layer, which results in a tensile stress. To get more insight into the processes that take place during the heating, a profound study of the morphology of the sample is needed before and after the heating process.

An adaptation of a model from Molfese et al. is proposed to determine the stress profile of a thin layer by measuring the deflection of cantilevers having a different layer thickness. From this cantilever deflection the linear stress gradient can be calculated. After determining the stress gradients at different thicknesses, a polynomial fit is used to describe the linear stress gradient. From this polynomial fit the stress profile can be calculated. The stress profile for a 4 µm thick poly-SiGe layer is determined by thinning the layers using a low power etching plasma. The model accurately determines the stress profile in the measured region. Outside this region the course of the stress profile is determined by the behaviour of the polynomial fit that was used to fit the linear stress gradient. The stress profile below a thickness of 0.9 µm is still uncertain. A method to achieve measurements at lower thickness is proposed. The stress at a certain part in the layer is almost fully determined by the deposition process of that part and is barely influenced when the rest of the layer is deposited. Stopping the deposition process at the required layer thickness would make the etching step superfluous and reduces the chance to damage the cantilever on the sample.

The last part of this thesis dealt with the transverse deflection of cantilevers with different width and length. In theory the Poisson ratio can be determined from the transverse deflection of a cantilever. For this study new samples were designed and processed. From these samples it could be concluded that the transversal deflection is dominated by the biaxial stress state of the layer. Also the underetching and the clamping play a role in the deflection profile. The transverse curvature undergoes a similar plate-like effect for wider beams. The center part of the tip remains flat. To get more insight in the transverse curvature some FEM simulations were performed. For future work samples should be designed in which the influence of clamping and underetching is minimized (using two masks instead of one). In that case, it should be possible to determine the Poisson ratio from the deflection profile according to FEM simulations as shown in this work.
References


[13] Invitation to the SEM World, JEOL LTD


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