Strain distribution analysis in Si/SiGe line structures for CMOS technology using Raman spectroscopy

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Abstract. Strained silicon underneath the field-effect transistor gate increases significantly the charge carrier mobility and thus improves the performance of leading-edge Complementary Metal Oxide Semiconductor (CMOS) devices. For better understanding of the structure-strain relationship on the nanoscale and for optimization of device structures, the measurement of the local strain state has become essential. Raman spectroscopy is used in the present investigation to analyze the strain distribution in and close to silicon/embedded silicon-germanium (SiGe) line structures in conjunction with strain modeling applying finite element analysis. Both experimental results and modeling indicate the impact of geometry on the stress state. An increase of compressive stress within the Si lines is obtained for increasing SiGe line widths and decreasing Si line widths. The stress state within the Si lines is shown to be a mixed one deviating from a pure uniaxial state. Underneath the SiGe cavities, the presence of a tensile stress was observed. To investigate a procedure to scale down the spatial resolution of the Raman measurements, tip-enhanced Raman scattering experiments have been performed on free-standing SiGe lines with 100nm line width and line distance. The results show superior resolution and strain information not attainable in conventional Raman scans.

1. Introduction

Strained silicon thin film structures have excited an increasing interest during the previous years in basic research as well as for applications in high-performance microprocessor devices. This interest is related to the significant performance gain attainable by utilizing strained films in active transistor regions [1], which will become more important as in future the scaling of device dimensions cannot be continued without changing materials, technology and device architecture. Thus strain has become a key approach for extending CMOS to the next technology nodes.

One potential technique for introducing strain into the channel silicon regions of CMOS devices is employing a lattice mismatch of epitaxially grown film structures. In particular, silicon-germanium (SiGe) solid solution allows the fabrication of films with tunable lattice constants, and thus, it has been used to generate dedicated strain in Si films for improved CMOS performance [2]. To understand the impact of strain on device structures and to be able to optimize it, local measurements of the mechanical strain in such structures are mandatory. A useful technique for strain determination in
silicon is Raman spectroscopy, enabling fast and nondestructive measurements with sub-µm resolution. This technique has the potential of sub-100 nm resolution in combination with near-field approaches [3]. Though still not downscaled to the lateral resolution of single MOSFET channel regions, Raman spectroscopy can be successfully applied to test structures with typical dimensions in the 100 nm range. For data evaluation, Raman measurements on patterned structures require combination with modeling, since usually the Raman signal does not yield the full tensor information related to the strain distribution. Such investigations taking into account the tensorial character of the strain state have been performed e.g. regarding the average strain state in series of parallel SiGe lines, where the asymmetric relaxation, i.e. the presence of larger strains parallel to lines and smaller strains perpendicular to lines was analyzed by ion scattering [4], X-ray scattering [5] and also Raman spectroscopy [6]. However, for understanding of the strain distribution in and close to structures relevant for strained devices, local strain profiles have to be measured, as achieved e.g. by Raman spectroscopy in silicon substrates underneath silicon oxide lines and silicon nitride lines with a µm-scale pitch [7,8]. The strain state in freestanding SiGe lines on a Si substrate was investigated by Jain et al. utilizing analytical modeling and Raman spectroscopy, showing compressive stresses in the lines increasing with reducing line heights [9,10]. This tendency is different for embedded SiGe line structures, as applied for strained Si CMOS technology. Here, an increasing height of the cavities supports the compressive strain in between the SiGe regions. However, above a critical thickness [11] defect formation leading to plastic relaxation can limit the strain level. Though less is known regarding the experimentally determined details of the strain distribution in such structures, valuable information has been obtained by TEM based approaches such as nano-beam diffraction [12] or electron holography [13], which require substantial sample preparation efforts.

In this study, we applied a combination of strain distribution determination by Raman spectroscopy and finite-element modeling (cf. e.g. [14]) on embedded SiGe / Si line structures with varying pitch and line widths ranging from the µm range down to 100 nm in order to study the impact of the line geometry onto the strain state. The combination of both techniques allows deriving predictions from the modeling also for smaller dimensions. This approach can thus provide helpful information to support technology progress and to optimize processes for CMOS manufacturing.

2. Experimental details
For sample preparation, a series of parallel SiO₂ lines was deposited onto (001) Si wafers, followed by etching of 45 nm deep cavities into the silicon between the lines and subsequent deposition of SiGe with a germanium content of 30 at% using a chemical vapour deposition (CVD) process. Thus, patterns of embedded SiGe/Si line structures were obtained with different SiGe line widths $w_{\text{SiGe}}$ varying between 1 µm and 3 µm and Si line widths $w_{\text{Si}}$ varying between 100 nm and 420 nm (cf. figure 1a). The lines with a length of 100 µm were arranged on pads of respective size (100 µm × 100 µm).

![Figure 1. SEM cross section of the Si/SiGe line structures (image source: ISMI).](image)

For the Raman measurements on these structures a Jobin Yvon HR800 spectrometer was used, equipped with 458 nm Ar excitation laser and a 100x objective (NA = 0.9) focusing the laser beam to
a spot size of about 1 µm. The penetration depth of the laser radiation is approximately 300 nm in the Si and about 200 nm in the regions capped with SiGe. Near-field Raman measurements were performed also in a backscattering setup on a MV 2000 system (Renishaw / Nanonics) using a 488 nm Ar-ion laser excitation and Au/Ag coated quartz tips for near-field enhancement.

Additional high resolution X-ray diffraction (XRD) reference measurements were performed utilizing a Bruker AXS D8 diffractometer equipped with copper rotating anode and video laser alignment system, enabling measurements with a beam size of 100 µm.

3. Measurement results

Figure 2 shows both the XRD measurement results and the Raman spectrum obtained on an unpatterned SiGe region. The XRD measurement of the Si and SiGe 004 reflections enables an accurate determination of the SiGe film thickness \( t \) and of the Germanium concentration \( x_{\text{Ge}} \). It indicates a fully strained state of the SiGe due to the pronounced film wiggles. This strain state is quantitatively confirmed by the relaxation scan performed on the SiGe 224 reflection (inset). For evaluation of the Raman data (figure 2b) with respect to composition and strain, the positions of the SiGe film related peaks denoted as “Si-Ge” and “Si-Si”, and of the reference Si peak “Si-Si bulk” were used. Whereas the positions of the film peaks are shifted with respect to those of an unstrained (fully relaxed) SiGe film, no shift of the Si bulk peak position with respect to that of an unstrained pure Si wafer was detected on this unpatterned SiGe region. Thus for scans on patterned structures, the shifts of the peaks compared to the unstrained Si bulk peak position given in figure 2b were determined.

![Figure 2](image)

**Figure 2.** XRD measurement of the SiGe 004 reflection and the 224 reflection (inset) as measured on an unpatterned SiGe pad without Si lines (a, left), and Raman spectrum measured as reference in the center of this pad (b, right) containing the Si bulk peak and three SiGe related main peaks. Apart from these first-order phonon modes, a weak SiGe-related peak at 440 cm\(^{-1}\) is observed (cf. [15]).

To investigate the strain profile of the Si and SiGe line structures, scans oriented perpendicular to the lines across structures with different line widths \( w_{\text{Si}} \) and \( w_{\text{SiGe}} \) were performed. The Raman peak intensities show maxima of the Si signal and minima of the SiGe signal on the Si line positions, matching with the SEM measured geometry. Accordingly, also a characteristic dependence of the Raman peak positions on the scan coordinates was observed as shown for the example of two patterns with different pitch and line width in figure 3a,b. The dashed and dotted horizontal lines represent the positions of the reference peaks measured on the unpatterned regions, corresponding to the positions of the unstrained silicon and fully strained SiGe, respectively. The wavenumber of the Si bulk peak (black squares, upper curves) is maximum on the Si line positions and minimum in between them,
with its average close to the reference bulk Si wavenumber. In contrast, the SiGe film peak position (grey circles, lower curves) is minimum at the Si lines and maximum on the SiGe cavity centers with a remaining offset to its reference position for all points on the pattern. The resulting question whether this offset is due to an onset of plastic relaxation or due to elastic strain in these structures has been analyzed making use of FEM modeling as shown below. Comparing figures 3a and b, it is clearly visible that the variation of the peak position depends sensitively on the line geometry. For smaller line widths (figure 3b), reduced variation of the peak positions is observed. Furthermore, also the average position of the film peak shifts towards the (fully-strained) reference value for smaller Si line widths.

\[ \sigma_{xx} = \sigma_{yy} = -235 \text{ MPa cm } \Delta \omega_3 \]  \hspace{1cm} (1)

**Figure 3.** Variation of the Raman wave number \( \omega \) for scans across two Si lines in between embedded SiGe regions for the geometry parameters \( w_{Si} = 420 \text{ nm}, w_{SiGe} = 2550 \text{ nm} \) (a, left) and \( w_{Si} = 100 \text{ nm}, w_{SiGe} = 1000 \text{ nm} \) (b, right). The upper curves show the Si bulk peak shift, and the lower ones the film peak shift. The coordinates \( x \) and \( y \) are aligned perpendicular and along the lines, respectively (cf. figure 1).

**4. Evaluation of Raman measurements and finite-element modeling**

To analyze the mechanical strain state related to the measured Raman shifts \( \Delta \omega \) in a silicon crystal, generally three eigenvalues of a matrix [16], leading to a cubic equation have to be determined. For the given geometry of backscattering from a Si (001) surface, only one mode (denoted as longitudinal phonon mode) \( \omega_3 \) is observable [17]. Whereas for the complex strain state within line structures the general secular equation has to be solved [16], for the special case of the unpatterned SiGe pad significant simplifications can be utilized. Assuming the silicon to be bisotropically strained, i.e. equal-axis biaxially strained with \( \sigma_{xx} = \sigma_{yy} \) (cf. [18]) and vanishing remaining stress components, a factor coupling the measured peak shift and the Si stress can be derived [3]:

\[ x_{Ge} = \frac{\beta_2 (\omega_{SiGe} - \omega_{SiSi,0}) - \beta_1 (\omega_{SiGe} - \omega_{SiGe,0})}{\alpha_1 \beta_2 - \alpha_2 \beta_1}, \]  \hspace{1cm} (2a)

\[ R = 1 - \frac{\omega_{SiSi,0} - \omega_{SiGe,0} - \alpha_x x_{Ge}}{\beta_x x_{Ge}}, \]  \hspace{1cm} (2b)
where $\alpha_1 = -62 \text{ cm}^{-1}$, $\beta_1 = 30.5 \text{ cm}^{-1}$, $\alpha_2 = 19.5 \text{ cm}^{-1}$ and $\beta_2 = 23.9 \text{ cm}^{-1}$ are fixed parameters. $\omega_{\text{Si-Si}}$ and $\omega_{\text{Si-Ge}}$ denote the SiGe film peak positions of the Si-Si and Si-Ge mode, respectively, and $\omega_{\text{Si-Si,0}}$ and $\omega_{\text{Si-Ge,0}}$ are the corresponding reference peak positions for vanishing Ge content. Thus, for the stress in the bisotropically strained SiGe results

$$\sigma_{xx} = \sigma_{yy} = (1-R) \sigma_0 , \quad (3)$$

where $\sigma_0$ denotes the stress for a fully strained SiGe film.

The application of the equations (2) to the measurement on the unpatterned position (figure 2b) yields a Ge content of 30.0 % and a relaxation parameter $R = 0$. Correspondingly, for the biaxial compressive stress within the SiGe we obtain a value of $\sigma_{xx} = \sigma_{yy} = -1910 \text{ MPa}$. To analyze also the Raman scans across the line structures, this information can be used to reduce the noise in the scans. If according to equations (2) both SiGe peaks are evaluated, due to the low intensity of the SiGe mode and the limited measurement time per spectrum during a line scan, a significant scattering of the obtained data for $x_{\text{Ge}}$ and $R$ results. The scattering of $R$ can be reduced when assuming the Ge content within the pattern to be constant and thus all variations of the Raman peak positions to be strain related. With this assumption used in the following, only the Si-Si modes are considered for strain evaluation on the pattern, and a significant noise reduction is achieved (cf. figure 4). Note that on the patterned structure the occurrence of $R$-values does not necessarily indicate the onset of plastic relaxation, which will be discussed in detail below (figure 7). Due to the averaging of the Raman signal across the laser spot, there also appears a remnant SiGe signal on the positions of the Si lines.

The shift of the SiGe curves on the positions of the Si lines towards lower wavenumbers (figure 3a,b) corresponds to a reduction of compressive stress within the SiGe, whereas the upshift of the Si curves at these positions indicates compressive stress within the Si lines (cf. equation (2b)). To analyze these features in more detail, FEM calculations were performed using ANSYS 9.0 with a geometry according to figure 1, i.e. a free surface on top and periodic boundary conditions on the right and left. The lattice mismatch between Si and SiGe was modeled by a thermal strain, i.e. by introducing different coefficients of thermal expansion and rising the temperature accordingly as initial condition. As a result of the modeling, nearly fully compressively strained SiGe regions with compressively stressed Si lines in between and regions of tensile strain underneath the layer were obtained (figure 5).

Within the Si line, the amount of stress $\sigma_{xx}$ reduces with increasing depth. At a depth of about 500 nm beneath the surface of the Si line, a change from compressive to tensile stress occurs. In contrast, the tensile stress in the silicon beneath the SiGe regions is concentrated only in a thin stripe. Thus, according to the penetration depth of the laser, only a small shift of the bulk silicon peak is observed in the Raman scans. At the edges of the SiGe regions, a stress concentration occurs, in agreement with the observed stress concentrations close to edges of patterned strained SiN film structures [8].
Figure 5. Calculated distribution of the stress component $\sigma_{xx}$ for a geometry according to figure 1 ($w_{Si} = 420$ nm, $w_{SiGe} = 2550$ nm). The Si line is on the top center surrounded by the (dark) SiGe regions.

For all measured line geometries, the experimentally derived stress data utilizing the bisotropic assumption (equations (2)) are matching the FEM calculations for the SiGe regions. The geometry of the SiGe cavities yields a stress state which is at their center close to that of an infinite biaxially strained film. However, a clear mismatch between the stress values derived from equation (1) and the FEM calculations results for the Si regions. This gives rise to reconsider the assumption of a simple bisotropic strain state within the Si for the Raman scan evaluation. For more detailed analysis of the stress tensor, we calculate a parameter $S$ with

$$S(x) = \frac{|\sigma_{xx}| - |\sigma_{yy}|}{|\sigma_{xx}| + |\sigma_{yy}|},$$

where $S = -1$ or $+1$ corresponds to a uniaxial stress state in $y$ or $x$ direction, respectively, and $S = 0$ results for the bisotropic stress state. The stress component $\sigma_{zz}$ is small compared to $\sigma_{xx}$ and $\sigma_{yy}$ (cf. figure 8b) and thus neglected in the following.

The contour plot of the parameter $S$ shows that the assumption of biaxial stress in SiGe is reasonable ($S \approx 0$), but not further valid for the silicon regions (figure 6). As the SiGe region gets narrower, the assumption of biaxial stress is not valid furthermore. However, in our experiments the width of the SiGe regions was always larger than the Si line width, yielding a deviation of less than 3% at the SiGe center and less than 30% at the edges from the bisotropic stress state ($|S| = 1$).

Figure 6. Contour plot of the stress distribution parameter $S$ for the geometry according to Figure 1.
The stress state in the silicon regions shows a different behaviour, i.e. $S$ varies between -1 and +1 there. According to the performed line scans, along horizontal paths the parameter $S(x)$ can be calculated and utilized for a generalization of equation (3), yielding for the component $\sigma_{xx}$

$$\sigma_{xx} = (1 + S) (-235 \text{ MPa cm}) \Delta \omega$$  \tag{5}$$

Using this approach for the experimentally derived stress distribution, both for the Si and for the SiGe regions, curve matching with the FEM modeling was obtained (figure 7). Consequently, the elastic strain state in the structures is concluded to be fully responsible for the measured Raman peak shifts; i.e. no onset of plastic deformation is detected (neither on the unstructured pad nor on the line structures). Therefore, the $R$ parameter calculated in equation (2b) is a formal quantity reflecting here the elastic strain state, in contrast to its usual interpretation on unpatterned films as parameter for the plastic deformation related strain relaxation.

![Figure 7](image_url)

**Figure 7.** Comparison of experimentally derived stress data and FEM results for a scan across the line structure according to figure 1. Evaluation of the Raman SiGe peak (a, left) and the Si peak (b, right) was performed. The dashed line represents the SiGe stress value as measured on the unstructured pad (fully strained SiGe film). Due to the averaging of the Raman signal across the laser spot, there appears also a remnant SiGe signal on the positions of the Si lines, representative for the edges of the SiGe regions.

According to the size of the laser spot of $\sim 1\mu$m, for the comparison with experimentally determined curves an intensity weighted average of all calculated local peak shifts was considered (cf. [19, 20]). The variation of the geometry parameters of the investigated line structures enabled to investigate directly the impact of geometry onto the mean stress within the Si and SiGe lines. For the SiGe lines, the absolute mean values of the compressive stress $\langle \sigma_{xx} \rangle$ are increasing with increasing width of the SiGe lines (figure 8a). Accordingly, a similar tendency is obtained for the stress components $\sigma_{xx}$ and $\sigma_{yy}$ within the Si lines, whereas $\sigma_{zz}$ is negligibly small (figure 8b). In real device structures the lateral extension of the SiGe regions is limited due to the positions of adjacent MOSFETs. However, the present experiments show also a gain of compressive Si line stress for reduced Si line widths. An upper limit of Si line stress is defined for a given Ge content in the SiGe regions by the strain of a correspondingly fully strained SiGe film. For small Si line widths below 50 nm, it has to be considered that the approximation of vanishing vertical stress $\sigma_{zz}$ is not longer valid. A significant amount of vertical stress in the tensile range is obtained, which has (beneficial) influence onto the hole mobility in the PMOS channel [14]. The performed Raman line scans give direct evidence for this impact of downscaling onto the silicon stress and prove experimentally that local stress introduction will be an important approach also for future technology nodes with further reduced channel dimensions.
Figure 8. Mean SiGe stress (a, left) and the stress at the center of the Si line in 20 nm depth (b, right) as a function of the SiGe line width $w_{SiGe}$ ($w_{Si}$=420 nm). Experimental values are marked by squares and error bars.

5. Raman investigation with enhanced spatial resolution

For strain measurements with enhanced spatial resolution, near-field approaches are increasingly considered, since they can maintain such advantages of optical techniques as low sample preparation effort and high strain sensitivity while having the potential for nanoscale spatial resolution. In particular, tip-enhanced Raman scattering (TERS) was utilized successfully on silicon structures, as shown e.g. by Sun and Shen on patterns with a relatively large periodicity length (>500 nm, cf. [21]). Improved resolution on patterns with a pitch down to ~250 nm pitch was obtained with Ag coated tips on strained silicon line structures [22]. Downscaling the strain resolution in silicon is difficult compared to other material systems not only due to technical issues (regarding e.g. an accurate control of the special tip geometry needed for backscattering and thus control of the near-field), but also due to the limited knowledge of the real strain distribution in the used silicon nanostructures. Thus, the above presented FEM approach was adapted to the samples used in the near-field experiments and carefully compared with the measurement results. For these experiments, on a fully strained SiGe film with 23at% Ge content, oxide lines were drawn by local anodic oxidation with an atomic force microscope (AFM) and used as mask for subsequent wet-chemical etching. As a result, a group of five free-standing SiGe lines with a height of 40 nm, a width of 100 nm and a line distance of 100 nm were obtained. Since the etching of the SiGe was stopped 10 nm above the interface to the silicon underneath, a thin fully strained SiGe film was retained on the sample surface as reference. Figure 9a shows the intensity distribution of Raman scans performed across these lines both without a tip in the laser beam and with the Au coated tip in feedback. Interestingly, not only the SiGe signal but also the Si signal is enhanced on the structures for both measurement modes. The enhancement of the Si signal can be explained by a scattering effect on the edges of the SiGe lines, resulting in an increased Raman scattering from the Si regions close to these edges. A striking feature is the clear resolution of all the lines in the measurements with the tip in feedback, which is not achievable in the conventional Raman scans. In the measurement performed with the tip in feedback, also in the Raman peak shift the signature of the single lines is visible. The increased spatial resolution of the scans with the tip in feedback can be explained by the excitation of plasmons in the apex of the Au tip, yielding an enhancement of the field in a region close to the tip. In the experiments, an enhanced SiGe film signal of about 25% compared to the conventional Raman measurement was obtained. By comparison of the measurement results with the FEM calculations (figure 10), a range for the field enhancement of about 200 nm has to be assumed to obtain reasonable agreement between the measurements and the strain calculations.
Figure 9. Conventional µRaman and TERS scans across free standing SiGe lines: Intensity (a) and peak shift (b). For details of the TERS scan setup cf. [22].

Figure 10. Average profiles, derived from the TERS-scan, for the Si stress (a) and the SiGe stress (b).

The strain distribution of free-standing lines differs essentially from that of embedded SiGe lines (figure 7). The downshift in the Raman signals for the freestanding lines indicates a relaxation of the compressive SiGe stress according to an average relaxation value of \( R = 20\% \) within the lines, and an average tensile stress in the silicon underneath. This tensile stress is enhanced at the positions just underneath the lines (figure 10). The results indicate that the description of the strain state with the used FEM approach reflects the measurement results appropriately and can thus be used for the analysis of the local strain distribution in strained silicon structures.

6. Summary and conclusions
Raman line scans across Si / SiGe line structures revealed local strain profiles in conjunction with finite element modeling, enabling a systematic investigation of stress relaxation effects compared to the stress in an unpatterned SiGe film. In the Si lines between the SiGe, a compressive stress is obtained, whereas underneath the SiGe a tensile Si stress was observed. As shown by careful comparison with modeling, the stress relaxation for the here investigated embedded SiGe structures is
of elastic nature, i.e. obtained without onset of additional plastic relaxation. The stress state within the SiGe filled cavities can be assumed roughly to be a bisotropic one with $\sigma_{xx} = \sigma_{yy}$, whereas in the silicon a mixed stress state is present which can be described by a parameter $S$. The measured compressive stress in the silicon lines is sensitive to the line geometry. It can be increased e.g. by increasing the SiGe cavity widths and by reducing the Si line widths, supporting an increase of charge carrier mobility and thus the performance of CMOS devices. Significantly increased spatial resolution can be obtained in Raman measurements utilizing tip-enhanced Raman scattering, as shown on free-standing SiGe line structures. A strain resolution for SiGe lines separated by a distance of 100 nm was obtained, which can be further improved by optimizing the tip geometry and still more accurately controlling the tip position within the laser beam.

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