Numerical investigations of the strain behavior in nanoscale patterned strained silicon structures

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Abstract

The physical properties of materials can be manipulated by applying stress or strain. For instance, the controlled introduction of strain in silicon (Si) devices was found to increase the charge carriers mobility and modify the Si optical properties. The exploitation of this potential technology raises fundamental questions on strain and stress stability and behavior during the fabrication and processing of strained Si devices. In this paper, we address this issue and provide detailed three-dimensional finite element simulations of strain redistribution upon nanoscale patterning that is a crucial step in the fabrication of devices. The shown calculated results give valuable insights into the relaxation phenomenon of nano-scale strained silicon mesa-structures and point out ways to modify the strain field in one-dimensional optical micro-cavity waveguides based on photonic crystal designs. Our calculations are augmented by experimental data obtained by UV μ-Raman spectroscopy analysis.

1. Introduction

"Stress engineering" is a promising approach to enhance the physical properties of semiconductor materials. Indeed, the controlled manipulation of strain or stress in semiconductor devices can lead to novel or improved functionalities [1, 2]. This phenomenon has been exploited to boost the performance of the complementary metal-oxide-semiconductor (CMOS) devices in the 65 nm technology node and below. This has sparked a surge of interest in both the implementation of processes for strain manipulation and the development of methods for accurate estimation of the strain within the devices. In this vein, strained silicon-on-insulator (sSOI) has attracted a great deal of attention as the material of choice for performance enhancement to respond to the relentless course towards device miniaturization.

Depending on the nature of the strain (tensile or compressive), the electron- or hole-mobility can be significantly increased with respect to their values in bulk silicon [3]. Uniaxial and biaxial strain are the two methods presently applied in the manipulation of the carrier mobility in the channels of Si field effect transistors. Each type of strain influences the performance in a different way, because each has a different effect on Si band structure. Both uniaxial and biaxial strain break the 12-fold symmetry of the unstrained Si band structure. For biaxially strained Si, the mobility enhancement originates from scattering reduction.

In a similar way, the optical properties of silicon—which is transparent in the infrared range - can be influenced by strain fields in optical devices. In contrast to semiconductor materials like gallium arsenide, Si is not suitable for optical active devices based on second order nonlinear light-matter interaction. This is due to the atomic lattice of Si, which shows an inversion-symmetry. This in turn implies that all even order contributions to the nonlinear susceptibility vanish. Here, the application of a strain gradient can remove the symmetry giving rise to a strain dependent second order nonlinear susceptibility [4]. This newly acquired property of silicon can be used to create devices based on second harmonic generation (SHG) or the electro-optical effect [5]. It is to be pointed out that contrary to strained electrical Si-structures, where a high strain is needed, in nonlinear photonic structures the important parameter is the strain gradient. The nonlinear effects can be further enhanced by using a proper photonic design like slow-light photonic crystals [5] or one-dimensional microcavity waveguides with high quality factors [6].

The introduction of strained materials in the fabrication process raises questions about the stability and the influence of the patterning of the structures to the resulting local strain tensor, because during the patterning, relaxation of the free edges occurs, which influences the strain field with implications for the performance as well as the design of strained devices.

Hence, the objective of this work is to predict the strain redistribution in sSOI nanostructures after patterning with a continuum mechanical approach, assuming dislocation-free monocrystalline silicon material with orthotropic mechanical behavior. The continuum numerical calculations were realized by the use of ANSYS V12.0 for the structure mechanical studies and COMSOL 3.5a with RF-module for the additionally shown electromagnetic field calculations. Despite that the dimensions are on the nanometer scale, atomistic and continuum mechanic methods remain valid even for layer thicknesses over five monolayers [7], assuming that there are no inhomogeneities in the investigated material.

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The presented results are relevant to Si-based electronic and photonic applications. In the first step, the strain relaxation in sSOI nanostructures is investigated in detail for rectangular structures with different aspect ratios. The calculated results are compared with the experimental data obtained from µ-Raman measurements. The second part deals with the design of nanoscale one-dimensional waveguides in comparison to different geometry ratios as well as the influence of the deposition of additional intrinsic strained layers.

The preparation of the sSOI substrates was realized by the heteropitaxial growth of Si thin layers on silicon-germanium (Si$_{0.84}$Ge$_{0.16}$) [8] and the transfer onto SiO$_2$/Si handle wafers by combining wafer bonding, hydrogen ion-induced thin layer transfer and etch-back techniques. The arrays of rectangular sSOI nanostructures were realized by electron-beam lithography and reactive etching. The initial biaxial tensile strain in the unpatterned layer is ~0.6%. The design studies for the optical components consider sSOI-wafer approaches for the strain generation as well as applied intrinsic layers. The strain investigations predict the strain modification options in a theoretical manner regardless of possible practical challenges like the realization of sufficiently thick strained Si layers.

2. The relaxation behavior of sSi-mesa structures

In order to get insight into the relaxation effects of nanoscale patterning processes, numerical investigations were performed and compared with measurements to get a deeper understanding of the current strain state. The described investigations include sSi nanostructures with lateral dimensions in the range of 80-400 nm and a thickness of 20-60 nm. A representative set of the investigated nanostructures is shown in Figure 1 displaying scanning electron microscopy images.

![SEM images of patterned nano-SSOI structures: a) 400 nm x 200 nm; b) 200 nm x 200 nm](image)

The strain measurements were performed by a UV µ-Raman system operating with a 325 nm He-Cd laser line, which has about 10 nm penetration depth in Si. Here Raman-shift is empirically correlated to the averaged biaxial strain ($\varepsilon_{xx} + \varepsilon_{yy}$) (Eq.1, $\omega_{\text{Si}}$ is the Raman shift frequency [9]), additional information of the strain distribution is needed.

$$\varepsilon_{xx} + \varepsilon_{yy} = 0.246 \times (\omega_{\text{bulk}} - \omega_{\text{strained}}) \quad (1)$$

By the use of a three dimensional FE-model of the nanostructures (Figure 2), the strain distribution for different dimensions is calculated. In order to compare the µ-Raman measurements with the calculations, the estimated strain was averaged over all sSi-elements in the model on the top 10 nm of the nanostructure.

![3D-FE quarter model of the mesa structure (400 x 200 x 60 nm)](image)

Because of the calculated local strain distribution of the strain tensor over the structure, a useful value, equivalent to the experiment is chosen. Figure 3 shows the graph of different strain values as a function of the structure width. All other parameters are constant (width x 200 nm x 60nm).

![Averaged strain for measured and calculated equivalent strain values (width x 200 nm x 60nm)](image)

For all data, the general trend is the increase in the post-pattering strain with the width. No absolute quantitative agreement is, however, observed between experiment and calculations. Especially in the smaller dimension range, where no uniform strain distribution exists, varieties of the behaviour and magnitude between measurement and calculation can be noticed. In this region, the homogenous strain state in the center (uniaxial or biaxial over a wide range) changes to a multiaxial state with a highly local dependence. Additionally, a non-linear behavior of the strain / structure-size relation could be found in the lower dimension range.

In addition, the influence of the thickness on the residual strain is experimentally and theoretically examined for a 120 nm x 200 nm structure with a height of 20 nm and 60 nm. The measured Raman-shift...
and the corresponding calculated strain distribution are shown in Figure 4 and Figure 5, respectively.

\[ \text{Figure 4: Measured Si-Si Raman shift} \]
\[ \text{(120 x 200 x 20 & 60 nm)} \]

\[ \text{Figure 5: 3D-FE results of the first principal strain} \]
\[ \text{(400 x 200 x 60 & 20 nm)} \]

Here, a high strain relaxation on the top of the thicker structure (Figure 5a) can be observed, whereas a nearly uniaxial strain distribution exists on the center of the lower structure in Figure 5b. In this case, the strain tendency is in good agreement with the calculations, nevertheless a small underestimation of the absolute strain magnitude is shown in Figure 6.

\[ \text{Figure 6: Influence of the structure height to the} \]
\[ \text{strain (400 x 200 x 20 & 60 nm)} \]

3. The relaxation behavior and design optimization of strained nano photonic devices

An additional potential application of stress-engineered Si deals with the simulation of strained nano photonic components namely SOI based ridge waveguides with photonic crystal micro-cavities, which can be used for optical switches and modulators in telecommunication devices.

In order to break the inversion symmetry of Si, the influence of the design parameters and the aspect ratio on the resulting strain gradient was determined. The created 2D finite element model of the cross-section of a one-dimensional ridge waveguide is shown in Figure 7.

\[ \text{Figure 7: 2-dimensional FE-model of the} \]
\[ \text{one-dimensional strained waveguide} \]

Because a large part of the propagating light is confined in the middle of the waveguide (shown by the magnetic field in Figure 8b), the strain in the symmetry plane and its gradient in x-direction were examined in the calculations. Thereby, the complexity and the local distribution of the strain tensor can be reduced to the first principal value (\( \varepsilon_1 \), in Figure 8a).

\[ \text{Figure 8: a) Sketch of the strain distribution (first} \]
\[ \text{principal); b) Distribution of the propagating light} \]
\[ \text{(correlating to the calculated magnetic field;} \]
\[ \text{TE-polarization)} \]

The numerical investigations contain three theoretical approaches for strain introduction:

I. using sSOI-wafer (the Si-layer is pre-strained by 0.6%),
II. using an unstrained SOI-wafer with the deposition of additional intrinsic strained Layers (SiO\(_2\), SiN: +/-300 MPa),
III. a combination of both (sSOI-wafer and the deposition of epitaxial strained layers).

The effect of the aspect ratio \( m \) (Eq.1) is shown in Figure 9 for the sSOI-design (I), where the remaining strain in the structure decreases with the thickness (\( h_{SS} \))

\[ m = \frac{b}{h_{Si}} \]
\[ n = \frac{h_{ss}}{h_{SiO2}} \]
of the sSi-waveguide. For a ratio of $m \sim 2.5-3.5$, a saturation of the strain relaxation is noticeable. In this case, the highest mean value of the strain gradient can be found (Figure 9b). Thereby, a homogenous and highly strained waveguide could be realized while keeping the thickness low.

Figure 9: Strain (a) and strain gradient (b) distribution under effect of aspect ratio $m$

In order to realize a strained waveguide only by the deposition of an intrinsic strained layer (II), the effect of the ratio between layer thickness and structure height ($n$) is shown for three waveguide heights and an intrinsic stress of $+300$ MPa in Figure 10a,b. According to this diagram, the maximal strain and the strain gradient could be increased by the enhancement of the deposition thickness, where saturation at about 100 nm layer thickness can be found. In this case, the parameter $m$ has no impact on the strain distribution.

Figure 10: Strain (a) and strain gradient (b) distribution under effect of the intrinsic layer thickness

When combining both concepts (III) to create a strained waveguide, a superposition of the resulting relaxation effects is possible. As presented in Figure 11a, a reduction of the strain relaxation in contrast to the concept (I) can be achieved by a tensile or compressive layer. Furthermore, for intrinsic tensile layers, it is possible to create a symmetrical strain field over the waveguide combined with a high mean value of the remaining strain, in comparison to the mean value of a strained structure without a deposited layer.

Figure 11: Strain (a) and strain gradient (b) distribution in combination of intrinsic layers and sSOI-wafer
The ascertained design rules for the waveguides can also be transferred to more complex components like the ridge waveguides with photonic micro-cavity shown in Figure 12a. Here, the holes forming the photonic micro mirrors, lead to an excessive increase of the electro-magnetic field in the cavity, as shown in Figure 12b, significantly enhancing the nonlinear light-matter interaction in the sSi.

Figure 12: a) 3D-model of the photonic micro cavity; b) Calculated electric field in the cavity

The first principal strain of the PhC is shown in Figure 13 for a) with a sSi-wafer design (I), b) a intrinsic strained layer design (II) and c) the combination (III). Especially in Figure 13a) and c), an additional strain concentration is observed in the region of the cavity with a maximum of the remaining mean strain in the design (III). In comparison with type (I) and (III), the relaxation of the holes can be prevented by the applied intrinsic layer. This insight of the strain state in the cavity of the PhC is one essential part to explain and correlate measured optical effects with the strain state.

Figure 13: First principal strain of the PhC: a) design (I); b) design (II); c) design (III)

4. Conclusions
This work shows that continuum mechanical approaches can be used advantageously to predict the effect of strain relaxation in pre-stressed Si substrates after nano-scale patterning. The calculated results were compared with μ-Raman measurements, and the general trend shows a close correlation between experimental data and calculated results, demonstrating the reliability of the applied approach. Moreover, theoretical investigations were also performed to use the numerical capabilities for the sample layout of optical components in order to reach high strain gradients and to consequently improve their non-linear optical properties.

The related results contribute to a better understanding of the complex strain behavior in functional nanotechnology components and can be applied to support their design in terms of optimized electrical or optical functionality.

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