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Closely spaced SiGe barns as stressor structures for strain-enhancement in silicon

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We present tensile and compressive strains realized within the same Si capping layer on an array of SiGe islands grown on pit-patterned (001) Si substrates. The strain distributions are obtained from synchrotron X-ray diffraction studies in combination with three-dimensional finite element calculations and simulations of the diffracted intensities. For barn-shaped islands grown at 720 °C with average Ge contents of 30%, the Si cap layer is misfit- and threading-dislocation free and exhibits compressive strains as high as 0.8% in positions between the islands and tensile strains of up to 1% on top of the islands. © 2013 American Institute of Physics. [<http://dx.doi.org/10.1063/1.4789507>]

Strain-induced modifications of the band structure of semiconductor hetero- and nanostructures and concomitant changes of their electronic transport and optical properties have been investigated experimentally and theoretically in great detail.^{1,2} Apart from basic physics considerations, the interest was triggered by the fact that strained systems allow for improved characteristics both in electronic³ and optoelectronic^{4,5} devices. In metal-oxide semiconductor (MOS) technology, strained Si-channels are used to enhance the performance of field-effect transistors (FET).⁶ Biaxial tensile strain is employed to increase electron mobility in n-channels, uniaxial compressive strain to enhance hole mobility.⁷ A comprehensive review on the influence of strain on groups IV and III-V channel MOSFETs for different crystallographic channel directions, including electric confinement and two-dimensional (2D) density of states was given by Sun *et al.*⁸

Following a concept suggested by Schmidt and Eberl,³ we have recently shown that quite high tensile strains in the order of 1% can be achieved in Si without introducing dislocations by depositing a Si cap layer on dome-shaped SiGe islands grown in the Stranski-Krastanow mode.^{9,10} With such structures, n-channel MOSFET devices were fabricated referred to as *Dot-FETs*, which were processed with the main gate segment above the strained Si layer on a single dot.¹² To prevent intermixing within the Si/SiGe/Si structure and degradation of its crystalline quality, a low-temperature FET fabrication procedure with all processing steps below 400 °C has been implemented. Despite deficiencies of the gate stack which led to degradation of strain values,¹¹ an average increase in the drain current of up to 22.5% was obtained compared to unstrained reference devices.¹³

Kar *et al.*¹⁴ suggested to improve Si p-channel characteristics by employing closely spaced dome-shaped SiGe

islands. Here, the lattice constant mismatch between the SiGe island and Si causes the region of the Si-cap between the islands to be under uniaxial compressive strain as shown by numerical strain simulations.

In this letter, we present investigations of a 30 nm Si layer featuring both biaxial tensile as well as uniaxial compressive strain based on that concept. Perfectly ordered 2D arrays of SiGe islands were grown on prepatterend Si substrates and capped with Si by molecular beam epitaxy (MBE). Here, barn-shaped islands with a higher aspect ratio (AR) and hence a larger elastic relaxation than domes are employed. We performed atomic force microscope (AFM) and transmission electron microscope (TEM) investigations to study the morphology and crystalline quality of the samples. X-ray diffraction (XRD) techniques combined with finite element method (FEM) calculations and simulations of the scattered X-ray intensities were used to determine the strain fields in the Si cap layer both in the regions between the islands and above the islands. Compressive strain values as high as 0.8% and tensile strains as high as 1% make it possible to implement CMOS devices on such closely spaced island structures with the n-channel situated in the tensile strained region above and the p-channel in the compressively strained areas between the islands.

Silicon (001) substrates were patterned by electron beam lithography and reactive ion etching resulting in circular holes with a diameter of 180 nm and a depth of 75 nm. The holes are arranged in a regular 2D pattern in a square-shaped alignment with 300 nm periodicity. After an *ex-situ* cleaning procedure,¹⁵ the samples were loaded into the MBE chamber. During the growth of the 45 nm Si buffer layer, the temperature was ramped up from 450 to 550 °C followed by the deposition of 26 ML Ge at a temperature of 720 °C and a growth rate of 0.05 Å/s. 30 nm of Si-cap was grown subsequently on one of the samples. The substrate temperature was kept at 400 °C for the first 10 nm and ramped up to 450 °C for the rest of the Si-cap (growth rate 1 Å/s).

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The surface morphology was studied by AFM operating in tapping mode, images and the corresponding surface orientation maps (SOM) as insets are shown in Fig. 1. The uncapped islands are of perfect barn-shape¹⁶ as seen in Fig. 1(a) with $\{105\}$, $\{113\}$, $\{15323\}$, $\{20423\}$, $\{23420\}$, and $\{111\}$ facets. The average height of the islands is 75 nm and their diameter 235 nm, resulting in an AR of 0.32. The morphology of the capped sample is shown in Fig. 1(b); the structures above the SiGe islands have an average diameter of about 237 nm and a height of 70 nm (AR=0.3). At their apex, the four $\{105\}$ top-facets are almost completely replaced by a $\{001\}$ facet. In between the islands, the Si cap-surface is defined by two sorts of $\{11n\}$ facets with inclination angles of about 6.5° and 12° , respectively, and $\{001\}$ plateaus in the center between four islands. For comparison, AFM line scans of both the uncapped and the capped samples are displayed in Fig. 1(c).

The structures were investigated using a JEOL FasTEM at 200 keV. The specimens were prepared along the $[110]$ direction by a focused ion beam instrument. The image shown in Fig. 2(a) was taken in bright field (BF) mode. The cross sectional TEM images show that the Si cap layer exhibits a nearly congruent overgrowth of the SiGe islands, and the barn shape of the buried islands is preserved perfectly, i.e., no evidence for significant intermixing between the island and Si cap was found.

XRD measurements were carried out at the beamline P08 at Petra III (DESY), Hamburg.¹⁷ Reciprocal space maps (RSM) around the (004) and (224) Bragg peak were recorded including the Si bulk peak as well as the SiGe island signal. The size of the incident beam was confined $200\ \mu\text{m}$ in horizontal and $100\ \mu\text{m}$ in vertical direction. The measurements were performed at an energy of 8048 eV corresponding to a

FIG. 1. AFM images showing the closely spaced barn-shaped islands before (a) and after capping with 30 nm Si (b) with the corresponding surface orientation maps as insets. Accordingly, linescans passing through the island center along the $[110]$ direction are displayed in (c) for both uncapped and capped islands.

FIG. 2. TEM images of capped barns. Sections (a) show an image recorded in bright field mode. The congruent overgrowth can be seen nicely, as well as the core-shell structure in the Ge composition inside the island. Panel (b) shows a dark-field image; bright regions close to the island rim are due to stacking faults located at $\{111\}$ facets.

wavelength of $1.5406\ \text{\AA}$. A MYTHEN 1D position sensitive detector was employed to record the data.

The RSMs feature well-resolved lateral intensity-oscillations from the pattern period in the vicinity of both the Si- and the SiGe-signals. This indicates a high uniformity of the pattern and the SiGe islands. Characteristic for uncapped SiGe islands is a rather large distribution of lattice constants and therefore strains due to their Ge-gradients and enhanced relaxation properties. The result is a smeared-out signal in reciprocal space as seen in the RSMs in Figs. 3(a) and 3(b).

FIG. 3. RSMs around the (004) and (224) Bragg peaks for the uncapped ((a) and (b)) and capped ((c) and (d)) barn-shaped SiGe islands. In (e) and (f), XRD simulations based on a FEM model of capped SiGe islands are shown.

After capping with Si, formerly relaxed sections of the islands are put under compressive strain, the width of the island signal in reciprocal space shrinks and its center shifts towards the Si peak as seen in Figs. 3(c) and 3(d).¹⁸ Furthermore, in the vicinity of the Si substrate peak, an oscillating pattern of diffuse intensity is seen for both the (004) and the (224) maps of the capped sample. In the asymmetrical (224) map, the wing-shaped signal is located at smaller Q_x values than the substrate peak, corresponding to tensile strained Si regions. These features actually originate from the strained Si capping layer and are replicated by XRD simulations based on our FEM model (Figs. 3(e) and 3(f)).

To calculate the strain distributions, a FEM model (COMSOL MULTIPHYSICS package) was set up with a $300 \times 300 \text{ nm}^2$ substrate block, defined by shallow {108} surfaces forming a pit (such surfaces consist of {105} and {001} microfacets¹⁹) and one barn-shaped island featuring all the facet sets as observed in the AFM data. For the model of the capped sample, the area between the islands is covered by two types of {111} facets according to the AFM scans. A 3D image of this model geometry featuring a surface plot of the in-plane strain ϵ_{xx} is shown in Fig. 4(a). To refine the Ge distribution for the strain calculations, the XRD measurements of the uncapped sample were used as reference and compared to kinematical XRD simulations^{20,21} based on the strains obtained from the FEM model. A Ge distribution with a core, a Ge-poor middle section, and a Ge-rich shell (see etching profiles shown by Zhang *et al.*²²) was used. The model for the capped sample features a core-shell Ge distribution with 24% Ge at the base, 22% in the middle section, and 35% Ge in the shell resulting in an average Ge

percentage of 28%. XRD simulations of the (004) and (224) Bragg peaks based on the FEM model of capped barns are shown in Figures 3(e) and 3(f). These calculated RSMs nicely display the oscillating pattern surrounding the respective Si (004) and (224) Bragg peaks we already saw in the measurements (Figs. 3(c) and 3(d)). Having a close look at the signals from strained Si and SiGe, we noticed that in a simulation where the SiGe signal is reproduced very well (as shown in the RSMs in Figs. 3(e) and 3(f)), the strained Si signal appears at slightly lower values in Q_x than the one seen in the experiment. This means that the Si cap in the actual sample is slightly more relaxed than the cap in the FEM model. This actually corresponds well to findings of the TEM investigations. In Fig. 2(b), brighter regions can be observed close to the rim of some of the islands. They actually appear due to stacking faults nucleating at the steep {111} facets of the barns, because of the compressive strain in these regions.^{23,24} To account for the additional relaxation due to these stacking faults, we have included an initial tensile strain within the cap domain of the FEM model. Strain values of only 0.1% are more than sufficient, which reduces the maximum tensile strain value in the Si cap by an insignificant amount of 0.02%. The region containing stacking faults is, however, very localized, and can be avoided by placing the n- and p-type channels into the defect-free regions on top of and in between the islands, respectively.

To investigate the compressively strained sections situated between the islands in more detail, and avoid any edge effects of the FEM domains, a further set of FEM models was set up including four of the original model blocks as shown in Fig. 4(a). A surface plot of the in plane strain along the x-coordinate ϵ_{xx} is displayed with the interchanging pattern of tensile strain above the island and compressive strain between the islands. Both tensile and compressive strains are in the order of 1%. In case of the biaxial tensile strain above the islands, the highest strain values of 0.95% within the cap are found close to the interface with the island. In Figure 4(b), we can see that ϵ_{xx} varies strongly between the SiGe islands. High compressive in-plane strain is found close to the side-walls of the buried SiGe island. Further regions with high compressive strain are situated close to the surface of the Si-capping layer between the islands, with values of 0.8%–1%. In Fig. 4(c), ϵ_{xx} values along horizontal lines at different heights (as indicated in Fig. 4(b)) are plotted. The irregularity of the line plots is a result of the FEM mesh.

In summary, we showed that high biaxial tensile strains as well as uniaxial compressive strains can be achieved within an epitaxially grown 30 nm thick Si layer with the proper spatial arrangement of SiGe islands as stressor structures. The samples shown in this paper feature arrays of highly uniform barn-shaped SiGe islands of excellent quality as confirmed by our XRD measurements. We also show that the strained sections of the Si capping layer give rise to unique intensity patterns in the RSMs. A wing-shaped signal in the RSMs of the capped sample was observed, which we could replicate in our XRD simulations. The sections of the Si-cap destined to form the p and n channels are defect-free and feature high strain values up to 0.8% and 1.0%, respectively, as proved by XRD measurements and FEM calculations.

FIG. 4. In image (a), the geometry of the FEM model of the capped sample is shown featuring a surface plot of the in plane strain component ϵ_{xx} . Please note the regions of biaxial tensile strain above the islands and the uniaxial compressive strain in between them. In (b), a 2D map of ϵ_{xx} of the cap-region confined between the {111} facets of two neighboring islands is shown. For clarity only the strain within the Si cap is highlighted. The dashed lines mark the positions where the strain data for the line plots shown in (c) were extracted (at height levels of 20, 30, and 40 nm from the island base). Compressive strains are the highest directly below the surface of the Si-cap with values around 0.8%.

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