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Systematic Characterization of Pseudomorphic (110) Intrinsic SiGe Epitaxial Films for Hybrid Orientation Technology with Embedded SiGe Source/Drain

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ABSTRACT

PFETs with embedded SiGe source/drain on HOT substrates have shown significant performance improvement compared to PFETs with embedded SiGe on (100) SOI substrates. In this paper, we report a systematic material characterization on the epitaxial SiGe films, both blanket and patterned, on (110) and (100) substrates, using an array of methods such as XRD AES, UV Raman, AFM, and TEM, and corresponding PFETs performance data.

INTRODUCTION

To exploit the higher mobility of holes on (110) and electrons on (100) substrates, two types of techniques have been developed in order to monolithically integrate different crystal orientations -- one is the hybrid orientation technology (HOT) [1]; and the other is the mixed orientation formed by direct silicon bonding (DSB) and followed by a solid phase epitaxy (SPE) [2]. Meanwhile, various techniques have been used to introduce uniaxial stress in MOSFET channel areas and improve the performance of the conventional devices. In particular, SiGe embedded in the source/drain (S/D) on HOT has been demonstrated to further enhance the pFET performance [3]. In this paper, we report a systematic study on the intrinsic pseudomorphic SiGe epi films on (110) Si substrate and explore the opportunities of fabricating strained channels on HOT substrates.

EXPERIMENTAL DETAILS

Commercially available semiconductor equipment for rapid thermal chemical vapor deposition (RTCVD) was used to deposit $Si_{(1-x)}Ge_x$ (where '*x*' is the Ge composition) thin films with basic germane and DCS chemistry. Blanket films of nominal 10% and 15% Ge and thicknesses 49-90 nm were deposited on 300 mm (100) and (110) silicon wafers at a temperature of 750^0C and well characterized before deposition on patterned device wafers. Epitaxial growth rate on (110) substrates was 30% lower than that of (100), while it was 30% higher on patterned wafers compared to blanket wafers because of loading effects.

These SiGe films were characterized using X-ray Diffraction (XRD), Auger and Raman to correlate different techniques for measuring Ge composition and the amount of strain. A Bede X-ray diffractometer using monochromatic CuKα (wavelength λ = 1.5406Å) radiation was used for rocking curve measurements around the Si (110) reflection. Auger Electron Spectroscopy (AES) data was collected on either a ULVAC-PHI SmartTool or Model 650 scanning Auger

microprobe, using 20 nA (ST) or 100 nA (650) at 10 kV. Alternate sputtering with a 2 kV Ar+ beam was used for depth profiling. For quantification, undoped blanket SiGe films, analyzed by Rutherford backscattering (RBS), were used to obtain average elemental sensitivity factors for each tool, correcting for instrumental response as well as preferential sputtering. Raman measurements were made using a HoribaJY LabRam 800 spectrometer system with microprobe capability. The excitation wavelength was 325 nm allowing for approximately 15 nm sampling depth into the SiGe. Using a 0.9NA UV objective (Leica), the lateral spatial resolution was approximately 0.7 μm. Atomic Force measurements (AFM) were performed on a Veeco Instruments Nanoscope D-5000 AFM, using an etched silicon tip with radius of 5-10 nm. The roughness calculations were taken from a 10 μm x 10 μm area. The Rmax represented the maximum peak to valley value within the area analyzed. The RMS value was calculated as the root mean square average of height deviations taken from the mean data plane. Transmission Electron Microscopy (TEM) was carried out on a JEOL 2010 field emission microscope, while the samples were prepared using industry standard focused ion beam technique.

DISCUSSION

Figure 1(a) shows the sample rocking curve scans around the (110) reflection for SiGe of different thicknesses. Clearly defined periodic fringes are seen in both symmetric scans suggesting that the film growth is pseudomorphic. The interference fringe spacing $\Delta\theta_p$ and the peak spacing $\delta\theta$ between the Si substrate and the SiGe peak were used to determine the film thickness and the perpendicular strain [4]. The fringe spacing $\Delta\theta_p$ was measured to be 190" and 360" and the thickness t of the film was calculated to be 49 nm and 90 nm using equation (1)

$$t = \lambda / \Delta\theta_p \cos\theta \qquad (1)$$

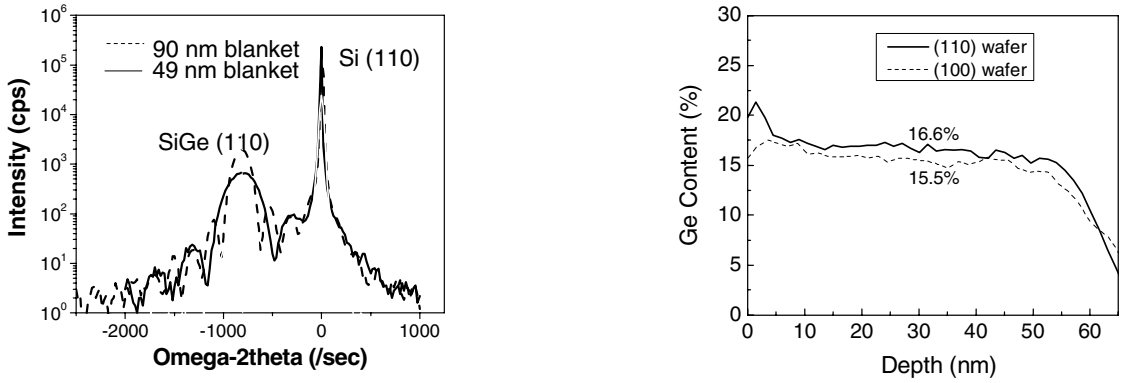
where θ is the angle of incidence and diffraction of the X-ray beam relative to the reflecting plane. The out-of-plane SiGe and Si lattice parameters, c_{SiGe} and a_{Si}, respectively, can be approximated by using the differential form of Bragg's law:

$$(c_{SiGe} - a_{Si})/a_{Si} \approx - (\theta_{SiGe} - \theta_{Si}) \cot(\theta_{Si}) \qquad (2)$$

Assuming a fully strained SiGe film on an unstrained Si substrate, c_{SiGe} can be related to the unstrained SiGe lattice parameter, a_{SiGe}, using linear elasticity theory:

$$c_{SiGe} = a_{SiGe}(1+\varepsilon_{zz}) = a_{SiGe}(1+ f\,\Delta\varepsilon) \qquad (3)$$

where ε_{zz} represents the out-of-plane SiGe strain, $\Delta\varepsilon$ the SiGe in-plane biaxial strain, and f is a parameter determined from the SiGe elastic constants. For an isotropic material, $f = -2\nu/(1-\nu)$ where ν is the Poisson's ratio of the SiGe film. However, f can be calculated for different orientations using a Vegard's law approximation for the components of the anisotropic elastic compliance tensor [5]. For a Ge fraction of 15%, f is calculated to be -0.501, resulting in an effective Poisson's ratio of 0.200 for a (110)-oriented SiGe film. These values are in contrast to those for a (100) oriented SiGe film, $f = -0.766$ and $\nu = 0.277$, possessing the same Ge fraction.



(a) (b)

Figure 1(a): (110) rocking curve scans around the Si (110) reflection for two blanket SiGe films on (110) Si wafers; (b) Ge depth profile on two patterned device wafers measured using Auger electron spectroscopy.

Because $\Delta\varepsilon$ can be calculated from the lattice mismatch between the SiGe film and the underlying Si: $\Delta\varepsilon = (a_{Si} - a_{SiGe}) / a_{SiGe}$, Eqn's 2 and 3 can be simplified to form:

$$(\theta_{Si} - \theta_{SiGe})\cot(\theta_{Si}) = (1-f)(a_{SiGe} - a_{Si}) / a_{Si} \qquad (4)$$

From the measured diffraction peak positions, we calculate a biaxial strain $\Delta\varepsilon$ of -0.61% and, from the unstrained SiGe lattice parameter, a corresponding Ge fraction of 15.5% according to Dismukes *et al.* [6].

The Ge profiles were also measured with AES on both blanket and patterned epi films. The results are very close to those of XRD. For patterned wafers, AES was done on 100 μm structures. As shown in Figure 1(b), the Ge concentrations of 15.5% on the (100) wafer and 16.6% on the (110) wafer were found to be fairly uniform throughout the films. The data were then used to extract the strain in the Raman measurements.

The Raman phonon spectrum consists of three first-order lines corresponding to the nearest neighbor Si-Si, Si-Ge, and Ge-Ge atomic vibrations. The Ge-Ge line is very weak and not shown in Figure 2(b). The peak positions and relative intensities of the phonon lines depend on the Ge fraction, and the peak positions also depend on the strain, according to Eqn's 5a–c

$$\omega_{SiSi} = 521.0 - 68\,x + \Delta_{Si}\Sigma \qquad (5a)$$
$$\omega_{SiGe} = 400.5 + 14.2\,x + \Delta_{SiGe}\Sigma \qquad (5b)$$
$$\omega_{GeGe} = 282.5 + 16\,x + \Delta_{GeGe}\Sigma \qquad (5c)$$

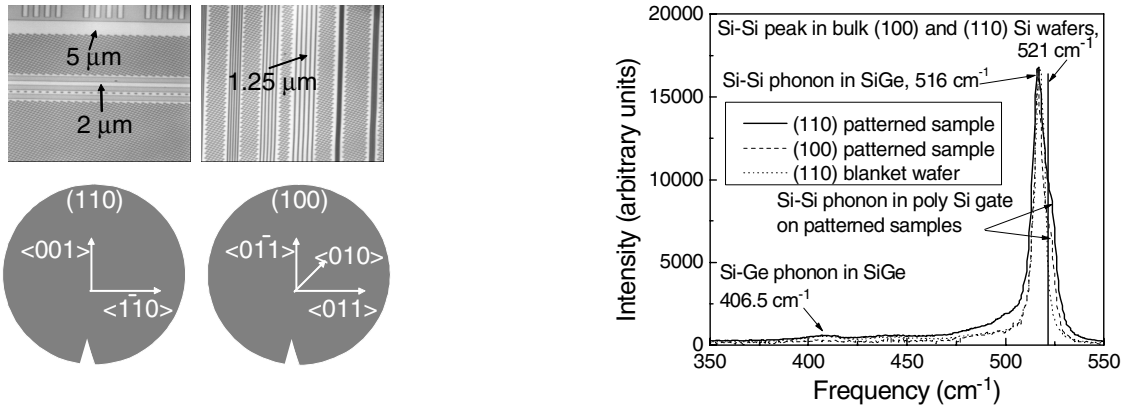
where ω_{SiSi} , ω_{SiGe} , and ω_{GeGe} are the measured phonon peak positions; x is the Ge concentration; Σ is the normalized strain, *i.e.* ε / 0.0417; and 0.0417 is the mismatch strain between pure Ge and Si, making $\Sigma = 1$ for pure Ge grown epitaxially on (100) Si wafers [7].

The coefficients Δ for determining both 'x' and strain have been reported in the literature [7-9] and also using our own reference samples of epitaxial SiGe films on (100) silicon in the range $0.15<x<0.35$, which were independently characterized by RBS and XRD for Ge concentration (x) and strain (ε). Using Equations (5) it is possible to determine both 'x' and

strain from the Raman spectrum, provided there is enough intensity in both the Si-Si and Si-Ge phonon lines. When the weaker Si-Ge line cannot be measured with adequate precision, the strain can still be determined from the Si-Si line, using the Ge composition from an independent measurement such as AES.

Raman measurements were made on both blanket and patterned SiGe films deposited on (100) and (110) Si substrates. In order to study the potential pattern-dependent effects, long horizontal (parallel to the notch) and vertical (perpendicular to the notch) stripes of SiGe epi films with width of 1.25, 2 and 5 μm, shown in Figure 2(a), were measured. While these epi stripes correspond to both <110> directions on (100) wafers, they are different on (110) wafers – the horizontal is along <110> direction, and the vertical is along <100> direction. The strain in the films along <110> and <100> directions with various width on the (110) patterned wafer are found to be 0.63~0.67% (only the data for 1.25μm epi strip is shown in Fig. 2(b)). The strain is the same as the strain on the (100) patterned sample, corresponding to fully strained $Si_{0.84}Ge_{0.16}$ films. Furthermore, the strain is in good agreement with those extracted from Raman and XRD on blanket films with the same alloy composition. All above is shown in Figure 2(b).

The surface roughness of the epi films was measured by AFM. Figure 3 shows the example AFM images of two blanket SiGe films grown on (110) and (100) Si substrates. RMS and Rmax comparison of blanket SiGe films with 15% are shown in the Table I. As the received Si wafers (out of box and no SiGe epi) had a RMS roughness of 0.061 and 0.095 nm for the (100) and (110) orientation, respectively, the (110) epi films had a 7x higher RMS roughness compared to the (100) epi films with the same deposition conditions.

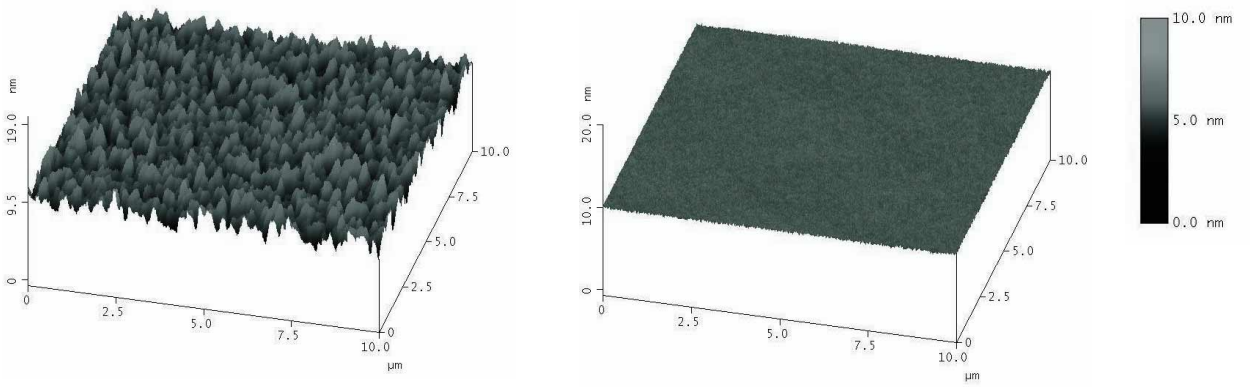


(a) (b)

Figure 2(a) Locations of Raman microprobe measurements for the SiGe epi stripe regions on a patterned (110) wafers, and illustration of channel directions on (110) and (100) wafers; (b) Raman spectra for the SiGe epi films on the (110) and (100) patterned (epi width of 1.25μm) and blanket wafers.

Table I: AFM RMS and Rmax for blanket SiGe films on (110) and (100) Si substrates

Subs. Orientation	(110)	(110)	(110)	(100)	(100)	(100)
SiGe thickness (nm)	50	90	none	50	90	none
RMS(nm)	0.518	0.679	0.095	0.083	0.090	0.061
Rmax(nm)	10.264	5.135	0.961	0.773	0.872	0.690



(a) (b)

Figure 3: AFM images of 90 nm thick SiGe films grown on (a): (110); and (b): (100) Si substrates.

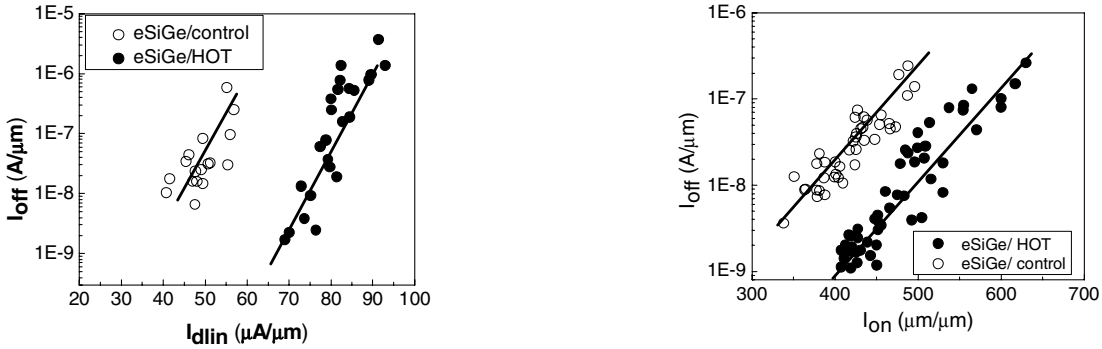
Figure 4(a) shows a weak beam dark field plan view TEM image of a blanket SiGe thin film grown on (110) Si substrate. Ge content is 15% and the thickness is 49 nm. No visible defects and no misfit dislocations were observed with a resolution of a few nanometers, indicating that the quality of the SiGe is very good, and that the film is fully strained. The same was true for a 90 nm thick film of similar Ge composition.

Devices with eSiGe S/D were fabricated using the 15% Ge epi process. Figure 4(b) shows a two-beam bright-field cross-sectional TEM image of a pFET device structure with embedded SiGe in the source/drain region on (110) Si. The epi has good quality and is fully strained. Only very low countable number of stacking faults was observed at the top corner of the SiGe source/drain.

Figure 5(a) and (b) show I_{dlin}-I_{off} and I_{on}-I_{off} for the 50 nm pFETs with <110>-oriented channels and eSiGe S/D on HOT and control substrates. I_{dlin} (I_d at V_{gs} = 1 V and V_{ds} = 50 mV) and I_{on} (I_d at V_{gs} = V_{ds} = 1 V) were improved by 57% and 30%, respectively, while threshold voltage and subthreshold swing were well matched between the devices on HOT and control substrates.

(a) (b)

Figure 4 (a): PTEM image of a blanket SiGe film on a 110 Si substrate; (b): XTEM image of a pFET structure with embedded SiGe S/D on a HOT substrate.



(a) (b)

Figure 5 (a): Measured I_{dlin}-I_{off} and (b) I_{on}-I_{off} for 50nm pFETs with embedded SiGe S/D on HOT and (100) SOI substrates. Channels are <110> oriented.

CONCLUSIONS

Systematic materials characterization has been performed to study both blanket and patterned SiGe films epitaxially grown on (110) and (100) Si substrates. Page: 6 Consistent results have been found in determining the Ge composition using XRD and Auger, and in determining the strain using Raman and XRD. High quality and fully strained films have been achieved. Device performance enhancement has been demonstrated with eSiGe source/drain on HOT substrates.

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