Fabrication of thick, high-quality strained SiGe layer on ultra-thin silicon-on-insulator and modeling of film strain

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Abstract

Fabrication of a thick strained SiGe layer on bulk silicon is hampered by the lattice mismatch and difference in the thermal expansion coefficients between Si and SiGe, and a high Ge content leads to severe strain in the SiGe film. When the thickness of the SiGe film is above a critical value (90 nm for 18% Ge), drastic deterioration of the film properties as well as dislocations will result. In comparison, a silicon-on-insulator (SOI) substrate with a thin top Si layer can mitigate the problems and so a thick SiGe layer with high Ge concentration can conceivably be synthesized. In the work reported here, a 110 nm thick high-quality strained Si\textsubscript{0.82}Ge\textsubscript{0.18} layer was fabricated on an ultra-thin SOI substrate with a 30 nm top silicon layer using ultra-high vacuum chemical vapor deposition (UHVCVD). The thickness of the SiGe layer is larger than the critical thickness on bulk Si. Cross-sectional transmission electron microscopy (XTEM) reveals that the SiGe layer is dislocation-free and the atoms at the SiGe/Si interface are well aligned, even though X-ray diffraction (XRD) data indicate that the SiGe film is highly strained. The strain factors determined from the XRD and Raman results agree well.

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1. Introduction

There has been considerable interest recently in the fabrication and properties of strained SiGe thin films due to mobility enhancement [1–4], bandgap reduction [5], as well as possible integration into standard silicon technology. Strained SiGe is useful in high performance vertical metal-oxide-semiconductor field-effect transistors (MOSFET), long-wavelength optical devices such as hetero-structure field effect transistors (HFET), hetero-junction bipolar transistors (HBT), and infrared detectors [6–10].

Several attempts have been made to fabricate high quality SiGe layers with high Ge concentration. Powell et al. utilized an ultra-thin silicon-on-insulator (SOI) substrate to achieve the synthesis of thick SiGe [11]. They fabricated a 70 nm thick Si\textsubscript{0.85}Ge\textsubscript{0.15} epilayer on SOI substrate with a 50 nm thick top Si layer by molecular beam epitaxy (MBE), but their SOI was not thin enough to grow thicker strained SiGe layer with a
high Ge fraction and the stress in SiGe layer was only partly relieved, and so its application has been limited. Mizuno [12] deposited thick strained SiGe directly on Si substrate, but the Ge concentration was quite low. Luo et al. [13] utilized a compliant substrate for the fabrication of high-quality SiGe by first producing a 20% boron borosilicate glass layer on the SOI wafers. In general, the lattice mismatch and difference in the thermal expansion coefficients between the Si and SiGe alloy with a high Ge content lead to severe strain in the SiGe film. When the thickness of the SiGe film is above a critical value, for instance, 90 nm for 18% Ge, drastic deterioration of the film properties and dislocations in the film will result [14]. For a hetero-structure with an epitaxial layer, the strain in the layer \( \varepsilon_f \) and substrate \( \varepsilon_s \) are both related to the misfit strain \( \varepsilon_0 \) by

\[
\varepsilon_f = \frac{h_s}{h_f + h_s} \varepsilon_0, \quad \varepsilon_s = -\frac{h_f}{h_f + h_s} \varepsilon_0,
\]

where \( h_s \) and \( h_f \) are the thickness of the substrate and the epilayer, respectively [15]. When considering a thin film deposited on a conventional bulk substrate, \( h_s \) is effectively infinite when compared to the epitaxial film, and so the strain is borne by the fabricated layer. As \( h_s \) approaches zero, \( \varepsilon_f \) is greatly reduced and an SOI substrate with an extremely thin top Si layer is perfectly suitable for this purpose [11,16]. This compliant substrate is much thinner than the epilayer and consequently bears most of the total strain [17]. Therefore, the thickness of the epitaxial SiGe layer on SOI can exceed the conventional critical thickness on bulk Si. In the work reported here, a 110 nm thick Si\(_{0.82}\)Ge\(_{0.18}\) layer was fabricated on an ultra-thin SOI substrate using ultra-high vacuum chemical vapor deposition (UHVCVD). The thickness of the SiGe layer was much larger than the critical thickness of SiGe on bulk Si and X-ray diffraction (XRD) and Raman spectroscopy were employed to assess the residual strain. They were also used to form the basis of a theoretical model to determine the strain in the SiGe epilayer.

2. Experimental

MBE and UHVCVD are the two main methods of low-temperature epitaxy of Si and SiGe alloys [18,19], and for best film uniformity, compatibility with large area processing, and relatively low apparatus costs, we adopted cold-wall UHVCVD (GSE 400) to fabricate the SiGe and Si layers. In our studies, the starting substrate was SIMOX SOI (separation by implantation of oxygen produced by SIMGUI, China) with a 380 nm SiO\(_2\) layer and a top 200 nm Si layer. The top Si layer was then thinned to 30 nm by repeated thermal oxidation and wet etching. Prior to SiGe film deposition, the native SiO\(_2\) layer on the ultra-thin SOI substrate was stripped using HF, followed by initial deposition of 10 nm of epitaxial Si to repair surface defects. A 110 nm thick Si\(_{0.82}\)Ge\(_{0.18}\) layer was then produced at 550 °C at a pressure of 1.2 × 10^{-7} Pa and flow rates of SiH\(_4\) and GeH\(_4\) at 6 and 1 sccm, respectively. The growth rate of SiGe layer was 0.1 nm/s. A relatively low substrate temperature of 550 °C was employed in our experiments to prevent possible strain relaxation, germanium segregation and diffusion. At low temperature and low strain, the Si/SiO\(_2\) interface behaves elastically and the SiGe grows pseudomorphically on the Si surface with the expected tetragonal distortion of the SiGe unit cell.

The concentration of Ge in the epitaxial layer was determined by Auger electron spectroscopy (AES) and the residual strain in the layers was measured using XRD and Raman spectroscopy. The microstructure of the SiGe epilayer was characterized by cross-sectional transmission electron microscopy (XTEM) using a Philips CM200FEG system.

3. Results and discussion

TEM was used to determine the location and densities of the dislocations introduced to relax the strain in the epitaxial layer and Fig. 1 shows the cross-sectional

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Fig. 1. Cross-sectional TEM image of the 110 nm Si\(_{0.82}\)Ge\(_{0.18}\) epilayer and 10 nm Si epilayer on a SIMOX substrate with a 30 nm top Si layer.
structure of the specimen except the bottom Si of the SOI substrate. The structure is composed of a 10 nm thick Si epilayer on top of 30 nm of unetched Si remaining on the SOI substrate. The SiGe epitaxial layer is about 110 nm which is larger than the conventional critical thickness (90 nm for 18% Ge) reported by Bean [14]. Fig. 2 depicts the high-resolution TEM image of the interface between the Si$_{0.82}$Ge$_{0.18}$ layer and Si layer. The interface is very sharp and atomically flat. The SiGe lattice matches that of Si very well, as inferred by our inability to detect any threading dislocations in the cross-sectioned specimen. The strain in the SiGe layer is thus not relieved by dislocations, and so in spite of the excellent crystalline quality demonstrated in the TEM micrographs, the SiGe layer is highly strained as corroborated by our XRD and Raman spectra to be shown later.

Fig. 3 displays the elemental depth profiles acquired by sputtering AES. The concentration of Ge in the SiGe epitaxial layer is about 18% and it remains almost constant throughout the entire SiGe epilayer. Some Ge signals were detected in the top Si layer of SOI and Si epilayer, these probably come from the Ge-sputtered SiGe film which still stayed in the detector. Because the Ge diffusion velocity is too low at 550°C and the growth time of SiGe (18 min) is very short, it is very difficult for Ge atoms to diffuse into the top Si layer. High-resolution symmetric (004) XRD scans were acquired from the 110 nm SiGe layer grown on bulk Si and ultra-thin SOI. In the bulk Si sample, the substrate thickness is effectively infinite when compared to the epitaxial SiGe film, and so the strain is mainly borne by the epilayer. Due to the presence of misfit dislocations generated by such strain at the SiGe/Si interface, the width of half-maximum (FWHM) of the SiGe peak in Fig. 4(a) is 0.20°, as broad as a result of the mosaic structure. In the ultra-thin SOI substrate sample, the much narrower FWHM is 0.15° and confirms that the SiGe layer is pseudomorphic to the SOI substrate, i.e., there is a negligible dislocation density at the SiGe/ SOI interface. From Fig. 4(b), the strain factor $S$ can be calculated [20] and we can also derive an “effective” lattice parameter $a_r$ from Vegard’s law:

$$a_r = a_{Si} + (a_{Ge} - a_{Si})x = a_{Si} + 0.2268x,$$

where $a_{Si}$ and $a_{Ge}$ are the lattice parameters of bulk Si and Ge alloy, respectively, and $x$ is Ge concentration of SiGe alloy.

$$\text{Fig. 2. High-resolution TEM micrograph of the interface between the Si}_{0.82}\text{Ge}_{0.18}\text{ epilayer and SIMOX substrate.}$$

$$\text{Fig. 3. AES depth profiles of the SiGe epilayer. The Ge concentration in the epilayer is about 18%.}$$

$$\text{Fig. 4(a).}$$
We can use the SiGe rocking curves from the (0 0 4) planes to calculate $a_\perp$:

$$a_\perp = 4d_{400} = \frac{n\lambda}{2\sin \theta}.$$  

(3)

The $a_{11}$ of the SiGe epilayer is calculated from the following equation:

$$a_\perp - a_{11} = -2 \left( \frac{c_{12}}{c_{11}} \right) (a_{11} - a_\parallel).$$  

(4)

Here, $a_\perp$ and $a_{11}$ are the perpendicular and in-plane lattice parameters of the SiGe tetragonal structure, respectively, and $c_{11}$ and $c_{12}$ are the elastic constants (Si: $c_{11} = 1.658$, $c_{12} = 0.639$, $c_{44} = 0.769$; Ge: $c_{11} = 1.285$, $c_{12} = 0.483$, $c_{44} = 0.668$, all in units of $10^{11}$ N m$^{-2}$) [21].

In a manner similar to Vegard’s law, we use an interpolated value for $c_{12}/c_{11}$ of approximately 0.38 for a Ge concentration of 18%. Finally, we can derive the strain factor $S$ to be 95.1% using the following formula [20]:

$$S = \frac{a_\parallel - a_{11}}{a_\parallel - a_0}$$  

(5)

where $a_0$ is the lattice parameter of Si and equal to 0.543 nm.

The strain factor $S$ can also be estimated from the Raman spectra. Fig. 5 displays the typical spectra in the range of 250–550 cm$^{-1}$ acquired from the Si$_{0.82}$Ge$_{0.18}$ on SOI sample. The shifts in the Si–Si phonon peak can be clearly observed. The peak at $\sim$512 cm$^{-1}$ is associated with the Si–Si vibrational mode in the SiGe epilayer. The Si–Si phonon peak from the SOI substrate emerges at $\sim$519 cm$^{-1}$ and the Si–Ge vibration peak appears at $\sim$404 cm$^{-1}$. Because the SiGe epilayer is very thin, the Ge concentration is relatively low and the base peak is relatively high, the Si–Si peak is very weak and Ge–Ge peak is difficult to observe. For $x \leq 0.2$, the Si–Si phonon mode has been shown to exhibit a linear dependence with composition in both the fully relaxed incommensurate pseudo-alloy [22,23] and fully strained commensurate superlattice [24]. Perry et al. have found that the relative shifts of the Si–Si phonon mode observed from the SiGe epilayer on Si at room temperature can be described as a function of the Ge fraction, $x$, using the following relationships: [25]

$$A_{p,a} = 69.0x({cm}^{-1}) [\text{fully-relaxed}],$$

$$A_{s,a} = 36.0x({cm}^{-1}) [\text{fully-strained}],$$  

(6)

where $A_{p,a}$ is this phonon shift for the fully relaxed pseudo-alloy and $A_{s,a}$ is that for the fully strained SiGe alloy. The strain ratio, $S$ can be derived from the
following equation:

\[ S = \frac{A_{p.a.} - A_{exp.}}{A_{p.a.} - A_{cl}}. \]  

Here, \( A_{exp.} \) is the frequency shift and the strain ratio \( S \) is calculated to be 94.3%.

The two independent methods yield a similar strain ratio \( S \). However, it should be noted that since the formulae adopted here are for bulk silicon, \( S \) may not reflect the strain in the epitaxial layer on SOI very accurately, but the error is expected to be small and the formalism discussed here should be applicable to most applications. Our results show that despite the high film strain, high crystalline quality and thick SiGe layers can be produced on ultra-thin SOI substrate.

4. Conclusion

We have successfully fabricated 110 nm thick strained Si\(_{0.82}\)Ge\(_{0.18}\) alloy of high crystalline quality on ultra-thin SOI substrate. The TEM micrographs reveal no detectable defects in the film and an excellent SiGe/Si interface. AES results indicate uniform Ge concentration throughout the entire SiGe epilayer. Two methods are employed to derive the strain ratio of the epilayer and the results agree very much showing that the SiGe layer is highly strained and the SiGe unit cell grows in the expected tetragonal distortion to match the Si lattice.

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