JOURNAL OF APPLIED PHYSICS **101**, 053501 (2007)

Thin strained layers inserted in compositionally graded SiGe buffers and their effects on strain relaxation and dislocation

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(Received 1 December 2006; accepted 11 January 2007; published online 1 March 2007)

The effect of inserting compressively or tensely strained layers into compositionally graded SiGe buffers on strain relaxation and threading dislocation density (TDD) was investigated. The samples having compressively strained layers showed lower TDD and more enhanced relaxation than those having tensely strained layers. In addition, dislocations were accumulated at the top part of the tensely strained layers within the graded buffers, while no accumulation was found at the compressively strained layers. These results might be due to the effect of strain from the thin inserted layers on the dislocation interactions in the compressively strained graded buffers. © *2007 American Institute of Physics*. [DOI: 10.1063/1.2710356]

I. INTRODUCTION

SiGe/Si heterostructures have been of considerable interest for their potential and technological significance in electronic and optical device applications.[1,2] Particularly, compositionally graded SiGe buffers have been successfully demonstrated for use as virtual substrates for the production of high mobility complementary metal-oxide semiconductor (CMOS) structures and for III-V integration on Si.[3–7] Some of the major requirements for use as high-quality virtual substrates include a low threading dislocation density (TDD), a low surface roughness, and a high degree of relaxation of the 4% lattice mismatch between Si and Ge. In this paper we show that improvements to the completeness of the relaxation of the SiGe graded buffer virtual substrates with little increase of TDD can be accomplished by inserting strained thin layers in graded SiGe buffers. Specifically, investigations involving the addition of both compressively strained layers and tensely strained layers showed improvements to the degree of relaxation of the graded buffer. However, only the case of the compressively strained layers was able to do so while maintaining or even slightly reducing the TDD. This study utilized etch-pit density (EPD) measurements to quantify the TDD, cross-sectional transmission microscopy (TEM) to characterize the dislocations, and x-ray diffraction techniques to investigate residual strain levels.

II. EXPERIMENT

All the SiGe layers in this research were produced through epitaxial growth at 1075 °C and at 80 Torr on *p*-type Si(001) wafers having a diameter of 200 mm using an industrial ASM Epsilon E2000 chemical vapor deposition system. The high growth temperature is enabled through the use of germanium tetrachloride as the germanium source[8] and the dichlorosilane as the silicon source. Figure 1 illustrates the experimental matrix used in this investigation where various compressive and tensile layers, defined by their Ge content, are inserted into the otherwise linearly graded buffer. In all experimental conditions the first strained layer was inserted at a depth of 0.6 μm and the second layer at a depth of 1.2 μm in the graded region (equivalently, at a Ge composition of 6% and 12%, respectively). The naming convention used in this paper will be the following: $X\%/Y\%$ where X is the Ge content of the first layer and Y is the Ge content of the second layer. These inserted strained layers were always 20 nm thick, which is below the equilibrium critical thickness,[9,10] and within each experimental trial the two layers were always of the same strain type (i.e., both compressive or both tensile). The control condition, having no inserted strained layers, consisted of a linearly graded 2 μm thick SiGe graded buffer where the Ge content increased from 0% to 20% at a grading rate of $10\%/\mu$m followed by a 0.5 μm thick $Si_{0.8}Ge_{0.2}$ cap layer. In the case of inserted tensely strained layers, the first condition consisted of 0% Ge (i.e., pure Si) in the first layer and 6% Ge in the second layer (or as expressed by our naming convention $0\%/6\%$) and the second condition consisted of both layers being of pure Si (or $0\%/0\%$). In the case of compressively strained layers, the two conditions were $(12\%/18\%)$ and $(12\%/24\%)$. Both in the control condition and in all of the inserted layer conditions, atomic force microscopy (AFM) analysis showed a consistent rms roughness of about 3–4 nm on 40×40 μm^2 area scan as shown in Fig. 2. All the samples exhibited the crosshatch morphology typical in SiGe graded buffers,[11] and the samples having compressively

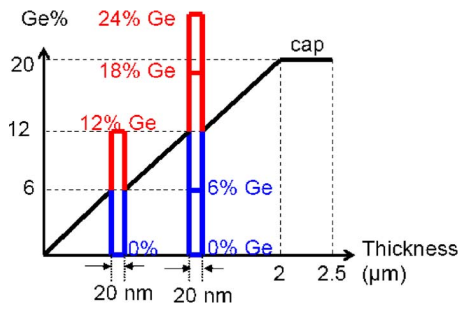

FIG. 1. (Color online) Schematic showing Ge content in SiGe graded buffer with thin tensely or compressively strained layers.

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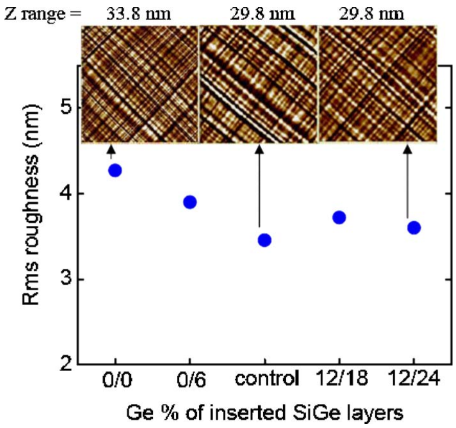

FIG. 2. (Color online) rms roughness of the samples with and without thin strained layers from 40×40 μm^2 AFM images. 40×40 μm^2 AFM images of 0%/0%, control, and 12%/24% samples were also inserted with their Z ranges.

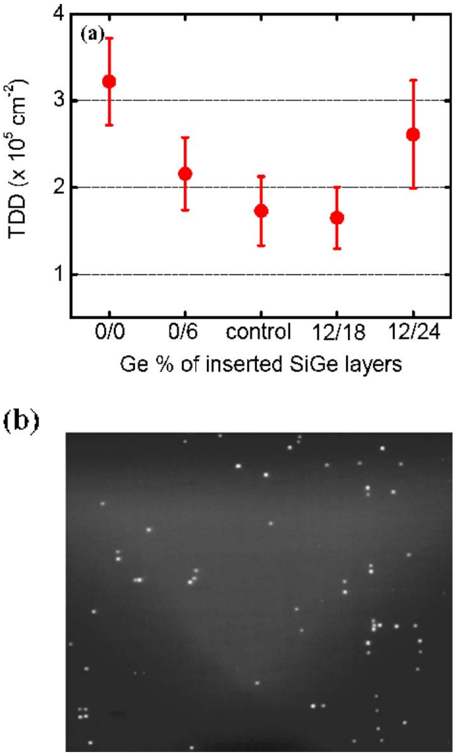

FIG. 3. (Color online) (a) TDD of the constant cap layers on graded SiGe buffers with and without thin strained layers (error bar shows ± standard deviation) and (b) 210×175 μm^2 dark field microscope image of control sample without thin strained layers after Secco etching.

strained thin layers showed slightly lower roughness and larger wavelength of crosshatch undulations than the ones having tensely strained layers. Wavelength of the crosshatch undulations of 0%/0% and 12%/24% sample was 0.75–1.6 and 2.5 μm, respectively. Strain relaxation of the constant composition cap layers was determined from high-resolution reciprocal space map (RSM) of asymmetric {224} peaks using a Panalytical X'Pert diffractometer. The TDDs were measured using an EPD counting technique with dark field microscopy after a decorative Secco ($HF:K_2Cr_2O_7:H_2O$) etch. EPD values were averaged over ten fields of view in each sample with samples taken from center regions of the wafer. Cross-sectional TEM (JEOL JEM 2100) was employed to characterize dislocations in the buffers.

III. RESULTS AND DISCUSSION

Figures 3(a) and 3(b) show TDD for the various conditions including the control condition (i.e., no strained layers) and a typical dark field image of control sample, respectively. TDD pileups were not observed. Only field threading dislocations were found. Comparison of TDD data from the tensile condition with the corresponding compressive condition having the same difference of Ge content in the inserted strained layers show on average a higher level of TDD in the samples having inserted tensile layers; 0%/0% and 0%/6% have higher TDD than 12%/18% and 12%/24%, respectively. The 0%/0% tensile condition showed particularly high TDD, while the 12%/18% compressive condition showed the lowest overall TDD.

The strain relaxation of the constant composition cap layers and typical RSM are expressed in Fig. 4. Usually, 1–2 μm thick cap layers are grown on graded buffers for the application in SiGe virtual substrates. However, we used a cap layer having only 0.5 μm thickness, which has somewhat lower strain relaxation than the typical thick cap layer in order to show the effect of the inserted thin stained layers more clearly. The control condition showed only 86% relaxation in the cap layer, while all the conditions having thin strained layers had a higher level of relaxation. Furthermore, samples having compressive layers showed higher levels of relaxation than those having tensile layers, with the 12%/24% structure having the greatest relaxation at 99%.

Cross-sectional TEM analysis helps elucidate these results. The control condition, having no inserted strained layers, shows a quite uniform distribution of dislocations throughout the graded buffer as shown in Fig. 5(a). However, inserting tensely strained layers appears to promote the accumulation of dislocations at the top interface of the inserted layer as shown in Fig. 5(b), where the 0%/0% condition is considered. Close scrutiny of this image indicates that this effect is even more substantial for the more highly strained tensile layer (i.e., the second layer in the 0%/0% case). In contrast, the sample of the compressively strained layers (12%/24%) did not show any accumulation of dislocations around the strained layers [Fig. 5(c)] and, in fact, has more similarities to the control condition.

In summary, the samples with compressively strained layers inserted in graded buffers show lower TDD with higher relaxation than those with tensely strained layers. This result may be explained by considering the interaction between these inserted layers and the linear, compressively strained, graded buffer having the glissile dislocation array. First let us consider the control condition: a continuous, linearly graded structure up to a terminal composition followed by a constant composition cap layer. In this case the relaxation of the graded structure is limited by dislocation interactions rather than by its glide.[12–17] Furthermore, the effect of dislocation blocking on limiting strain relaxation has been reported to be closely related to the residual background strain in the graded buffer, where the associated residual

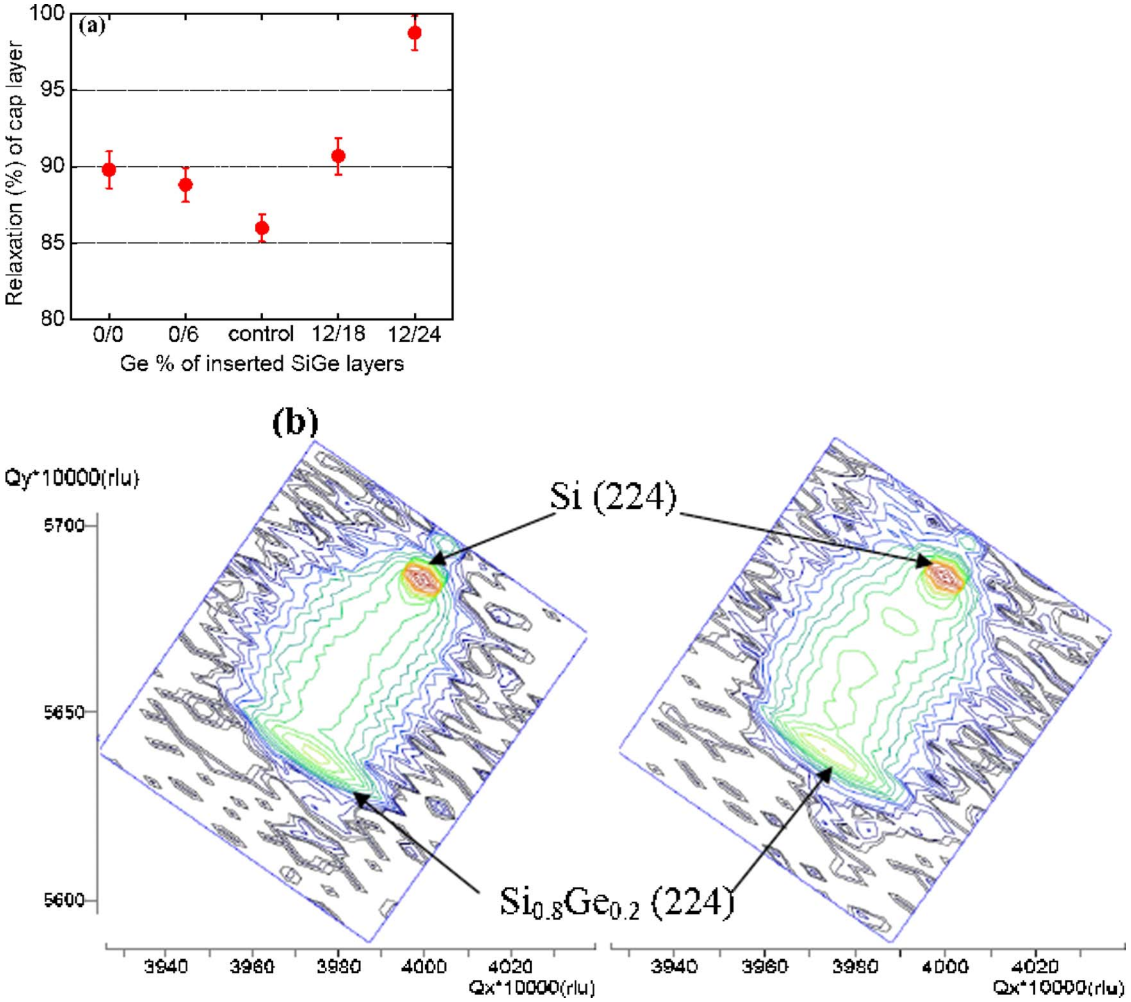

FIG. 4. (Color online) (a) Relaxation of the constant composition cap layers on graded SiGe buffers with and without thin strained layers (error bar shows ± standard deviation) and (b) typical (224) RSM of the control (left) and 12%/24% sample (right).

background stress acts as a driving force for relaxation and, by extension, dislocation movement.[15–17] It has been shown that when a moving thread dislocation is blocked by an orthogonally oriented misfit dislocation, the misfit's associated stress field negates the relaxation-driving stress field from the residual background strain and, thus, immobilizes the thread.[15] In order for a threading dislocation to glide further it must overcome this impediment by passing through a restricted channel between the film surface and the stress field from the underlying misfit dislocation, a stress field that decays inversely with the distance from the originating misfit.

In considering the samples with compressively strained layers (12%/18% and 12%/24%), it is hypothesized that the increased background compressive strain in the graded buffers resulting from the insertion of the compressively strained layers, provides an additional driving force sufficient to overcome dislocation blocking. This results in higher overall levels of relaxation with little or no increase in TDD. Considering the same mechanism for the samples having tensely strained layers, the background compressive strain in the graded buffer should be reduced by the tensile strain from the thin strained layers resulting in a reduced driving force to overcome dislocation.

The TEM analysis shown in Fig. 5 reveals an interesting difference in distribution of the dislocation network between the compressive and tensile layer samples. In the cross-sectional TEM images of Fig. 5(a), a control sample shows fairly uniform distribution of dislocations. In the case of the sample having tensely strained layers (0%/0%), dislocations are accumulated only at the top part of the tensely strained layers [Fig. 5(b)]. This accumulation is not found in compressively strained layers (12%/24%) [Fig. 5(c)]. It has been proposed that the dislocation half loops are nucleated at the growth surface when the thickness of SiGe graded buffer is over the critical thickness and then propagates until reaching the interface with Si substrate, at which point a misfit dislocation and two threading dislocations exist.[18,19] This process repeats until all misfit dislocations distribute uniformly from the interface to a certain thickness of the layer. In the case of tensely strained layers, the dislocation half loops, having been formed at the growth surface and propagating into the compressively strained SiGe buffer may become pinned at the thin tensely strained layers leaving a dislocation accumulation near the top surface of the tensile layer. Moreover, the tensile strain from these layers might work as a kinetic barrier impeding the ability of the underlying dislocations from contributing to the strain relaxation

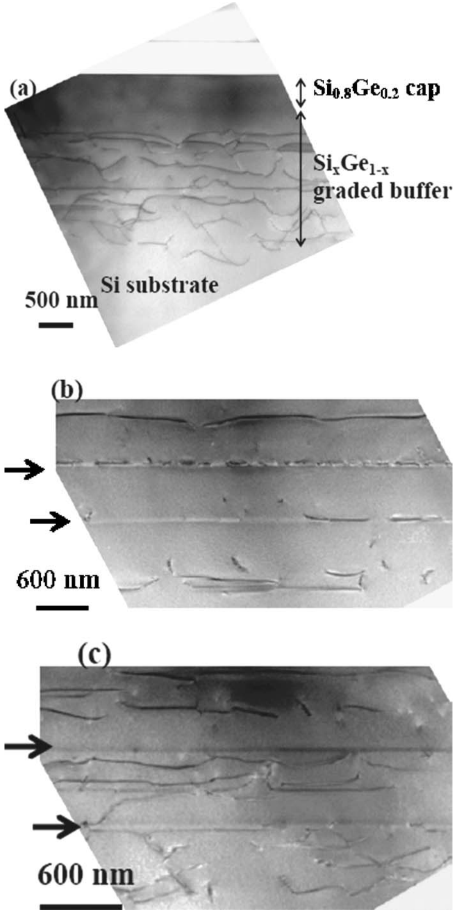

FIG. 5. Bright-field cross-sectional TEM images of (a) the control sample without the thin strained layers, (b) 0%/0%, and (c) 12%/24% sample. Arrows indicate the thin strained layers inserted in graded SiGe buffers.

by propagating through the compressively strained SiGe buffer.[20] The impediment of dislocation propagation will result in higher TDD with lower relaxation due to the enhanced dislocation interaction. However, this explanation does not account for the tensely strained layer samples having a higher degree of relaxation than the control sample.

IV. SUMMARY

We have investigated the effect of thin strained layers inserted into SiGe graded buffers. The samples having compressively strained layers showed lower TDD and more enhanced relaxation than those having tensely strained layers. In addition, dislocations were accumulated at the top part of the tensely strained layers in the graded buffers, while no accumulation was found at the compressively strained layers. These results may be able to be explained by considering the interaction between the strain introduced by the inserted layer and the background compressive strain present in the standard SiGe graded buffer. In this paper we have presented two such possible explanations.

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