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Dislocation structure formation in SiGe/Si(001) heterostructures with low-temperature buffer layers

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Abstract

Mechanisms of misfit dislocation generation as well as peculiarities of dislocation structure formation in $Si_{0.7}Ge_{0.3}$/Si multilayer heterostructures grown by molecular beam epitaxy with low-temperature (LT) SiGe and (SiGe + Si) buffer layers were studied. Full strain relaxation in the heterostructures with 200–250 nm thick buffer layers has been achieved. In the heterostructures with both types of LT layer, misfit dislocation generation is found to proceed similarly to heterostructure growth at high temperatures; however, the rate of dislocation nucleation is higher due to the high vacancy concentration near the interface. Threading dislocations, which are not connected with misfit dislocation network, are generated in the epitaxial layers apart from the SiGe–Si interface to form a dislocation density of 10^7–10^8 cm^{-2} on the surface.

1. Introduction

Fully relaxed $Si_{1-x}Ge_x$/Si heterostructures are currently of great interest for use in a variety of microelectronic devices due to the higher mobilities of charge carriers in the highly strained channels in multilayer heterostructures grown on virtual substrates [1, 2]. The silicon substrates with compositionally graded $Si_{1-x}Ge_x$ layers as virtual substrates provide high Ge content (up to $x = 1$) on the surface and high degree of misfit strain relaxation in such heterostructures. The main issue in growing virtual substrates is concerned with getting fully relaxed buffer layers with threading dislocation densities as low as $\leqslant 10^5$ cm^{-2} at minimal layer thickness. Using the intermediate layers grown at low temperatures (LTs) within multilayer buffer heterostructures opens new possibilities in this area [3]. For single-layer SiGe/Si heterostructures, the main difference is concerned with the kind of LT layer which is grown directly on the high-temperature buffer Si layer. In $Si_{0.7}Ge_{0.3}$(550 °C)/LT-Si(50 nm, 400 °C)/Si heterostructure, it has been shown that the degree of strain relaxation in the heterostructure is affected by

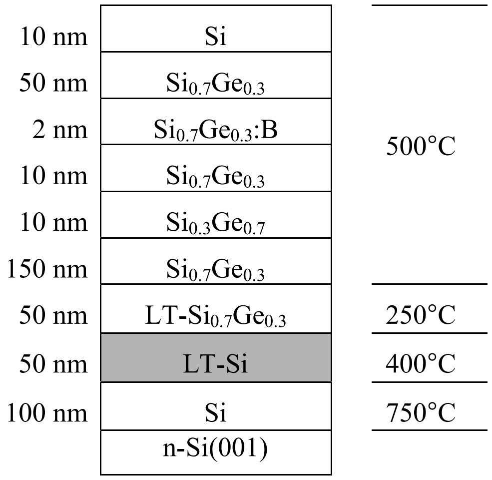

Figure 1. A schematic representation of the samples and nominal parameters of layer growth. The highlighted LT-Si layer is absent in sample I and exists in sample II.

the SiGe layer thickness, and achieves a value of 90% at 500 nm [3]. Another type of LT layer has been suggested in [4] based on the use of LT-SiGe of the same alloy composition as the other part of the layer grown at high temperature. In $Si_{0.72}Ge_{0.28}$(44 nm, 550 °C)/LT-$Si_{0.72}Ge_{0.28}$(26 nm, 200 °C)/Si heterostructure, a full strain relaxation has been achieved while a rather high density of threading dislocations has been observed.

Using the LT layers provides a high degree of misfit strain relaxation in thinner buffer layers in comparison with the similar heterostructures grown at conventional temperatures. Apparently, this effect is related to the high concentration of intrinsic point defects in the LT layers; however, their role in the strain relaxation processes is still unclear. Transmission electron microscopy (TEM) investigations of the cross-sectional specimens have shown that dislocations are predominantly located within the LT layers and under them, while dislocation density in the SiGe layer above proves to be significantly lower than that in similar heterostructures without LT layers [3]. On the basis of these data, the authors of [3] have concluded that the presence of the LT layers changes the misfit dislocation nucleation mechanism and/or rate of the dislocation nucleation. In the present paper we have carried out a comparative analysis of the structural features and degree of strain relaxation in the $Si_{0.7}Ge_{0.3}$/Si(001) heterostructures containing both single LT-$Si_{0.7}Ge_{0.3}$ and combined LT-($Si_{0.7}Ge_{0.3}$ + Si) layers. The aim of the work was to study mechanisms of misfit dislocation generation as well as the peculiarities of dislocation structure formation in heterostructures with different kinds of LT layer.

2. Experiments

Modulation-doped heterostructures with single quantum wells were used for the experiments. The scheme of the samples studied as well as layer thicknesses and growth temperatures are shown in figure 1. The LT-SiGe(250 °C) layer is the main part of the buffer layer in both heterostructures, whereas the LT-Si(400 °C) layer is used only in one of them. The heterostructures were grown by molecular beam epitaxy (MBE) using the ‘RIBER SIVA 45’ installation. Prior to epitaxial growth, the substrates were cleaned with a standard RCA process

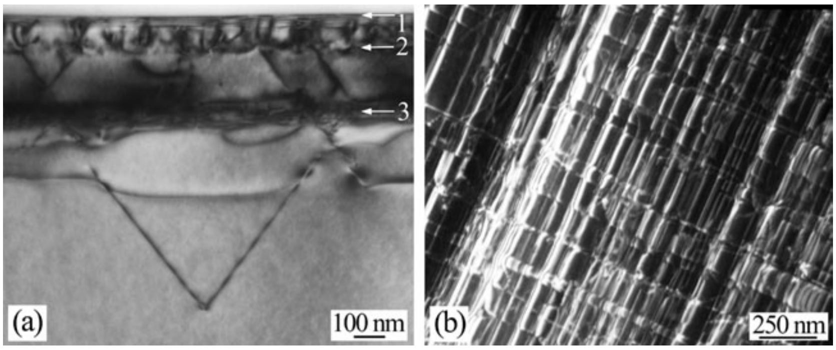

Figure 2. TEM cross-sectional (a) and plan-view (b) micrographs of the heterostructure with a LT-SiGe layer (sample I). Arrows indicate the positions of the surface (1), $Si_{0.3}Ge_{0.7}$ channel (2) and SiGe–Si interface (3).

followed by an annealing at 1035 °C for 15 min in a growth chamber to remove the native oxide. An undoped Si buffer layer was initially grown directly on the substrates at 750 °C. After growing the LT layers, the growth temperature was increased without interruption of the molecular beams. Structural investigations of the samples grown were carried out by high-resolution x-ray diffraction (HRXRD), chemical selective etching and TEM. For studying the dislocation distribution by optical microscopy, the samples were prepared by selective chemical etching so that an oblique section was formed and dislocation etch pits were revealed on its surface simultaneously.

3. Results and discussion

The degree of strain relaxation in the samples was determined through the HRXRD data obtained for (004) and (115) Bragg diffraction reflections. Strain relaxations of 100 and 80% have been obtained for the heterostructures with LT-SiGe (sample I) and LT-(SiGe + Si) (sample II) layers, respectively. A distinctive cross-hatch pattern was observed by optical microscopy on the surface for both as-grown samples. After selective chemical etching, patterns with long orthogonal lines and dislocation etch pits with a density of about (2–3) $\times$ 10^7 cm^{-2} were revealed again on the surfaces of both heterostructures. This distinct difference in etch patterns was observed in the near-interface substrate region of the samples, i.e. in the Si buffer layer close to the interface. For sample I, a pattern with orthogonal lines and dislocation etch pits with a density of 4 $\times$ 10^7 cm^{-2} was revealed. In contrast, a pattern with smoothed orthogonal lines and shallow dislocation etch pits was revealed for sample II. This relief is caused by the memory effect of the etchant and reflects the material above being removed. This indicates that there are no dislocations in the near-interface substrate region in sample II.

Figures 2 and 3 show TEM micrographs of the cross-sectional and plan-view samples. Plan-view micrographs were taken for thick parts of the foils, with thickness $\geqslant 0.3$ μm. Thus all defects in the epitaxial layers were observed in these micrographs. In sample I (LT-SiGe), a highly developed three-dimensional MD network is observed at the SiGe–Si interface (figure 2(a)). Its dense multilevel part is positioned near the interface, encompassing some adjacent regions of both the layer and substrate, and its width is about 100 nm. Thus, misfit dislocations are not located within the LT-SiGe layer. Threading dislocations with a density of about 10^7 cm^{-2} as well as dislocation semiloops propagating deeply into the substrate are

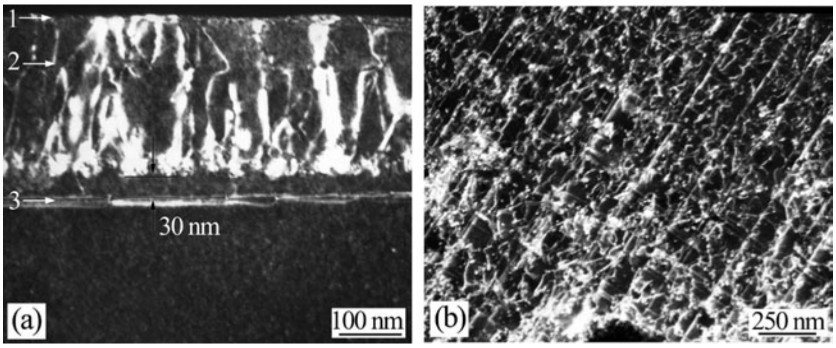

Figure 3. Dark-field TEM cross-sectional (a) and plan-view (b) micrographs of the heterostructure with a LT-(SiGe + Si) layer (sample II). Arrows indicate the positions of the surface (1), $Si_{0.3}Ge_{0.7}$ channel (2) and SiGe–Si interface (3).

observed above and under the MD network, respectively. As seen in figure 2(b), a dense MD network with a linear density of $\sim 3 \times 10^5$ cm^{-1} is observed in the plan-view micrograph. Threading dislocations can hardly be distinguished against this background. Such dislocation structure is typical for heterostructures without LT layers. Similar dislocation structure has been observed in $Si_{0.5}Ge_{0.5}$/Si heterostructures grown by MBE at 450 °C [5]. However, it is noteworthy that threading dislocations with a density of $\geqslant 10^9$ cm^{-2} are usually generated due to the island growth regime in $Si_{1-x}Ge_x$ ($x \geqslant 0.25$)/Si heterostructures grown at usual temperatures, >550 °C [6]. The typical shape of dislocation semiloops in the substrate indicates that an active MD multiplication has occurred at the interface in this heterostructure through the modified Frank–Read mechanism [7]. In sample I, a sharp jump in the threading dislocation density is observed in the active region, which is a highly strained 13.5 nm thick $Si_{0.3}Ge_{0.7}$ layer. This indicates that additional threading dislocation generation has occurred in this region to produce the dislocation density of $\geqslant 10^8$ cm^{-2} on the surface.

In sample II with LT-(SiGe + Si) layers, a practically flat MD network is observed at the SiGe–Si interface (figure 3(a)). There is an ≈30 nm thick band with a low threading dislocation density (10^5–10^6 cm^{-2}) over it. A sharp jump in the threading dislocation density is observed at the top edge of this band. Once generated in this region, these dislocations thread through the upper part of the heterostructure. A plan-view TEM micrograph shows the existence of a regular dense MD network ($\sim 1.5 \times 10^5$ cm^{-1}) and highly curved threading dislocations with the density of $\sim(5$–$7) \times 10^8$ cm^{-2} in the epitaxial part of the heterostructure (figure 3(b)). A MD network does not form in the active layer; however, some decreasing threading dislocation density is observed above it (figure 3(a)). Dislocation semiloops are absent in the near-interface substrate region, which indicates that MD multiplication at the interface has not occurred.

We have found distinct differences between the dislocation distributions over similar heterostructures with different kinds of LT buffer layer. The results obtained can be partly explained in terms of the influence of vacancies on dislocation nucleation. In sample I, growing the LT-$Si_{0.7}Ge_{0.3}$ layer at 250 °C on the high-temperature buffer Si layer provided the two-dimensional epitaxial growth regime and results in a metastable state of the SiGe alloy. Misfit dislocation generation occurred during subsequent growth of the high-temperature $Si_{0.7}Ge_{0.3}$ layer and was accompanied by the formation of a regular MD network at the interface at the initial stages of strain relaxation [8]. The most plausible mechanism of MD generation is the mechanism proposed by Perovic and Houghton [9] for the heterostructures grown at conventional temperatures. For this mechanism, the nucleation of vacancy-type prismatic dislocation loops at the stress concentrators, which are proposed to be sub-nanometre-sized Ge-rich platelets, localized at the interface is the starting stage of strain relaxation. In sample I, relatively high vacancy concentration has been produced in the LT-SiGe layer during its epitaxial growth, which promotes the high rate of dislocation nucleation in the alloy near the interface. However, the fact of MD multiplication at the interface indicates that the MD density in the network formed initially proved to be insufficient to provide full strain relaxation in the heterostructure. As has been recently shown by Szeles *et al* [10], in LT-Si(150 nm, 300 °C)/Si epitaxial structure the first part of the LT-Si layer is defect free up to thickness of 80 nm (the vacancy concentration is $\leqslant 10^{19}$ cm^{-3}). As the layer thickness increases, the vacancy concentration increases nearly exponentially and changes by over two orders of magnitude within the subsequent 70 nm to reach the concentration of $\sim 10^{21}$ nm^{-3} on the surface. From these data, one can suppose that, in sample I, the vacancy concentration in the LT-SiGe(50 nm) layer was not extremely high, although it was higher than the value appropriate for a high-temperature alloy. Thus, we can conclude that a full strain relaxation in this sample has been achieved as a result of subsequent MD multiplication at the interface. As regards the additional generation of the threading dislocations in the region of the active layer, observed in sample I, we will not discuss this in this paper because the process is not obviously connected with the presence of the LT-SiGe layer in the sample.

For sample II, the situation with intrinsic point defects is different because high vacancy concentrations exist in both regions close to the SiGe–Si interface. Over the interface in the LT-SiGe(50 nm, 250 °C) layer, the vacancy concentration is as high as that in sample I, but may be much higher due to the growing of this layer on the LT-Si(50 nm, 400 °C) layer. Under the interface, a relatively high vacancy concentration exists near the surface of the LT-Si layer. These vacancies diffuse into the LT-SiGe layer through the interface under the action of misfit strains [11]. As a result, the rate of dislocation nucleation through the Perovic–Houghton mechanism is higher than that in sample I due to the higher vacancy concentration near the interface. Thus, a flat regular MD network can be formed at the interface with very high MD density (80% strain relaxation) to prevent MD multiplication through the modified Frank–Read mechanism.

The additional generation of threading dislocations, found in sample II, is worthy of special notice. The region of their nucleation is positioned about 30 nm above the interface; i.e. it is in the middle of the LT-SiGe layer. Recently it has been found that corrugated relief is formed on the surface of the LT-Si layer growing on the high-temperature buffer Si layer at temperatures less than 400 °C, which can be a source of threading dislocation generation in a subsequent SiGe layer [12]. The consecutive growth of two LT layers realized in this sample appears to produce sufficient conditions for the corrugated surface of the LT-SiGe layer to start forming. The nature of the sources of these threading dislocations is still unclear.

4. Conclusions

Multilayer $Si_{0.7}Ge_{0.3}$/Si heterostructures with LT-$Si_{0.7}Ge_{0.3}$(50 nm, 250 °C) and LT-$Si_{0.7}Ge_{0.3}$(50 nm, 250 °C) + Si(50 nm, 400 °C) buffer layers have been grown by MBE. Practically full strain relaxations, 100 and 80%, have been achieved in these heterostructures, respectively, at a total buffer layer thickness of about 200 nm. For both types of LT layer, an initial MD generation was proposed to occur through the Perovic–Houghton mechanism. High vacancy concentration close to the SiGe–Si interface, arising due to the LT epitaxial growth, promotes the active operation of this mechanism. For a single LT-$Si_{0.7}Ge_{0.3}$(50 nm, 250 °C) buffer layer, the vacancy concentration achieved in this layer proves to be insufficient to provide a high enough rate of dislocation nucleation for the full misfit strain relaxation. As a result, an additional MD multiplication through a modified Frank–Read mechanism occurs in the sample. Embedding the intermediate LT-Si layer in a similar heterostructure leads to the significant increase of the vacancy concentration near the interface, which leads to the formation of a dense flat MD network without dislocation multiplication. The results obtained indicate that in the heterostructures studied with both types of LT layer, the MD generation occurred through mechanisms typical for SiGe/Si heterostructures grown at conventional temperatures; however, the rate of dislocation nucleation was very much higher due to the high vacancy concentration near the interface. A possible role of the Si self-interstitials in the dislocation structure formation has not been found.

It is noteworthy that the use of a combined LT-(SiGe + Si) layer has at least two drawbacks. The absence of MD multiplication leads to incomplete misfit strain relaxation. The corrugation of the growing surface of the LT-SiGe layer is accompanied by additional threading dislocation generation during the growth of the high-temperature part of the SiGe alloy. Their nucleation centres are located in the middle of the LT-SiGe layer; however, the nature of these centres is still unclear. High threading dislocation density, 10^7–10^8 nm^{-2}, was detected on the surface for both heterostructures because of their additional generation without the connection with a MD network.

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