Si/SiGe modulation-doped structures with thin buffer layers: Effect of substrate orientation

G. L. Zhou, Z. Ma, M. E. Lin, J. Reed, L. H. Allen, and H. Morkoç
Coordinated Science Laboratory and Material Research Laboratory, University of Illinois at Urbana-Champaign, 104 South Goodwin Avenue, Urbana, Illinois 61801

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High quality Si (strained)/$Si_{0.7}Ge_{0.3}$ (relaxed) modulation-doped structures incorporating unusually thin (700 nm) buffer layers were grown with molecular beam epitaxy at 700 °C. By utilizing (100) substrates misoriented toward (011) by 4°, the density of threading dislocations was reduced by over an order of magnitude as compared with conventional techniques. These layers produced exceptionally high Hall mobilities of 1790 cm^2/V s at 300 K and 19 000 cm^2/V s at 77 K on *n*-type modulation-doped heterostructures. The effect of substrate misorientation on threading dislocation density was investigated using transmission electron microscopy and Nomarski microscopy.

In *n*-type modulation-doped Si-SiGe structures, the band structure is type II where the Si layer is under tensile strain. The lowest Si conduction band in such a structure is twofold degenerate. The electrons occupying the low energy conduction band valleys have a small in-plane mass of $m_l=0.19m_0$ and a large mass of $m_t=0.92m_0$ in the direction perpendicular to the growth plane.[1,2] A thin SiGe layer, generally on top of the strained Si, is intentionally doped leaving the adjacent Si layer essentially free of impurities. Due to the favorable discontinuity in the conduction band, electrons transfer to the lower conduction-band states in the Si layer, leading to the spatial separation of electrons from their parent impurities. To realize this structure, a high quality SiGe buffer layer, with an in-plane lattice constant larger than that of Si, is required. The typical single-step buffer layers with Ge contents around 30% are grown at temperatures below 550 °C and produce threading dislocation densities usually on the order of 10^8–10^9 cm^{-2}. This is the major impediment to achieving high electron mobility in Si/SiGe *n*-type modulation-doped heterostructures.

Most recently, substantial progress has been made in improving the quality of strained Si-SiGe structures by employing graded SiGe buffer layers.[3,4] Modulation-doped Si-SiGe structures, made by molecular beam epitaxy (MBE) and ultrahigh vacuum chemical vapor deposition (UHV-CVD), have shown dramatic enhancement of electron mobilities.[5–7] The samples with the highest mobilities thus far employed a thick (3000 nm) graded $Si_{0.95}Ge_{0.05}$-$Si_{0.7}Ge_{0.3}$ buffer layer, followed by a constant composition SiGe buffer layer both of which were grown at temperatures between 750 and 900 °C.[5] Obviously, these thick buffer layers present problems in field effect transistor (FET) applications, such as parallel conduction and the unacceptably long-time required for growth. Furthermore, the thick layers and high growth temperature may cause wafer warpage, and create obstacles to future heterointegration. Consequently, this necessitates lower temperature processing and thinner buffer layers.

The use of misoriented substrates for the heteroepitaxy of compound semiconductors on Si has led to substantial improvement in the dislocation density of the epitaxial layers due to a uniform distribution of steps and ledges which act as nucleation sites.[8] The interfaces are smoother, the composition of ternary compounds is more uniform, and the anisotropy in lateral growth is reduced.[9,10] However, there are scant reports on using misoriented substrates for SiGe epitaxial growth. In this letter, we present the results of high quality $Si_{0.7}Ge_{0.3}$ layers grown on misoriented Si (100) substrates with relatively thin, 700 nm, SiGe graded buffer layers which are grown at comparatively low (650–700 °C) temperatures by MBE.

The samples in this study were grown in a Perkin–Elmer SiGe MBE system equipped with electron beam evaporators for Si and Ge and an effusion cell for Sb doping. The base pressure was 5×10^{-11} Torr while the pressure during the growth was in the mid 10^{-10}–10^{-9} Torr range. On-axis (100) *p*-type substrates with 3 in. diameters as well as ones misoriented by 4° toward (011) or (001) were cleaned using the RCA method and treated in a dilute (10:1) HF solution prior to loading into the UHV system. The substrate temperatures were measured by a thermocouple calibrated by an infrared pyrometer. The growth rate, measured by a quartz crystal monitor and Sentinel III electron impact emission spectroscopy (EIES), was around 0.2 nm/s for SiGe buffer layers and 0.05–0.1 nm/s for modulation-doped active layers. The thickness calibration was done with a Dektak 3030 surface profilometer. The growth temperatures employed were in the range of 650–700 °C for buffer layers, 500 °C for strained Si channel layers and SiGe spacer layers, and 400 °C for Sb-doped layers. In order to produce the $Si_{0.95}Ge_{0.05}$-$Si_{0.7}Ge_{0.3}$ linearly graded buffer layer, the temperature of both the Ge and Si sources was ramped while keeping the aggregated growth rate at 0.2 nm/s. For this study the graded buffer layer thickness was 700 nm. The graded buffer layer was followed by a constant composition $Si_{0.7}Ge_{0.3}$ layer having a thickness of 400–450 nm.

Figure 1 shows a cross-sectional transmission electron microscopy (XTEM) image of a linearly graded $Si_{1-x}Ge_x$ with x from 5% to 30% capped with a 400-nm-thick uniform composition $Si_{0.7}Ge_{0.3}$ layer. As the micrograph shows, many dislocations form at the SiGe graded buffer and Si substrate interface. Initially, threading dislocations

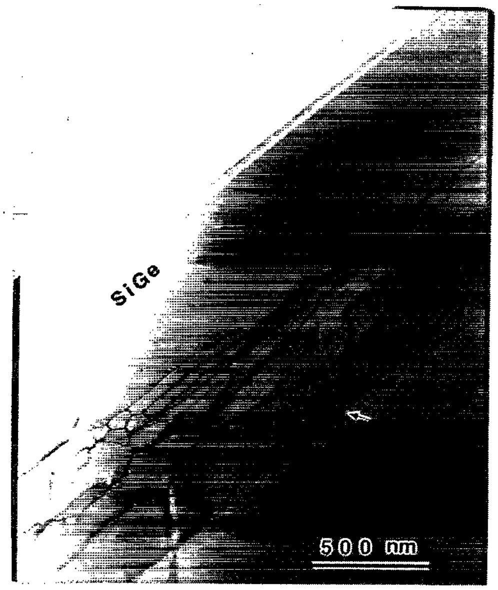

FIG. 1. TEM cross section of a 400 nm uniform $Si_{0.7}Ge_{0.3}$ layer grown on a 700 nm graded $Si_{1-x}Ge_x$ layer on [011] 4° off cut Si.

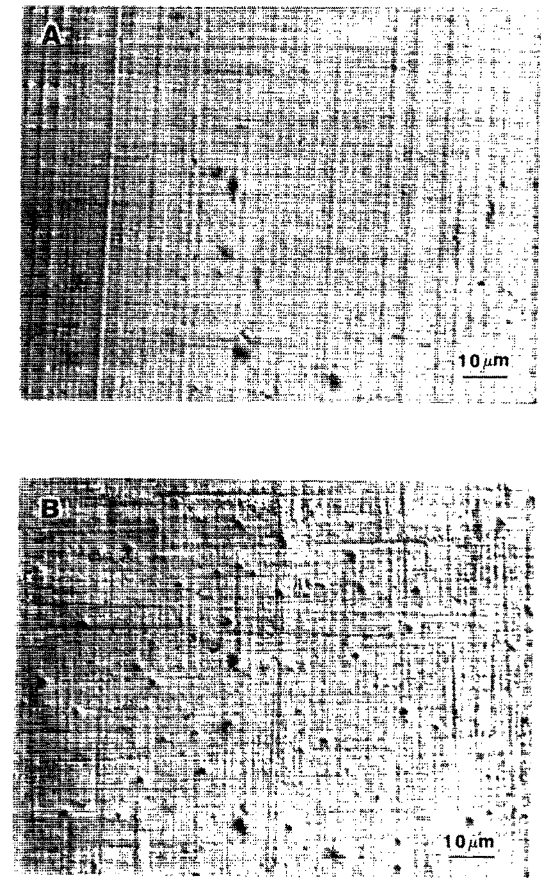

FIG. 2. High magnification Nomarski micrograph of two 700 nm graded $Si_{1-x}Ge_x$ layers on (011) 4° off cut (a) and (001) 4° off cut (b) Si substrates followed by 600 nm uniform $Si_{0.7}Ge_{0.3}$ layers. The arrow indicates the interface of SiGe buffer layers and Si substrates.

are launched with a 60° angle to the interface and then are bent to threads parallel to it. Moreover many of the dislocations propagate into the substrate, as observed by LeCoues *et al.*[3] The lack of threading dislocations detected in the cap layer implies that the buffer layer is effective in relieving the strain and blocking the propagation of emitted threading dislocations. Because the field of observation in XTEM is small (1 μm^2), the absence of threading dislocations only implies that the dislocation density is less than 10^8 cm^2. To more accurately determine the threading dislocation densities, we used a chemical etch to produce etch pits and then counted them by using standard Nomarski optical micro-scopy. Figures 2(a) and 2(b) show the Nomarski optical micrographs from two SiGe buffer layers, similar to those used in Fig. 1, after etching the sample in Wright™ solution for 30 s. To avoid etching away the $Si_{1-x}Ge_x$ graded buffer layers (the etch rate in our case is around 15–20 nm/s), the thickness of SiGe cap layers was 600 nm.

The growth conditions for both samples are identical. However, the substrate used in Fig. 2(a) was (100) Si tilted toward (011) by 4°, whereas the substrate used in Fig. 2(b) was (001) by 4°. Note that the density of threading dislocations which appear as black dots in the images are quite different. By counting the dots and dividing by the area, we obtained values for the dislocation densities of 3×10^5 and 7×10^6 cm^{-2}, respectively. Similar SiGe buffer layers were also grown using on-axis (100) Si substrate and again the dislocation densities were found to be high, similar to that shown in Fig. 2(b). We deduce from this that the thickness of graded SiGe buffer is too thin or the gradient of Ge composition is too large to block the threading dislocations. In addition to the etch pits, cross-hatch patterns can be clearly observed. These patterns are caused by the inhomogeneous strain fields associated with the misfit dislocations combined with strain-dependent etch rate.

In Table I, we compare the dislocation densities as well as Hall mobilities for modulation-doped heterostructures grown on SiGe buffer layers on Si substrates with different

TABLE I. Etch-pit densities and electron mobilities of modulation-doped heterostructures grown on different silicon substrates.

Samples number	1	2	3	4	5	6
Substrate	[011] off	[011] off	[011] off	[001] off	[001] off	on-axis
Thickness of graded buffer (nm)	700	700	700	700	700	700
Thickness of $Si_{0.7}Ge_{0.3}$ (nm)	400	400	400	400	400	400
SiGe spacer (nm)	50	100	150	100	150	100
Etch-pit density (cm^{-2})	4.5×10^5	5.0×10^5	3.5×10^5	5.6×10^6	7.2×10^6	2.5×10^6
300 K mobility (cm^2/V s)	1 140	1 600	1 790	1 140	1 080	1 030
77 K mobility (cm^2/V s)	8 970	13 800	19 000	6 360	5 640	7 404

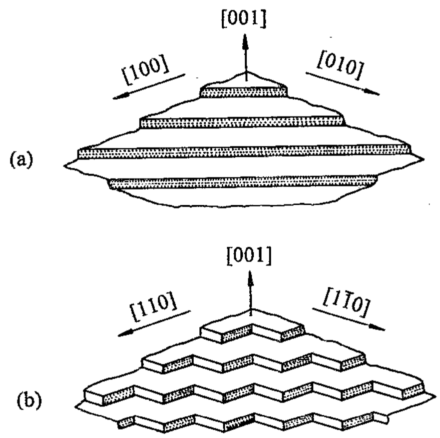

FIG. 3. Schematic representation of step configurations for (100) Si surface misoriented by 4° toward (a) (011), and (b) (001).

miscuts. In these samples, the thickness of strained Si channel layers is 20 nm, and of Sb-doped SiGe layers is 30 nm with a doping level of 1×10^{18} cm^{-3}. The results for various undoped SiGe spacer layers are also listed in Table I. The Hall mobilities are typically higher for samples grown on substrates tilted toward (011) with the highest values being 1790 cm^2/V s at 300 K and 19 000 cm^2 V s at 77 K. These results clearly indicate that the particular tilt employed is responsible for reducing the threading dislocation density in the $Si_{0.7}Ge_{0.3}$ buffer layer and thus the associated scattering centers. By contrast, the samples grown on substrates with on-axis and tilt toward (001) characteristically exhibit lower mobilities, and the optical microscopy examination shows higher etch-pit densities.

A possible explanation is that surface steps affect the propagation of dislocations. There are two types of steps on (100) Si surfaces: Steps A, perpendicular to the dimerization direction, and steps B, parallel to the dimerization direction.[11] The step edges always run straight along the [110] directions, so the steps formed on the substrate tilted toward (011) are more likely to have straight edges, as shown in Fig. 3(a). This step configuration may guide dislocations to propagate to the wafer edge, thus reducing the threading branches on top of the film. But, for the substrate tilted toward (001), the kinks are much more irregularly spaced along the step edges, as shown in Fig. 3(b). Consequently, the situation is similar to the film grown on on-axis substrates. Additional investigations are required to determine in more detail the exact nature of dislocation reduction in samples grown on (100) Si tilted by 4° toward (011).

In summary, we have investigated MBE growth on SiGe graded buffer layers using on-axis (100) Si wafers and those tilted toward (011) and (001) by 4°. The film quality gauged by the density of dislocations and Hall mobility was observed to be consistently enhanced in samples grown on substrates tilted toward (011). High quality $Si_{0.7}Ge_{0.3}$ layers with very low dislocation densities (in the range of 10^5 cm^{-2}) were reproducibly grown on relatively thin (700 nm) SiGe graded buffers. *n*-type modulation-doped heterostructures grown on such buffers exhibited mobilities of 1 790 cm^2/V s at 300 K and 19 000 cm^2/V s at 77 K.

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