The elimination of surface cross-hatch from relaxed, limited-area $Si_{1-x}Ge_x$ buffer layers

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The influence of lateral dimensions on the relaxation and surface topography of linearly graded $Si_{1-x}Ge_x$ buffer layers has been investigated. A dramatic change in the relaxation mechanism has been observed for depositions on Si mesa pillars of lateral dimensions 10 μm and below. Misfit dislocations are able to extend unhindered and terminate at the edges of the growth zone, yielding a surface free of cross-hatch. For lateral dimensions in excess of 10 μm orthogonal misfit interactions occur and relaxation is dominated by the modified Frank–Read (MFR) mechanism. The stress fields associated with the MFR dislocation pile-ups result in a pronounced cross-hatch topography. © *1997 American Institute of Physics.* [S0003-6951(97)04443-4]

An essential requirement for the complete exploitation of strained layer SiGe heterostructures is the growth of relaxed, defect free virtual substrates to any Ge content. The use of compositionally graded buffer layers has led to a dramatic decrease in the threading dislocation density in such substrates.[1] Such buffer layers have enabled two-dimensional electron mobilities, confined within tensile strained Si channels, of 5.2×10^5 and 2600 $cm^2/V\,s$ to be achieved at 0.14 and 300 K, respectively.[2,3] Such high mobility heterostructures are of great interest for metal-oxide semiconductor (MOS) and microwave applications.

However, as a consequence of plastic buffer layer relaxation the stress fields associated with the underlying misfit dislocations cause a roughening of the epilayer surface, resulting in a cross-hatch surface topography with a periodicity of around 1 μm.[4,5] Such roughening of the buffer layer is detrimental to carrier mobilities and is not compatible with planar integrated circuit technologies. In order to reduce this effect thick buffer layers, often 2–5 μm thick, are generally used which are both time consuming and expensive to produce.

By reducing the lateral dimension of the growth zone defect densities may be reduced,[6–8] but there have been no previous studies on how lateral dimensions influence the cross-hatch surface topography. In the present letter we discuss for the first time the relaxation mechanism of limited-area, linearly graded $Si_{1-x}Ge_x$ buffer layers. We report a mechanism by which relaxation occurs by complete misfit extension across the growth zone, enabling misfit termination at the growth zone edge without orthogonal misfit interactions.

Arrays of square Si(001) mesa pillars, orientated along ⟨110⟩ directions and of lateral dimensions ranging from 3 to 20 μm, were anisotropically plasma-etched to a depth of 2 μm on Si(001) substrates. Effectively ''infinite-area'' unpatterned regions of area 1 cm^2 were also included for comparison. A 100 nm pure Si layer was deposited by solid-source molecular beam epitaxy (MBE) followed by a graded $Si_{1-x}Ge_x$ buffer region with x varying linearly from 5% to 23% over 500 nm. A 200 nm uniform $Si_{0.77}Ge_{0.23}$ buffer followed by a 10 nm tensile-strained pure Si channel and a 50 nm uniform $Si_{0.77}Ge_{0.23}$ cap layer completed the structure. All MBE deposition was performed at a substrate temperature of 550 °C so as to inhibit three-dimensional growth.

The limited-area $Si_{1-x}Ge_x$ epilayers were characterized using a JEOL JEM-2000fx transmission electron microscope (TEM) operating at an accelerating voltage of 200 keV. Scanning electron micrographs (SEMs) were obtained using a JEOL JSM 6100 system and atomic force micrograph (AFM) images were obtained using a M5 Park Scientific Instruments microscope. Cross-sectional TEM samples were prepared by mechanical thinning followed by Ar-ion sputtering. The degree of relaxation of the individual limited-area depositions was determined using micro-Raman spectroscopy. The 488 nm line of an Ar-ion laser was focused to a spot of diameter less than 2 μm using a microscope objective. In addition, the Ge content of the infinite-area deposition was determined using high and low incidence x-ray[115] rocking curves.

Figure 1 shows a cross-sectional TEM image of the graded $Si_{1-x}Ge_x$/Si heterostructure deposited on a 10-μm-wide Si mesa pillar and is typical of depositions of 10 μm and below. For graded depositions relaxation occurs by misfit extension upon different atomic planes. In the case of graded, limited-area buffers a reduction in orthogonal ⟨110⟩ misfit interactions enables misfit dislocations to extend unhindered and terminate at the edges of the growth zone. In addition, since orthogonal pinning events are avoided, a reduction in the threading dislocation density of the epilayer is to be expected.

A similar view of an identical epilayer deposited on a 20-μm-wide mesa pillar is depicted in Fig. 2. In both Figs. 1 and 2 the dislocations are of the 1/2⟨110⟩60° type. The large

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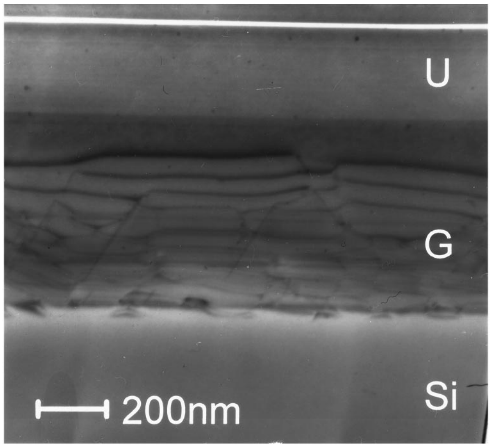

FIG. 1. Cross-sectional TEM (XTEM) image of the Si/SiGe heterostructure deposited on a 10-μm-wide Si mesa pillar. The misfit dislocations are clearly confined within the linearly graded region (denoted G) with no dislocations penetrating the growth mesa (Si) or the uniform $Si_{0.77}Ge_{0.23}$ buffer layer (U).

number of dislocation pile-ups penetrating deep into the Si growth pillar clearly demonstrates a different relaxation mechanism in operation. Such pile-ups are characteristic of the modified Frank–Read (MFR) relaxation mechanism proposed by LeGoues.[1] As the lateral dimension of the growth zone increases, an increased number of misfit dislocations are required to traverse the mesa in order to relax the structure. This results in an increased probability of an extending misfit encountering a pre-existing orthogonal dislocation on the same atomic plane of the graded buffer. The MFR mechanism is a direct consequence of such interactions.

The co-operative stress fields associated with such dislocation pile-ups considerably influence the surface morphology of the epilayer. The effect of such stress fields is demonstrated in the AFM profiles of Figs. 3 and 4. Figure 3(a) shows the smooth surface topography typical of a non-MFR relaxed deposition on a 6 μm mesa, while Fig. 3(b) depicts the height profile across the mesa. The speckle contrast evident in Fig. 3(a) is thought to be due to post-growth contamination. The corresponding AFM image of a MFR relaxed

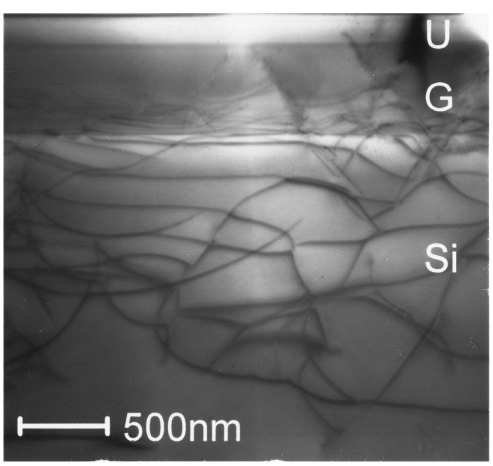

FIG. 2. XTEM image of an identical heterostructure to that of Fig. 1, except deposited on a 20-μm-wide Si mesa pillar. Note the massive dislocation network penetrating deep into the actual growth mesa (Si).

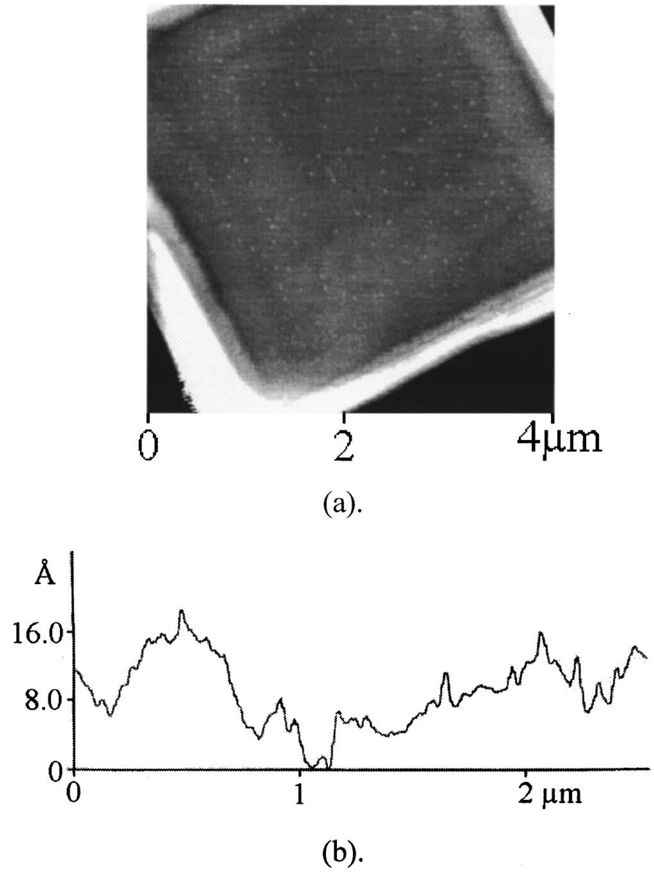

FIG. 3. AFM surface profile of the Si/SiGe heterostructure deposited on a 6-μm-wide mesa (a) and the corresponding height profile across the growth zone (b) indicating peak undulations of approximately 16 Å.

buffer deposited on a 20-μm-wide mesa is given in Fig. 4. The surface topography of the MFR relaxed mesa depositions are similar to that of the infinite-area control depositions. Lutz *et al.*[9] have demonstrated that a single 60° dislocation at the epilayer/substrate interface results in an atomic step at the intersection of the associated glide plane and the epilayer surface. Further, since the MFR mechanism results in dislocation pile-ups along a common (111) glide plane the resulting surface morphology is simply the sum of the individual surface step displacements of the dislocations involved in the pile-up. This results in a pronounced surface cross-hatch to the MFR relaxed depositions as shown in Fig. 4.

Figure 5 shows the Si–Si Raman spectrum obtained from the center of each of the individual mesa depositions. Due to the penetration depth of the laser light ($\sim$120 nm), such backscattered spectra arise primarily from the uniform $Si_{0.77}Ge_{0.23}$ layer of the heterostructure. The Si–Si peak positions obtained from the 3 and 4 μm depositions are seen to coincide with the spectra obtained from the infinite area deposition and correspond to approximately 77% relaxation.[10] However, for 6, 10, and 20 μm mesa depositions a shift in the Si–Si peak is observed indicating an increased residual strain, with the maximum residual strain occurring in the 10 μm deposition and corresponding to approximately 50% relaxation. For depositions in excess of 10 μm relaxation occurs due to the onset of the MFR mecha-

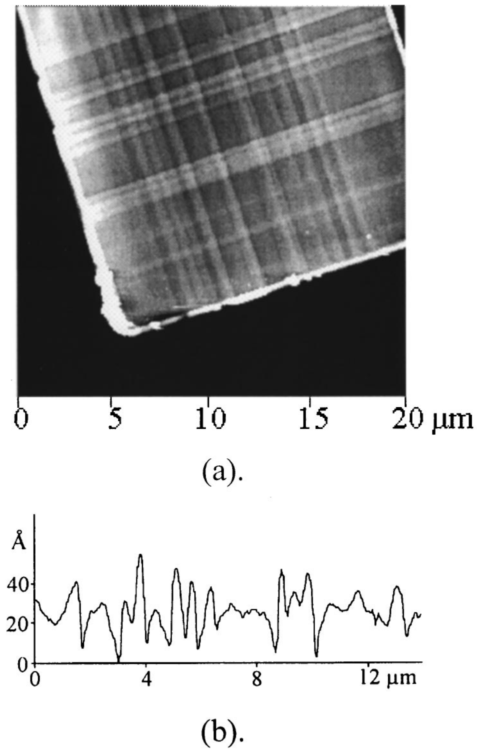

FIG. 4. AFM surface profile of the 20 μm deposition (a) showing a highly developed cross-hatch and the corresponding height profile (b) with peak undulations of approximately 60 Å.

nism and the Si–Si peak of the epilayer again shifts towards that of relaxed infinite area deposition. The broadening of the spectra from the 3 and 4 μm depositions can be attributed to elastic relaxation effects which occur at the edges of the growth zone.[11–13]

In summary, we have investigated the effect of lateral dimensions on the surface morphology of linearly graded $Si_{1-x}Ge_x$ buffer layers. For lateral dimensions of less than 10 μm, non-MFR relaxation is observed with misfit dislocations traversing the whole of the growth zone and terminating at the mesa edges without orthogonal misfit interactions occurring. This results in a relaxed epilayer with a smooth surface morphology. With increasing lateral dimension, orthogonal misfit interactions occur and relaxation is dominated by the MFR mechanism. This results in a pronounced surface cross-hatch morphology. It is postulated that the use of limited-area, linearly graded $Si_{1-x}Ge_x$ buffer layers offers the opportunity of obtaining relaxed buffer layers to any Ge content while avoiding threading dislocations and the problematic cross-hatch roughening.

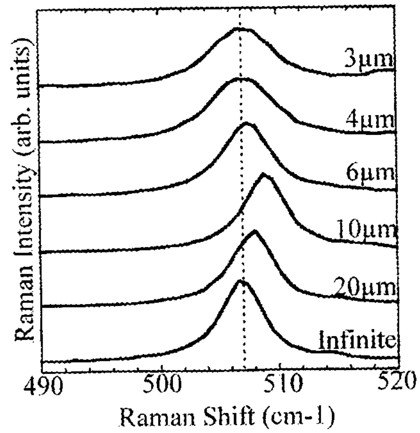

FIG. 5. Si–Si Raman frequency shift as a function of lateral dimension of the uniform $Si_{0.77}Ge_{0.23}$ epilayer deposited on the linearly graded buffers. The dashed line corresponds to ~80% relaxation whilst the residual strain within the 10 μm deposition indicates ~50% relaxation.

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