Identification of a Mobility-Limiting Scattering Mechanism in Modulation-Doped Si/SiGe Heterostructures

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High electron mobilities in modulation-doped Si/SiGe in the range of $(1.5-1.8) \times 10^5$ cm^2/V s at 0.4–1.4 K have been achieved by several groups. Those numbers fall short of the expected theoretical value. We have examined how strain in the Si channel affects the low temperature electron mobility by systematically varying the Ge content in the relaxed buffer underneath, and by changing the Si channel thickness. A clear reduction in mobility is observed at a critical layer thickness, which is identified as the thickness at which remaining threading dislocations glide in the Si channel, resulting in misfit dislocations at the bottom interface. Understanding and control of this mechanism have led to the growth of samples with mobility values in the range of $(3-4) \times 10^5$ cm^2/V s.

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An essential requirement for n-type modulation-doped Si/SiGe structures is that the Si channel be under tensile strain, which lowers the twofold degenerate conduction band of Si with respect to the sixfold degenerate band in relaxed SiGe. The use of a graded Ge-content buffer layer [1] grown on a Si substrate has allowed the growth of strained Si imbedded between relaxed SiGe layers with a low density of threading dislocations (1×10^5–1×10^7 cm^{-2}). The implementation of this technique resulted in the increase in electron mobility at 4.2 K from 2000 cm^2/V s as reported in 1985 by Abstreiter *et al.* [2] to 20 000 cm^2/V s [3]. Subsequently, thicker buffer and spacer layers have led to an increase in mobility in the range of $(1.5-1.8) \times 10^5$ cm^2/V s as reported by various groups [4]. The main scattering mechanism limiting the mobility in those samples was not clearly identified. While ionized impurity scattering and background impurities would eventually limit the mobility, theoretical calculations by Stern and Laux [5] concluded that the mobility should have been significantly higher than the measured values, especially for the case of a thick spacer layer and low background doping. Monroe *et al.* [6] have considered various scattering mechanisms such as alloy scattering, surface roughness, strain field, and threading dislocations. Their calculations predict that the scattering due to threading dislocations in the Si channel should not limit the mobility unless the density of threads is several orders of magnitude higher than in our current samples.

However, Monroe *et al.* [6] assumed that the dislocations were only threading, i.e., there are no misfit segments at all along the buffer-channel interface. We find that this is not true, nor should it be expected to be the case, at any channel thickness in excess of the Matthews-Blakeslee critical thickness [7]. Reported buffer layers have threading dislocation densities on the order of 10^5 to 10^7 cm^{-2}. Each of these will glide as soon as the Matthews-Blakeslee critical thickness is exceeded, resulting in a misfit dislocation at the bottom interface of the Si channel. We have investigated the effect of the presence of these dislocations on the electron mobility by varying the buffer layer Ge content x and the channel thickness d. We find excellent agreement with the Matthews-Blakeslee critical thickness, and identify the array of misfits at the bottom interface of the channel as the major cause for low temperature mobility degradation. By suppressing this effect we have achieved electron mobilities in excess of 400 000 cm^2/V s at 0.4 K. This is more than double the previous record value, and agrees well with the upper limit predicted by theoretical calculations.

The layers under study were grown by ultrahigh vacuum chemical vapor deposition (UHV-CVD) in the temperature range of 500–550 °C. A schematic of the layer structure is shown in Fig. 1. First, a step-graded $Si_{1-x}Ge_x$ layer is grown, reaching a 30%–40% Ge composition. This is followed by the growth of a 1 μm thick $Si_{1-x}Ge_x$ buffer layer, where x is in the range of 0.25–0.35. A strained Si channel is then grown to a thickness in the range of 8–15 nm, followed by an undoped 15 nm $Si_{1-x}Ge_x$ spacer layer, an n-type doped $Si_{1-x}Ge_x$ supply layer, and a 4 nm thick Si cap layer. The Ge fraction and the degree of relaxation of the buffer layer were determined by high resolution x-ray diffraction. The measurement of layer thickness and the identification of defects were achieved by cross-sectional and planar-view transmission electron microscopy (TEM), and the mobility measurements were performed in the range of 0.4–300 K using standard van der Pauw and Hall bar geometries.

Figure 2 shows the dependence of electron mobility at 20 K on the Si channel thickness for three different values of buffer layer composition x. The three arrows in the figure (from left to right) correspond to the Matthews-Blakeslee critical thickness for Si grown on relaxed $Si_{1-x}Ge_x$, with $x = 0.34$, 0.30, and 0.25, respectively (the corresponding percentage lattice mismatch is indicated

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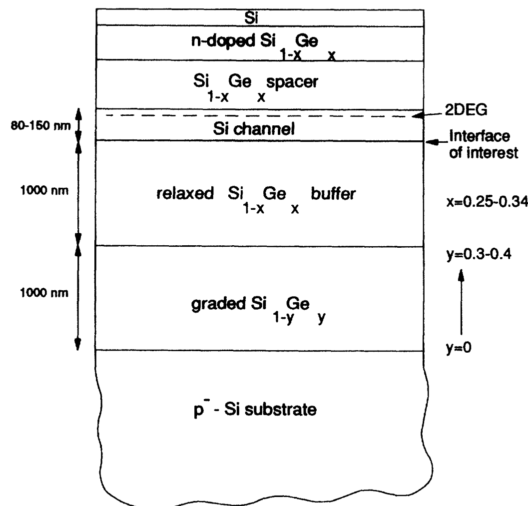

FIG. 1. Schematic of the layer structure grown by UHV-CVD.

below each arrow). For each x value, a clear reduction in mobility is observed as the channel thickness is increased. Also, for the same channel thickness, a reduction in mobility is observed as x increases.

The critical thickness beyond which misfit dislocations are created is predicted for the case of strained layer growth by Matthews and Blakeslee [7], under the assumption that there are no nucleation barriers to such dislocations. For strained SiGe on Si, the existence of a nucleation activation energy [8] allows growth of layers whose critical thickness considerably exceeds the predicted critical thickness, without the generation of misfit dislocations. In the samples studied here, on the other hand, where strained Si is grown on relaxed SiGe, *pre-existing* threading dislocation densities are on the order of 10^5 to 10^7 cm^{-2}. Thus, this is one of the rare instances for which the theoretical Matthews-Blakeslee critical thickness should apply exactly. Consequently, if the channel is grown below this critical thickness, the dislocations continue to thread through the Si channel. When the critical thickness is reached, however, an array of misfit dislocations is formed by glide of the threading segments along the heterojunction interface. The length of the resulting misfit segments depends on the growth conditions, such as growth temperature (which determines the glide velocity) and the time it takes to grow the remaining layers. It is important to note that the average reduction of strain in the Si channel is less than 2%, corresponding to the worst case of 2×10^4 cm^{-1} density of misfit dislocations at the channel interface. Such an insignificant relaxation has a negligible effect on the strain in the Si channel, and thus cannot be responsible for the dramatic decrease in mobility observed in Fig. 2.

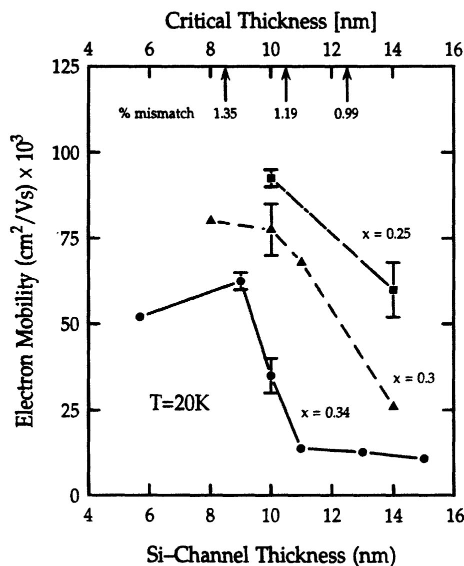

FIG. 2. Electron mobility as a function of channel thickness for three different values of x (the Ge content in the underlying buffer) measured at 20 K. The arrows indicate the Matthews-Blakeslee critical thickness for the given amount of percentage lattice mismatch, which agrees well with the bending point in the mobility curves.

Figure 3 shows a planar-view TEM picture of three cases: $x = 0.35$ and $d = 11$ nm, $x = 0.25$ and $d = 14$ nm, and $x = 0.25$ and $d = 10$ nm. The corresponding mobility at 20 K is 14 000, 60 000, and 95 000 cm^2/V s, respectively. In the first case, the array of misfit dislocations is obvious and the separation between two segments is on the average about 1 μm. The length of each segment is on the order of 100 μm. In the second case, the average separation between threading segments is about 2 μm, and in the third case, they are completely absent within our detection limit.

This one-to-one correspondence between mobility degradation and density of misfit segments is clear evidence that these misfits play a dominant role in limiting the electron mobility in the Si channel at low temperature. The array of 60° misfits causes a strain field in the Si channel. Since, in our case, the dislocations are very near to the free surface, the image force has to be considered, and the strain field around a dislocation decays along the channel with a characteristic length that is equal to the distance between the dislocation and the surface of the channel [9] (10 nm in our case). Since the average separation of the misfit dislocations in the worst sample [corresponding to Fig. 3(a)] is about 1 μm, and the characteristic decay length of the strain field is 10 nm, the dislocations can be treated independently. The edge component of the dislocation affects the transport most, since it is the only component that can modify the conduction band offset by relaxing the Si lattice around it. This, in turn, leads to a fluctuating potential and a local charge density variation. A self-consistent calculation is needed to fully account for this effect, but is beyond the scope of this work.

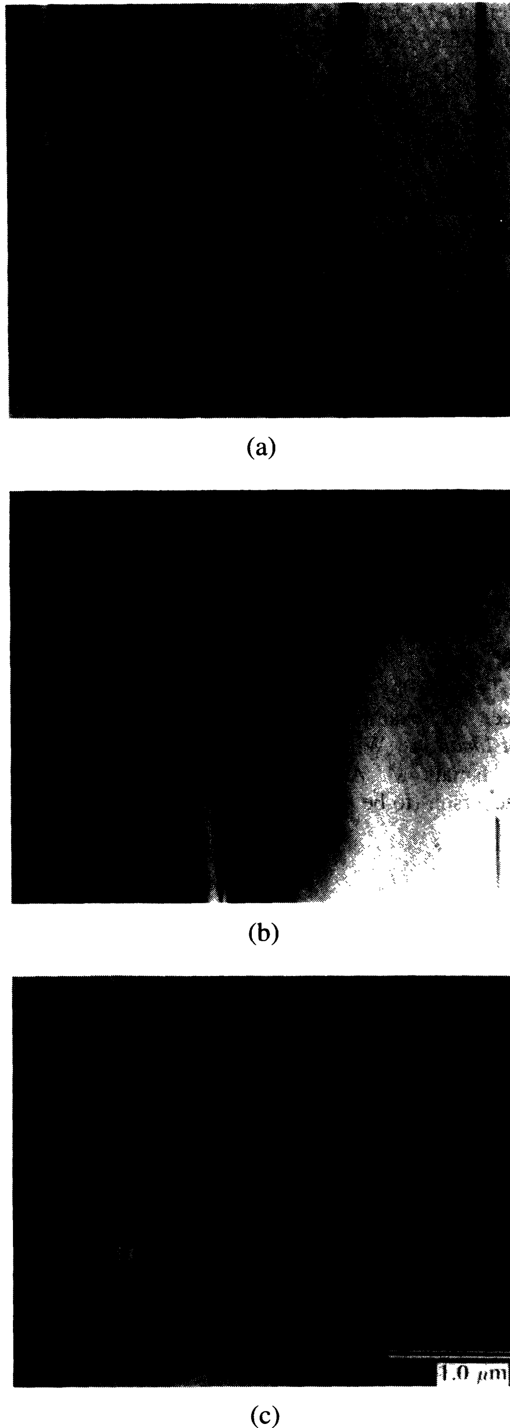

FIG. 3. Planar-view TEM picture of (a) $x = 0.35$ and $d = 11$ nm, (b) $x = 0.25$ and $d = 14$ nm, and (c) $x = 0.25$ and $d = 10$ nm. The arrow in (c) indicates a threading segment, which has not extended along the interface.

We have calculated the strain along the Si channel 2 nm below the upper interface (Fig. 4), where the centroid of the electron charge is expected to be for the sample shown in Fig. 3(a). The resulting change in the

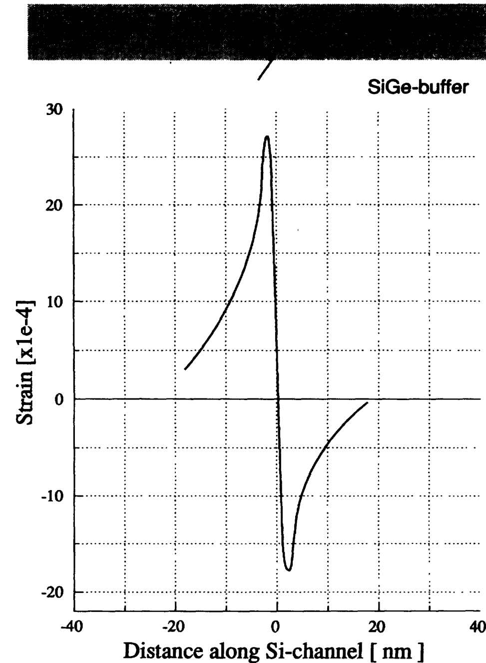

FIG. 4. Calculated in-plane strain variation, 2 nm below the top of the Si channel, due to the presence of a 60° misfit dislocation at the buffer-channel interface.

rms strain in the Si channel due to the misfit dislocations is 2.0×10^{-5}. Using this value, the mobility derived from the calculations of Monroe *et al.* [6] would be 17 000 $cm^2/V\,s$, slightly higher than the measured value of 14 000 $cm^2/V\,s$. The higher value may be attributed to the fact that the misfit dislocations are assumed in our calculation to be uniformly distributed, whereas in reality they are not. The same calculation estimates the mobility of the sample in Fig. 3(b) to be 76 000 $cm^2/V\,s$. It is interesting to note that the calculation and the measurement both show a factor of 4 reduction in mobility for a reduction in the dislocation spacing by a factor of 2.

In order to confirm the above results, the sample corresponding to Fig. 3(a) was backgated, which allowed varying the charge density in the channel as well as modifying the position of the charge centroid within the quantum well [10]. As a function of negative gate bias, the electron density is reduced and the electrons are pushed toward the top interface. We have observed an increase in the electron mobility by 10% at 4.2 K as the electron density was reduced by 15%. Since the mobility in all our ungated high mobility samples decreases almost linearly with the reduction in electron density, the observed mobility enhancement with the backgate is actually equivalent to more than 20%. This is attributed to shifting the centroid of the charge away from the bottom interface by about 0.7 nm.

From the discussion above, one can easily conclude that the ideal sample would be one with a thin Si channel and/or low x. Lowering the x value beyond a certain

limit can be detrimental since it results in a reduction of the conduction band offset. A thinner channel would be useful, but eventually surface roughness scattering (which varies with the channel thickness as d^{-6}) would become dominant and reduce the mobility. The onset of such a reduction is seen in Fig. 2 for the 5.7 nm thick channel case at $x = 0.34$. As a compromise, one might expect a value of $x = 0.2$–0.25 and $d = 10$ nm to be optimum. Indeed, mobility values in the range of $(3-4) \times 10^5$ cm^2/V s have been measured at 0.4–1.4 K in ungated structures [10]. This is more than a factor of 2 larger than the previous record value [4], and agrees well with the theoretical predictions [5]. Furthermore, a record mobility of 526 000 cm^2/V s at 0.4 K was obtained by backgating such a structure.

In summary, we have identified a major scattering mechanism limiting the low temperature electron mobility in modulation-doped Si/SiGe. Once the channel thickness exceeds the critical thickness, preexisting threading dislocations glide, forming an array of misfits at the channel-buffer interface. The associated strain field results in a clear reduction in the electron mobility. By avoiding this scattering mechanism, we have managed to grow structures with electron mobility values up to 4×10^5 cm^2/V s.

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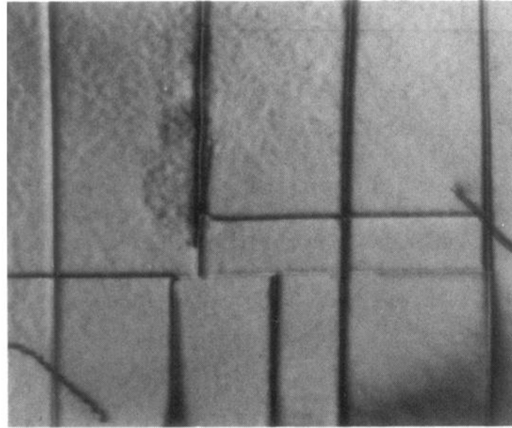
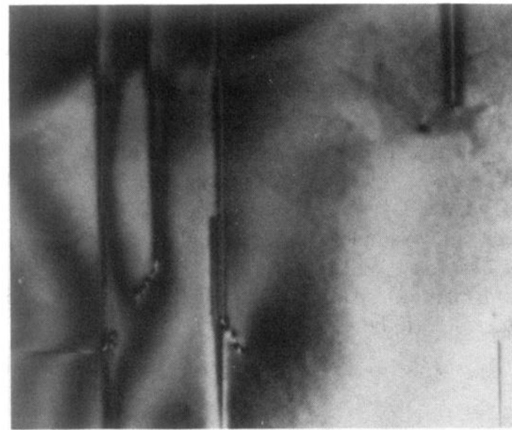


(a)



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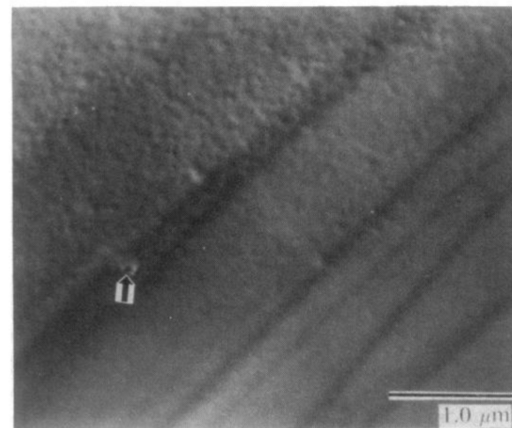

(c)

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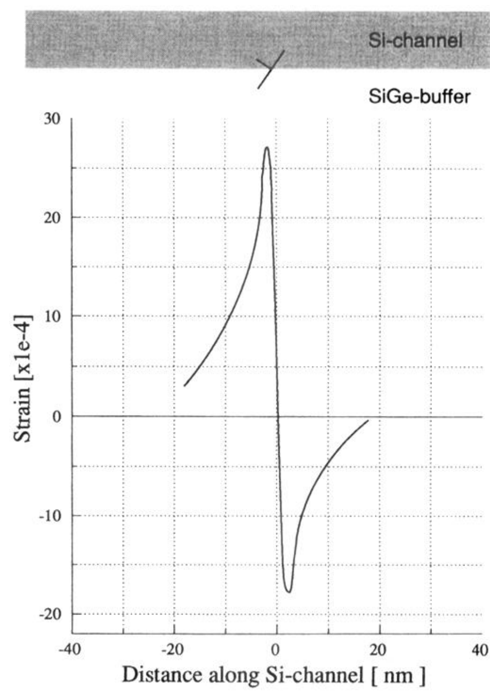

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