

Velocity overshoot in a modulation-doped Si/Si_{1-x}Ge_x structure

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Abstract. The in-plane transport properties of a strained (100) Si layer on a relaxed Si_{1-x}Ge_x substrate are studied for an ungated modulation-doped structure. We use an ensemble Monte Carlo technique. These results are then used to study a gated device structure with a moment equation method. Similar velocity–field characteristics are found for ungated strained Si with any valley splitting energy $\Delta E \geq 0.1$ eV. These phonon-limited electron mobilities reach $4000 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ at 300 K, and $23\,000 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ at 77 K. There is only a slight increase in the saturation velocity at both temperatures. However, a significant overshoot peak transient velocity is found to depend upon ΔE , and for $\Delta E = 0.4$ eV it reaches $4.1 \times 10^7 \text{ cm s}^{-1}$ at 300 K, and $5.2 \times 10^7 \text{ cm s}^{-1}$ at 77 K. Impact ionization increases with ΔE , due to the reduction in the bandgap. For the gated device structure, our numerical simulation of a deep submicrometre modulation-doped device shows velocity overshoot with a peak velocity of $2.6 \times 10^7 \text{ cm s}^{-1}$ in the quantum well at 300 K, which is important in achieving a high transconductance of about 300 mS mm^{-1} .

Owing to the recent developments in epitaxial growth techniques of Si/Si_{1-x}Ge_x heterostructures, extremely high mobilities have been reported in an n-type modulation-doped heterostructure, typically $1600 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ at 300 K and $96\,000 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ at 4.2 K [1], or $1500 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ at 300 K and $9500 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ at 77 K [2]. Peak mobilities of $175\,000 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ have been achieved at a low temperature [3, 4]. A high-transconductance n-type Si/Si_{1-x}Ge_x modulation-doped field-effect transistor has been created and exhibits 600 mS mm^{-1} at 77 K with a gate length of $0.25 \mu\text{m}$ [2]. In these later experiments, a two-dimensional electron gas was realized in a strained Si (100) layer grown on a relaxed Si_{1-x}Ge_x (100) substrate, where the Si layer acts as a potential well and the Si_{1-x}Ge_x substrate acts as a potential barrier.

The strain at the heterointerface raises four valleys parallel to the interface, and lowers the two perpendicular valleys. This creates an energy splitting ΔE [5, 6]. (In a modulation-doped heterostructure, quantization in the channel adds to the valley splitting [7], so that we use this simple parameter to characterize the layer.) The splitting is expected to suppress the intervalley phonon scattering of electrons from lower valleys to upper valleys, and effectively reduces the intervalley phonon scattering rate. In the lowered valleys, electrons show the smaller transverse mass in the in-plane transport. These are the main mechanisms for the high mobility and the high transconductance in the above devices [1, 2]. The strain

also causes a reduction in the bandgap, and affects impact ionization and the channel electron density.

We have adopted an ensemble Monte Carlo technique [8] to study the in-plane transport property of an ungated modulation-doped structure. The effect of strain is included only in the band structure as the valley splitting energy ΔE . The two-dimensional nature of the scattering in the quantized layer is neglected, since we treat high-field properties. In order to model the smaller transverse-mass transport properly, we use the Herring–Vogt transformation with a three-valley model. We use zeroth-order f- and g-phonons and first-order f- and g-phonons for intervalley scattering as well as acoustic phonons. The usual set of coupling constants for phonon modes is adopted, which recovers the measured velocity–field characteristics of unstrained Si [9]. Impact ionization is included with the soft ionization model of Ridley [10] and is influenced by the strain through the reduced bandgap. Non-parabolicity also depends on the bandgap and is subject to the strain effects. The simulation for a gated structure has been performed with a moment equation method [11], which can incorporate quantum effects. The Monte Carlo results of velocity–field and energy–field characteristics for an ungated structure are used as input data to characterize the material in the moment equation method.

At 300 K, the calculated mobility for strained Si is almost triple the low field mobility ($4000 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$, compared with that of unstrained Si, $1500 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$) due to the smaller transverse mass transport. In fields larger than 20 kV cm^{-1} , all curves approach one another

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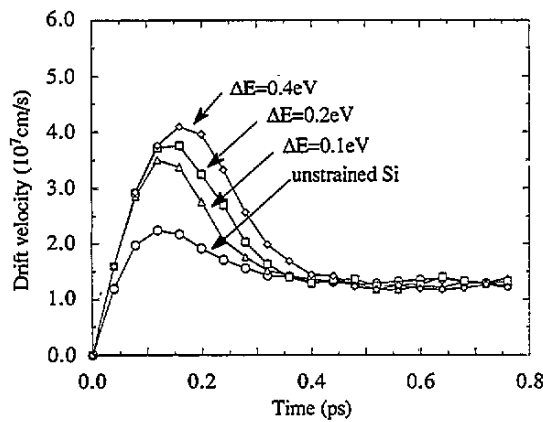


Figure 1. Transient overshoot velocity with a sudden application of a field of 50 kV cm^{-1} at 300 K for various valley splitting values ΔE .

and have a similar saturation velocity $\sim 1.0 \times 10^7 \text{ cm s}^{-1}$, although strained Si tends to show a slightly higher value. At 77 K, the mobility is higher, $17\,000 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ for unstrained Si and $23\,000 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ for strained Si, and the saturation velocity is reached for fields larger than $\sim 5 \text{ kV cm}^{-1}$. Again, there is no significant difference between them, although strained Si tends to show a slightly higher value. The saturation velocity is estimated to be $\sim 1.3 \times 10^7 \text{ cm s}^{-1}$ at 77 K.

Figure 1 shows the transient change of the drift velocity when an electric field of 50 kV cm^{-1} is applied suddenly at time $t = 0$ at 300 K. The velocity shows a significant overshoot, which is larger for larger ΔE . Around $t = 0.3$ to 0.35 ps , the velocity reaches its steady-state value. The peak velocity for $\Delta E = 0.4 \text{ eV}$ is $4.1 \times 10^7 \text{ cm s}^{-1}$ and the overshoot lasts for 0.35 ps . Their product is $\sim 0.1 \mu\text{m}$, and this gives an estimation for the device size for which the electrons run from source to drain without reaching the steady-state velocity. This length is of the same order of magnitude as the gate length of $0.25 \mu\text{m}$ in the reported experiment [2], and the high transconductance measured there can be attributed to this overshoot effect, which is more enhanced at 77 K, as shown in figure 2. The overshoot peak velocity again

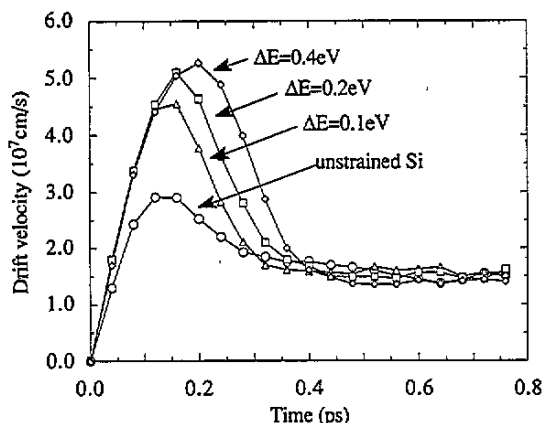


Figure 2. Transient overshoot velocity with a sudden application of a field of 50 kV cm^{-1} at 77 K for various valley splitting values ΔE .

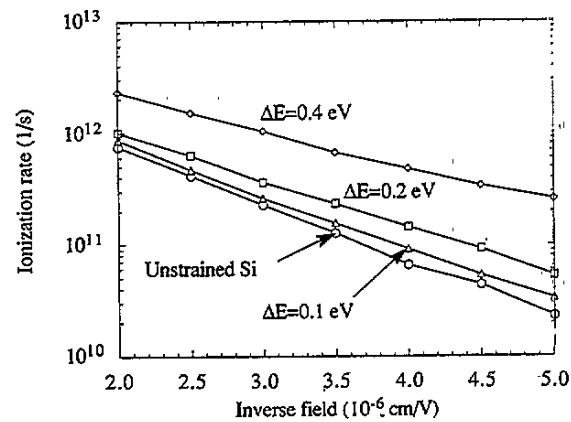


Figure 3. Impact ionization rate at 300 K.

increases with ΔE , and for $\Delta E = 0.4 \text{ eV}$ it is now $5.2 \times 10^7 \text{ cm s}^{-1}$ and the transient behaviour lasts for 0.4 ps , so that the product is larger ($\sim 0.2 \mu\text{m}$). The effect of the overshoot is therefore enhanced compared with that at 300 K, and compares well with the effects in the device of [2]. Figure 3 shows the carrier generation rate at 300 K. The unstrained Si results are consistent with those of [9]. As expected, the ionization rate increases with ΔE , due to the reduction of the bandgap. The ionization increases with the field and decreases with the temperature and this is the same trend as unstrained Si. Figure 4 illustrates the longitudinal velocity as a function of position in the quantum well of a $0.18 \mu\text{m}$ modulation-doped device. The ΔE for this device is 0.2 eV . The bias condition is $V_g = 0.5 \text{ V}$ and $V_d = 1.5 \text{ V}$. The velocity overshoot in the gate region results in a peak velocity of $2.6 \times 10^7 \text{ cm s}^{-1}$. The overshoot is important in achieving the high transconductance for the device, for it introduces a larger current flow along the quantum well. The transconductance for this device is found to be 300 mS mm^{-1} , which is comparable to the experimental result in [2]. The first velocity peak near the source is due to the structure model we used for the change of interface discontinuity [11], and is probably not realistic. Nevertheless, these results suggest that the structure can increase the electron velocity between source and gate,

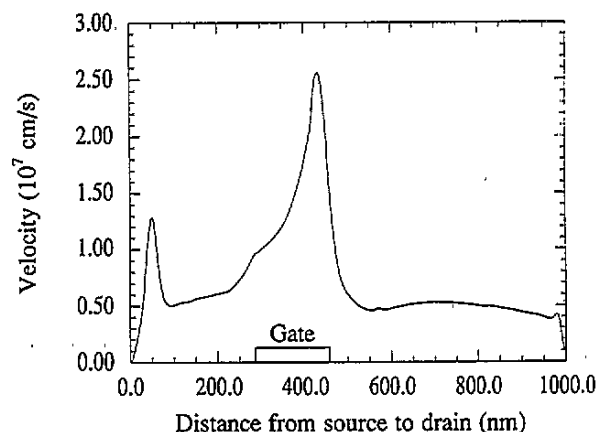


Figure 4. Longitudinal velocity as a function of position in the quantum well of a $0.18 \mu\text{m}$ modulation-doped device.

which in turn will raise the average velocity through the device and enhance the device performance.

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