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Reduced intervalley scattering rates in strained Si/Si_xGe_{1-x} quantum wells and enhancement of electron mobility: A model calculation

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In a $Si/Si_{0.5}Ge_{0.5}$ quantum well grown on a [100] oriented $Si_{0.75}Ge_{0.25}$ buffer, the four valleys having longitudinal mass normal to the [100] direction are lifted from the remaining two valleys. As a consequence, the intervalley f scattering between these two groups of valleys, the strongest in bulk Si, occurs only when the electrons in the subbands reach a high threshold energy. A high value of mobility limited mainly by acoustic phonon scattering is thus expected and is also obtained from the model calculation described in the present work. It is shown that higher values of the mobility may be obtained for wider wells.

Electronic transport in strained Si/Si_xGe_{1-x} heterojunctions, quantum wells (QWs), and superlattices has been studied by several workers[1–10] in recent years. An enhancement of the mobility over the values in pure bulk silicon has been observed in these studies both at low temperatures[1–5] and at room temperature.[6,7] The enhancement at low temperature is due to reduced impurity scattering[8] in modulation doped samples. However, at room temperature neither the impurity scattering nor the interface roughness scattering plays a significant role. It has also been proved[9] that when the two-dimensional electron gas (2DEG) is confined in the Si layer in type II band alignment,[3,10] the alloy-disorder scattering also becomes weak. The mobility in Si/SiGe systems at room temperature is therefore limited by phonon scattering. It has been found earlier,[11–13] that the phonon scattering mechanisms operative in bulk Si[14,15] may be employed for the calculation of the mobility of 2DEG in Si–SiO_2 systems. The mobility in Si/SiGe system may thus be calculated in a similar way when the band alignment is type II in nature; however, in the calculation the alteration of the band structure caused by lattice-mismatch-generated strain[10] should be taken into account.

In the present work, we undertake a calculation of the mobility in strained Si layers considering growth of a $Si/Si_{0.5}Ge_{0.5}$ QW on a $Si_{0.75}Ge_{0.25}$ buffer layer along the [100] direction. In this case, the conduction band of the $Si_{0.5}Ge_{0.5}$ layer is above that of the Si layer by an amount $\Delta E_c = 0.15$ eV.[10] The mismatch-generated strain lowers the two valleys (termed as group I valleys hereafter) having the longitudinal mass along the growth axis, i.e., [100] direction (z axis hereafter), from the remaining four valleys (termed as group II valleys hereafter). The scattering mechanisms in the subbands belonging to group I valleys are the deformation potential acoustic phonon scattering and the weak intervalley scattering involving g phonons. The scattering between group I and group II valleys is via f phonons, the interaction being the strongest in the bulk.[14,15] In the present case the subbands belonging to group I valleys and the states (continuum) due to group II valleys are widely separated in energy approximately by ΔE_c. The electrons in the lowest subband can absorb and emit a f phonon only when their energy reaches an approximate threshold of $\Delta E_c - k_B\theta_f$ and $\Delta E_c + k_B\theta_f$, respectively, where $k_B\theta_f$ is the energy of the f phonon ($\theta_f = 630$ K). The corresponding relaxation time when multiplied by the probability of occupancy of electrons [$\sim\exp(-E/k_BT)$] (Refs. 11 and 12) makes almost no contribution to the mobility. This reduced scattering rate coupled with lower conductivity mass in the subbands is expected to give a high value of the mobility. In this communication, we present a model calculation of the mobility for different phonon scattering mechanisms to support the above arguments in favor of the mobility enhancement. Our calculation is based on simplified envelope functions and some other approximations. We believe, however, that the conclusions derived will not be drastically altered if a more refined calculation is made. In our calculation, the energies of the subbands are obtained for $\Delta E_c = 0.15$ eV with $m^*_{zb} = 0.19m_0$ and $m^*_{zw} = 0.916m_0$, where m^* is the effective mass and w and b refer, respectively, to the well and the barrier. It is found that for a 6-nm-wide well four subbands with energy E_1, E_2, E_3, and E_4 (the subbands and their energies are denoted by the same symbol) belonging to group I valleys lie below ΔE_c. The states belonging to group II valleys are above the heterobarrier and therefore form a continuum.

The expressions for the relaxation time for deformation potential scattering within E_i subband and between E_i and E_j subbands are taken from the paper by Ridley.[16] The intervalley scattering mediated by g phonons between two degenerate E_i subbands and between E_i and E_j subbands is a first-order process and the expression for the relaxation time is derived following earlier work[12] on Si inversion layers by using sine functions. The scattering rate from a bound state to the continuum states induced by f phonon is calculated by following a model developed for polar optic phonon scattering.[17] In all the derivations, parabolic $E-k$ relationship is assumed.

In our calculation, we have assumed a 2D carrier density (n) of 10^{12} cm^{-2}, and calculated the populations (n_i's) in the subbands (E_i's) by using standard expressions.[18] For each subband, the mobilities limited by deformation potential scattering alone (μ_{DP}), by interval-

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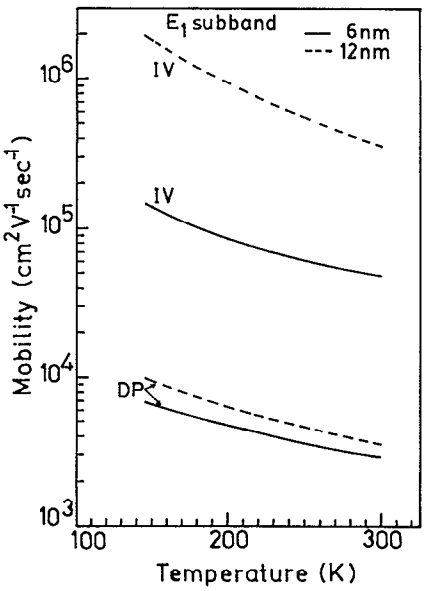

FIG. 1. Mobility in the lowest (E_1) subband in a QW vs temperature limited by deformation potential acoustic phonon (DP) scattering only and by intervalley (IV) scattering only.

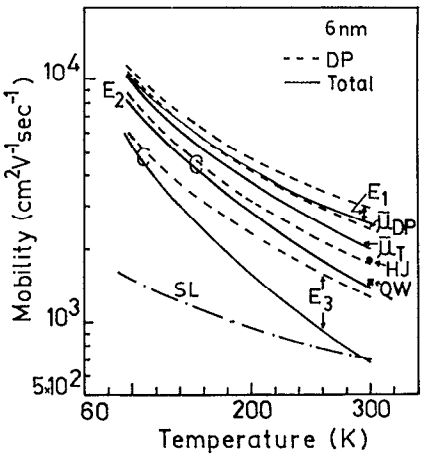

FIG. 2. Mobility values in three subbands (E_1, E_2, and E_3) as a function of temperature in a 6-nm QW. The dashed and solid curves represent the values limited by DP and total (DP + IV) scattering, respectively. $\bar{\mu}$ denotes the average value considering populations in all the subbands. The experimental data for a superlattice (SL), a quantum well (QW), and a heterojunction (HJ) are shown.

ley scattering alone (μ_{IV}), and the total mobility (μ_T) by considering all the scattering rates exactly (not by using Mathiessen rule) are calculated. The calculated values of the mobility μ_{DP} and μ_{IV} for electrons in the lowest subband (E_1) of 6- and 12-nm-wide wells are plotted in Fig. 1 as a function of temperature. The curves indicate that the mobility due to deformation potential scattering is lower by more than one order of magnitude, confirming that the intervalley scattering is suppressed in strained Si layers. In bulk Si, intervalley scattering alone can account for the observed mobility at room temperature.[14,15] Although the results for E_1 subband are given in Fig. 1, the above conclusions apply to other subbands also.

In Fig. 2, we have plotted the values of mobility in each subband limited by deformation potential scattering alone (μ_{DP}) and by all scattering mechanisms (μ_T). As pointed out in the earlier paragraph and supported by the results in Fig. 1, the weak intervalley scattering hardly alters the overall mobility μ_T from μ_{DP}. The average values of the mobility $\bar{\mu}(=\Sigma_i n_i \mu_i/n)$, for deformation potential and total scattering are also calculated and included in the figure. As expected $\bar{\mu}_{DP}$ does not differ from $\bar{\mu}_T$. The results indicate that a value of 2000 $cm^2/V\,s$ is obtained at room temperature, which is larger than the value in pure bulk Si ($\sim$1470 $cm^2/V\,s$).[14,15] For the sake of comparison the mobility data for a 6-nm/6-nm superlattice,[3] a 10-nm QW (Ref. 6) and a heterojunction[7] are included in Fig. 2.

The expression for the mobility limited by deformation potential scattering[16] indicates that the value for each subband should increase linearly with well width L. The energy of a subband decreases with increasing well width, increasing the energy separation between a subband and the continuum states. Thus f scattering becomes more weak and the net effect of using a wider well is an increase in the mobility. On the other hand, the subbands are closer in wider wells and more subbands are allowed within the well. The scattering rate will thereby increase with a decrease in mobility. To examine which of these two opposite effects dominates, we have repeated the calculation for a value of $L = 12$ nm. The calculations indicate that eight subbands are allowed within the QW. The mobility values limited by deformation potential and intervalley scatterings in the lowest subband are compared in Fig. 1. From the curves it is apparent that while doubling of the well width increases the value of μ_{DP} by about 20%, the corresponding increase in μ_{IV} is nearly by a factor of 8 to 10, depending on temperature. We conclude that the intervalley scattering is indeed weaker in a wider well and the values of μ_{DP} do not scale as L, since more subbands are involved in wider wells. The values of μ_{DP} and μ_T for different subbands in a 12-nm-wide well are plotted as a function of temperature in Fig. 3 for a carrier density of 10^{12} cm^{-2}. It is found that for this case the population in the five lowermost subbands is significant. It is again observed that the mobility in each subband effectively equals μ_{DP}, since intervalley scattering rate is drastically reduced. The average values $\bar{\mu}_T$ and $\bar{\mu}_{DP}$ are also included in Fig. 3. The overall mobility $\bar{\mu}_T$ is 2300 $cm^2\,V\,s$ at room temperature and is slightly larger than the value for a 6-nm well.

It appears from Fig. 2 that the experimental data[3] for a 6-nm/6-nm superlattice are quite low compared with our calculated values for a 6-nm QW. Although in a superlattice the conduction occurs in a miniband, a Kronig–Penney calculation[19] for the above superlattice indicates that the wells are essentially uncoupled and the width of the miniband is negligible. The value of the mobility in the 12-nm superlattice should not therefore deviate much from the values calculated for a QW. The lower experimental

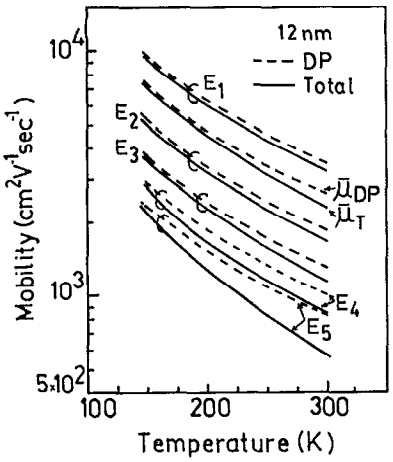

FIG. 3. Mobility values in five subbands (E_1,...,E_5) as a function of temperature in a 12-nm QW. The dashed and solid curves represent the values limited by DP and total (DP + IV) scattering, respectively. $\bar{\mu}$ denotes the average value considering populations in all the subbands.

values suggest therefore, that the samples were not of very high quality. Recently obtained values of the mobility for QWs (Ref. 6) are comparable to the value in intrinsic bulk silicon. The values slightly decrease with increase in well width. Nevertheless, the values are still lower than the calculated values and the calculation predicts a larger increase of the mobility with well width. Our calculation does not use the eigenvalues and envelope functions obtained self-consistently and the exact overlap function for phonon scattering. Yet the approximations involved are not likely to account for the gross difference between the experimental value of 1470 cm^2/V s and the calculated value of 2300 cm^2/V s. The value of 1800 cm^2/V s for a heterojunction[7] is closer to the calculated value, but the present calculation does not apply to this case. The subbands in heterojunctions are more densely packed and a realistic calculation involves extensive computation. It is, however, justified to conclude that the enhancement of mobility in heterojunctions from the bulk value is due to the reduction in f scattering, since the states belonging to types I and II valleys are widely separated in energy.

In conclusion, we have shown that in a strained Si–$Si_{0.5}Ge_{0.5}$QW, the strain alters the energy of the subbands in such a way that the IV scattering, the most dominant scattering mechanism in bulk Si, becomes insignificant. The most important scattering mechanism is then the deformation potential scattering. Our estimate for $L = 12$ nm indicates that the mobility in a QW is about 60% higher than the value in pure bulk Si at room temperature.

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