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Electron mobility in a Si_xGe_{1-x} quantum well limited by alloy-disorder scattering

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A calculation has been made of the mobility of a two-dimensional electron gas in a quantum well composed of Si and Si_xGe_{1-x}. Both the type-I and type-II band alignments are assumed and the strain-induced splitting of the six-fold degenerate conduction-band minima is considered. For a type-I alignment, the electrons are confined in the alloy layer and the mobility is severely limited by alloy-disorder scattering. In the case of type-II alignment, the electrons confined in the Si layer are scattered by alloy disorder in the barrier and the mobility becomes higher.

Strained-layer superlattices made of Si_xGe_{1-x} and Si are being investigated for the study of novel physical phenomena related to the reduced dimensionality of the carrier gas as well as for the fabrication of electronic and photonic devices.[1,2] An enhancement of the mobility[3] has been observed in modulation-doped (MD) heterostructures made of these materials, much in the same way as is found in GaAs-AlGaAs systems.

Theoretical calculation of the mobility for quantum wells (QWs) has so far been performed for the case of ionized impurity scattering[4] only. In high-mobility MD samples, the limiting values of the mobility will be governed by phonon and alloy-disorder scattering mechanisms. Recent calculation by Krishnamurthy, Sher, and Chen[5] for bulk Si_xGe_{1-x} alloy has indicated that the alloy-disorder scattering is quite significant. The results lead us to believe that this scattering mechanism will be the most dominant if the two-dimensional electron gas (2DEG) is confined in the lower-gap alloy material. The band alignment for this situation is type I in nature and is shown in Fig. 1(a). If, however, the band alignment is type II in nature as shown in Fig. 1(b) and as proposed in some recent studies,[6] the carriers confined in the Si layer will be scattered by alloy-disorder potential in the barrier alloy layer. In any case, it is worthwhile to have an idea of the proper magnitude of this mobility in order to evaluate the overall mobility in the Si-Si_xGe_{1-x} system. In the present work, we have considered both types of band alignment and have calculated the mobility of 2DEG in QWs due to alloy-disorder scattering. In the calculation, the lowest subband is considered to be occupied. We have taken into consideration the splitting of the six-fold degenerate conduction-band minima due to the effect of strain arising out of the lattice mismatch between Si and Si_xGe_{1-x}.

The scattering probability of the 2DEG due to random alloy-disorder potential has been calculated by different workers either by using a spherically symmetric square potential[7–9] or by considering a short-range δ potential.[10,11] The calculated values of the mobility for the two methods do not differ much. Since the present work employs the potential values given by Krishnamurthy and co-workers,[5] we follow their prescription of the δ potential. The transition probability from a state $\mathbf{k}$ to another state $\mathbf{k}'$ is given by[7,9]

$$P(\mathbf{k},\mathbf{k}') = (2\pi/\hbar)x(1-x)\Delta E^2 I \delta(E_{\mathbf{k}'} - E_{\mathbf{k}}), \tag{1}$$

where $I = \int |\chi(z)|^4 dz$, $\mathbf{k}$ and $\mathbf{k}'$ are the 2D wave vectors for electrons, ΔE is the measure of alloy-potential fluctuations, and $\chi(z)$ is the wave function of the 2DEG along the direction (z axis) of quantization in the QW of half width a. The relaxation time is

$$\frac{1}{\tau} = \frac{1}{(2\pi)^2} \int P(\mathbf{k},\mathbf{k}') \ (1 - \cos\theta) d\mathbf{k}', \tag{2}$$

where θ is the angle between $\mathbf{k}$ and $\mathbf{k}'$.

The wave function $\chi(z)$ is assumed to have the usual form

$$\chi(z) = \begin{cases} A\cos\alpha z, & |z| < a, \\ B\exp(-\beta z), & |z| > a \end{cases}, \tag{3}$$

where $\alpha^2 = 2m_z^* E_1/\hbar^2$ and $\beta^2 = (2m_z^*/\hbar^2)(\Delta E_c - E_1)$. ΔE_c is the conduction-band offset and E_1 is the subband energy. It may be noted that in type-II QWs made of GaSb and InAs, the electron and hole subbands are quite close in energy and the envelope functions are admixtures of the functions for the two bands.[12] In the present Si-SiGe system the electron and hole subbands are wide apart in type-II alignment, so that we employ the simplified envelope function following Ref. 4. It is pointed out that the effective masses for Si and Si_xGe_{1-x} are identical.[5] The constants A and B are therefore obtained by matching χ's and $d\chi/dz$'s at the heterointerfaces. Using Eqs. (1)–(3), it is straightforward to show that

$$\frac{1}{\tau_w} = \left(\frac{2m_D^* x(1-x)\Delta E^2}{\hbar^3 N_0}\right)\left(\frac{\beta^2}{\alpha(1+\beta a)^2}\right) \times \left[\frac{\sin(\alpha a)\cos(\alpha a)}{6}\left(\cos^4(\alpha a) + \frac{5}{4}\cos^2(\alpha a) + \frac{15}{8}\right) + \frac{5}{16}\alpha a\right], \tag{4}$$

and

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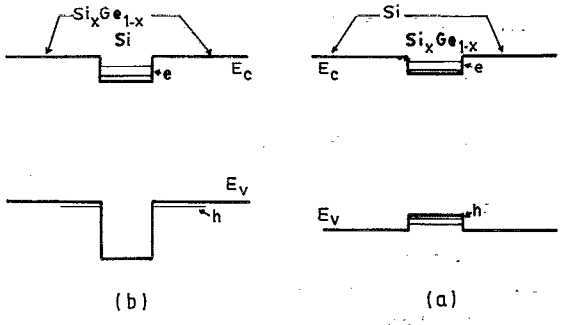

FIG. 1. Band diagrams for a Si-Si$_x$Ge$_{1-x}$ QW: (a) type-I and (b) type-II alignment. $E_{c(v)}$ refers to the conduction-(valence) band edge.

$$\frac{1}{\tau_b}=\left(\frac{m_D^{*}x(1-x)\Delta E^2}{2\hbar^3 N_0}\right)\left(\frac{\beta\alpha^4}{(1+\beta a)^2(\alpha^2+\beta^2)^2}\right), \qquad (5)$$

where N_0 is the number of anion sites per unit volume of the alloy, m_D^* is the density-of-states effective mass, and w and b denote, respectively, the situation when the alloy material forms the well and the barrier. As noted earlier,[7] the relaxation time is independent of energy and hence the mobility is independent of temperature.

In our calculation, we consider the z axis along the (100) direction. It has been argued[1,6] that when Si and $Si_{0.5}Ge_{0.5}$ are grown on a $Si_{0.75}Ge_{0.25}$ substrate, the band alignment is type II in nature. In this case the conduction band of $Si_{0.5}Ge_{0.5}$ is above that of Si by an amount $\Delta E_c = 0.15$ eV. Due to mismatch-generated strain the two valleys in Si having longitudinal mass along the z axis (growth axis) are lowered from the remaining four valleys. In this case, therefore, $m_z^* = 0.916m_0$ and both the density-of-states effective mass m_D^* and the conductivity effective mass m_c^* along the [100] plane is $0.19m_0$.[13] On the other hand, when growth is on a Si substrate, the band alignment is type I, the conduction band of the $Si_{0.5}Ge_{0.5}$ layer, in which the 2DEG is formed is lower than that of Si by an amount $\Delta E_c = 0.02$ eV.[1] In this case, the four valleys are lowered from the remaining two valleys. The appropriate masses are therefore[13] $m_z^* = 0.19m_0$, $m_D^* = 0.417m_0$, and $m_c^* = 0.315m_0$. As pointed out earlier,[5] the effective mass in Si_xGe_{1-x} is not much different from the values in Si.

The alloy-disorder scattering potential is given by $\Delta E^2 = (f_s\Delta E_s)^2 + (f_p\Delta E_p)^2$, where $f_s(f_p)$ are the fraction of time an electron spends in the cation $s(p)$ orbital in the alloy.[5,14] Krishnamurthy and co-workers[5] concluded that the contribution by the p-orbital term is insignificant for $x=0.5$. Using Eq. (8) and the value of the mobility for $x=0.5$ given in Fig. 1 of Ref. 5, we have obtained a value of $\Delta E=1.058$ eV and have used this value in Eqs. (4) and (5) of the present work to calculate the 2D mobility. The value of N_0 is taken to be 2.346×10^{28} m^{-3}.

Figure 2 shows the values of the mobility calculated from Eq. (4), when the $Si_{0.5}Ge_{0.5}$ layer is treated as the well material. It appears that the mobility for a thin well is quite high; the values then sharply decrease with increasing well width, attain a minima at about 85 Å, and then slowly increase. For thin wells, the wave function penetrates more into the nonalloy barrier; the alloy scattering is then less significant so as to make the mobility quite high. With an increase in thickness, the wave functions are more confined into the alloy region and the alloy-scattering rate increases. When the well is thick enough to confine the electrons entirely into the well, the mobility increases due to the

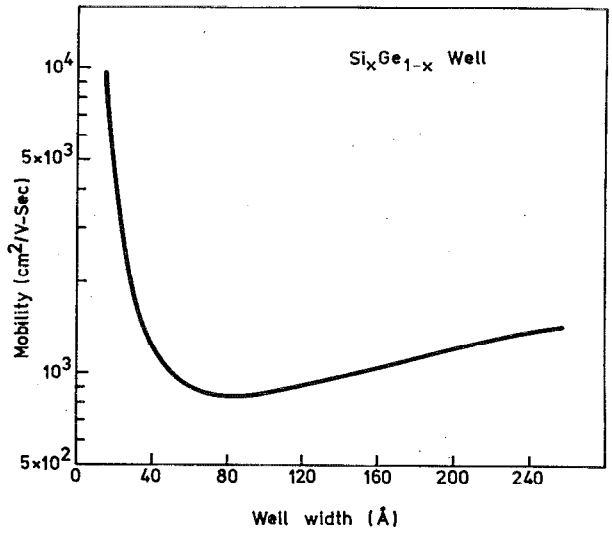

FIG. 2. Dependence of the alloy-disorder scattering limited electron mobility on the width of the quantum well. The electrons are assumed to be confined in the $Si_{0.5}Ge_{0.5}$ layer.

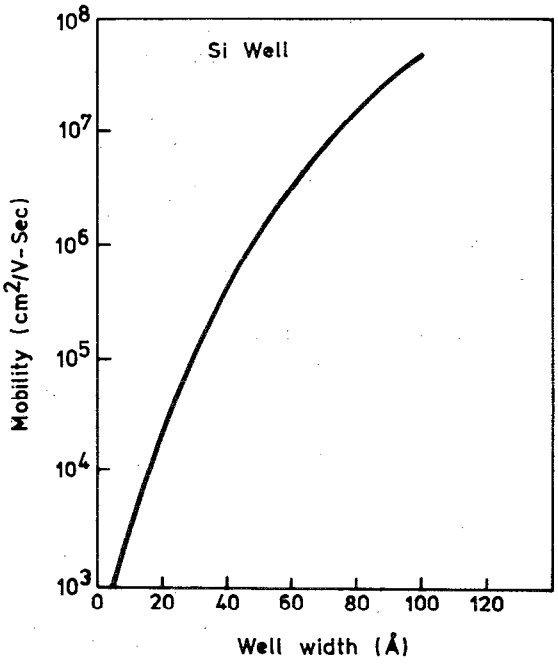

FIG. 3. Dependence of the alloy-disorder scattering limited electron mobility on the width of the quantum well. The electrons are assumed to be confined in the Si layer.

decrease of the scattering probability with well width governed by the term $\int|\chi(z)|^4 dz$ in Eq. (1). We have considered in the present work only the lowest subband. Even in that situation the alloy-scattering limited mobility is quite low (~ 800 cm^2/V s) and is expected to be comparable to the mobility values limited by phonon or impurity scattering.

The values of the mobility for 2D electrons confined in the Si QW with $Si_{0.5}Ge_{0.5}$ as the barrier, are shown in Fig. 3 and are found to increase monotonically with the increase in the well width. This is expected, because for thinner wells the wave functions penetrate more into the alloy barrier and the scattering rate is consequently higher. As the well thickness increases, the electrons are confined more into the well and the barrier alloy-disorder scattering becomes less, so as to make the mobility higher. The values indicate that for well widths of about 100 Å, the alloy-scattering limited mobility may be weak in comparison to the impurity-scattering limited mobility.

In summary, we have obtained the expressions for the alloy-disorder scattering limited mobility for strained $Si\text{-}Si_xGe_{1-x}$ QWs and obtained the numerical values considering the alloy material to form either the well or the barrier. The mobility is quite low when the $Si\text{-}Si_xGe_{1-x}$ alloy acts as the well.

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