Carrier velocity-field characteristics and alloy scattering potential in $Si_{1-x}Ge_x/Si$

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The alloy scattering potential is an important parameter in SiGe alloys since it not only affects the velocity-field characteristics for carrier transport, but also allows increased optical transitions by relaxing *k*-selection rules. In this letter, we report on the velocity-field measurements for relaxed and coherently strained SiGe alloys. The alloy scattering potential is obtained from a careful fit to the data. The hole velocity at any field is found to have a bowing behavior as a function of alloy composition. This reflects a strong alloy scattering potential which is calculated to be 0.6 eV for the valence band.

Coherently strained $Si_{1-x}Ge_x$ alloys and SiGe/Si heterostructures are currently of immense interest due to their potentially useful electronic and optical properties and compatibility with existing Si technology.[1-3] The built-in mismatch strain dramatically alters the band structure and carrier transport properties. Although some reports of improved device performance in this material system have been made, numerous important experimental issues in transport of both minority and majority carriers are still not clear. Alloy scattering is an important factor in determining the transport properties and luminescence from these materials and is not known at present. In this letter we report the measured velocity-field characteristics of electrons and holes in relaxed and pseudomorphic $Si_{1-x}Ge_x/Si$ ($0<x<1.0$) heterostructures. The measured data have been analyzed in detail and the alloy scattering potential U_0 has been estimated. To our knowledge, this is the first experimental determination of carrier velocities and U_0 in these alloys.

The experimental $Si_{1-x}Ge_x$ samples were grown on high resistivity ($>1000\ \Omega$ cm) (001) Si substrates by molecular beam epitaxy using gaseous disilane (Si_2H_6) and solid Ge as sources. Details of our growth system and procedures have been published elsewhere.[4] Two types of samples were grown. The first are approximately 1-μm-thick undoped (*n*-type) and B-doped (*p*-type) $Si_{1-x}Ge_x$ ($0.1<x<1.0$) layers which are relaxed. Cross-sectional transmission electron microscopy (XTEM) measurements on these samples show that most of the misfit dislocations are contained and localized at the substrate-epilayer interface. We therefore believe that the transport measurements reflect the intrinsic properties of SiGe. The second type of sample is a pseudomorphic $Si_{1-x}Ge_x/Si$ ($0.06\leq x\leq 0.20$) structure in which the alloy layer is doped *p* type with B and is of thickness less than the critical thickness. Depending on the composition, the thickness of the alloy layer in the various structures vary from 1000 Å ($x=0.06$) to 400 Å ($x=0.20$). The composition in the alloy films were confirmed by double-crystal x-ray measurements.

The velocity-field characteristics at room temperature were determined from pulsed current-voltage measurements[5] on planar H-shaped devices shown in Fig. 1, where the dimensions of the device are also indicated. The electric field is determined from the measured potential profile in the bridge region of the device. Ohmic contacts were made with Al. The applied field is derived from the uniform distribution between the contacts in the center region. The voltage pulse width is fixed at 0.2 μs. The input voltage and output current pulses were recorded on a sampling scope. The velocity is computed from the measured current (density) by taking into account the carrier density obtained from Hall measurements on the same samples.

The measured hole velocity-field characteristics in the relaxed and coherently strained p-$Si_{1-x}Ge_x$ samples are shown in Figs. 2(a) and 2(b), respectively. For each sample, accurate measurements were not possible beyond the highest field point shown in the data due to the development of current instabilities during measurements. The exact cause of such instabilities cannot be ascertained but domain nucleation due to any carrier transfer effect can be a likely cause. The low-field mobilities extrapolated from these data agree fairly well with those obtained from Hall data.

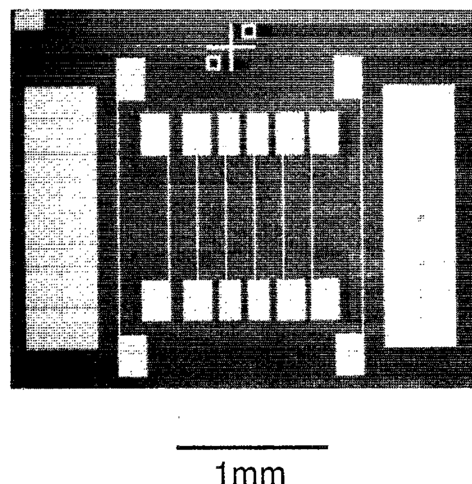
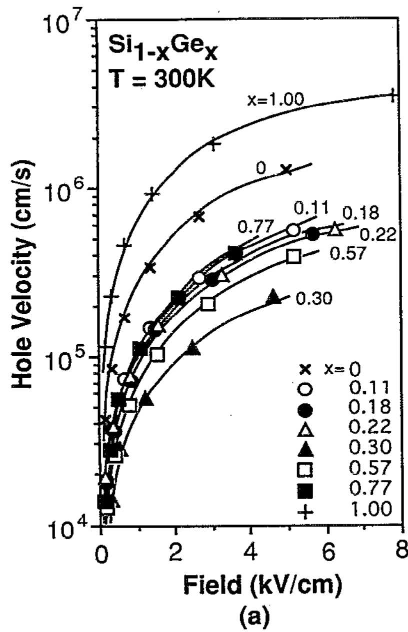


FIG. 1. Photomicrograph of the H-device with contacts for measurement of current and potential profile in the bridge region.



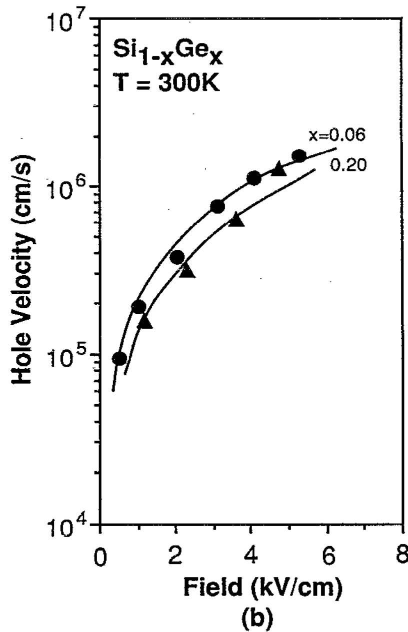


FIG. 2. Measured velocity-field characteristics of (a) relaxed and (b) coherently strained p-$\mathrm{Si}_{1-x}\mathrm{Ge}_x$ alloys. Hall factors given by Eq. (4) have been used to calculate the data.

It should be noted that in calculating the relevant parameters from Hall data, the value of the Hall factor r needs to be known. The Hall factor for unstrained p $\mathrm{Si}_{1-x}\mathrm{Ge}_x$ was estimated in the following way. For the two-band system (heavy and light holes), the observed Hall factor r bears the following relation to the individual band Hall factors r_{hh} and r_{lh}:[6]

$$r=\frac{\mathrm{f}_{\mathrm{hh}}r_{\mathrm{hh}}\mu_{\mathrm{hh}}^2+\mathrm{f}_{\mathrm{lh}}r_{\mathrm{lh}}\mu_{\mathrm{lh}}^2}{(\mathrm{f}_{\mathrm{hh}}\mu_{\mathrm{hh}}+\mathrm{f}_{\mathrm{lh}}\mu_{\mathrm{lh}})^2}, \tag{1}$$

where f_{hh} and f_{lh} are the fractions of carriers in the heavy-

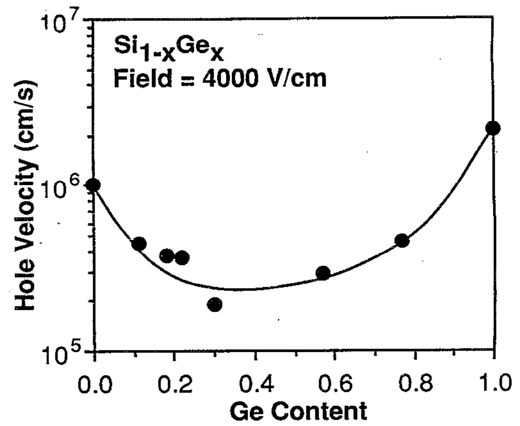


FIG. 3. Variation of hole velocities in relaxed p $\mathrm{Si}_{1-x}\mathrm{Ge}_x$ as a function of alloy composition.

hole and light-hole bands, and μ_{hh} and μ_{lh} are the corresponding heavy- and light-hole mobilities. The individual quantities are calculated accordingly:

$$r_{\mathrm{hh}}=\frac{\langle\tau_{\mathrm{hh}}^2\rangle}{\langle\tau_{\mathrm{hh}}\rangle^2},$$

$$\mu_{\mathrm{hh}}=\frac{e\langle\tau_{\mathrm{hh}}\rangle}{m_{\mathrm{hh}}^*}, \tag{2}$$

$$\mathrm{f}_{\mathrm{hh}}=\frac{n_{\mathrm{hh}}}{n_{\mathrm{hh}}+n_{\mathrm{lh}}},$$

with corresponding expressions for the light-hole terms. The average of the nth power of the relaxation time τ is[7]

$$\langle\tau_{hh}^n\rangle=\frac{\int_0^\infty\tau^n(E)D_{\mathrm{hh}}(E)E\exp(-E/kT)dE}{\int_0^\infty D_{\mathrm{hh}}(E)E\exp(-E/kT)dE}, \tag{3}$$

where $D_{\mathrm{hh}}(E)$ is the heavy-hole density of states. A similar expression pertains to the light hole relaxation time. The relaxation time was approximated as the inverse of the total scattering rate. This is an approximation and the re-

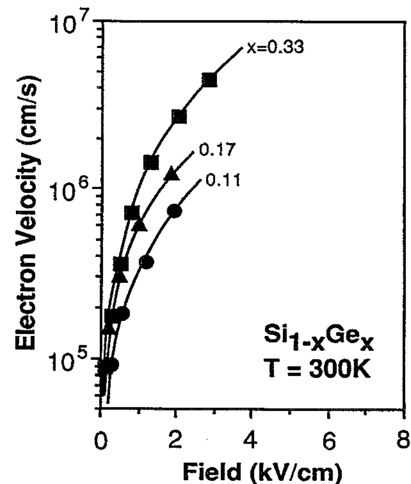


FIG. 4. Measured electron velocity-field characteristics is relaxed n $\mathrm{Si}_{1-x}\mathrm{Ge}_x$. $r=1$ has been used to calculate the data.

sulting Hall factors for Si and Ge were roughly a factor of 2 larger than measured values. This is to be expected as a consequence of the approximation of using spherical bands with anisotropic scattering.[8] However, the values calculated for the alloy were found to vary nearly linearly as a function of Ge fraction x, between the calculated r values for Si and Ge. This is the justification for our using a linear interpolation between known measured values of r for Si and Ge to estimate r values for the alloy $Si_{1-x}Ge_x$. The experimental values of Hall factor used are $r=0.73$ (Si)[9–11] and $r=1.7$ (Ge).[12] For the alloy, we used

$$r(x)=(1-x)(0.73)+x(1.7). \tag{4}$$

The same values are also used for the pseudomorphic alloys. The data of Figs. 2(a) and 2(b) indicate that there is a bowing of the transport properties in the alloys between the Si and Ge end points. This is illustrated in Fig. 3, where the measured velocity at a fixed E are plotted against alloy composition. The Si and Ge hole velocities are slightly smaller than previously published data, probably because of higher carrier density in our samples. The electron velocity-field characteristics in the various samples are shown in Fig. 4. Here, a value of $r=1$ is used to compute the data.

The alloy scattering potential for unstrained p $Si_{1-x}Ge_x$ was obtained using the following approach. Using the Hall factor for $x=0.22$ ($r=0.94$), we obtain the conductivity mobility from our measured velocity-field results. This value is 95 cm^2/V s. The corresponding mobility for Si at similar doping values is 150 cm^2/V s.[13] To find the dependence of mobility on alloy scattering potential, we have carried out a detailed six-band $k\cdot p$ Monte Carlo study of hole transport.[14] We find that the effect of alloy potential on the mobilities can be summarized as

$$\mu_{\text{alloy}}(U_0)=\frac{\mu_{\text{alloy}}(0)}{1+aU_0^2}, \tag{5}$$

where, based on the Monte Carlo results, $a=2.3\ \text{eV}^{-2}$. Our Monte Carlo results also show that if a value of $U_0=0.3$ eV is used, the alloy mobility is essentially similar to that of undoped Si. Thus, we have

$$\frac{\mu_{\text{alloy}}(U_0=0.3)}{\mu_{\text{alloy}}(U_0)}=\frac{150}{95}, \tag{6}$$

which then give us $U_0=0.6$ eV. This value is quite large and is different from the value which explains the electron mobility (U_0 for the conduction band is ~ 0.2 eV). This may reflect the fact that the differences in Si and Ge manifest themselves more in the valence band than in the conduction band. This is also consistent with the fact that the band offset in the SiGe system is almost entirely in the valence band.

In conclusion, we have measured the high-field carrier velocities and the alloy scattering potential U_0 in $Si_{1-x}Ge_x$. A value of $U_0=0.6$ eV is estimated for $x=0.22$ for scattering of holes.

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