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Author(s): T. E. Whall, A. D. Plews, N. L. Mattey, and E. H. C. Parker
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Hole effective mass in remote doped $Si/Si_{1-x}Ge_x$ quantum wells with $0.05 \leqslant x \leqslant 0.3$

T. E. Whall, A. D. Plews, N. L. Mattey, and E. H. C. Parker
Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom

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The effective masses in remote doped $Si/Si_{1-x}Ge_x$ hole quantum wells with $0.05 \leqslant x \leqslant 0.3$, have been determined from the temperature dependence of the Shubnikov–de Haas oscillations. The values are lower than previously observed by other workers, but still somewhat higher than the theoretical Γ-point values for the ground-state heavy hole subband. The differences are attributed to finite carrier sheet densities and can be satisfactorily accounted for by nonparabolicity corrections. © *1994 American Institute of Physics.*

The two-dimensional hole gas (2DHG) formed at the SiGe/Si heterointerface in a pseudomorphic Si/SiGe/Si structure is of considerable technological interest since it is likely to offer a viable route to fast p-channel metal–oxide–semiconductor (MOS) devices. Unfortunately, there is little agreement in the literature as to the value of hole effective mass m^* and its dependence on Ge concentration (x). Cheng *et al.*[1] report m^* (measured by cyclotron resonance) falling from 0.4 to $0.29m_e$, where m_e is the free electron mass, as x is increased from 13% to 37%, while Kiehl *et al.*[2] find, from magnetotransport measurements, no Ge concentration dependence with an average $m^* \sim 0.36m_e$ for x in the range 15%–35%. These values are considerably larger than might be expected from band structure calculations of m^* for decoupled bands at the zone center, $k=0$. For example m^*, is predicted to fall to $\sim 0.2m_e$ for Si in the completely decoupled limit.[3]

We have recently observed m^* as low as $(0.23 \pm 0.02)m_e$ for $x=0.13$ from a detailed analysis of the thermal damping of the Shubnikov–de Haas oscillations.[4] This value is in reasonable agreement with theoretical predictions which range between $0.20m_e$ and $0.25m_e$.[5,6] In the present work we have determined the hole effective masses for $0.05 \leqslant x \leqslant 0.3$. The most important feature of this investigation is that measurements have been made on samples of lower carrier sheet densities than hitherto. A novel form of analysis of the data is adopted in which the effects of temperature dependent screening, weak localization, and hole–hole interactions are accounted for. It is demonstrated that the experimentally deduced masses are independent of magnetic field and temperature. Good agreement is obtained with band structure calculations of zone center effective masses,[5,6] when sensible corrections for band nonparabolicity are made.

A range of samples was grown using solid-source molecular beam epitaxy (MBE) each consisting of an n^-Si (100) substrate with ~300 nm undoped Si followed by a $Si_{1-x}Ge_x$ alloy layer of thickness L_a, an undoped Si spacer of thickness L_s and a 50 nm B-doped cap. The nominal layer thicknesses and Ge content deduced from x-ray diffraction (XRD) measurements, assuming the SiGe is fully strained, are summarized in Table I. Also shown are the carrier sheet densities obtained from the periods of the Shubnikov–de Haas oscillations and the 4 K Hall mobility. The electrical measurements were made on samples of standard Hall bar geometry.

According to theory the Shubnikov–de Haas oscillations in the longitudinal resistivity $\Delta\rho_{xx}$ are described by:[7]

$$\frac{\Delta\rho_{xx}}{\rho_0} = R_s V \frac{\xi}{\sinh \xi} e^{-\pi/\omega_c \tau_q} \cos\left(2\pi \frac{E_F}{\hbar\omega_c} + \Phi\right), \quad (1)$$

where ρ_0 is the Boltzmann resistivity, R_s is the spin reduction factor,[8] V depends on the scattering mechanism being equal to 4 for short range scattering as has been shown to be the case for the present samples,[9] $\xi = 2\pi^2 kT/\hbar\omega_c$, $\omega_c = eB/m^*$ and τ_q is the quantum lifetime. Typical oscillations are shown in Fig. 1, the periodicity in $1/B$ confirming the occupation of a single subband as anticipated for this sheet density. To obtain the effective mass we plot

$$\ln[\Delta\rho_m(T)/\rho_0(T)] \quad \text{vs} \quad \ln(\xi/\sinh \xi) - [\pi/\omega_c \tau_q(T)] \qquad (2)$$

for various T at fixed B, where $\Delta\rho_m$ is the peak value of $\Delta\rho_{xx}$, m^* is used as an adjustable parameter to obtain a gradient of unity for each value of B, confirming that m^* is independent of B. In order to extract $\Delta\rho_m$ a cubic spline interpolation and a rectangular digital filter[10] are used to remove the B^2 background term associated with hole–hole interactions.[11] The temperature dependence of the Boltzmann

TABLE I. Properties of remote doped Si/SiGe hole quantum wells. x: Ge composition, $Si_{1-x}Ge_x$; L_a: alloy thickness; L_s: dopant setback; N_s: carrier sheet density; m^*: measured effective mass; and m_e: free electron mass.

Sample	x (measured)	L_a (nm)	L_s (nm)	N_s (Shubnikov–de Haas) (10^{11} cm^{-2})	Hall mobility at 4 K (cm^2 V^{-1} s^{-1})	m^*/m_e
1	0.052	30	20	0.95	9 200	0.28
2	0.081	30	20	1.32	10 500	0.33
3	0.081	30	20	1.60	8 850	0.29
4	0.12	30	20	2.46	9 600	0.27
5	0.12	30	20	2.05	10 500	0.27
6	0.13	30	20	2.00	11 100	0.23
7	0.17	50	20	2.93	3 600	0.31
8	0.19	22	30	3.30	3 500	0.26
9	0.29	20	20	5.80	2 200	0.24

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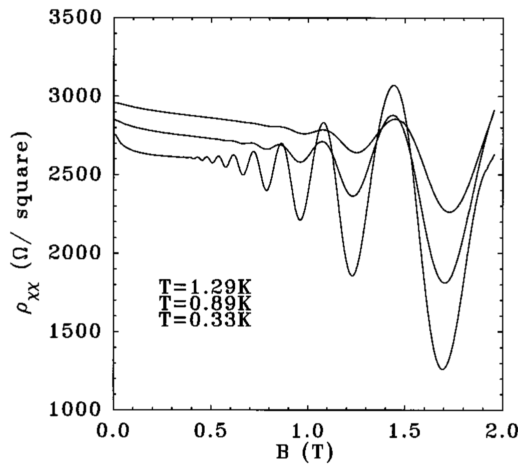


FIG. 1. Temperature dependence of the Shubnikov–de Haas oscillators for sample 5.

resistivity ρ_0 is obtained by fitting the temperature dependence of the zero magnetic field conductivity to the form:

$$\sigma_{xx}(T)=\frac{1}{\rho_0(T=0)}\,(1-\gamma T/T_F)+A\,\ln\left(\frac{kT\tau}{\hbar}\right). \quad (3)$$

γ is a screening parameter calculated by Gold,[12] who finds $\gamma\sim 1$ for interface roughness and interface charge scattering, which have been found to dominate in the present materials.[4,9] We have estimated the interface charge densities in these materials and find that they vary between 2×10^{11} cm^{-2} for a sample having a 4 K mobility of about 2000 cm^{-2} V^{-1} s^{-1} and 2×10^{10} cm^{-2} for a mobility of about 18 000 cm^2 V^{-1} s^{-1}.[4,19,13] The coefficient A is a measure of the effects of weak localization and hole–hole interactions. $\tau_q(T)$ is then found by putting $\tau_q\approx\tau$ the elastic scattering time, with $\tau\alpha\rho_0^{-1}$, which should be a reasonable approximation in the present case where the scattering is of the short range type. In our analysis we neglect any temperature or magnetic field dependence of R_s. Figure 2 shows the temperature dependence of σ_{xx} and the corresponding fit to Eq. (2) for sample 7 (Table I) and Fig. 3(a) illustrates the determination of the effective mass for temperatures in the range 0.3–1.6 K giving a magnetic field independent value of $m^*=0.31m_e$. It is important to note that the screening corrections (in ρ_0 and τ_q) have been found to be essential in order to obtain the linear behavior shown in Fig. 3(a). To determine that the measured m^* is also temperature independent, Fig. 3(b) shows a Dingle plot of

$$\ln[(\Delta\rho_m \sinh\xi)/\rho_0\xi] \quad \text{vs } 1/B \quad (4)$$

for various values of T for this sample. The gradient of the line may be written as $-\pi\tau/\tau_q\mu_0$ giving τ/τ_q=0.96. The good straight lines obtained in Fig. 3 justify our assumptions that V and R_s are temperature and magnetic field independent.

In Table I we summarize our data. The somewhat lower values of m^* we observe as compared to those reported by previous workers.[1,2,14,15] are attributed to the fact that our samples are, on average, of significantly lower sheet density. Figure 4 shows the present experimental results compared with the cyclotron mass of bulk unstrained SiGe[1] and the theoretically predicted masses at the zone center of strained SiGe alloys.[5,7] The error bars give the estimated experimental errors in the present measurements. Although our masses show clearly the effects of strain, and are lower than previously published results, the deviations from the theoretical values at the Γ point ($k=0$) are substantial. To correct for

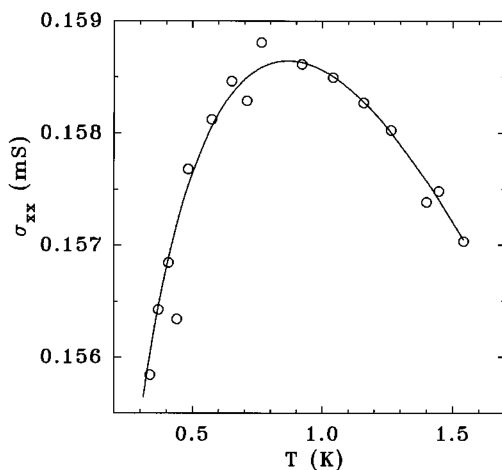
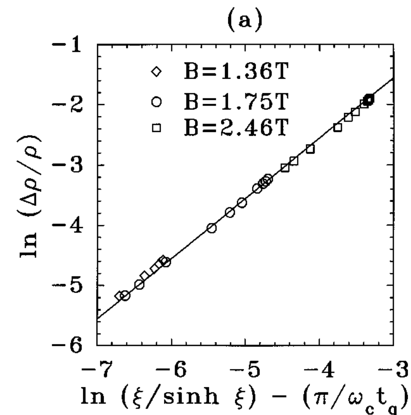


FIG. 2. Temperature dependence of electrical conductivity σ_{xx} in zero magnetic field, between 0.3 and 1.8 K for sample 7.



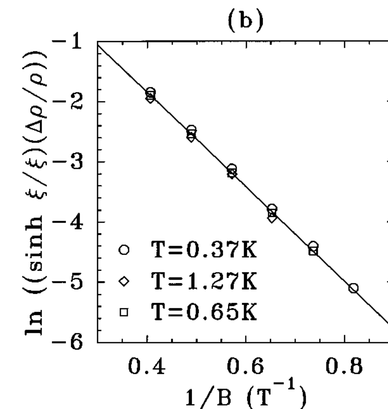


FIG. 3. (a) $\ln(\Delta\rho_m/\rho_0)$ plotted vs $\ln(\xi/\sinh\xi)$ for sample 7 in the temperature range 0.3–1.3 K, at various magnetic fields. (b) Dingle plots of $\ln[(\Delta\rho_m \sinh\xi)/(\rho_0\xi)]$ vs $1/B$ for sample 7 at various temperatures.

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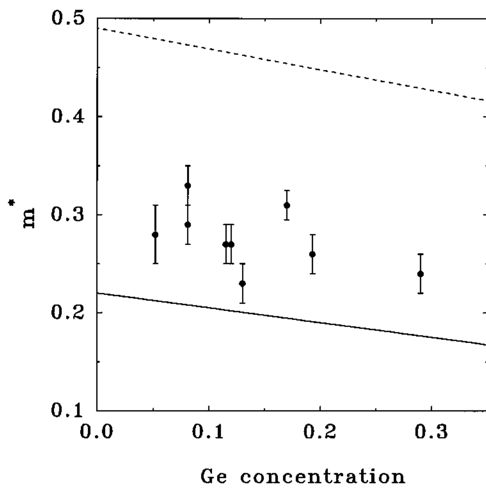

FIG. 4. Experimental effective mass values m^* compared with average mass in unstrained bulk SiGe alloy (dashed line) and calculated band edge ($k=0$) mass (solid line) for strained alloys.

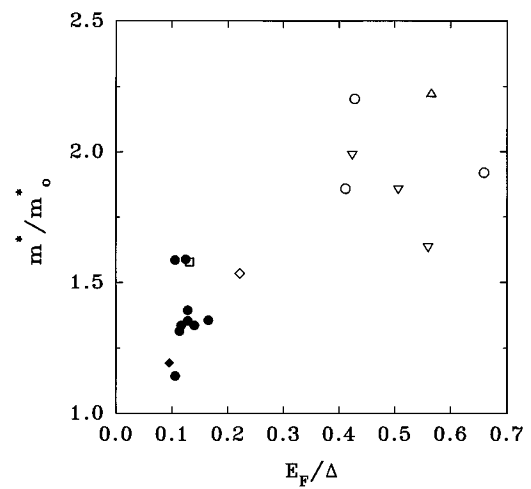

FIG. 5. Variations of effective mass with strain and sheet density in the SiGe two-dimensional hole gas. m_0^* theoretical $k=0$ value, E_F Fermi energy. Δ light hole-heavy hole splitting. ●: present work, ◆: present samples Nicholas (see Ref. 18); ▽: Cheng *et al.* (see Ref. 1); ○: Kiehl *et al.* (see Ref. 2); △: Wang *et al.* (see Ref. 14); ◇: Fang *et al.* (see Ref. 15); □: People *et al.* (see Ref. 19).

the fact that m^* has been measured at finite sheet density we use the forms[16,17]

$$\hbar^2 k_{xy}^2/2m_0^* = \epsilon[1+c\epsilon/\Delta] \quad \text{and} \quad m^* = \hbar^2/d^2\epsilon/dk_{xy}^2, \tag{5}$$

where k_{xy} is the 2D wave vector, ϵ is the hole energy, m_0^* is the $k_{xy}=0$ effective mass, Δ is the splitting of the $n=1$, $m_j=\pm\frac{3}{2}$ and $n=1$, $m_j=\pm\frac{1}{2}$ valence maxima, and c is a nonparabolicity factor. The discrepancy between the experimental values and the theoretical band edge values can be accounted for by choosing an average value of c equal to 0.5. This comparison ignores, of course, the effects of confinement and a possible germanium concentration dependence of c.[17] However, the magnitude of the nonparabolicity agrees with that obtained by Cheng *et al.*[1] from cyclotron resonance measurements on samples of higher sheet density, and by Osbourn *et al.*[16] from magnetotransport measurements on InGaAs strained layers. Their deduced values of c are larger than obtained here, presumably because of a factor of 3 error in Eq. (1) of Ref. 17. As supporting evidence for the present interpretation, we have plotted the normalized effective mass (m^*/m_0^*) obtained by various authors[1,2,14,15,18,19] versus E_F/Δ in Fig. 5, where E_F is the Fermi energy. Although there is appreciable scatter in the data, an increase in m^*/m_0^* is evident which is consistent with the effects of band nonparabolicity [see Eq. (5)]. More detailed analysis must await theoretical calculations of nonparabolicity in SiGe, although the present experimental values of c are believed to be of the right order of magnitude.[16,17]

Finally, the average value of τ/τ_q deduced for the present samples is 1.0 ± 0.3. This value is consistent with that found previously[4] and with that expected for short range interface charge and/or interface roughness scattering.[14]

In conclusion, the measured effective mass values are substantially smaller than those in unstrained SiGe alloys, but larger than the theoretical Γ point values in strained alloys. Good agreement with the theoretical values is obtained when corrections are made for the finite sheet density of the measured samples. Our results and those of other workers are indicative of significant nonparabolicity in the ground-state heavy-hole subband.

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