Theory of the channel-width dependence of the low-temperature hole mobility in Ge-rich narrow square Si/SiGe/Si quantum wells

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(Received 6 November 2006; revised manuscript received 26 December 2006; published 22 February 2007)

A theory is given of the mobility of a two-dimensional hole gas (2DHG) at low temperature in narrow square $Si/Si_{1-x}Ge_x/Si$ quantum wells at high Ge content. Different from the previous treatment, we have carried out a proper calculation of the misfit deformation potential and 2DHG screening. As a result, the scattering mechanisms due to surface roughness, misfit deformation potential, and alloy disorder are found to dominate the 2DHG mobility. Our theory enables a very good quantitative description of recently measured data about the dependence of the 8 K mobility of holes in a $Si/Si_{0.2}Ge_{0.8}/Si$ quantum well on the channel width varying from 25–70 Å. Further, this provides evidence in favor of screening of short-range interactions such as alloy disorder.

DOI: 10.1103/PhysRevB.75.073305 PACS number(s): 73.50.Bk, 73.63.Hs

I. INTRODUCTION

Ge-rich Si/SiGe/Si and SiGe/Ge/SiGe quantum wells (QWs) prepared on virtual substrates have recently been intensively studied for application for *p*-type metal-oxide-semiconductor field-effect transistors.[1] The sandwich heterostructures have also attracted attention for optoelectronic application such as quantum cascade lasers.

The mobility of a two-dimensional hole gas (2DHG) in *p*-channel QWs is one of the most important parameters fixing its performance, however, limited by various scatterings. To improve the performance one needs to identify the key scattering mechanisms. It is well known[1] that the best way for this purpose is to study the dependence of 2DHG mobility on the experimental conditions such as sample temperature, carrier density, and well width.

It should be stressed that the key scattering mechanisms limiting low-temperature 2DHG mobility in the above QWs remain as a subject under debate. Indeed, from its temperature dependence some authors[2,3] assumed surface roughness scattering to be a key mechanism. However, from its carrier density dependence, the others[4,5] assumed ionized impurity scattering to be dominant. It is to be noted that in their calculations the misfit deformation potential scattering induced by interface roughness is ignored, which has been proven to be important for SiGe heterostructures.[6] So far, the well-width dependence has been less studied and the interpretation of some experimental findings is unsatisfactory.

Indeed, Tsujino *et al.*[7] have recently reported experimental data about the curve describing the evolution of the 8 K mobility of holes in a *p*-type $Si/Si_{0.2}Ge_{0.8}/Si$ QW versus the well width varying from $L=25$–70 Å. The authors found a noticeable decrease of its steepness from $L=45$ Å on. They explained the finding in terms of surface-roughness scattering (for $L<45$ Å) and misfit deformation potential one (for $L>45$ Å), ignoring the Matthiessen's rule. This is unreasonable because the scattering rates are of the same order of magnitude. The misfit deformation potential for holes was taken in the very form for electrons, which is shown to be invalid.[6,8,9] The amplitude of misfit deformation potential scattering from the barrier was taken in the form of that from the well. This is not plausible because the hole distribution is mainly located in the well, decaying rapidly into the barrier. In addition, the screening of alloy disorder scattering was omitted. So, the key scattering sources for holes in the quoted system are still unclear.

Thus, the goal of this paper is to present a rigorous treatment of the low-temperature 2DHG mobility in a Ge-rich narrow square Si/SiGe/Si QW. Our theory must be based on a proper calculation of scattering mechanisms, especially, misfit deformation potential scattering and 2DHG screening of alloy scattering.

II. BASIC EQUATIONS

A. Finite square quantum well

We will be dealing with a Si/SiGe/Si QW, which is composed of a SiGe layer grown pseudomorphically in the [001] (z) direction between two pure Si ones. The alloy layer forms a *p*-channel in the interval: $-L/2 \leq z \leq L/2$.

As well known,[10] disorder present in a heterostructure is usually a scattering source affecting its transport properties. The disorder is described by some random field, which is

1098-0121/2007/75(7)/073305(4)

characterized by an autocorrelation function in wave-vector space $\langle|U(\mathbf{q})|^2\rangle$, where the angular brackets stand for averaging over the randomness. Here $U(\mathbf{q})$ means a two-dimensional (2D) Fourier transform of the unscreened scattering potential $U(\mathbf{q},z)$ weighted with the hole envelope wave function of a subband

$$U(\mathbf{q}) = \int_{-\infty}^{+\infty} dz|\zeta(z)|^2 U(\mathbf{q},z). \quad (1)$$

At very low temperature the holes are assumed to primarily occupy the ground-state valence subband.

It was shown[11] that the realistic model of finitely deep QWs should be adopted to describe narrow conduction channels. Accordingly, for a square QW the ground-state wave function is given by

$$\zeta(z) = \begin{cases} A\kappa^{1/2}e^{\kappa(z+L/2)} & \text{for } z < -L/2 \\ Bk^{1/2}\cos(kz) & \text{for } |z| < L/2 \\ A\kappa^{1/2}e^{-\kappa(z-L/2)} & \text{for } z > L/2. \end{cases} \quad (2)$$

Here A and B are dimensionless constants determined by the continuity of the wave function and its derivative and the normalization

$$Ab^{1/2} = Ba^{1/2}\cos(a/2), \quad b = a\tan(a/2) \quad (3)$$

and

$$A^2 + \frac{B^2}{2}(a + \sin a) = 1, \quad (4)$$

where $a=kL$ and $b=\kappa L$ are dimensionless wave numbers in the well and barrier, respectively. These are fixed by Schrödinger's equation for a square QW of any well thickness L and any barrier height V_0,

$$a = \frac{L\sqrt{2m_z V_0}}{\hbar}\cos(a/2), \quad (5)$$

with m_z as the out-of-plane hole effective mass.

B. Low-temperature hole mobility due to single-subband scattering

In what follows, we assume that the well width is small enough that the energy separation between the ground and excited hole states is large compared, e.g., with the Fermi energy. Therefore, we are to restrict ourselves to a single-subband scattering model.

At very low temperature the mobility is determined via the momentum relaxation time τ by a familiar relation: $\mu = e\tau/m^*$, with m^* as the in-plane hole effective mass. Here the inverse relaxation time, i.e., the scattering rate for zero temperature is expressed in terms of the autocorrelation function of disorder,[12,13]

$$\frac{1}{\tau} = \frac{1}{(2\pi)^2\hbar E_F}\int_0^{2k_F} dq \int_0^{2\pi} d\varphi \frac{q^2}{(4k_F^2 - q^2)^{1/2}} \frac{\langle|U(\mathbf{q})|^2\rangle}{\varepsilon^2(q)}, \quad (6)$$

where $\mathbf{q}=(q,\varphi)$ means a 2D wave vector in the in-plane (in polar coordinates), $E_F=\hbar^2k_F^2/2m^*$ is the Fermi energy, and k_F the Fermi wave number fixed by the sheet hole density: $k_F = \sqrt{2\pi p_s}$.

The dielectric function $\varepsilon(q)$ figuring in Eq. (6) takes account of the screening of a scattering potential by the 2DHG. Within the random-phase approximation, this is supplied at zero temperature by[10]

$$\varepsilon(q) = 1 + \frac{q_{TF}}{q}F_S(qL)[1 - G(q)] \quad \text{for } q \le 2k_F. \quad (7)$$

Here $q_{TF}=2m^*e^2/\varepsilon_L\hbar^2$ is the inverse 2D Thomas-Fermi screening length, with ε_L as a dielectric constant of the QW. The function $G(q)=q/[2(q^2+k_F^2)^{1/2}]$ allows for local field corrections due to a many-body exchange effect.

The screening form factor $F_S(qL)$ in Eq. (7) takes account of the extension of hole states along the growth direction, defined by

$$F_S(qL) = \int_{-\infty}^{+\infty} dz \int_{-\infty}^{+\infty} dz' |\zeta(z)|^2 |\zeta(z')|^2 e^{-q|z-z'|}. \quad (8)$$

By means of Eq. (2) for the lowest-subband wave function, this may be written in terms of the dimensionless in-plane wave number $t=qL$ as follows:[14]

$$\begin{aligned} F_S(t) = \frac{B^4a^2}{4}\Bigg\{ & \frac{2}{t}\left(1 + \frac{\sin a}{a}\right) + \frac{t}{t^2+4a^2}\left[1 + 2\frac{\sin a}{a} + \frac{\sin(2a)}{2a}\right] - 4e^{-t/2}\left(\frac{1}{t} + \frac{t\cos a - 2a\sin a}{t^2+4a^2}\right) \\ & \times \left[\left(\frac{1}{t} + \frac{t\cos a}{t^2+4a^2}\right)\sinh\frac{t}{2} + \frac{2a\sin a}{t^2+4a^2}\cosh\frac{t}{2}\right]\Bigg\} \\ & + 4A^2B^2ab\frac{e^{-t/2}}{t+2b}\left[\left(\frac{1}{t} + \frac{t\cos a}{t^2+4a^2}\right)\sinh\frac{t}{2} + \frac{2a\sin a}{t^2+4a^2}\cosh\frac{t}{2}\right] + 2\frac{A^4b^2}{t+2b}\left[\frac{e^{-t}}{t+2b} + \frac{1}{2b}\right], \end{aligned} \quad (9)$$

with a and b given by Eqs. (3) and (5).

III. HOLE-SCATTERING MECHANISMS IN A Si/SiGe/Si QW

In the case when the 2DHG experiences simultaneously several sources of scattering, viz., alloy disorder, surface roughness, and misfit deformation potential, the total relaxation time is determined by the Matthiessen's rule

$$\frac{1}{\tau_{\text{tot}}} = \frac{1}{\tau_{AD}} + \frac{2}{\tau_{SR}} + \frac{2}{\tau_{DP}}, \quad (10)$$

where we introduced a factor of 2 in the last two terms on the right-hand side to include the effects from both interfaces of the QW. Thus, according to Eq. (6) we ought to specify the autocorrelation function in wave-vector space $\langle|U(\mathbf{q})|^2\rangle$ for these scattering sources.

A. Alloy disorder

We begin with scattering of the 2DHG from alloy disorder located inside of the $Si_{1-x}Ge_x$ well layer. The autocorrelation function for the scattering is supplied in the familiar form

$$\langle|U_{AD}(\mathbf{q})|^2\rangle = x(1-x)u_{al}^2\Omega_0\int_{-L/2}^{+L/2} dz|\zeta(z)|^4, \tag{11}$$

in which x is the Ge content, u_{al} is the alloy potential, and L is, as before, the $Si_{1-x}Ge_x$ well width. The volume occupied by one alloy atom is given by $\Omega_0=a^3(x)/8$, with $a(x)$ the lattice constant of the alloy.

By means of Eq. (2) for the lowest-subband wave function, this is rewritten in terms of the dimensionless wave number in the well $a=kL$ as follows:

$$\langle|U_{AD}(\mathbf{q})|^2\rangle = x(1-x)u_{al}^2\Omega_0\frac{B^4a^2}{L}\left[\frac{3}{8}+\frac{\sin a}{2a}+\frac{\sin(2a)}{16a}\right]. \tag{12}$$

B. Surface roughness

Next, we are dealing with scattering of the 2DHG from a rough potential barrier. The scattering potential is due to roughness-induced fluctuations in the position of the barrier.[10] The autocorrelation function for surface-roughness scattering in a square QW of an arbitrary depth was derived in Ref. 14. The result reads as follows:

$$\langle|U_{SR}(\mathbf{q})|^2\rangle = \left(\frac{\hbar^2B^2a^3}{2m_zL^3}\right)^2\langle|\Delta_{\mathbf{q}}|^2\rangle, \tag{13}$$

where $\Delta_{\mathbf{q}}$ is a Fourier transform of the interface profile.

C. Misfit deformation potential

Lastly, interface roughness was shown[14,15] to produce fluctuations in a strain field in a lattice-mismatched heterostructure. These in turn act as a scattering source on charge carriers. Further, it was proven[6,8,9] that the misfit deformation potentials for two kinds of carrier are quite different, viz., the one for electrons is fixed by a single normal diagonal component of the strain field, whereas the one for holes is fixed by all its components. The 2D Fourier transform of the hole deformation potential due to roughness of an interface, e.g., at $z=-L/2$ is derived to be[6]

$$U_{DP}(\mathbf{q},z) = \frac{\alpha\varepsilon_\parallel}{2}\left\{\frac{3}{2}[b_s(K+1)]^2(1+\sin^4\varphi+\cos^4\varphi) + \left(\frac{d_sG}{4c_{44}}\right)^2(1+\sin^2\varphi\cos^2\varphi)\right\}^{1/2} q\Delta_{\mathbf{q}}e^{-q(z+L/2)}, \tag{14}$$

in the well ($|z|\leq L/2$), and zero elsewhere. Here b_s and d_s are the shear deformation potential constants of the well layer, and $\varepsilon_\parallel$ is the lattice mismatch specified by the Ge content and the widths of the well and barrier.[16] The anisotropy ratio of the well is given by $\alpha=2c_{44}/(c_{11}-c_{12})$, and the elastic constants are given by

$$K=2\frac{c_{12}}{c_{11}}, \quad G=2(c_{11}+2c_{12})\left(1-\frac{c_{12}}{c_{11}}\right), \tag{15}$$

with c_{ij} as the elastic stiffness constants of the well.

As clearly seen from Eq. (14), the misfit deformation potential connected with a rough interface decays rapidly (exponentially) with an increase of the distance far away therefrom. As a result, this scattering from the barrier is much weaker than that from the well since the holes are mainly located in the well.

Averaging Eq. (14) by means of the lowest-subband wave function from Eq. (2), we get the autocorrelation function for scattering of interest in the form

$$\langle|U_{DP}(\mathbf{q})|^2\rangle = \left(\frac{\alpha\varepsilon_\parallel B^2a}{2L}\right)^2\left\{\frac{3}{2}[b_s(K+1)]^2(1+\sin^4\varphi+\cos^4\varphi) + \left(\frac{d_sG}{4c_{44}}\right)^2(1+\sin^2\varphi\cos^2\varphi)\right\}t^2e^{-t} \times\left[\left(\frac{1}{t}+\frac{t\cos a}{t^2+4a^2}\right)\sinh\frac{t}{2}+\frac{2a\sin a}{t^2+4a^2}\cosh\frac{t}{2}\right]^2\langle|\Delta_{\mathbf{q}}|^2\rangle. \tag{16}$$

IV. RESULTS AND CONCLUSIONS

We are applying our theory to explain the channel width dependence of the low- (8 K) temperature hole mobility in a narrow $Si/Si_{0.2}Ge_{0.8}/Si$ QW reported in Ref. 7. As indicated,[7,13] for narrow wells ($L\lesssim 100$ Å) we may adopt the single-subband model as a good approximation since the energy separation between the lowest and excited subbands ($\gtrsim$80 meV) is much larger than the Fermi energy ($\sim$20 meV). Further, the rate of impurity scattering was estimated to be much (two orders of magnitude) smaller than the measured one, so omitted.

For numerical calculation, we used the lattice constants, elastic stiffness constants, and shear deformation potentials for Si and Ge listed in Ref. 9. The barrier height depends on the Ge content x as $V_0=0.74x$ eV.[16] The alloy potential is $u_{al}=0.9$ eV.[17] The out-of-plane and in-plane effective hole masses at $x=0.8$ are $m_z=0.22\ m_e$,[17] and $m^*\sim 0.18\ m_e$.[7] The interface profile is described by a Gaussian autocorrelation function with, as x-ray reflectivity shown,[7] a roughness amplitude $\Delta=3.5$ Å and correlation length $\Lambda=23$ Å.

To quantify the effect of the finiteness of a potential barrier on the mobility, we examine the ratio of the mobilities of a QW with a finite and an infinite barrier: $R=\mu^{\rm fin}/\mu^{\rm infin}$. This is plotted in Fig. 1 for diverse scattering mechanisms, viz., alloy disorder, surface roughness, and deformation potential at $x=0.4$ and 0.8.

The partial and overall 2DHG mobilities limited by the above-quote scatterings are plotted at a hole density $p_s=1.5\times10^{12}$ cm^{-2} versus well width L in Fig. 2, where the measured data[7] are also represented for a comparison.

From Figs. 1 and 2 we may draw the following conclusions.

(i) Figure 1 reveals that the commonly used model of infinite QWs[12,13] overestimates the scattering in narrow QWs. The error is increased with a decrease of the well width and large for surface roughness scattering. For in-

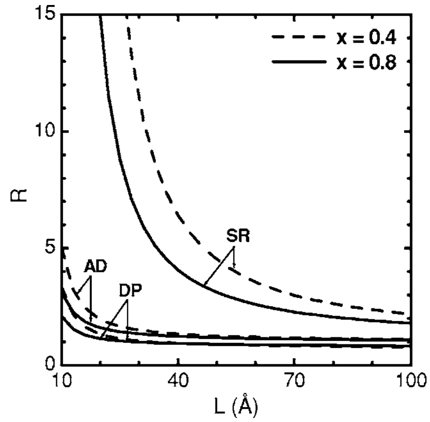

FIG. 1. Mobility ratio $R=\mu^{\text{fin}}/\mu^{\text{infin}}$ for holes in a $Si/Si_{1-x}Ge_x/Si$ square QW vs well width L for diverse scattering sources: alloy disorder R_{AD}, surface roughness R_{SR}, and misfit deformation potential R_{DP}. The solid and dashed lines refer to $x=0.4$ and 0.8, respectively.

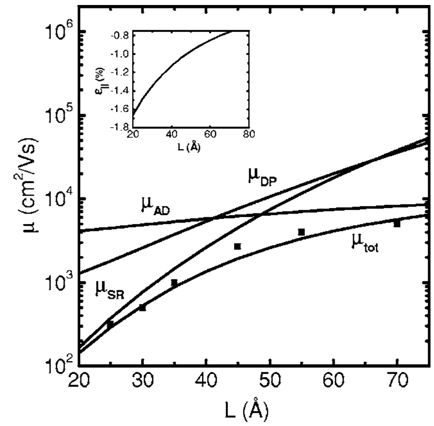

FIG. 2. Mobilities μ of holes in a $Si/Si_{0.2}Ge_{0.8}/Si$ square QW vs well width L. The lines refer to the mobilities limited by alloy disorder μ_{AD}, surface roughness μ_{SR}, misfit deformation potential μ_{DP}, and overall μ_{tot}. The 8 K experimental data[7] are marked by squares. The well-width dependence of the lattice mismatch is shown in the inset for a barrier width of 18 Å.

stance, at $L=25$ Å, $R_{DP}\sim 1$, $R_{AD}\sim 2$, $R_{SR}\gtrsim 10$. The last error is serious in view of the fact that with some practical attempts at structural optimization the hole mobility can be upgraded by a few times only.

(ii) An inspection of Fig. 2 indicates that the overall 2DHG mobility in the $Si/Si_{0.2}Ge_{0.8}/Si$ QW, calculated within the realistic model of finite QWs, reproduces very well the recent experimental data about its dependence on the channel width varying from $L=25-70$ Å. Different from the previous belief, this mobility is dominated not only by surface-roughness scattering but by misfit deformation potential and alloy disorder as well.

(iii) The role of scattering mechanisms changes with the well width. The surface roughness and deformation potential are, in essence, responsible for the steepness of the total-mobility curve at $L\lesssim 45$ Å, and the alloy disorder for its steepness at $L\gtrsim 45$ Å. With an increase of L, the screening effect is reduced.[12] The partial mobility limited by screened alloy scattering is then seen as increased, but remarkably more slowly than those by surface roughness and deformation potential. Therefore, becoming more dominant for $L\gtrsim 50$ Å this leads to a decrease of the steepness of the total mobility. The screening of alloy scattering turns out to be important.

(iv) It is worth mentioning that screening of alloy scattering is still a matter of some debate in virtue of its short-range nature. A study[18] of the temperature dependence of the 2DHG mobility has shown the importance of screening of this scattering. Our study of its well-width dependence provides additional evidence in favor of the screening of short-range interactions such as alloy disorder.

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