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Strain fluctuations in a real [001]-oriented zinc-blende-structure surface quantum well

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A theoretical study is presented of effects from strain fluctuations in a surface quantum well (SQW), which is composed of a strained zinc-blende-structure layer grown on a (001) substrate. It is found that in analogy to a zinc-blende quantum well (QW) with buried interfaces there always exist in the SQW a large fluctuating density of bulk piezoelectric charges and a high random piezoelectric field. However, in contrast to the buried QW case, roughness at a free surface of the SQW causes random fluctuations in the dilatation, which give rise to perturbing deformation potentials. The piezoelectric field and deformation potentials supply strong disorder interactions as new important scattering mechanisms for confined charge carriers in SQW's. A comparison of their effects in a SQW and the QW under equal conditions is given.

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In the last years, the two-dimensional electron gas (2DEG) has been formed at a surface of several semiconductor heterostructures.[1–5] The free surface in a surface quantum well (SQW) exhibits a distinction from buried interfaces in a quantum well (QW). Accessibility of one face of a SQW enables gradual etching of the well width to study the width dependence of its observable properties. Moreover, the free surface of a SQW imposes a boundary condition for elastic lattice deformation in the well, which is strikingly different from that by a buried interface in a QW.

On the other hand, elastic lattice deformation due to lattice mismatch between various layers of a semiconductor heterostructure is known[6] to result in both microscopic effects, e.g., change of the band gap and lifting of the degeneracy of the valence band, and in macroscopic ones, e.g., piezoelectric field. Therefore, a wide variety of basic properties of a QW is expected to significantly change if its boundaries are modified, in particular, if a SQW is formed, for instance, by removing the top barrier layer of the QW by selective chemical etching.[4]

Up to now, SQW's have been studied much less than QW's and mainly in conjunction with passivation[2,3] and optical phenomena.[4] A thorough study of diverse physical properties of SQW's is, therefore, of some interest. The understanding of them is also of benefit for the modeling of lateral quantization effects in etched quantum wires and quantum dots,[2–4,7] where the lateral barriers are defined by open surfaces.[8,9]

Recently, it has been pointed out[10–12] that interface roughness in a semiconductor heterostructure causes random fluctuations in the strain field. Feenstra and Lutz[11] proved that for Si/SiGe systems strain variations generate random deformation potentials as a new scattering mechanism, which yields much better agreement with experimental data than the well-known scatterings do. Further, Quang and coworkers[12] found that for a QW made of zinc-blende material strain variations generate a random piezoelectric field. This field is a new scattering mechanism and offers an accurate way to explain the mobility of strained InGaAs-based QW's, which cannot be understood by the well-known scattering sources.

Thus, the aim of this paper is to extend our earlier theory of effects due to strain fluctuations in QW's (Ref. 12) to the case of SQW's that are made of zinc-blende material, especially grown on a (001) substrate. Thereby, we explore which of the above-mentioned disorder interactions exists in a SQW and compare their impacts from a free rough surface in a SQW and from a buried one in a QW.

To start with, we recall the main arguments for ideal SQW's, which are composed of a strained zinc-blende layer grown pseudomorphically on a substrate, where the well thickness is much smaller than the critical one but the substrate thickness is larger. It is known[6] that if the substrate has been oriented along a high symmetry direction, e.g., [001] and the open surface is assumed to be ideal, i.e., absolutely flat, the stress field inside of the well is uniform and biaxial. Accordingly, the strain field is uniform and has no shear components, i.e., with zero off-diagonal ones. Consequently, ideal SQW's present neither a piezoelectric polarization nor any piezoelectric field.

However, as mentioned above, interface roughness can cause drastic modification in the strain field. This turns out to depend very sensitively on the condition of the interface to be open or buried. Indeed, in a QW with buried interfaces a fraction of the elastic strain energy in the well is transmitted during growth to unstrained barriers, so lowering the total energy of the well, whereas in a SQW with an open surface (vacuum or air/well) the surface evolution is dictated by a boundary condition that the surface is traction free.[13]

The effect from a rough open surface on the stress field inside of a well was derived by Srolovitz[10] for a medium of elastic isotropy. With the use of Hooke's law, the strain field within the well is supplied in a crystal reference system in terms of the surface profile $\Delta_{\mathbf{q}}$ by the following 2D Fourier expansion:

$$\epsilon_{xx}(\mathbf{r},z)=\epsilon_{\parallel}+\epsilon_{\parallel}\sum_{\mathbf{q}} q\Delta_{\mathbf{q}}e^{-qz}[(K+2)\cos^2\theta-K\sin^2\theta -(K+1)qz\cos^2\theta]e^{i\mathbf{qr}},$$

$$\epsilon_{yy}(\mathbf{r},z)=\epsilon_{\parallel}+\epsilon_{\parallel}\sum_{\mathbf{q}} q\Delta_{\mathbf{q}}e^{-qz}[(K+2)\sin^2\theta-K\cos^2\theta -(K+1)qz\sin^2\theta]e^{i\mathbf{qr}},$$

$$\epsilon_{zz}(\mathbf{r},z)=\epsilon_{\perp}+\epsilon_{\parallel}\sum_{\mathbf{q}} q\Delta_{\mathbf{q}}e^{-qz}[(K+1)qz-K]e^{i\mathbf{qr}},$$

$$\epsilon_{xy}(\mathbf{r},z)=\frac{G\epsilon_{\parallel}}{8c_{44}}\sum_{\mathbf{q}} q\Delta_{\mathbf{q}}e^{-qz}(2-qz)\sin 2\theta\, e^{i\mathbf{qr}}, \quad (1)$$

$$\epsilon_{yz}(\mathbf{r},z)=\frac{G\epsilon_{\parallel}}{4c_{44}}\sum_{\mathbf{q}} q\Delta_{\mathbf{q}}e^{-qz}(1-qz)\sin\theta e^{i(\mathbf{qr}+\pi/2)},$$

$$\epsilon_{zx}(\mathbf{r},z)=\frac{G\epsilon_{\parallel}}{4c_{44}}\sum_{\mathbf{q}} q\Delta_{\mathbf{q}}e^{-qz}(1-qz)\cos\theta e^{i(\mathbf{qr}+\pi/2)},$$

where $0\leqslant z\leqslant L$, with L as the well thickness. Hereafter, $\mathbf{r}=(x,y)$ denotes a 2D position vector in the surface plane $z=0$, z the growth direction, and (q,θ) are the polar coordinates of a 2D wave vector $\mathbf{q}$. The in-plane and normal components of the strain field in the absence of roughness is given in terms of the lattice constants of the substrate and well: $\epsilon_{\parallel}=(a_{\rm s}-a_{\rm w})/a_{\rm w}$, and $\epsilon_{\perp}=-K\epsilon_{\parallel}$. The elastic constants of the well are $K=2c_{12}/c_{11}$, and $G=2(K+1)(c_{11}-c_{12})$, with c_{11}, c_{12}, and c_{44} as its stiffness constants. For simplicity, the interface profile is chosen in a Gaussian form with a roughness amplitude Δ and correlation length Λ.

It is clearly seen from Eq. (1) that because of surface roughness the strain field in SQW's is fundamentally changed, subjected to random nonuniform fluctuations in the well. Moreover, it is distinctive of actual SQW's that the strain field has nonvanishing off-diagonal components although grown on a (001) substrate. The strain variations are found[12] to be largest on the surface plane and then decay rather rapidly. Their maximal rms values are

$$\overline{\Delta\epsilon_{\parallel}}(0)=\sqrt{2(K^2+2K+3)}|\epsilon_{\parallel}|(\Delta/\Lambda),$$

$$\overline{\Delta\epsilon_{\perp}}(0)=2K|\epsilon_{\parallel}|(\Delta/\Lambda), \quad (2)$$

$$\overline{\epsilon_{xy}}(0)=\overline{\epsilon_{yz}}(0)=\overline{\epsilon_{zx}}(0)=(G/\sqrt{8}c_{44})|\epsilon_{\parallel}|(\Delta/\Lambda).$$

We now turn to the study of macroscopic effects from strain fluctuations. The nonzero off-diagonal strain components induce a polarization vector inside of the well via its piezoelectric constant e_{14}: $P_i=2e_{14}\epsilon_{jk}$ $(i\neq j\neq k)$, with ϵ_{jk} given by Eq. (1). The polarization is then strongly nonuniform in the well and, hence, creates a density of fixed charges according to $\rho(\mathbf{r},z)=-\boldsymbol{\nabla}\mathbf{P}(\mathbf{r},z)$:

$$\rho(\mathbf{r},z)=\frac{e_{14}G\epsilon_{\parallel}}{4c_{44}}\sum_{\mathbf{q}} q^2\Delta_{\mathbf{q}}e^{-qz}(5-3qz)\sin 2\theta\, e^{i\mathbf{q}\cdot\mathbf{r}}. \quad (3)$$

In contrast to the previous theories,[6,14] due to surface roughness there always exist piezoelectric charges in a real strained zinc-blende SQW even with a (001) substrate. The charges are bulklike and randomly distributed within the well with a zero average density, but a nonzero rms density. The latter is seen to be largest on the surface plane with

$$\overline{\rho}(0)=5(G/c_{44})|e_{14}\epsilon_{\parallel}|(\Delta/\Lambda^2). \quad (4)$$

The bulk piezoelectric charges generate an electric field. The potential energy of an electron of charge $-e$ in the field may be represented in terms of an integral extended over the well layer by

$$U_{\rm PE}(\mathbf{r},z)=\int d\mathbf{r}'dz'\rho(\mathbf{r}',z')v(\mathbf{r}'-\mathbf{r};z',z), \quad (5)$$

where $v(\mathbf{r}'-\mathbf{r};z',z)$ stands for Green's function of Poisson's equation.

The dielectric discontinuity through vacuum/well surface exerts a drastic influence on the electric-field distribution, which is to be involved in terms of image charges.[15] Green's function of interest is then specified on the semiconductor side $(z>0)$ by

$$v(\mathbf{r}'-\mathbf{r};z',z)=\frac{-e}{\varepsilon_{\rm L}[(\mathbf{r}'-\mathbf{r})^2+(z'-z)^2]^{1/2}} +\frac{\varepsilon_{\rm L}-1}{\varepsilon_{\rm L}+1}\frac{-e}{\varepsilon_{\rm L}[(\mathbf{r}'-\mathbf{r})^2+(z'+z)^2]^{1/2}} \quad (6)$$

and on the vacuum side $(z<0)$ by

$$v(\mathbf{r}'-\mathbf{r};z',z)=\frac{1}{(\varepsilon_{\rm L}+1)/2}\frac{-e}{[(\mathbf{r}'-\mathbf{r})^2+(z'-z)^2]^{1/2}}, \quad (7)$$

with $\varepsilon_{\rm L}$ as the dielectric constant of the system.

On the substitution of Eq. (3) for the piezoelectric charge density, Eqs. (6) and (7) for Green's function into Eq. (5), and with the subsequent use of a 2D Fourier transform of the Coulomb potential,[15] we are able to get a 2D Fourier expansion for the piezoelectric potential:

$$U_{\rm PE}(\mathbf{r},z)=-\frac{\pi e e_{14}G\epsilon_{\parallel}}{2\varepsilon_{\rm L}(z)c_{44}}\sum_{\mathbf{q}} q\Delta_{\mathbf{q}}F(q,z;L)\sin 2\theta\, e^{i\mathbf{qr}}. \quad (8)$$

The dielectric constant varies along the growth direction as $\varepsilon_{\rm L}(z)=\varepsilon_{\rm L}$ for $z>0$, and $\varepsilon_{\rm L}(z)=\frac{1}{2}(\varepsilon_{\rm L}+1)$ for $z<0$.

The form factor entering Eq. (8) depends on the well thickness L, fixed on the semiconductor side $(z>0)$ by

$$F(q,z;L)=\int_0^L dz'(5-3qz')e^{-qz'}\left[e^{-q|z'-z|}+\frac{\varepsilon_{\rm L}-1}{\varepsilon_{\rm L}+1}e^{-q|z'+z|}\right] \quad (9)$$

and on the vacuum side $(z<0)$ by

$$F(q,z;L)=\int_0^L dz'(5-3qz')e^{-q(z'+|z'-z|)}. \quad (10)$$

Next, we are concerned with the strength of the piezoelectric field. By means of $\mathbf{E}(\mathbf{r},z)=-\boldsymbol{\nabla}[U_{\mathrm{PE}}(\mathbf{r},z)/-e]$, with $U_{\mathrm{PE}}(\mathbf{r},z)$ given by Eq. (8), we may easily argue that the field in question has both in-plane and normal components although the substrate has been oriented in a high-symmetry direction, e.g., [001]. In addition, both components undergo random fluctuations with a zero average but a nonzero rms (see Fig. 2).

We are now examining microscopic effects, namely, the impact of strain fluctuations on the energy band structure of the system in question. It has been shown[16] that the strains bring about a shift of the band edges of the conduction and valence bands, defined by

$$\Delta E_c = a_c \frac{\Delta V}{V},$$

$$\Delta E_v^{\mp} = a_v \frac{\Delta V}{V} \pm \sqrt{\frac{b^2}{2}A + d^2 B}, \tag{11}$$

with a_l $(l=c,v)$, b, and d as the deformation potential constants. The upper and lower signs refer to the heavy and light holes, respectively, and

$$\frac{\Delta V}{V} = \epsilon_{xx}(\mathbf{r},z)+\epsilon_{yy}(\mathbf{r},z)+\epsilon_{zz}(\mathbf{r},z), \tag{12}$$

and

$$\begin{aligned} A &= [\epsilon_{xx}(\mathbf{r},z)-\epsilon_{yy}(\mathbf{r},z)]^2+[\epsilon_{yy}(\mathbf{r},z)-\epsilon_{zz}(\mathbf{r},z)]^2 \\ &\quad +[\epsilon_{zz}(\mathbf{r},z)-\epsilon_{xx}(\mathbf{r},z)]^2, \\ B &= \epsilon_{xy}^2(\mathbf{r},z)+\epsilon_{yz}^2(\mathbf{r},z)+\epsilon_{zx}^2(\mathbf{r},z). \end{aligned} \tag{13}$$

Because of strain variations, the volume dilatation $\Delta V/V$ is subjected to random fluctuations. These produce band-edge fluctuations as perturbing deformation potentials acting on the electrons in the conduction band and the holes in the valence one. Inserting Eqs. (1) and (12) into Eq. (11) yields

$$U_{\mathrm{DP}}^{(l)}(\mathbf{r},z) = a_l \epsilon_{\parallel}(2-K)\sum_{\mathbf{q}} q\Delta_{\mathbf{q}} e^{-qz} e^{i\mathbf{q}\cdot\mathbf{r}}, \tag{14}$$

which describes disorder interactions with a zero average but a nonzero rms potential. The latter is maximal on the surface plane with

$$\overline{U_{\mathrm{DP}}^{(l)}}(0) = 2\,|a_l \epsilon_{\parallel}(2-K)|(\Delta/\Lambda). \tag{15}$$

Thus, the impact from a free surface in zinc-blende SQW's is similar to that from a buried interface in Si/SiGe heterostructures.[11] However, this is quite different from the influence from a buried interface in zinc-blende QW's, where strain fluctuations produce no random deformation potentials.[12]

Finally, we estimate the order of magnitude of the valence band splitting due to strain variations. By virtue of the randomness of the quantities $\Delta V/V$, A, and B, it is suggested to replace them with their configuration averages. By definition $\overline{\delta E} = \langle \Delta E_v^- \rangle - \langle \Delta E_v^+ \rangle$, it holds

$$\overline{\delta E}(z) = 2\sqrt{\frac{b^2}{2}\langle A\rangle + d^2\langle B\rangle}, \tag{16}$$

where the angular brackets mean the configuration average. This is also maximal on the surface plane with

$$\begin{aligned} \overline{\delta E}(0) = 2|\epsilon_{\parallel}|\{&b^2(K+1)^2[1+10(\Delta/\Lambda)^2] \\ &+3d^2(G/\sqrt{8}c_{44})^2(\Delta/\Lambda)^2\}^{1/2}. \end{aligned} \tag{17}$$

To illustrate the foregoing theory, we have carried out numerical calculations for a SQW made of $\mathrm{In_{0.2}Ga_{0.8}As}$ grown pseudomorphically on GaAs with a lattice mismatch $\epsilon_{\parallel}=-0.0145$. The effects from strain fluctuations are to be measured by the rms of the physical properties of interest as a function of the distance z (in units of the correlation length Λ). Numerical results for the QW under equal conditions are reproduced[12] for a comparison.

The maximal rms fluctuations of shear strains in a SQW with a ratio for the surface profile $\Delta/\Lambda=0.1$ are estimated by Eq. (2): $\overline{\epsilon_{xy}}(0)=\overline{\epsilon_{yz}}(0)=\overline{\epsilon_{zx}}(0)=0.59|\epsilon_{\parallel}|$, while those in the reference QW are less than $0.28|\epsilon_{\parallel}|$.

In accordance with large shear strains, the maximal rms density of piezoelectric charges is fixed by Eq. (4) to be high. For instance, for a SQW with $\Delta=5$ Å, $\Lambda=50$ Å: $\bar{\rho}(0)=2.1\times10^{19}\ e/\mathrm{cm}^3$, while for the QW: $\bar{\rho}(0)=6.3\times10^{18}\ e/\mathrm{cm}^3$.

In accordance with a large density of piezoelectric charges, their field is found to be high. For a SQW with $\Delta=5$ Å, $\Lambda=50$ Å, the maximal rms piezoelectric potential within the well is 9 meV (see Fig. 1). The maximal rms for the in-plane field component within the well is 1.36×10^6 V/cm, and for the normal component 8×10^6 V/cm (Fig. 2), while that in the QW less than 10^5 V/cm.

It is worth remarking that at distances rather deep into the

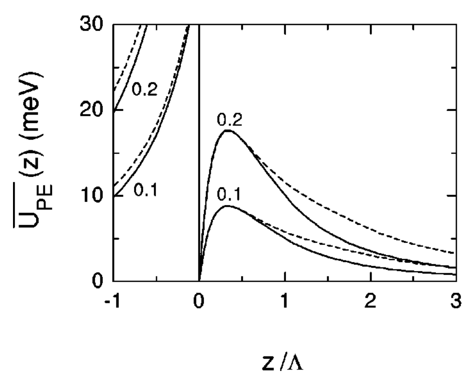

FIG. 1. Root-mean-square piezoelectric potential $\overline{U_{\mathrm{PE}}}(z)$ in a SQW vs distance z under different well widths $L=50$ (solid lines), 150 Å (dashed ones), a correlation length $\Lambda=50$ Å, and different ratios $\Delta/\Lambda=0.1$, 0.2.

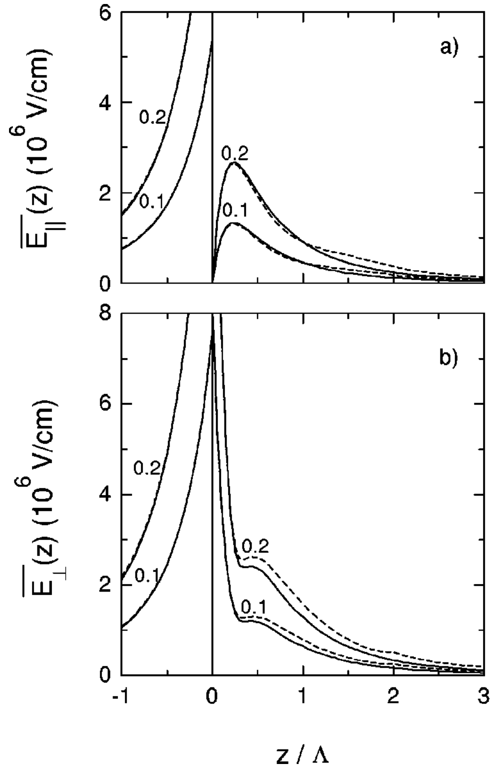

FIG. 2. Root-mean-square piezoelectric field strength in the SQW of Fig. 1 vs distance z for (a) the in-plane component $\overline{E_{\parallel}}(z)$ and (b) the normal component $\overline{E_{\perp}}(z)$.

well, the piezoelectric field is still rather strong. For a SQW of width $L = 50–100$ Å, in the region of $z = 25–50$ Å, where the majority of charge carriers are located, for $\Delta = 5$ Å, $\Lambda = 50$ Å the in-plane component $\overline{E_{\parallel}} = 10^6 – 5 \times 10^5$ V/cm [Fig. 2(a)]. Therefore, 2D excitonic states may be unstable and two types of electron-hole pair (free and bound) are simultaneously present in a SQW.

For a SQW with $\Delta = 5$ Å, $\Lambda = 50$ Å, the maximal rms deformation potentials are estimated by Eq. (15): $\overline{U_{\rm DP}^{(c)}}(0) = 19$ meV and $\overline{U_{\rm DP}^{(v)}}(0) = 3.3$ meV. These are of the order of magnitude of the rms piezoelectric potential.

Disorder interactions have been shown[17] to give rise to 2D density-of-state tails, which lead to a broadening of optical spectra of the order of magnitude of the rms potentials. The broadening in SQW's is due to the deformation potential and the piezoelectric one as well as conventional surface roughness potential, whereas that in QW's due merely to the latter two. As seen above, the piezoelectric field in a SQW is remarkably stronger than that in the QW. Therefore, the photoluminescence linewidth from a zinc-blende SQW is to be much larger than that from the reference QW, which is in a good agreement with the experimental data (four times larger).[4] Further, inclusion of the former two potentials may also offer a way to explain the measured linewidth with a smaller (likely realistic) roughness amplitude than that used previously in Ref. 4 ($\Delta = 12$ Å), when basing on surface roughness potential only.

Lastly, the maximal rms valence band splitting is fixed by Eq. (17): $\overline{\delta E}(0) = 150$ meV, which causes an additional redshift of optical spectra.

The random piezoelectric and deformation potentials present new scattering mechanisms for confined charge carriers in SQW's. The mobility calculation reveals that these are predominant over surface roughness scattering in rather thick SQW's with a width greater than 200 Å.

To summarize, in this paper we have demonstrated that strain fluctuations due to roughness at a free surface of zinc-blende SQW's create a high-random piezoelectric field even with a high symmetry growth axis, e.g., [001]. This is analogous to the case of zinc-blende QW's.[12] However, in difference from the QW's with buried interfaces, these also create high random deformation potentials.

The disorder effects from strain variations in a SQW are remarkably larger than those in the QW under equal conditions. So, the mobility of a QW is expected to drastically reduce when removing its top barrier to form a relevant SQW.

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