Random Piezoelectric Field in Real [001]-Oriented Strain-Relaxed Semiconductor Heterostructures

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We work out a theory of piezoelectricity in an actual semiconductor heterostructure which is composed of a lattice-mismatched zinc-blende layer grown on a [001]-oriented substrate. In contrast to earlier theories, we predict a large density of fixed bulk piezoelectric charges, which are induced by strain fluctuations connected with interface roughness. The piezoelectric charges create a high electric field. The random piezoelectric field presents a conceptually new important scattering mechanism. The system of charge carriers in such a heterostructure becomes strongly disordered and includes generally both free electron-hole pairs near the interface and excitons far from it.

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It is well known [1] that the elastic lattice deformation due to lattice mismatch between different layers of a semiconductor heterostructure can lead both to microscopic effects, e.g., change of the band gap and lift of the degeneracy of the valence band, and to macroscopic effects, e.g., piezoelectric field. An exact knowledge of the lattice mismatch-induced strain field and its impacts is, therefore, of vital importance to the interpretation of observed phenomena as well as the design and development of new electronic and optoelectronic devices. Strain fields in two-dimensional (2D) epilayers have intensively been studied both experimentally and theoretically [1].

The strain field in a system is closely related to its boundaries. It was shown that because of strain release via additional free surfaces in a semiconductor structure with reduced spatial dimensions, e.g., 1D quantum wire [2–4] and 0D quantum dot [2,4], the strain field is considerably changed. Recently, it has been pointed out [5,6] that the roughness of an interface between lattice-mismatched layers in a 2D semiconductor structure is an important mechanism for strain relaxation. This means the roughness may bring about a drastic modification of the stress field. This in turn implies according to Hooke's law [7] a radical redistribution of the strain field.

Thus, the aim of this Letter is to present a theory of the strain field and its effects, especially the piezoelectric field, in a real zinc-blende heterostructure grown especially on a (001) substrate, taking adequate account of strain release by interface roughness. It is to be noted that the roughness-induced piezoelectric field has been addressed in [8,9]. In Ref. [8] the piezoelectric polarization was, however, assumed to exist only with a *non*-[001] oriented substrate and to take a constant flat-interface value.

As a model system, we are examining a quantum well composed of a strained layer sandwiched between two unstrained layers, where the well thickness is smaller but the barrier ones larger than the critical thickness. It was proved [1,7] that if the substrate has been oriented along a high symmetry direction, e.g., [001] and the interface is supposed to be ideal, i.e., absolutely flat, the stress field within the well is uniform and biaxial. Accordingly, the strain field is uniform and has no shear components, i.e., with zero off-diagonal components.

It should be emphasized [8] that actual layered semiconductor systems always exhibit lateral feature in the form of interface roughness. This is shown [5,6] to result in a modification of the stress field. The effect from a rough buried interface (barrier/well) located at $z = 0$ on the stress field inside of a strained layer was derived by Feenstra and Lutz [6]. With the use of Hooke's law for a medium of elastic isotropy [7], the strain field inside of the well is determined in a crystal reference system to be

$$\begin{aligned}
\epsilon_{xx}(\mathbf{r}, z) &= \epsilon_{\parallel} + \frac{(K+1)\epsilon_{\parallel}}{2}\sum_{\mathbf{q}} q\Delta_{\mathbf{q}} e^{-qz}\cos^2\theta e^{i\mathbf{q}\cdot\mathbf{r}},\\
\epsilon_{yy}(\mathbf{r}, z) &= \epsilon_{\parallel} + \frac{(K+1)\epsilon_{\parallel}}{2}\sum_{\mathbf{q}} q\Delta_{\mathbf{q}} e^{-qz}\sin^2\theta e^{i\mathbf{q}\cdot\mathbf{r}},\\
\epsilon_{zz}(\mathbf{r}, z) &= \epsilon_{\perp} - \frac{(K+1)\epsilon_{\parallel}}{2}\sum_{\mathbf{q}} q\Delta_{\mathbf{q}} e^{-qz} e^{i\mathbf{q}\cdot\mathbf{r}},\\
\epsilon_{xy}(\mathbf{r}, z) &= \frac{G\epsilon_{\parallel}}{4c_{44}}\sum_{\mathbf{q}} q\Delta_{\mathbf{q}} e^{-qz}\sin 2\theta e^{i\mathbf{q}\cdot\mathbf{r}},\\
\epsilon_{yz}(\mathbf{r}, z) &= \frac{G\epsilon_{\parallel}}{2c_{44}}\sum_{\mathbf{q}} q\Delta_{\mathbf{q}} e^{-qz}\sin\theta e^{i(\mathbf{q}\cdot\mathbf{r}+\pi/2)},\\
\epsilon_{zx}(\mathbf{r}, z) &= \frac{G\epsilon_{\parallel}}{2c_{44}}\sum_{\mathbf{q}} q\Delta_{\mathbf{q}} e^{-qz}\cos\theta e^{i(\mathbf{q}\cdot\mathbf{r}+\pi/2)},
\end{aligned} \tag{1}$$

where $0 \le z \le L$, with L the well thickness. Hereafter, $\mathbf{r} = (x, y)$ represents a 2D position vector in the interface plane, z the [001] growth direction; q, θ are the polar coordinates of a wave vector $\mathbf{q}$ in the plane, and $\Delta_{\mathbf{q}}$ is

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the Fourier transform of the interface profile. The elastic constants of the strained layer are defined by $K = 2c_{12}/c_{11}$ and $G = 2(K+1)(c_{11} - c_{12})$, with c_{11}, c_{12}, and c_{44} as its elastic stiffness constants.

Equation (1) reveals because of the randomness of $\Delta_{\mathbf{q}}$, the strain field in a real lattice-mismatched quantum well are fundamentally changed, being random in nature and microscopically nonuniform in the well. This is quite different from the case of ideal interfaces [1,7]. Moreover, it is distinctive of a heterostructure with rough interface that the strain field has *nonvanishing* off-diagonal components although grown on a (001) substrate.

To characterize the magnitude of fluctuations in the strain field we determine their rms. For simplicity, the interface profile is chosen in a Gaussian form [10]. Then, we obtain for the rms fluctuation of the in-plane strain:

$$\frac{\overline{\Delta\epsilon_{\parallel}}(z)}{|\epsilon_{\parallel}|} = \frac{3(K+1)}{2\sqrt{2}}\frac{\Delta}{\Lambda}\left[Q_4^0\left(\frac{z}{\Lambda}\right)\right]^{1/2}. \tag{2}$$

with Δ and Λ being the roughness amplitude and correlation length, respectively. Hereafter, we introduce a special function of the dimensionless variable $t = z/\Lambda$ in terms of a parabolic cylinder function

$$Q_n^m(t) = (2\sqrt{2}\,t)^m \exp(2t^2) D_{-n}(2\sqrt{2}\,t). \tag{3}$$

We now turn to the study of macroscopic properties of a system made of zinc-blende material. The off-diagonal components of a strain field induce a polarization vector via the piezoelectric constant e_{14}: $P_i = 2e_{14}\epsilon_{jk}$. It has been pointed out [1,8] that a strained layer of zinc-blende material grown on a [001]-oriented substrate exhibits neither a piezoelectric polarization nor any piezoelectric field. Nevertheless, it should be stressed that this conclusion was, in fact, drawn simply for the case of *ideal* interfaces. All experimentally accessible structures are real quantum wells with rough interface and, as quoted above, have nonzero shear strains. With the aid of Eq. (1) for ϵ_{jk} $(j \neq k)$, one may arrive at

$$P_x(\mathbf{r}, z) = \frac{e_{14}G\epsilon_{\parallel}}{c_{44}}\sum_{\mathbf{q}} q\Delta_{\mathbf{q}} e^{-qz}\sin\theta e^{i(\mathbf{q}\cdot\mathbf{r}+\pi/2)},$$
$$P_y(\mathbf{r}, z) = \frac{e_{14}G\epsilon_{\parallel}}{c_{44}}\sum_{\mathbf{q}} q\Delta_{\mathbf{q}} e^{-qz}\cos\theta e^{i(\mathbf{q}\cdot\mathbf{r}+\pi/2)}, \tag{4}$$
$$P_z(\mathbf{r}, z) = \frac{e_{14}G\epsilon_{\parallel}}{2c_{44}}\sum_{\mathbf{q}} q\Delta_{\mathbf{q}} e^{-qz}\sin 2\theta e^{i\mathbf{q}\cdot\mathbf{r}}.$$

Equation (4) shows that in difference from [8], the roughness-induced polarization is strongly nonuniform. Therefore, a density of bound charges is generated within the well. According to $\rho(\mathbf{r}, z) = -\nabla\mathbf{P}(\mathbf{r}, z)$, it holds

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

It is clearly observed from Eq. (5) that in opposition to previous theories [1,8], owing to roughness there always exist piezoelectric charges in an actual strain-relaxed heterostructure even with a (001) substrate. These are bulklike and randomly distributed inside of the well with a zero average but a nonzero rms density, given by

$$\overline{\rho}(z) = 6\sqrt{15}\,\frac{|e_{14}G\epsilon_{\parallel}|}{c_{44}}\frac{\Delta}{\Lambda^2}\left[Q_6^0\left(\frac{z}{\Lambda}\right)\right]^{1/2}. \tag{6}$$

The piezoelectric charges create an electric field. Upon solving Poisson's equation for the charge density fixed by Eq. (5), we may get a 2D Fourier expansion for the piezoelectric potential of an electron of charge $-e$:

$$U(\mathbf{r}, z) = -\frac{3\pi e e_{14}G\epsilon_{\parallel}}{\varepsilon_L c_{44}}\sum_{\mathbf{q}} q\Delta_{\mathbf{q}} F(q, z; L)\sin 2\theta e^{i\mathbf{q}\cdot\mathbf{r}}. \tag{7}$$

Here ε_L is the dielectric constant of the system, and the form factor is defined by

$$F(q, z; L) = \int_0^L dz' e^{-q(z'+|z'-z|)}. \tag{8}$$

Equation (7) indicates the piezoelectric potential is random with a zero average but a nonzero rms. The latter is supplied inside of the well by

$$\overline{U}(z) = \frac{3\pi}{2\sqrt{2}}\frac{e|e_{14}G\epsilon_{\parallel}|}{\varepsilon_L c_{44}}\Delta\left[Q_2^0\left(\frac{z}{\Lambda}\right)+4Q_3^1\left(\frac{z}{\Lambda}\right)+6Q_4^2\left(\frac{z}{\Lambda}\right)-2Q_2^0\left(\frac{L}{\Lambda}\right)-4\frac{z}{L}Q_3^1\left(\frac{L}{\Lambda}\right)+Q_2^0\left(\frac{2L-z}{\Lambda}\right)\right]^{1/2}. \tag{9}$$

Next, we calculate the strength of a random piezoelectric field with the aid of $\mathbf{E}(\mathbf{r}, z) = -\nabla[U(\mathbf{r}, z)/-e]$. The field has, following Eq. (7), both in-plane and normal components even with a (001) substrate. Further, these undergo random fluctuations with a zero average but a nonzero rms. The latter is supplied within the well by

$$\overline{E_{\parallel,\perp}}(z) = \frac{3\sqrt{3}\,\pi}{\alpha_{\parallel,\perp}}\frac{|e_{14}G\epsilon_{\parallel}|}{\varepsilon_L c_{44}}\frac{\Delta}{\Lambda}\left[Q_4^0\left(\frac{z}{\Lambda}\right)\pm 8Q_5^1\left(\frac{z}{\Lambda}\right)+20Q_6^2\left(\frac{z}{\Lambda}\right)-2Q_4^0\left(\frac{L}{\Lambda}\right)\mp 8\frac{z}{L}Q_5^1\left(\frac{L}{\Lambda}\right)+Q_4^0\left(\frac{2L-z}{\Lambda}\right)\right]^{1/2}, \tag{10}$$

where $\alpha_{\parallel} = 2$, $\alpha_{\perp} = \sqrt{2}$, the upper (lower) signs refer to the in-plane (normal) component of the field.

Finally, we examine microscopic effects from strain relaxation in a real [001]-oriented strained heterostructure of zinc-blende material. We calculate the impact of strain fluctuations on its energy band structure. An inspection of Eq. (1) reveals that the conduction and valence band edges undergo no shift associated with the volume dilatation since it remains unchanged under strain fluctuations. This means that the charge carriers experience no random perturbing deformation potential. One needs to evaluate merely a splitting between the heavy and light hole valence bands, defined by [11]: $\delta E = 2E_S$, where

$$E_S^2 = \frac{b^2}{2}A + d^2B, \tag{11}$$

with b and d as deformation potential constants. A and B are given in Ref. [11] in terms of the diagonal and nondiagonal components of the strain field, respectively.

As evidently seen from Eq. (1), because of roughness A and B become random functions of spatial coordinates. To estimate the order of magnitude of the roughness-induced splitting energy, it is suggested to replace them by their configuration averages. The calculation of the latter is easily done, yielding

$$\overline{E_S}^2(z) = [b\epsilon_\parallel(K+1)]^2 + [\Delta\epsilon_\parallel(z)]^2\left[\frac{51}{9}b^2 + 11\left(\frac{c_{11}-c_{12}}{c_{44}}\right)^2 d^2\right]. \tag{12}$$

The first term appearing in Eq. (12) describes the homogeneous splitting due to the lattice mismatch-induced strain $\epsilon_\parallel$ studied previously [1], whereas the second term refers to an inhomogeneous splitting due to the roughness-induced strain fluctuation $\Delta\epsilon_\parallel(z)$.

To illustrate the foregoing theory, we have carried out numerical calculations for a quantum well made from $GaAs/In_{0.2}Ga_{0.8}As/GaAs$. The lattice mismatch is $\epsilon_\parallel = -0.014$. We calculate the effects arising from the strain fluctuations related to roughness of the interface at $z = 0$ as a function of the distance from the interface plane. The distance is clearly scaled in units of the correlation length Λ.

Figures 1–4 reveal the strain fluctuations and relative phenomena occur mainly within a near-interface region of a few correlation lengths ($z \lesssim 3\Lambda$), decaying rather rapidly far from the interface plane $z = 0$. Thereon, the rms of the strain fluctuations, valence band splitting, and piezoelectric charge density are maximal. The latter is found to be large, up to $5 \times 10^{19}\ e/\mathrm{cm}^3$. Accordingly, the piezoelectric field is high with a rms potential of up to 20 meV and a rms strength up to 10^5 V/cm. This supplies a strong *ad hoc* disorder interaction affecting the in-plane motion of confined charge carriers. In opposition to the flat-interface case this field exists even outside of the well, in the unstrained GaAs barrier, as experimentally justified in [8]. Figure 5 shows this field presents a key scattering source, which is

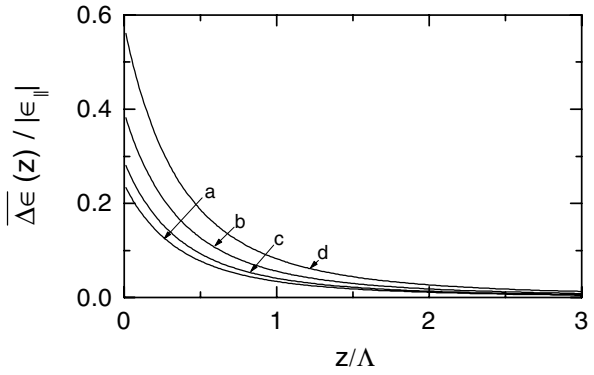

FIG. 1. rms fluctuations of the strain components vs distance z for a ratio of $\Delta/\Lambda = 0.2$: (*a*) $\overline{\Delta\epsilon_\parallel}(z)$; (*b*) $\overline{\Delta\epsilon_\perp}(z)$; (*c*) $\overline{\Delta\epsilon_{xy}}(z)$; and (*d*) $\overline{\Delta\epsilon_{yz}}(z) = \overline{\Delta\epsilon_{zx}}(z)$.

predominant (about 1 order of magnitude) over conventional surface roughness under a well width $L \gtrsim 150$ Å.

The strain fluctuations lead, via splitting energy (up to 85 meV), to an additional redshift in optical spectra connected with electron transitions between the conduction and heavy hole bands. It was indicated [12,13] that the disorder owing to a random piezoelectric potential gives rise to a density-of-state tail in 2D and 1D semiconductor structures, which result in a broadening of optical spectra [8]. Further, since under a high electric field excitonic states are unstable, two types of electron-hole pair may be simultaneously present in a quantum well: free pairs near to the interface and 2D excitons deep in the well.

It is worthy to recall [14] the so-far-known scattering mechanisms fail in the interpretation of low-temperature mobilities measured in lattice-mismatched quantum wells made, e.g., from $In_{0.2}Ga_{0.8}As/GaAs$ (Ref. [14]): $\mu^{(1)}_{\mathrm{expt}} \approx 3 \times 10^4\ \mathrm{cm}^2/\mathrm{V\,s}$, and $In_{0.15}Ga_{0.85}As/Al_{0.23}Ga_{0.77}As$ (Ref. [15]): $\mu^{(2)}_{\mathrm{expt}} = 7.3 \times 10^4\ \mathrm{cm}^2/\mathrm{V\,s}$. Therefore, Lyo and Fritz [14] proposed another source of scattering which stems from strain fluctuations created by a random distribution of In atoms. However, their theory was found to fail in explaining a large difference in mobility ($\approx 240\%$)

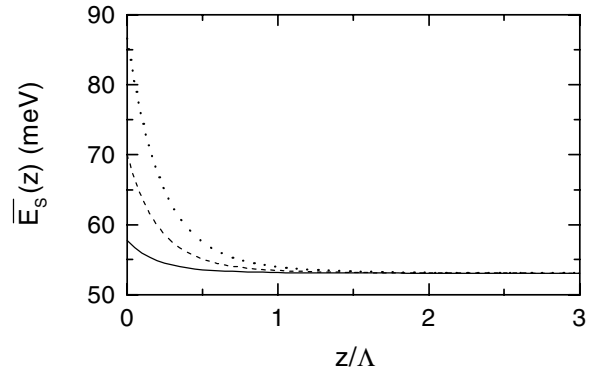

FIG. 2. rms valence band splitting $\overline{E_S}(z)$ vs distance z for different ratios $\Delta/\Lambda = 0.1$, 0.2, and 0.3 marked by solid, dashed, and dotted lines, respectively.

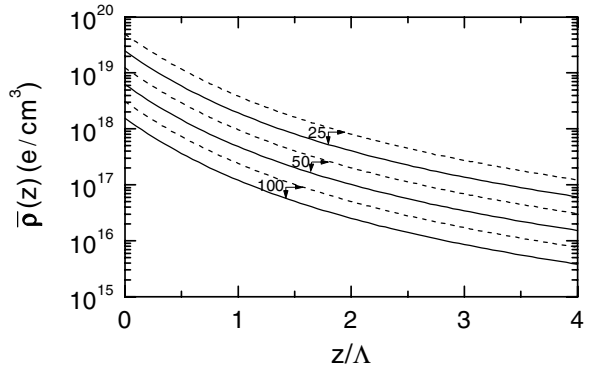

FIG. 3. rms density of piezoelectric charges $\overline{\rho}(z)$ vs distance z under $\Delta = 5$ (solid lines), 10 Å (dashed ones), and various correlation lengths Λ denoted on lines in units of Å.

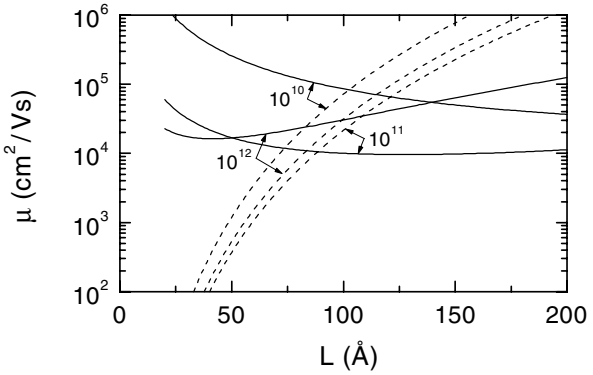

FIG. 5. Mobilities vs well width L under a roughness of $\Delta = 5$ Å, $\Lambda = 50$ Å, and different sheet electron densities denoted on lines in units of cm^{-2}. Solid and dashed lines refer to the mobilities limited by piezoelectric and surface roughness scattering, respectively.

despite a small difference in In content (only 5%). So, this remains as a challenging problem in the mobility theory.

We suggest the above difference in electron mobility is due primarily to scattering by a roughness-induced piezoelectric field. We have calculated the mobility with an inclusion of piezoelectric scattering. Using an experimental data [16] with $\Delta = 5.4$ Å and $\Lambda = 50$ Å, for the sample in [15] we obtained: $\mu^{(1)}_{\text{theor}} = 3.2 \times 10^4$ cm^2/V s, while for the one in [16]: $\mu^{(2)}_{\text{theor}} = 7.6 \times 10^4$ cm^2/V s. So, the theory is found in an excellent agreement with experiment.

In summary, we have proved for the first time that because of interface roughness a high random piezoelectric field always exists in real strained heterostructures of zinc-blende material even with a high symmetry growth axis, e.g., [001]. This turns out to be a conceptually new important scattering mechanism governing the mobility of real lattice-mismatched heterostructures. The system of charge carriers becomes strongly disordered and generally consists of both free and bound electron-hole pairs.

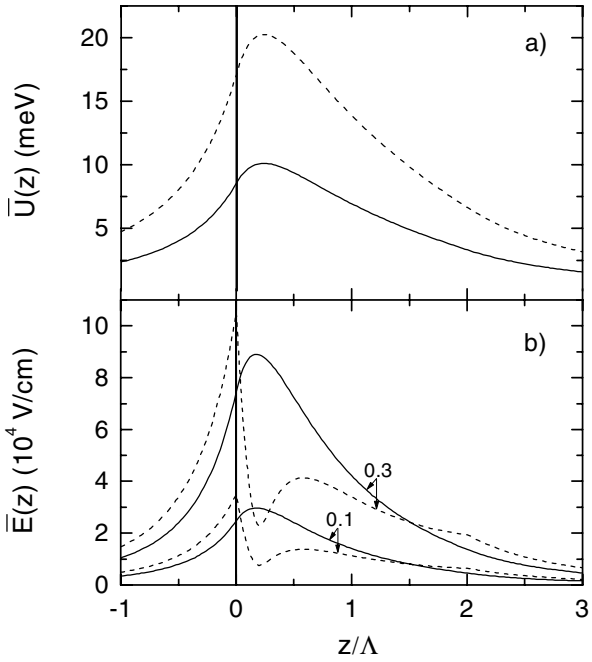

FIG. 4. Piezoelectric field in a quantum well of a thickness $L = 100$ Å and a correlation length $\Lambda = 50$ Å vs distance z with: (a) rms potential $\overline{U}(z)$ for $\Delta = 5$ (solid line), 10 Å (dashed line); and (b) rms field strength: $\overline{E_{\parallel}}(z)$ (solid lines), $\overline{E_{\perp}}(z)$ (dashed lines) for different ratios $\Delta/\Lambda = 0.1, 0.3$.

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