Analytic solutions of the effective-mass equation in strained Si-$Si_{1-x}Ge_x$ heterostructures applied to resonant tunneling

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(Received 14 August 1989)

The tunnel current in the valence band of Si-$Si_{1-x}Ge_x$ double-barrier structures is calculated within the framework of the three-band effective-mass equation including the spin-orbit split-off band and the built-in strain. We present analytic solutions of the effective-mass equation in each bulk constituent and use them to calculate the transmission coefficient and tunnel current via a transfer-matrix technique. Though the tunnel current originates only from incoming heavy-hole states, these are strongly mixed into light-hole (LH) and spin-orbit split-off (SO) states, and several resonances in the tunnel current are even dominated by outgoing LH or SO states. An estimate is done to compare the calculated resonant bias values with experimental results.

I. INTRODUCTION

Lattice-matched semiconductor heterostructures have been extensively investigated[1] and significant progress in understanding the electronic structure has been realized.[2,3] Fortunately, it turned out that the restriction to lattice-matched materials for realizing heterostructures without misfit defects is not necessary, as long as the layers under consideration are sufficiently thin, so that the lattice mismatch can be accommodated by built-in biaxial elastic strain.[4–7] Consequently, Si and $Si_{1-x}Ge_x$ alloys become extremely attractive candidates for lattice-mismatched semiconductor heterostructures.[8]

The extensive work on resonant tunneling through lattice-matched double-barrier heterostructures[9] has been followed by much experimental research concerning resonant tunneling in the valence band of lattice-mismatched Si-$Si_{1-x}Ge_x$ double-barrier structures.[10–15] However, a theoretical description, including the built-in strain and the spin-orbit split-off (SO) band, which for Si lies close to the heavy-hole (HH) and light-hole (LH) bands, has not yet been developed.

In this paper we calculate the tunnel current in the valence band of Si-$Si_{1-x}Ge_x$ double-barrier structures, within the framework of the six-component envelope-function approximation.[2,3,16] The Luttinger-Kohn Hamiltonian,[17] including the spin-orbit split-off band and the built-in strain,[18] can be decoupled into two independent 3×3 blocks[19] by a unitary transformation similar to that used in Ref. 20. This Hamiltonian is the starting point of our calculations.

In Sec. II we present the analytic solutions of the effective-mass equation in the bulk and use them in Sec. III to calculate the transmission coefficients through the Si-$Si_{1-x}Ge_x$ double-barrier structures via a transfer-matrix technique.[21–24] The tunnel current is derived in Sec. IV and the results are compared with experiment.[10–15] Finally, in Sec. V we summarize the results and conclusions.

II. ANALYTIC SOLUTION OF THE EFFECTIVE-MASS EQUATION

The three highest valence bands (doubly degenerate) of Si and $Si_{1-x}Ge_x$ are described by the 6×6 Luttinger-Kohn Hamiltonian.[17] This Hamiltonian incorporates the heavy-hole (HH), light-hole (LH), and split-off (SO) bands. Since the spin-orbit splitting Δ for Si ($\Delta=44$ meV) is smaller than or of the order of the confinement energy and the strain parameter S, the SO band must be retained. The 6×6 Hamiltonian matrix can be decoupled into two independent 3×3 matrices[6,19] by a unitary transformation similar to that used in Ref. 20.

The lattice constants of the pure elements Si and Ge are mismatched by about 4%. However, for thin layers composed of Si and $Si_{1-x}Ge_x$ alloys the lattice constants parallel to the interfacial plane adjust so that perfect matching of the two materials is obtained. To compensate for this strain, the lattice constants perpendicular to the interface adjust independently for the two materials to minimize the elastic energy.[4,5] The influence of the lattice deformation on the electronic properties is described within the concept of deformation potentials by additional terms S in the effective-mass Hamiltonian.[4,5,6,18]

In summary, the Hamiltonian matrix, including the HH, LH, and SO bands and the strain, is[19]

$$\underline{H}=\begin{bmatrix} A_+ +S & C\mp iB & \sqrt{2}C\pm(i/\sqrt{2})B \\ C\pm iB & A_- -S & F+\sqrt{2}S\mp i\sqrt{3/2}B \\ \sqrt{2}C\mp(i/\sqrt{2})B & F+\sqrt{2}S\pm i\sqrt{3/2}B & D \end{bmatrix}, \tag{1}$$

where

$$A_\pm=-\tfrac{1}{2}(\gamma_1\mp 2\gamma_2)k_z^2-\tfrac{1}{2}(\gamma_1\pm\gamma_2)k_\parallel^2 , \tag{2a}$$

$$B=\sqrt{3}\gamma_3 k_\parallel k_z , \tag{2b}$$

$$C=\frac{\sqrt{3}}{2}k_\parallel^2[\gamma_2^2\cos^2(2\theta)+\gamma_3^2\sin^2(2\theta)]^{1/2} , \tag{2c}$$

$$D=-\Delta-\tfrac{1}{2}\gamma_1(k_z^2+k_\parallel^2) , \tag{2d}$$

$$F=\gamma_2\left[\sqrt{2}k_z^2-\frac{1}{\sqrt{2}}k_\parallel^2\right] . \tag{2e}$$

k_z is the wave vector along the growth direction, $k_\parallel$ the magnitude of the wave vector in the interface plane, θ the angle between the direction of $k_\parallel$ and the [100] direction, and the γ's the Luttinger parameters of the material.

For $k_\parallel=0$ the HH state remains decoupled from the LH and SO states and the strain S splits the HH and LH bands. The LH and SO states are coupled by the strain S. This coupling becomes important for materials with small spin-orbit coupling Δ such as in the case of Si ($\Delta=44$ meV). For the interpretation of the resonances in the tunnel current, it is essential to notice that for $k_\parallel\neq 0$ all states are mixed via the $k_\parallel$ terms in the off-diagonal elements of $\underline{H}$.

In the bulk the components of the wave vector $\mathbf{k}$ are good quantum numbers and the solutions of the effective-mass equation,

$$\underline{H}(-i\nabla)\mathbf{F}=E\mathbf{F} , \tag{3}$$

can be taken to be of the form[25]

$$\mathbf{F}(\mathbf{r})=\mathbf{f}e^{i\mathbf{k}\cdot\mathbf{r}} , \tag{4}$$

where $\mathbf{f}=(f_1,f_2,f_3)$ is an eigenvector of the Hamiltonian matrix (1). An explicit form of the eigenvectors is obtained with a Gauss algorithm:

$$\mathbf{h}=\begin{bmatrix} (A_- -S-E)(D-E)-(F+\sqrt{2}S\mp i\sqrt{3/2}B)(F+\sqrt{2}S\pm i\sqrt{3/2}B) \\ -(C\pm iB)(D-E)+\left[\sqrt{2}C\mp\frac{i}{\sqrt{2}}B\right](F+\sqrt{2}S\mp i\sqrt{3/2}B) \\ -\left[\sqrt{2}C\mp\frac{i}{\sqrt{2}}B\right](A_- -S-E)+(F+\sqrt{2}S\pm i\sqrt{3/2}B)(C\pm iB) \end{bmatrix}, \tag{5a}$$

$$\mathbf{l}=\begin{bmatrix} -(C\mp iB)(D-E)+\left[\sqrt{2}C\pm\frac{i}{\sqrt{2}}B\right](F+\sqrt{2}S\pm i\sqrt{3/2}B) \\ (A_+ +S-E)(D-E)-\left[\sqrt{2}C\pm\frac{i}{\sqrt{2}}B\right]\left[\sqrt{2}C\mp\frac{i}{\sqrt{2}}B\right] \\ -(F+\sqrt{2}S\pm i\sqrt{3/2}B)(A_+ +S-E)+(C\mp iB)\left[\sqrt{2}C\mp\frac{i}{\sqrt{2}}B\right] \end{bmatrix}, \tag{5b}$$

$$\mathbf{s}=\begin{bmatrix} -\left[\sqrt{2}C\pm\frac{i}{\sqrt{2}}B\right](A_- -S-E)+(C\mp iB)(F+\sqrt{2}S\mp i\sqrt{3/2}B) \\ -(F+\sqrt{2}S\mp i\sqrt{3/2}B)(A_+ +S-E)+(C\pm iB)\left[\sqrt{2}C\pm\frac{i}{\sqrt{2}}B\right] \\ (A_- -S-E)(A_+ +S-E)-(C\mp iB)(C\pm iB) \end{bmatrix} . \tag{5c}$$

In deriving the eigenvectors, the linear equation system has been arranged so that the results are purely HH-, LH-, or SO-like (corresponding to the nomenclature **h**, *l*, and **s**, respectively) in the limit of infinite spin-orbit coupling Δ and vanishing in-plane wave vector $k_\parallel$.

In the case of a heterostructure, the potential $V(z)$ breaks translational symmetry along z; however, k_x and k_y remain good quantum numbers. The potential $V(z)$ is a constant in each layer, and for each energy E and in-plane wave vector $k_\parallel$ the bulk secular equation gives six values of k_z, which are denoted $\pm k_h$, $\pm k_l$, and $\pm k_s$. In the barrier the energy E is replaced by $E-V_0$, where V_0 is the band offset.

The potential $V(z)$ mixes the bulk solutions (4) and (5) with different values of k_z, and the general solution in each layer of constant potential is a linear combination of them, e.g., in layer b (see Fig. 1):

$$\mathbf{F}(\mathbf{r})=[b_1\mathbf{h}(+k_h)e^{ik_hz}+b_2\mathbf{l}(+k_l)e^{ik_lz}+b_3\mathbf{s}(+k_s)e^{ik_sz}$$
$$+b_4\mathbf{h}(-k_h)e^{-ik_hz}+b_5\mathbf{l}(-k_l)e^{-ik_lz}+b_6\mathbf{s}(-k_s)e^{-ik_sz}]e^{i(k_xx+k_yy)}$$
$$\equiv\mathbf{F}(z)e^{i(k_xx+k_yy)} . \tag{6}$$

The stationary states of a heterostructure are derived by imposing appropriate boundary conditions[16,26] at each interface, which enforce the continuity of the envelope function and the conservation of the probability current. In the approximation that the periodic part of the Bloch functions are equal on both sides of the interface at z_m, the boundary conditions are[16,26]

$$\mathbf{F}(z) \text{ continuous at } z_m , \tag{7a}$$

$$\underline{\beta}\mathbf{F}(z) \text{ continuous at } z_m . \tag{7b}$$

The matrix $\underline{\beta}$ is derived by integrating the effective-mass equation across an interface[26] and its explicit form is

$$\underline{\beta}=\begin{bmatrix} (\gamma_1-2\gamma_2)(\partial/\partial z) & -\sqrt{3}\gamma_3k_\parallel & \sqrt{3/2}\gamma_3k_\parallel \\ \sqrt{3}\gamma_3k_\parallel & (\gamma_1+2\gamma_2)(\partial/\partial z) & -2\sqrt{2}\gamma_2(\partial/\partial z)-(3/\sqrt{2})\gamma_3k_\parallel \\ -\sqrt{3/2}\gamma_3k_\parallel & -2\sqrt{2}\gamma_2(\partial/\partial z)+(3/\sqrt{2})\gamma_3k_\parallel & \gamma_1(\partial/\partial z) \end{bmatrix} . \tag{8}$$

In the case of a quantum well (Si-$Si_{1-x}Ge_x$-Si) the stationary states are derived from a linear equation system consisting of 18 coefficients that is constructed by use of Eqs. (6)–(8) at the two interfaces. In each Si barrier three coefficients vanish by the condition of vanishing envelope function at infinity. Hence the subband dispersion $E(k_\parallel)$ is determined in implicit form by the condition of a vanishing coefficient determinant, which is of order 12.

However, the emphasis of this paper is on resonant tunneling, and therefore it is the transmission coefficient through double barriers that is calculated in the following section.

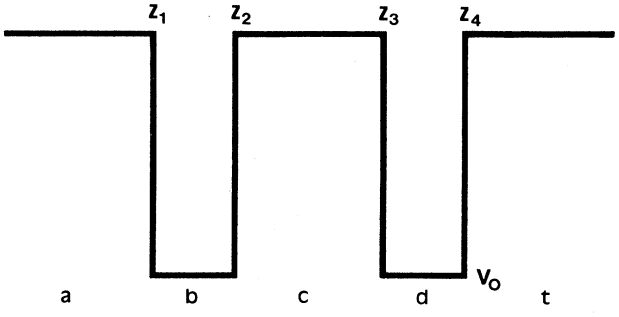

FIG. 1. Valence-band-edge profile for HH in a double-barrier structure. The regions b and d consist of Si and the regions a, c, and t of $Si_{1-x}Ge_x$.

III. TRANSMISSION COEFFICIENT VIA A TRANSFER-MATRIX TECHNIQUE

The transfer-matrix technique has been applied extensively to calculate the transmission coefficient through double-barrier structures,[21–24] and the extension to the $j=\frac{3}{2}$ valence bands has been presented.[27,28]

At each interface we get from (6)–(8) an equation for the amplitudes, e.g., at $z=z_2$ (see Fig. 1)

$$\underline{M}_3\mathbf{b}=\underline{M}_4\mathbf{c} , \tag{9}$$

where $\underline{M}_3$ is a complex 6×6 matrix which contains the coefficients of b_i in (6). Analogous equations at each interface give the transmission amplitudes $\mathbf{t}$ as a function of the incoming amplitudes, included in the vector $\mathbf{a}$:

$$\mathbf{t}=\underline{M}_8^{-1}\underline{M}_7\underline{M}_6^{-1}\underline{M}_5\underline{M}_4^{-1}\underline{M}_3\underline{M}_2^{-1}\underline{M}_1\mathbf{a} , \tag{10}$$

where $\mathbf{t}=(t_1,t_2,t_3,0,0,0)$ and $\mathbf{a}=(a_1,a_2,a_3,r_1,r_2,r_3)$ and the r_i are the reflection amplitudes.

Attention must be paid in two cases. First, for E small compared to the terms containing $k_\parallel$, S, or Δ, the secular equation gives imaginary or complex values for k_z in the $Si_{1-x}Ge_x$ regions. In these cases only bulk solutions that vanish at infinity must be taken into account in the electrodes. Secondly, for large $k_\parallel$, the bulk LH dispersion $E(k_z)$ becomes "camelback"-like, i.e., it has two solutions for $|k_z|$ at the same energy. The smaller one has to be inserted into the $\mathbf{s}$ eigenvector. Since the velocity is proportional to $\partial E/\partial k_z$, the two solutions with the same sign of k_z have opposite velocities, and this must be prop-

erly accounted for by modifying the assignment of the components of the **t** and **a** vectors: $\mathbf{t}=(t_1,t_2,0,0,0,t_3)$ and $\mathbf{a}=(a_1,a_2,r_3,r_1,r_2,a_3)$.

The transmission coefficient D_n through channel n (i.e., HH, LH, or SO) is, for example, in the case of an incoming HH state,

$$D_n=\frac{\langle \mathbf{F}_n^t|j_z|\mathbf{F}_n^t\rangle}{\langle \mathbf{F}_1^a|j_z|\mathbf{F}_1^a\rangle}=\frac{|t_n|^2}{|a_1|^2}N\ , \tag{11}$$

where N is a normalization factor. The general formula for the probability current density is given in Ref. 26 and its explicit form is

$$\langle \mathbf{F}|j_z|\mathbf{F}\rangle=|\alpha|^2\left[i\gamma_3 k_\parallel\left[\sqrt{3}(f_1f_2^*-f_1^*f_2)+\sqrt{3/2}(f_1^*f_3-f_1f_3^*)+\frac{3}{\sqrt{2}}(f_2f_3^*-f_2^*f_3)\right]\right.$$
$$\left.-k_z[\gamma_-|f_1|^2+\gamma_+|f_2|^2+\gamma_1|f_3|^2-2\sqrt{2}\gamma_2(f_2^*f_3+f_2f_3^*)]\right]\ , \tag{12}$$

where $\gamma_\pm=\gamma_1\pm2\gamma_2$, and α is the amplitude.

An example for the transmission coefficient as a function of energy in the case of an incoming HH state is shown in Fig. 2. In the energy range considered three HH resonances occur. The third shows up at an energy larger than the barrier height and is therefore a virtual one. Already for the chosen value of the in-plane wave vector, $k_\parallel=0.01$ Å^{-1}, the incoming HH state is strongly mixed into the outgoing LH and SO channels. Due to the strain-induced and spin-orbit splitting the transmission coefficient for the LH and SO states is only defined at higher energies, when the corresponding k_z in the electrodes become real. With the parameters used in Fig. 2, the k_z in the electrodes become real at about 50 meV for a LH state and at about 180 meV for a SO state. The first resonance in the SO channel occurs at an energy slightly higher than the barrier height. With increasing $k_\parallel$ the effects of mixing increase and the line shapes of the resonances become strongly asymmetric (also see Ref. 28).

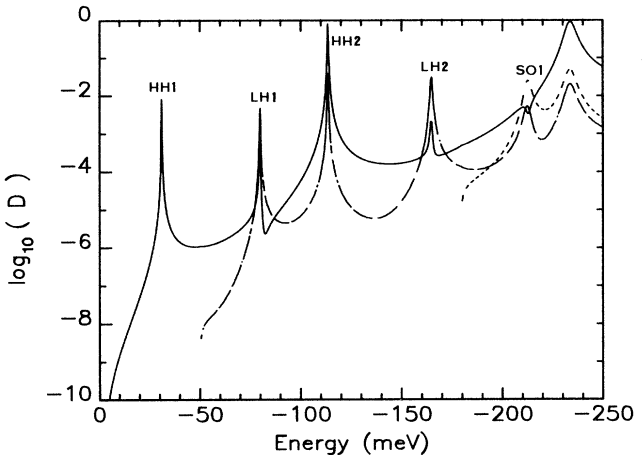

FIG. 2. Transmission coefficient of an incoming HH state through a Si-$Si_{1-x}Ge_x$ double-barrier structure grown on Si substrate and with $x=0.25$, as has been used in Ref. 10. The well width is 55 Å. For numerical reasons a barrier width of 30 Å has been chosen instead of the 100 Å used in the experiment. The γ parameters for Si ($\gamma_1=4.285$, $\gamma_2=0.339$, and $\gamma_3=1.446$) are taken from Ref. 30, and those for the $Si_{0.75}Ge_{0.25}$ alloy ($\gamma_1=6.559$, $\gamma_2=1.314$, and $\gamma_3=2.507$) are derived by linear interpolation between the values for Si (Ref. 30) and Ge (Ref. 31). The valence-band offset $V_0=210$ meV is taken from Ref. 32 by linear interpolation. Since the structure is grown on Si substrate, the Si layers are unstrained and the strain parameter $S=40$ meV for the $Si_{0.75}Ge_{0.25}$ layers is taken from Ref. 33. The spin-orbit splitting Δ is, for Si, $\Delta=44$ meV, and for Ge, $\Delta=290$ meV. In a linear interpolation the alloy value is $\Delta=106$ meV. The magnitude of the in-plane wave vector is $k_\parallel=0.01$ Å^{-1} and the calculation is done in an axial approximation, i.e., $\gamma_2=\gamma_3=(\gamma_2+\gamma_3)/2$ in Eq. (2c). The solid, dotted-dashed, and dashed lines show the outgoing HH, LH, and SO channels, respectively.

IV. TUNNEL CURRENT

The current density through a double-barrier structure between two p^+-type electrodes in each outgoing channel n is, at zero temperature,[29]

$$j_n=\frac{e}{(2\pi)^2/\hbar}\int_{E_F}^{\min\{E_F+eU,\,0\}}dE\int_{k_\parallel(0)}^{k_\parallel(E)}dk_\parallel k_\parallel D_n\ . \tag{13}$$

The total current density is the sum over all three outgoing channels n, i.e., HH, LH, and SO.

The Fermi energy E_F has been chosen to be 20 meV. Due to the strain-induced and spin-orbit splitting there are no occupied incoming LH or SO states at $T=0$ K. For E up to the Fermi energy, the LH and SO states have no real k_z in the electrodes. As a result, the whole tunnel current originates from incoming HH states. Though experimentally it is only possible to measure the total tunnel current, for the interpretation of the resonances it is of interest to show the tunnel current density for each outgoing channel individually, as is done in Fig. 3.

Five resonances occur. The first and the third are HH-like, while the second and fourth is dominated by outgoing LH states. Since, in the current, states with $k_\parallel$ up to about 0.04 Å^{-1} are involved for $E_F=20$ meV, the incoming HH states are strongly mixed into the outgoing LH and SO states. At a bias of about 160 mV the bulk SO band in the right electrode with real k_z appears at the Fermi energy of the electrode and the incoming HH states get heavily mixed into SO states. The fifth reso-

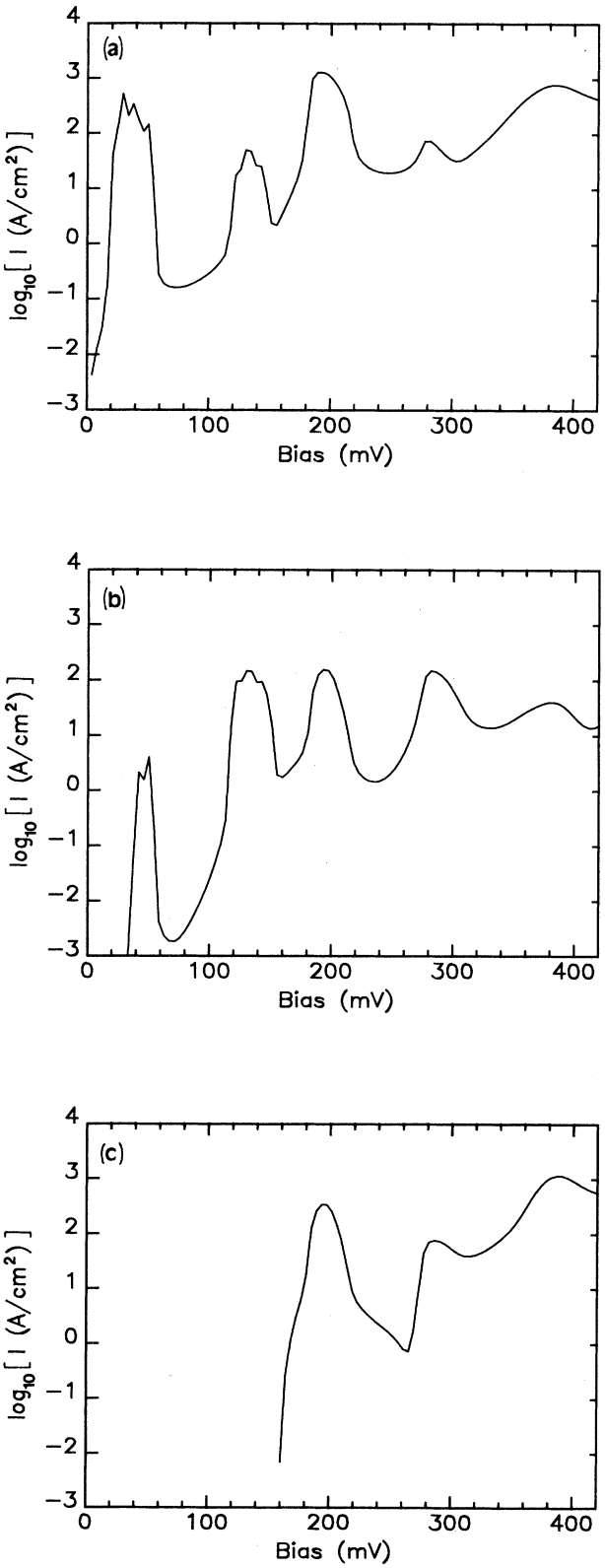

FIG. 3. Tunnel current through a Si-$Si_{0.75}Ge_{0.25}$ double-barrier structure with the same parameters as in Fig. 2 and with a chosen Fermi energy of 20 meV. (a) outgoing HH channel, (b) outgoing LH channel, and (c) outgoing SO channel.

TABLE I. Comparison of the calculated bias value U^R_{theor} at resonances with the experimental values U^R_{expt} of Ref. 10. The fitted factor 1.64 accounts for voltage drops outside the double-barrier region.

U^R_{expt} (mV)	$1.64U^R_{\text{theor}}$ (mV)
30	56
160	213
320	316
490	461
630	633

nance is even dominated by outgoing SO states.

In Table I we compare the calculated bias values at the resonances with the maximum of the broad peaks of Ref. 10. The calculated resonance voltages are brought into reasonable agreement with the experimental values by multiplying with a fitted factor of 1.64. This factor accounts for the fact that the voltage drops occurring outside the double-barrier region contribute to the measured bias. When considering Table I, one should keep in mind that the Fermi energy has only been estimated and that the barriers and the well under bias are each approximated by one region of constant potential. To our knowledge all other experiments show only two or three resonances, and therefore a quantitative comparison taking into account a fixed scaling function for the bias is less significant in those cases; nevertheless, the scaling factors are of the same order, for all experiments analyzed.

V. SUMMARY AND CONCLUSIONS

The relevant valence bands of Si and $Si_{1-x}Ge_x$ are described by the 6×6 Luttinger-Kohn Hamiltonian, which can be decoupled into two independent 3×3 blocks by a unitary transformation. The lattice mismatch between layers of Si and $Si_{1-x}Ge_x$ can be accommodated by built-in biaxial elastic strain, for which the influence on the electronic properties is described by additional terms in the effective-mass Hamiltonian. The analytic solutions of the effective-mass equation are found and, together with the appropriate boundary conditions at interfaces, the transmission coefficient is calculated via a transfer-matrix technique for three-component envelope functions. For nonzero in-plane wave vector all states are strongly mixed.

The tunnel current density is calculated and the results are shown for each outgoing channel individually. Due to the strain-induced and spin-orbit splitting the tunnel current originates at zero temperature only from incoming HH states. These states are strongly mixed into outgoing LH and SO channels and several resonances are even dominated by outgoing LH and SO states. The calculated resonance voltages are brought into agreement with the experimental values by multiplying with a fitted scaling factor, which accounts for voltage drops outside the double-barrier region.

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