# Boundary condition for the interface between silicon and silicon oxide

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A boundary condition is formulated for the interface of a quantum well embedded in a material of large energy barrier. Distinct differences are pointed out between a free-standing film and the quantum well. The boundary condition for the effective-mass and envelope-function approach includes the property of the transition layer between the well and the barrier in the form of an adjustable parameter. A full-zone $\mathbf{k}\cdot\mathbf{p}$ method is used along with the boundary condition to calculate the energy gap of the quantum well as a function of the well thickness. The model fits well the experimental data on multiple $Si/SiO_2$ quantum wells.

## I. INTRODUCTION

The observance[1] of room-temperature photoluminescence (PL) of porous silicon has attracted a great deal of theoretical and experimental studies[2] on this material since its discovery. The experimental studies usually involve the silicon quantum well embedded in silicon dioxide[3–5] or silicon nitride.[6] Lu, Lockwood, and Baribeau[3] reported that the origin of the PL is quantum confinement. They also found that the maximum PL peak is related to the quantum-well thickness by an inverse square power law, i.e., $E_{\mathrm{PL}}-E_g^{\mathrm{bulk}}\propto d^{-2}$, where $E_g^{\mathrm{bulk}}$ is the bulk energy gap. But others[4–6] found that there is a size-insensitive PL band. Theoretical studies include the effective-mass approach[7,8] (EMA) and first-principle calculation,[9,10] among others.[11] The first-principle calculation for the free-standing quantum film that is surrounded by vacuum shows that the energy gap is related to the quantum film thickness by a different power law, i.e., $E_g\propto d^{-1.39}$. Kim and Lee[8] suggested a boundary condition that can explain this dependence of the energy gap on the film thickness.

While theoretical studies deal with the free-standing quantum structure surrounded by vacuum, experimental studies are based on the quantum structure embedded in a material with a large band gap such as silicon dioxide. It is not yet fully explained what effect this difference in the medium surrounding the silicon quantum structure has on the energy gap. Furthermore, an interfacial transition layer exists between silicon and silicon dioxide because of the intermediate oxidation states at the interface.[12] This transition layer has not been taken into account so far in determining the band gap.

In this article, differences between the experiment and the theory are examined and a boundary condition appropriate for the embedded quantum structure is derived with the EMA and the envelope-function approach (EFA). In Sec. II, the differences between the free-standing quantum film and the quantum well embedded in a large-energy-gap material are discussed. In Sec. III, a boundary condition for the imbedded quantum structure is derived for the sharp interface as well as for the interface with a transition layer. In Sec. IV, the boundary condition is applied to the silicon quantum well and the present model is compared with the experimental result in the literature for the dependence of the PL band on the film thickness.

## II. FREE-STANDING FILM VERSUS EMBEDDED FILM

The infinite barrier boundary condition has usually been used for calculating the energy gap of a quantum structure that is confined by vacuum or by a large-energy-gap material.[7] The infinite boundary condition, however, neglects the effect of the environment in which the quantum film is confined.

There are a number of distinct differences between the free-standing film surrounded by vacuum and the embedded film as shown in Fig. 1. First, vacuum has no electrons. The vacuum is described in terms of vacuum state, whereas the large-energy-gap material surrounding the quantum film is described in terms of the ground state.[13] The vacuum state involves only electrons but the ground state involves not only electrons but also holes. As for the confined film, it can be described in terms of the ground state or the vacuum state.

Continuity of the envelope functions of electrons and holes is used in the EMA. In the vacuum state, however, holes cannot be defined and thus the continuity condition for the hole cannot be used. Therefore, the continuity condition on the electron must be used both in the conduction and valence bands. The total wave-function approach used in this work requires relationships between electron and holes for the wave vector and the energy:[14]

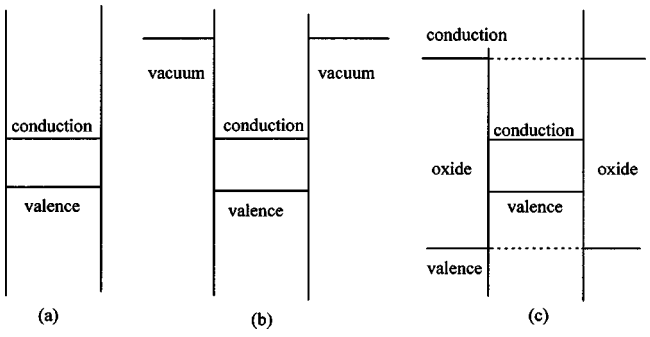


FIG. 1. Band diagrams for (a) an infinite energy barrier, (b) a free-standing film surrounded by vacuum, and (c) a quantum well embedded in a large-energy-gap material.

 

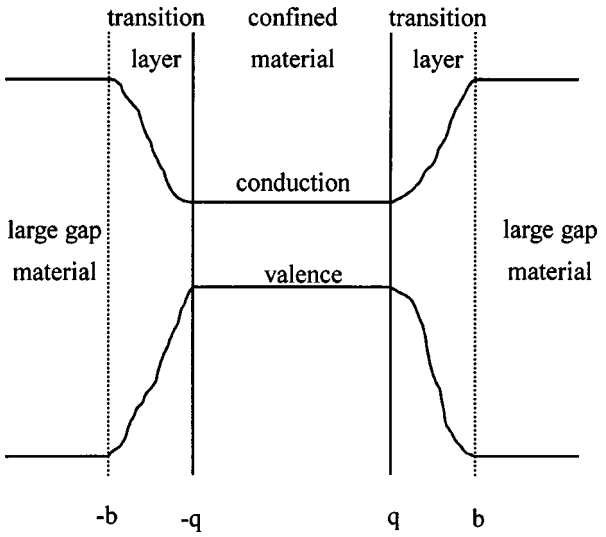


FIG. 2. General band scheme of the quantum well embedded in an oxide.

$$\mathbf{g}=-\mathbf{k}, \quad E^{\mathrm{hh}}=-E^{\mathrm{el}}, \tag{1}$$

where $\mathbf{g}$ and $\mathbf{k}$ are the wave vectors for the hole and electron, respectively, and $E^{\mathrm{hh}}$ and $E^{\mathrm{el}}$ are the energies. This total wave-function approach leads to the same result as with the typical EMA.[15]

### III. BOUNDARY CONDITION

The quantum-well structure being considered consists of a confined material, a large-energy-gap material and a transition layer, as depicted in Fig. 2. Consider first the case where there is no transition layer such that $b=q$ in Fig. 2. The total wave function of electron in the large-energy-gap material, henceforth referred to as the barrier material, in the energy range of interest may be written as follows:

$$\Psi_b(\mathbf{r})=A_b e^{i\mathbf{k}_\perp\cdot\mathbf{r}_\perp}e^{\kappa z}+B_b e^{i\mathbf{k}_\perp\cdot\mathbf{r}_\perp}e^{-\kappa z}, \tag{2}$$

where $\mathbf{k}_\perp$ and $\mathbf{r}_\perp$, respectively, are the wave vector and the coordinate perpendicular to the quantum well and $\kappa$ is the imaginary wave vector longitudinal to the quantum well. The confinement here is in the $z$ direction. The equation suggests that the state in the barrier layer decays in the energy range of interest.

The Schrödinger equation for the confined material is

$$[-\nabla^2+V_p(\mathbf{r})+U(\mathbf{r})]\Psi_c(\mathbf{r})=E\Psi_c(\mathbf{r}), \tag{3}$$

where $\Psi_c(\mathbf{r})$ is the total wave function of electron in the confined material, $V_p(\mathbf{r})$ and $U(\mathbf{r})$, respectively, are the periodic potential and the perturbation potential, and $E$ is the energy. Here atomic units are used throughout, i.e., the rydberg for energy and the Bohr radius for length. With the EMA and the EFA Eq. (3) is rewritten as

$$[\mathbf{H}^m(-i\nabla)+\mathbf{I}U(\mathbf{r})]\mathbf{F}^m(\mathbf{r})=E\mathbf{F}^m(\mathbf{r}), \tag{4}$$

where $\mathbf{H}^m(\mathbf{k})$ is an $n\times n$ Hamiltonian matrix for the $m$ state, i.e., the conduction band, etc, in the $\mathbf{k}\cdot\mathbf{p}$ perturbation scheme, $\mathbf{I}$ is an $n\times n$ identity matrix, and $\mathbf{F}^m(\mathbf{r})$ is an $n\times 1$ column vector of envelope functions. The total wave function of electron in the $m$ state in the confined material[16] becomes

$$\Psi_c^m(\mathbf{r})=\sum_j \mathbf{F}_j^m(\mathbf{r})u_j^m(\mathbf{r}), \tag{5}$$

where $u_j^m(\mathbf{r})$ is the periodic function at the zone center in the full-zone $\mathbf{k}\cdot\mathbf{p}$ perturbation scheme and $F_j^m(\mathbf{r})$ is the element of $\mathbf{F}^m(\mathbf{r})$ corresponding to $u_j^m(\mathbf{r})$.

The condition that the continuity[8] with respect to the total wave function be satisfied everywhere within the unit cell gives

$$\Psi_c^m(\mathbf{r}_\perp,q)=\Psi_b(\mathbf{r}_\perp,q), \quad \Psi_{c,z}^m(\mathbf{r}_\perp,q)=\Psi_{b,z}(\mathbf{r}_\perp,q), \tag{6}$$

where $z$ denotes the differentiation with respect to $z$, and $q$ represents the points within the outermost unit cell of the confined material. For the transverse direction in the interface plane, the connection rules of the wave function are accomplished. Equation (2) and the connection rules of the total wave function along with the condition that the total wave function vanishes at infinity lead to the following boundary condition:

$$\Psi_{c,z}^m(\mathbf{r}_\perp,q)+\kappa\Psi_c^m(\mathbf{r}_\perp,q)=0 \quad \text{at } z=q, \tag{7}$$

$$\Psi_{c,z}^m(\mathbf{r}_\perp,-q)-\kappa\Psi_c^m(\mathbf{r}_\perp,-q)=0 \quad \text{at } z=-q. \tag{8}$$

Consider now the case where the transition layer is taken into consideration. The total wave function in the transition layer may be written as follows:

$$\Psi_t(\mathbf{r})=A_t e^{i\mathbf{k}_\perp\cdot\mathbf{r}_\perp}f_p(z)+B_t e^{i\mathbf{k}_\perp\cdot\mathbf{r}_\perp}f_d(z), \tag{9}$$

where $f_p(z)$ and $f_d(z)$ represent the functions for the state in the confined material to propagate in the transition layer and to decay, respectively. These functions are linearly independent. Since the electron has the properties of both the propagation state and the evanescent state in the energy range of interest in the transition layer, the total wave function in the layer may be of an Airy function.

Combining Eqs. (5) and (9), the connection rules at the interface between the silicon and the transition layer in the longitudinal direction become

$$\Psi_c^m(\mathbf{r}_\perp,q)=A_t e^{i\mathbf{k}_\perp\cdot\mathbf{r}_\perp}f_p(q)+B_t e^{i\mathbf{k}_\perp\cdot\mathbf{r}_\perp}f_d(q), \tag{10a}$$

$$\left.\frac{\partial\Psi_c^m}{\partial z}\right|_{(\mathbf{r}_\perp,q)}=A_t e^{i\mathbf{k}_\perp\cdot\mathbf{r}_\perp}\left.\frac{\partial f_p}{\partial z}\right|_{z=q}+B_t e^{i\mathbf{k}_\perp\cdot\mathbf{r}_\perp}\left.\frac{\partial f_d}{\partial z}\right|_{z=q}. \tag{10b}$$

Here, Eqs. (10a) and (10b) are satisfied in the outermost unit cell of the confined material. Combining Eqs. (2) and (9) and using the condition that the total wave function vanishes at infinity yields the connection rules at the interface between the transition layer and the barrier material:

$$A_t e^{i\mathbf{k}_\perp\cdot\mathbf{r}_\perp}f_p(b)+B_t e^{i\mathbf{k}_\perp\cdot\mathbf{r}_\perp}f_d(b)=A_b e^{i\mathbf{k}_\perp\cdot\mathbf{r}_\perp}e^{-\kappa^b}, \tag{11a}$$

$$A_t e^{i\mathbf{k}_\perp\cdot\mathbf{r}_\perp}\left.\frac{\partial f_p}{\partial z}\right|_{z=b}+B_t e^{i\mathbf{k}_\perp\cdot\mathbf{r}_\perp}\left.\frac{\partial f_d}{\partial z}\right|_{z=b}=-A_b\kappa e^{i\mathbf{k}_\perp\cdot\mathbf{r}_\perp}e^{-\kappa^b}. \tag{11b}$$

The properties of the transition layer, i.e., the functions $f_p(z)$ and $f_d(z)$, and the parameter $\kappa$ are difficult to determine. Therefore $A_t$ and $B_t$ in Eqs. (10) and (11) are eliminated to obtain

$$\begin{bmatrix} \Psi_c^m(\mathbf{r}_\perp,q) \\ \left.\dfrac{\partial\Psi_c^m}{\partial z}\right|_{(r_\perp,q)} \end{bmatrix}=A_b\begin{bmatrix} f_p(q) & f_d(q) \\ \left.\dfrac{\partial f_p}{\partial z}\right|_{z=q} & \left.\dfrac{\partial f_d}{\partial z}\right|_{z=q}\end{bmatrix}\begin{bmatrix} f_p(b) & f_d(b) \\ \left.\dfrac{\partial f_p}{\partial z}\right|_{z=b} & \left.\dfrac{\partial f_d}{\partial z}\right|_{z=b}\end{bmatrix}^{-1}\begin{bmatrix} e^{i\mathbf{k}_\perp\cdot\mathbf{r}_\perp}e^{-\kappa^b} \\ -\kappa e^{i\mathbf{k}_\perp\cdot\mathbf{r}_\perp}e^{-\kappa^b}\end{bmatrix}.$$

If $\lambda$ is defined by

$$\lambda=-\frac{[f_{p,z}(q)f_{d,z}(b)-f_{d,z}(q)f_{p,z}(b)]-[f_{d,z}(q)f_p(b)-f_{p,z}(q)f_d(b)]\kappa}{[f_p(q)f_{d,z}(b)-f_d(q)f_{p,z}(b)]-[f_d(q)f_p(b)-f_p(q)f_d(b)]\kappa},$$

the above relationship can be simplified as follows:

$$\frac{\Psi_c^m(\mathbf{r}_\perp,q)}{\left.\dfrac{\partial\Psi_c^m}{\partial z}\right|_{(\mathbf{r}_\perp,q)}}=-\frac{1}{\lambda}. \tag{12}$$

The parameter $\lambda$ is undoubtedly dependent on the energy but is assumed to be constant. The lumped parameter contains in it the quality of the interface. Equation (12) essentially states that the wave function in the confined material decays exponentially in the transition layer as well as in the barrier material. This boundary condition written for the quantum well $2q$ in length that is embedded in the barrier is

$$\Psi_{c,z}^m(\mathbf{r}_\perp,q)+\lambda\Psi_c^m(\mathbf{r}_\perp,q)=0 \quad \text{at } z=q. \tag{13}$$

The value of $\lambda$ can range from about 0.1 to $\infty$ depending on the type of barrier; its value being infinity for infinite barrier height. Equation (13) is of the same form as Eq. (7) except that $\kappa$ is replaced with $\lambda$. Therefore the boundary condition for the total wave function at the left-hand side of the quantum well involving the transition layer can be written as follows:

$$\Psi_{c,z}^m(\mathbf{r}_\perp,-q)-\lambda\Psi_c^m(\mathbf{r}_\perp,-q)=0 \quad \text{at } z=-q. \tag{14}$$

This condition is deduced from the symmetry of the quantum well and the similarity with the case of no transition layer, i.e., Eq. (8).

From theoretical point of view, the parameters $\kappa$ in Eqs. (7) and (8) and $\lambda$ in Eqs. (13) and (14) can be regarded as the imaginary wave vector of electron. Therefore the boundary condition of Eqs. (13) and (14) can be considered applicable to both cases of a quantum well with and without the transition layer.

The boundary condition is of the same form as that for the free-standing film.[8] However, the confinement conditions resulting from the boundary condition are different as will be seen in the next section. The difference lies in the fact that the hole in the valence band and the electron in the conduction band are confined by the barrier in the case of embedded quantum well, whereas the electron is confined both in the conduction and valence bands by the vacuum surrounding the free-standing film. This difference leads to a large difference in the dependence of the energy gap on the film thickness.

## IV. APPLICATION TO SILICON QUANTUM WELL

We now apply the boundary condition, Eqs. (13) and (14), to the calculation of the dependence of the photoluminescence energy gap of silicon quantum well on the well thickness. The Hamiltonian matrix $\mathbf{H}^\nu(\mathbf{k})$ for the electron in the valence band is the $\Delta_5$ bands,[17]

$$\Delta_5=\begin{bmatrix} E(\Gamma_{25'}^i)+k_z^2 & Qk_z & 0 \\ Qk_z & E(\Gamma_{15})+k_z^2 & Q'k_z \\ 0 & Q'k_z & E(\Gamma_{25'}^u)+k_z^2\end{bmatrix} \tag{15}$$

and $\mathbf{H}^c(\mathbf{k})$ for the electron in the conduction band is the $\Delta_1$ bands,[17]

$$\Delta_1=\begin{bmatrix} E(\Gamma_{15})+k_z^2 & Tk_z & T'k_z \\ Tk_z & E(\Gamma_1^u)+k_z^2 & 0 \\ T'k_z & 0 & E(\Gamma_1^l)+k_z^2\end{bmatrix}, \tag{16}$$

where $E(\Gamma_j)$ is the energy of the $j$ state at the zone center and the $Q$'s and the $T$'s are the matrix elements of the linear momentum. Here, the crystal momentum is neglected in the transverse direction. Since the full-zone $\mathbf{k}\cdot\mathbf{p}$ perturbation scheme is used, the periodic functions for the wave function correspond to those at the zone center.

The envelope functions of the electron in the valence band $F_j^\nu$ become

$$F_1^\nu=A_1^\nu e^{ikz}+B_1^\nu e^{-ikz}, \tag{17a}$$

$$F_2^\nu=\frac{iQ(E_{25}^u+k^2)}{(E_{15}+k^2)(E_{25}^u+k^2)-Q'^2k^2}F_{1,z}^\nu\equiv -i\eta_2^\nu F_{1,z}^\nu, \tag{17b}$$

$$F_3^\nu=\frac{QQ'k^2}{(E_{15}+k^2)(E_{25}^u+k^2)-Q'^2k^2}F_1^\nu\equiv\eta_3^\nu F^\nu, \quad (17c)$$

where the $E$'s are defined by

$$E_{15}=E(\Gamma_{15})-E^{\rm el}, \quad E_{25}^u=E(\Gamma_{25}^u)-E^{\rm el}.$$

Since the present $\mathbf{k}\cdot\mathbf{p}$ perturbation scheme can expand the full-zone Bloch function in terms of Bloch functions associated with $\mathbf{k}=\mathbf{0}$, the total wave function of the electron in the conduction band is

$$\begin{aligned}\Psi^\nu(\mathbf{r})&=F_1^\nu(z)u_{25'}^l(\mathbf{r})+F_2^\nu(z)u_{15}(\mathbf{r})+F_3^\nu(z)u_{25'}^u(\mathbf{r})\\&=F_1^\nu(z)u_{25'}^l(\mathbf{r})-i\eta_2^\nu F_{1,z}^\nu(z)u_{15}(\mathbf{r})+\eta_3^\nu F_1^\nu(z)u_{25'}^u(\mathbf{r}).\end{aligned} \quad (18)$$

According to the EFA, the value of the envelope function is constant in the unit cell. Thus, the wave function in the outermost unit cell of the confined material is written as

$$\begin{aligned}\Psi^\nu(\mathbf{r}_\perp,q)&=F_1^\nu(q)u_{25'}^l(\mathbf{r})+F_2^\nu(q)u_{15}(\mathbf{r})+F_3^\nu(q)u_{25'}^u(\mathbf{r})\\&=F_1^\nu(q)u_{25'}^l(\mathbf{r})-i\eta_2^\nu F_{l,z}^\nu(q)u_{15}(\mathbf{r})\\&\quad+\eta_3^\nu F_1^\nu(q)u_{25'}^u(\mathbf{r}),\end{aligned} \quad (19)$$

and its partial derivative with respect to $z$ is

$$\begin{aligned}\Psi_{,z}^\nu(\mathbf{r}_{\perp,q})&=F_{1,z}^\nu(q)u_{25'}^l(\mathbf{r})+F_1^\nu(q)u_{25',z}^l(\mathbf{r})\\&\quad-i\eta_2^\nu F_{1,zz}^\nu(q)u_{15}(\mathbf{r})-i\eta_2^\nu F_{1,z}^\nu(q)u_{15,z}(\mathbf{r})\\&\quad+\eta_3^\nu F_{1,z}^\nu(q)u_{25'}^u(\mathbf{r})+\eta_3^\nu F_1^\nu(q)u_{25',z}^u(\mathbf{r}),\end{aligned} \quad (20)$$

where the subscript $zz$ represents the second-order partial derivative with respect to $z$. Combining Eqs. (5), (13), and (14), and using the orthogonality between the periodic functions and the matrix elements of the momentum[17] yields:

$$\frac{2\lambda km^\nu}{k^2(m^\nu)^2-\lambda^2}=\tan(2kq), \quad (21)$$

where $m^\nu$ is defined by $m^\nu=1+(Q\eta_2^\nu)/2$. Here Eq. (21) must be rewritten in terms of the heavy hole:

$$-\frac{2\lambda gm^\nu}{g^2(m^\nu)^2-\lambda^2}=\tan(2gq), \quad (22)$$

where Eq. (1) is used and the imaginary wave vector of the heavy hole is negative of that of the electron. Equation (22) is the confinement condition of the heavy hole in the valence band. Equations (21) and (22) show that the confinement of the electron is different from that of the hole in the valence band.

The envelope functions of the electron in the conduction band are

$$F_1^c=A_1^ce^{ik_1z}+B_1^ce^{-ik_1z}+A_2^ce^{ik_2z}+B_2^ce^{-ik_2z}, \quad (23a)$$

$$F_2^c=\eta_{21}^cA_1^ce^{ik_1z}-\eta_{21}^cB_1^ce^{-ik_1z}+\eta_{22}^cA_2^ce^{ik_2z}-\eta_{22}^cB_2^ce^{-ik_2z}, \quad (23b)$$

$$F_3^c=i\gamma_1F_{1,z}^c+\gamma_2F_2^c, \quad (23c)$$

where the $\eta$'s and $\gamma$'s are defined by

$$\gamma_1=\frac{\eta_{32}^c\eta_{21}^c-\eta_{31}^c\eta_{22}^c}{k_1\eta_{22}^c-k_2\eta_{21}^c}, \quad \gamma_1=\frac{\eta_{32}^c\eta_{21}^c-\eta_{31}^c\eta_{22}^c}{k_1\eta_{22}^c-k_2\eta_{21}^c},$$

$$\eta_{21}^c=\frac{-Tk_1}{E_1^u+k_1^2}, \quad \eta_{22}^c=\frac{-Tk_2}{E_1^u+k_2^2}, \quad \eta_{21}^c=\frac{-Tk_1}{E_1^u+k_1^2},$$

$$\eta_{32}^c=\frac{-T'k_2}{E_1^l+k_2^2}.$$

The wave function of electron in silicon is

$$\begin{aligned}\Psi^c(\mathbf{r})&=F_1^c(z)u_{15}(\mathbf{r})+F_2^c(z)u_1^u(\mathbf{r})+[i\gamma_1F_{1,z}^c(z)\\&\quad+\gamma_2F_2^c(z)]u_1^l(\mathbf{r}).\end{aligned} \quad (24)$$

By the same procedure as for the electron in the valence band, the confinement condition of the electron in the conduction band is

$$\begin{aligned}&2(\zeta_{21}^2-\zeta_{22}^2\lambda^2)\cos(2k^-q)+4\zeta_{11}\zeta_{12}\lambda\sin(2k^+q)\\&-2(\zeta_{11}^2-\zeta_{12}^2\lambda^2)\cos(2k^+q)-4\zeta_{21}\zeta_{22}\lambda\sin(2k^-q)\\&-8(\eta_{21}^e\lambda^2+m_{11}m_{21})(\eta_{22}^e\lambda^2+m_{12}m_{22})=0,\end{aligned} \quad (25)$$

where the $\zeta$'s, $k^\pm$, and $m$'s are defined by

$$\zeta_{11}=m_{12}m_{21}-m_{11}m_{22}+(\eta_{22}^c-\eta_{21}^c)\lambda^2,$$

$$\zeta_{21}=-m_{12}m_{21}-m_{11}m_{22}-(\eta_{22}^c+\eta_{21}^c)\lambda^2,$$

$$\zeta_{12}=m_{22}-m_{21}+m_{11}\eta_{22}^c-m_{12}\eta_{21}^c,$$

$$\zeta_{12}=m_{22}-m_{21}-m_{11}\eta_{22}^c+m_{12}\eta_{21}^c,$$

$$k^\pm=k_1\pm k_2,$$

$$m_{11}=\left(1-\frac{T'\gamma_1}{2}\right)k_1+\frac{T+T'\gamma_2}{2}\eta_{21}^c,$$

$$m_{11}=\left(1-\frac{T'\gamma_1}{2}\right)k_1+\frac{T+T'\gamma_2}{2}\eta_{21}^c,$$

$$m_{21}=\frac{T'}{2}+\eta_{21}^ck_1, \quad m_{22}=\frac{T'}{2}+\eta_{22}^ck_2.$$

The energy gap is calculated from $E_g=E^{\rm hh}+E^{\rm el}$, where $E^{\rm hh}$ is the energy level of the heavy hole and $E^{\rm el}$ is that of electron state including the bulk energy gap. The value of $E^{\rm hh}$ is obtained for given film thickness $2q$ and the parameter $\lambda$ by iteration based on Eq. (22). For the calculation, a value is assumed for $E^{\rm hh}(>0)$, which in turn gives $E_\nu^{\rm el}$ as $(-E^{\rm hh})$, where $E_\nu^{\rm el}$ is the energy level of electron in the valence band and $\mathrm{Det}[\Delta_5-E_\nu^{\rm el}\mathbf{I}]=0$ is then solved for $k$ and $-k$ from which four spurious solutions are excluded. The value of $g$ is $|k|$. The value of $\eta_2^\nu$ is obtained from Eq. (17b) and that of $m^\nu$ from its definition. These values are used in Eq. (22) to check whether the equation is satisfied. This it-

TABLE I. Parameters used for the calculation (energy and matrix elements of the momentum are in rydbergs and atomic units, respectively).

| Parameter | Value | Parameter | Value |
|---|---|---|---|
| $E(\Gamma^{c}_{25'})$ | 0.00 | $Q$ | 1.050 |
| $E(\Gamma^{u}_{25'})$ | 0.940 | $Q'$ | −0.807 |
| $E(\Gamma_{15})$ | 0.252 | $T$ | 1.080 |
| $E(\Gamma^{u}_{1})$ | 0.520 | $T'$ | 0.206 |
| $E(\Gamma^{l}_{1})$ | −0.950 | λ | 0.30 |

eration is repeated until the equation is satisfied. The calculation procedure for $E^{\mathrm{el}}$ is similar. The only difference is in solving this time $\mathrm{Det}[\Delta_1 - E^{\mathrm{el}}\mathbf{I}]=0$ for $k_1$, $k_2$, $-k_1$, and $-k_2$ from which two spurious solutions are removed that are larger in absolute value than the wave vector corresponding to the first Brillouin zone. The iteration this time is based on Eq. (25).

The results in this section are used to compare the theoretical results with the experimental data by Lu, Lockwood, and Baribeau.[3] Their experimental data are based on six-period, multiple quantum wells, each well being amorphous silicon surrounded by $SiO_2$ 1 nm thick. The parameters used for the calculation are given in Table I. The usual energy gap displacement of 0.32 eV (Δ in Fig. 3) was used between amorphous silicon and crystalline silicon. The comparison in Fig. 3 shows that the present model fits the experimental data well. The best-fit value of λ is 0.30. Also shown in Fig. 3 as a dotted curve is the best-fit result based on the confinement conditions for the free-standing film, which involves choosing the best-fit value of work function $W$. It is apparent that the confinement conditions of the free-standing film cannot represent the experimental data. Furthermore, the thickness dependence of the energy gap for the embedded film is seen to be quite different from that for the free-standing film.

The theoretical results are also applied to the data by Kanemistsu and Okamoto.[4] They formed single quantum wells on a SIMOX wafer and found that both the size-sensitive and size-insensitive bands exist. Since our confinement conditions are for the size-sensitive band, the comparison shown in Fig. 4 is only for this size-sensitive band. The figure shows that the present model with $\lambda = 0.15$ fits the experimental data well except when the well thickness is less than 10 Å. This fact suggests that the bulk properties cannot represent the well that is less than 10 Å in size and the EMA fails.

The parameter λ is the imaginary wave vector and a measure of quality of the barrier material including the transition layer. The higher the value, the larger the barrier height. Shown in Fig. 5 is the energy gap as a function of the well thickness with λ as the parameter. For small values of λ,

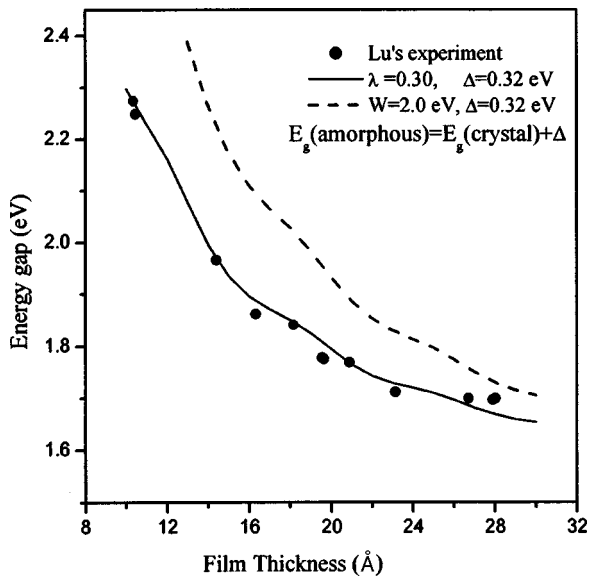


FIG. 3. Dependence of the energy gap on the well thickness for the amorphous silicon quantum well.

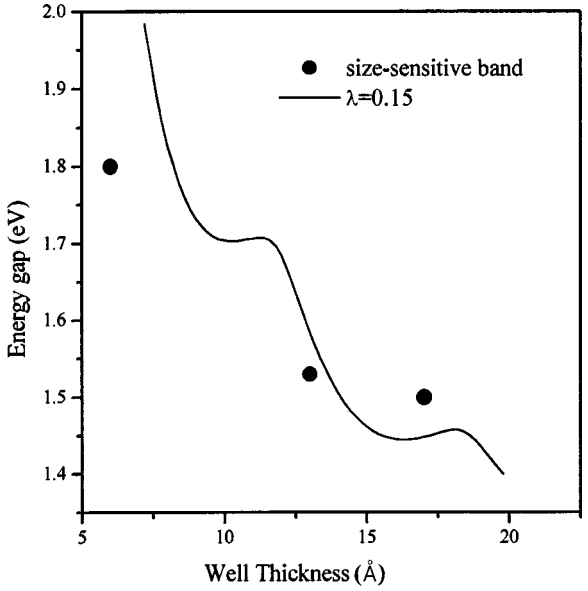


FIG. 4. Dependence of the energy gap on the well thickness for the silicon quantum well fabricated from a SIMOX wafer.

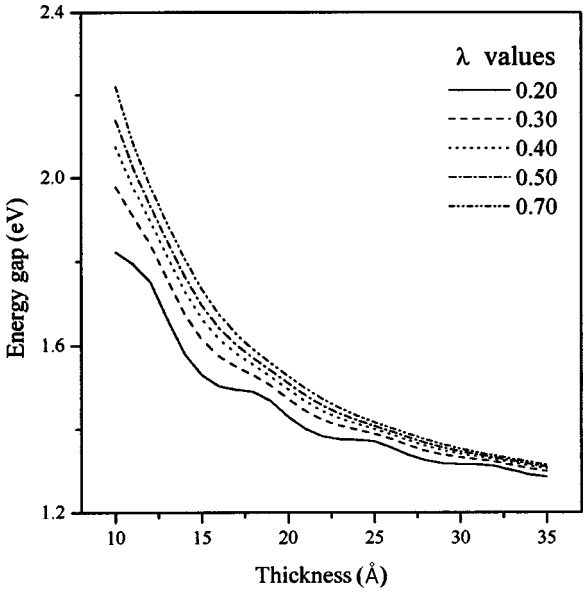


FIG. 5. Effect of the parameter λ on the size dependence of the energy gap.

even and odd solutions of electron are a significant factor and therefore steplike plateaus appear in Fig. 5, as in Fig. 4. As the value of λ increases, however, the hole energy shift dominates and smooth curves result.

Our calculation results show that the power $n$ in the power law for the thickness dependence, $(E_g - E_g^{\text{bulk}}) \propto d^{-n}$, approaches 2 as the value of λ increases or as the barrier height increases. The power $n$ decreases with decreasing λ, the value approaching $-1.2$ as λ approaches 0.15.

In summary, a boundary condition has been derived for the interface between silicon and silicon dioxide that can be used with the effective-mass and envelope-function approximations. The boundary condition takes into account the effects of the transition layer at the interface. The confinement conditions for the quantum well resulting from the boundary condition lead to an entirely different dependence of the energy gap on the thickness compared with that for the free-standing film.

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