

Band structure and confined energy levels of the $\text{Si}_3\text{N}_4/\text{Si}/\text{GaAs}$ system

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The band structure of strained Si (4–10 ML) on (001) GaAs, band lineups of the strained Si/(001)GaAs heterojunction, and confined energy levels of the $\text{Si}_3\text{N}_4/\text{Si}/\text{GaAs}$ quantum well have been calculated via a pseudopotential method. It has been found that in this technically important $\text{Si}_3\text{N}_4/\text{Si}/(001)\text{GaAs}$ structure, strained Si has a very narrow band gap (0.34 eV) at the $\Delta_\perp$ point in the Brillouin zone. For the strained Si/(001)GaAs heterojunction, the conduction band offsets from the $\Delta_\perp$ for Si to the Γ valley for GaAs is 0.83 eV, and that from the $\Delta_\perp$ valley for Si to the X valley for GaAs is 1.21 eV. The valence band offset is 0.25 eV. The lowest confined energy level in the conduction band of the $\text{Si}_3\text{N}_4/\text{Si}/\text{GaAs}$ quantum well ranging from 4 to 10 monolayers is found to be 0.22–0.28 eV above the conduction band edge of strained Si, or 0.57–0.61 eV below the conduction band edge of GaAs, while the first confined energy level in the valence band is barely above the valence band maximum of GaAs. The accumulation and inversion take place at these confined energy levels. © 1997 American Institute of Physics. [S0021-8979(97)05213-4]

I. INTRODUCTION

The critical task in the development of metal-insulator-semiconductor field-effect transistors (MISFETs) employing GaAs is to obtain a nearly ideal interface between the insulator and GaAs, which has been unsuccessful for several decades. Recently, by incorporating a strained Si interlayer (several monolayers) between the insulator and (001)GaAs, GaAs MIS structures with minimum interface trap densities in the mid $10^{10} \text{ cm}^{-2} \text{ eV}^{-1}$ have been achieved.^{1–3} Realization of GaAs MISFETs in the near future appears quite promising.

However, incorporation of a narrower band gap Si interlayer between GaAs and the insulator leads to the formation of a quantum well which confines the electrons. Thus, the strained Si interlayer, which improves the interface between the insulator and GaAs may have significant adverse effects. Although many experimental investigations were carried out on $\text{Si}_3\text{N}_4/\text{Si}/(001)\text{GaAs}$ MIS structures, no attempt has been made to understand the fundamental properties of this system, e.g., the band structure. Some investigators^{4–6} explained the results using the band structure of bulk Si instead of strained Si. This undoubtedly causes misunderstanding and misguidance. Therefore, it is important to investigate the band structure of the strained Si interlayer and quantum well energy levels, so that we can clearly understand the electrical properties of the MIS system.

Van de Walle and Martin^{7–9} proposed a first-principle approach, called the model-solid theory, to calculate the heterojunction band discontinuities at semiconductor interfaces, which includes the effects of strain. The model-solid theory

has two main aspects: first, it generates an accurate band structure, and second, it aligns this band structure on an “absolute” energy scale. The first part is accomplished by performing density-functional calculations on individual bulk semiconductors. Since the density-functional theory fails to produce the correct band gap, we use the band gap calculated by the pseudopotential method, and then add it to the valence band in order to obtain the conduction band position. The valence band discontinuity of a heterojunction can be accurately derived using the Van de Walle and Martin approach. In comparison with other model theories, e.g., Frensky–Kroemer theory¹⁰ and Harrison’s theory,¹¹ Van de Walle and Martin’s model-solid theory yields better predictions.

This article is organized as follows. First, we present the band structure of a coherently strained Si layer calculated using the real space pseudopotential and considering the lattice distortion in the strained layer. Next, we use the model-solid theory to derive the valence band discontinuity and obtain the conduction band offset using the calculated band gap. Finally, we calculate the energy levels in the quantum well using the pseudopotential method and the effective mass approximation.

II. BAND STRUCTURE OF COHERENTLY STRAINED Si ON (001) GaAs

There are several approaches to calculate the band structures of semiconductors, e.g., the local-density function method and the pseudopotential method. Although the local density function method is quite accurate for ground-state properties and some excitation energies, it does not give an accurate energy gap.¹² The pseudopotential method using several parameters to fit the experimental data may produce accurate energy bands. For the empirical pseudopotential method, the pseudopotential parameters in the k space are

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TABLE I. Coefficients for the pseudopotential in Gaussian form as in Eq. (1) (in atomic units).

Coefficients	v_1	v_2	v_3	α_c	α_3
From Ref. 15	2.454	-1.585	-0.934	0.6102	0.3
Modified Si	2.554	-1.635	-0.954	0.6102	0.3
Ga in GaAs	2.529	-1.327	-1.932	0.61	0.35
Ga in GaAs	1.562	-1.544	-0.138	0.61	0.35

used.^{13,14} For the band structure of coherently strained Si, we use the pseudopotential in real space Gaussian form derived by Kane¹⁵ and consider the effect of strain on the crystal structure. In order to obtain the energy gap of 1.12 eV for unstrained Si, the coefficients which form the pseudopotential are slightly modified as shown in Table I. The pseudopotential in Gaussian form is given by¹⁵

$$V_{\text{tot}}(\mathbf{r}) = \sum_{\mathbf{R}} (v_1 + v_2|\mathbf{r} - \mathbf{R}|^2)e^{-\alpha_c|\mathbf{r} - \mathbf{R}|^2} + v_3e^{-\alpha_3|\mathbf{r} - \mathbf{R}|^2}. \quad (1)$$

The coefficients are given in Table I.

Using the modified coefficients in Table I, we calculated the band structure of bulk Si (unstrained) as shown in Fig. 1. The energy splitting of bulk Si at several symmetry points in the k space is listed in Table II. It can be seen from Table II that, after modification, the energy splitting is still in good agreement with the experimental data. The two important points, i.e., L_1 and Δ , are more accurate.

For the band structure calculation of a strained Si layer, the distortion of the crystal structure needs to be considered. The detailed results of the atomic structure of strained semiconductors were summarized by Van de Walle.⁹ For strained Si on GaAs (001), the in-plane lattice constant $a_{\parallel}$ is the same as the lattice constant of GaAs, i.e., $a_{\parallel} = 5.65$ Å, and the out-of plane lattice constant $a_{\perp}$ can be calculated using the scheme described in Ref. 9. The out of plane lattice constant $a_{\perp}$ is found to be 5.26 Å. Using these lattice constants and the modified coefficients, we obtained the band structure of

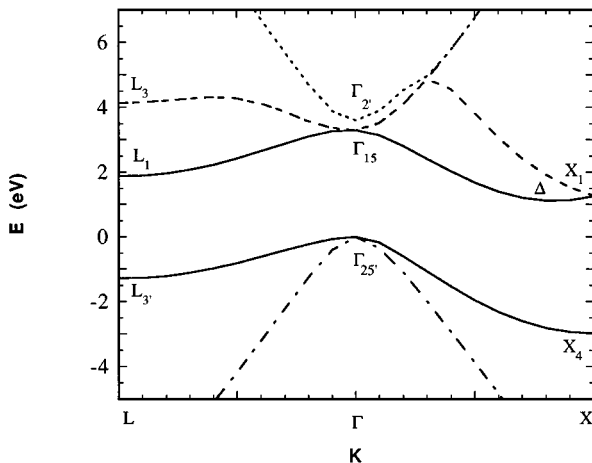


FIG. 1. Band structure of bulk Si (unstrained) from Γ to X calculated using the modified coefficients listed in Table I.

strained Si on (001) GaAs as shown in Fig. 2. The spin-orbit splitting is not considered, because it is only 0.04 eV at the Γ point of the valence band.⁷ Strained Si on (001) GaAs has a face-centered tetragonal lattice. Consequently, the six X points in the Brillouin zone split into four X points and two Z points. Correspondingly, there are four $\Delta_{\parallel}$ and two $\Delta_{\perp}$ points. The four L points remain equivalent. Therefore, the strain along $[001]$ induces a splitting of the energy bands from Γ to X as shown in Fig. 2. From Γ to L , there is no splitting at the same band. However, the degenerate bands are separated now, e.g., $\Gamma_{15} - L_3$ and $L_{3'} - \Gamma_{25'} - X_4$ bands (See Figs. 1 and 2 and Table III). Let us take a closer look at the L and Δ points. The conduction band minimum along $[001]$ direction in the Brillouin zone ($\Delta_{\perp}$) decreases significantly (0.34 eV above $\Gamma_{25'}$), while that along $[100]$ direction ($\Delta_{\parallel}$) does not change by any appreciable extent (0.97 eV). At the L point, those degenerate bands are separated. Thus $L_{3'}$ becomes $L_{3'a}$ and $L_{3'b}$, and L_3 changes to L_{3a} and L_{3b} . The separation between $\Gamma_{25'a}$ and L_1 becomes 1.17 eV. (That of bulk Si is 1.89 eV.) The band gap of strained Si is 0.34 eV, and the separation between $\Delta_{\parallel}$ and $\Delta_{\perp}$ is 0.63 eV. There are not any direct experimental data supporting these points. We may compare our results with those from other methods. Rieger *et al.*¹² reported the energy gap of strained Si on (001) Ge, which is 0.34 eV, calculated by empirical pseudopotential method. The band structure of strained Si on (001) Ge is the same as that on (001) GaAs. Van de Walle *et al.*⁷ calculated the band splitting due to strains using deformation potentials. The separation between $\Delta_{\parallel}$ and $\Delta_{\perp}$ is about 0.67 eV for strained Si on (001) Ge, which is very close to our result (0.63 eV) for strained Si on (001) GaAs.

III. BAND LINE UPS FOR THE STRAINED Si/(001) GaAs HETEROJUNCTION

The band lineups can be accomplished using Van de Walle's model-solid theory.⁹ According to the model-solid theory, the absolute energy level of the valence band can be derived using the data provided in Ref. 9. The first step is to calculate the average position of valence bands using⁹

$$E_{v,av} = E_{v,av}^0 + a_v \frac{\Delta\Omega}{\Omega}, \quad (2)$$

where $E_{v,av}^0$ is the average of valence bands without strain. The fractional volume change $\Delta\Omega/\Omega = \text{Tr}(\vec{\epsilon}) = (\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz})$, where ϵ_{xx} , ϵ_{yy} , and ϵ_{zz} are strains. The energy shifts with respect to $E_{v,av}^0$ are given by⁸

$$\Delta E_{v,2} = \frac{1}{3} \Delta_0 - \frac{1}{2} \delta E_{001}, \quad (3)$$

$$\Delta E_{v,1} = -\frac{1}{6} \Delta_0 + \frac{1}{4} \delta E_{001} + \frac{1}{2} [\Delta_0^2 + \Delta_0 \delta E_{001} + \frac{9}{4} (\delta E_{001})^2]^{1/2}, \quad (4)$$

TABLE II. Comparison of energy splitting (in eV) of bulk Si calculated using the modified coefficients with those from the experiments and from the empirical pseudopotential method.

	$\Gamma_{25'}-\Gamma_{2'}$	$\Gamma_{25'}-\Gamma_{15}$	$\Gamma_{25'}-L_1$	$\Gamma_{25'}-\Delta_1$	$L_{3'}-L_1$	$L_{3'}-L_3$	X_4-X_1
The present work	3.6	3.3	1.89	1.12	3.17	5.42	4.25
Cohen <i>et al.</i> (Ref. 13)	3.8	3.4	1.9	0.8	3.1	5.2	4.0
Experimental (Ref. 13)		3.4	1.9	1.12	3.2	5.3	4.1

$$\Delta E_{v,3} = -\frac{1}{6} \Delta_0 + \frac{1}{4} \delta E_{001} - \frac{1}{2} \left[\Delta_0^2 + \Delta_0 \delta E_{001} + \frac{9}{4} (\delta E_{001})^2 \right]^{1/2}, \quad (5)$$

where Δ_0 is the spin-orbit splitting, which is negligible for Si, and $\delta E_{001} = 2b(\varepsilon_{zz} - \varepsilon_{xx})$. b is given in Ref. 9. Using this scheme, we obtained the absolute valence band energy levels at Γ , i.e., $E_{v1} = 6.55$ eV, and $E_{v2} = E_{v3} = -7.06$ eV. This means that one valence band is degenerated at Γ and another one is 0.51 eV above the degenerated band at Γ . This is in good agreement with the results from the pseudopotential calculation (See Fig. 2), where the separation between $\Gamma_{25'a}$ and $\Gamma_{25'b}$ is 0.6 eV (See Table III). The absolute valence band energy for bulk GaAs is given by⁹

$$E_v = E_{v,av} + \frac{\Delta_0}{3}, \quad (6)$$

and we obtain $E_v = -6.81$ eV. Using these absolute energy levels and the energy gap calculated in Sec. I, we obtain the band lineups for the heterojunction of strained Si/(001) GaAs as shown in Fig. 3. Bratina *et al.*¹⁶ reported the valence band offsets for strained Si/(001) GaAs using x-ray photospectroscopy (XPS) measurements. They obtained the valence band offset of 0.39 ± 0.1 eV. However, their results were corrected using some theoretical results, and this can not be regarded as direct experimental measurements. Costa *et al.*¹⁷ measured the Schottky barrier of the diode, Al/6 Å-

Si/*p*-GaAs(001), and found that the barrier height is only 0.28 eV. This result indicates that the valence band discontinuity of strained Si/(001) GaAs should be smaller than or equal to 0.28 eV. This result agrees with our results (0.25 eV). In addition, the band discontinuity between $\Delta_\perp$ for Si and X for GaAs is also presented, which is useful for calculations of energy levels in the quantum well in the following section.

IV. CONFINED ENERGY LEVELS OF THE $\text{Si}_3\text{N}_4/\text{Si}/(001)\text{GaAs}$ SYSTEM

Based on the above calculations, the band alignment of the $\text{Si}_3\text{N}_4/\text{Si}/\text{GaAs}$ system is constructed as shown in Fig. 4. In this section, we present theoretical calculations of energy levels of the quantum well of $\text{Si}_3\text{N}_4/\text{Si}/\text{GaAs}$ based on both the pseudopotential and the effective-mass methods. It is not convenient to carry out the full calculation based on the pseudopotential method every time. If the results from the simple effective mass method do not completely deviate from the more reliable pseudopotential calculation, we may gain qualitative understanding by performing the simple effective mass calculation.

One of the major problems is the thickness of the Si interlayer. The initial thickness of the Si interlayer is ~ 10 Å (8 ML). After the deposition of Si_3N_4 , a part of the Si interlayer is consumed by nitridation. The actual thickness of the Si interlayer is less than 10 Å. Zheng *et al.*¹⁸ reported that the optimal thickness of the Si interlayer is ~ 4 Å (3 ML) determined by transmission electron microscopy (TEM). Our recent XPS and TEM measurements¹⁹ suggest that the thickness of the Si interlayer may be 2–6 monolayers, which depends on the process parameters, or 2.6–7.9 Å, considering $a_\perp = 5.26$ Å. Here we consider Si quantum wells ranging from 2 to 10 ML.

In the pseudopotential calculation, we consider $(\text{Si})_1(\text{GaAs})_8$, $(\text{Si})_2(\text{GaAs})_8$, and $(\text{Si})_x(\text{GaAs})_7$ (001) superlattices ($x = 3-5$). Here the subscript indicates the number of diatomic layers in each period. The parameters for GaAs empirical pseudopotentials are listed in Table I. The parameters are adjusted to give both the correct band gaps for bulk GaAs and, at the same time, a valence-band offset with respect to strained Si as close as possible to that given in Fig. 3. We obtain a value of 0.267 eV (0.25 eV) when the energy cut off used is 8 Ry (18 Ry). For the superlattice calculation, we used the 8 Ry energy cut off to reduce the computing time. The details of the method for calculating superlattice band structures with real-space pseudopotentials can be found in Ref. 20. The dispersion curves so obtained for a $(\text{Si})_3(\text{GaAs})_7$ superlattice (6 ML Si interlayer) are shown in

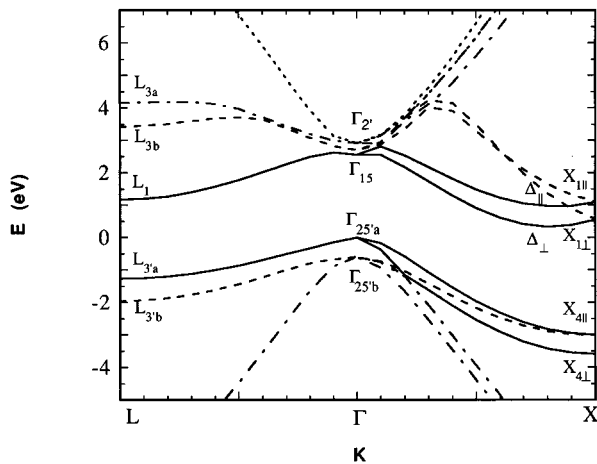


FIG. 2. Band structure of strained Si on (001) GaAs using the same modified pseudopotential as that for bulk Si and the [001]-strained crystal structure.

TABLE III. Energy splitting (in eV) of strained Si on (001) GaAs.

$\Gamma_{25'a}-\Gamma_{2'}$	$\Gamma_{25'a}-\Gamma_{15}$	$\Gamma_{25'a}-L_1$	$\Gamma_{25'a}-\Delta_{\perp}$	$\Gamma_{25'a}-\Delta_{\parallel}$	$\Gamma_{25'a}-\Gamma_{25'b}$	$L_{3'a}-L_1$
2.93	2.56	1.17	0.34	0.97	0.6	2.43
$L_{3'a}-L_{3'b}$	L_1-L_{3b}	$L_{3b}-L_{3a}$	$X_{1\perp}-X_{4\parallel}$	$X_{4\parallel}-X_{4\perp}$	$X_{1\perp}-X_{1\parallel}$	
0.7	2.26	0.74	3.58	0.59	0.53	

Fig. 5. (The dispersion curves for the other superlattices are similar to those in Fig. 5.) Note that the first conduction band is nearly dispersionless, indicating good confinement. The energy zero is set at the valence-band maximum (VBM) of bulk GaAs. We found that this Si quantum well level is not sensitive to the thickness of GaAs, provided it is sufficiently thick. The valence band, however, has substantial dispersion due to weak confinement. In the limit of very thick barrier, the first confined electron level should be close to the average position of the first conduction band in Fig. 5, which is at 0.88 eV. Comparing with the conduction band minimum of strained Si (also obtained by the same energy cut off), the confinement energy for electron is found to be 0.29 eV.

In the effective mass calculation, the Schrödinger-like equation is solved for a band-edge discontinuity between the $\Delta_{\perp}$ valley for Si and the X valley for GaAs (not the Γ valley). The detailed calculation can be found in the Appendix.

The detailed results for 2–10 ML calculated from both the pseudopotential method and the effective mass method are summarized in Table IV and Fig. 6. It can be found that for the quantum wells with large thickness (more than 6 ML), with decrease in thickness of the Si interlayer, the confinement energy level in the conduction band increases (we do find the same trend as the effective-mass theory as shown in Fig. 6). However, for quantum wells with thickness smaller than 6 ML, the confinement energy decreases, a counter-intuitive result when compared with the effective-mass theory. So, the anomalous behavior only occurs for quantum wells with widths thinner than 6 ML. Similar anomalous behavior was found in previous pseudopotential calculations for short-period SiGe superlattices.²¹ Therefore, for Si interlayers thicker than 6 ML, the results from the effective mass method are very close to those from the

pseudopotential calculation. For the Si interlayers thinner than 6 ML, the effective mass method is no longer valid. From the pseudopotential calculation, it can be found that electrons are still strongly confined for Si interlayers even thinner than 6 ML. It should be noted that the result from the two monolayer Si is not very reliable because the crystal structure of the two monolayer Si might not be real Si (Si atoms are not surrounded by four other Si atoms). However, the tendency that it shows is reasonable.

With these confined energy levels in both the conduction band and the valence band determined by the pseudopotential calculation and with the use of the correct valence-band offset, the complete band structure is constructed and shown in Fig. 4. The separation between the two closest energy levels is 0.81–0.88 eV for 4–10 ML Si. If the Fermi level is completely unpinned, the maximum range in which the Fermi level can reach is from the valence band to the first confinement level in the conduction band. In our previous experimental work,³ we measured the C – V characteristics of $\text{Al}/\text{Si}_3\text{N}_4/\text{Si}/p\text{-GaAs}$ MIS capacitors, and found that the total band bending of this structure is 0.84 eV, which is in good agreement with the result obtained by the pseudopotential method. Considering that usually higher interface trap density appears at the band edge, this band bending can be well explained using the above theoretical band structure. In addition, Mui *et al.*²² measured the C – V characteristics of $\text{Al}/\text{Si}_3\text{N}_4/\text{Si}/n\text{-GaAs}$, and found that the band bending ranges from 0.75 to 0.89 eV, all in reasonable agreement with our calculations. In an earlier investigation, we proposed that the band gap of the strained Si layer might be 0.7 eV, based on the experimental results of the heterojunction and empirical pseudopotential calculation.²³ Using the band

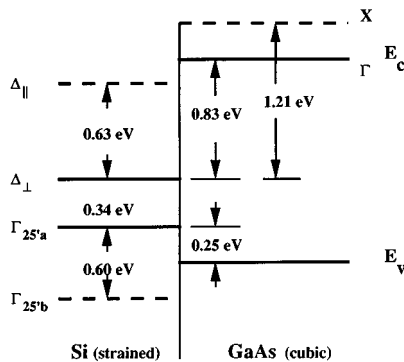
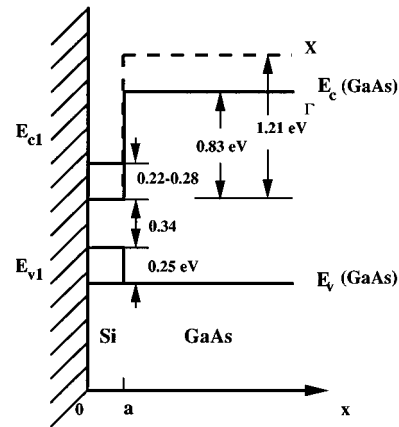


FIG. 3. Band lineups of the heterojunction of strained Si/(001) GaAs using the deformation potentials and the calculated band structure.

FIG. 4. The complete band structure of the $\text{Si}_3\text{N}_4/\text{Si}/\text{GaAs}$ system which includes a quantum well (4–10 ML) and confined energy levels.

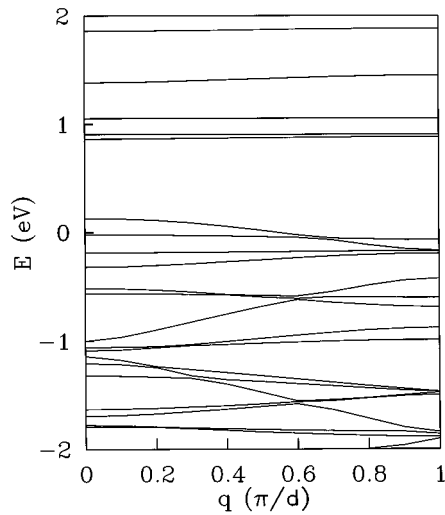


FIG. 5. Band structures of a $(\text{Si})_3(\text{GaAs})_7$ superlattice (6 ML Si) obtained by a real-space pseudopotential method.

gap of 0.7 eV, and the band-edge discontinuities proposed in Ref. 23, the separation between the two energy levels is 1.20 eV, which seems to be too large compared to the band bending experimental data. In that investigation, the experimental data were treated with partially relaxed Si layer, and in the theoretical calculation, we considered only the average effect of strain. This is probably the reason why we could not obtain reasonable quantum energy levels using that band structure.

In Fig. 4, it is shown that the lowest confined energy level in the conduction band (obtained by the pseudopotential method) is 0.22–0.28 eV above the conduction band edge of strained Si or 0.57–0.61 eV below the conduction band edge of GaAs. The confined energy level in the valence band is barely above that of GaAs. For the $\text{Al}/\text{Si}_3\text{N}_4/\text{Si}(001)/\text{GaAs}$ MIS structure, in accumulation and inversion, electrons should thus be completely confined in the strained Si layer and the Fermi level would not reach the GaAs conduction band edge.

TABLE IV. Energy levels (in eV) of quantum wells in the conduction band with various Si interlayers from 2 to 10 ML calculated by both the pseudopotential method and the effective mass approach.

Si thickness (Å)	Pseudopotential calculation		Effective mass calculation	
	$E_{c1} - E_v(\text{GaAs})$	$E_{c1} - E_c(\text{Si})$	$E_{c1} - E_v(\text{GaAs})$	$E_{c1} - E_c(\text{Si})$
2.63 (2 mono)	0.59	0	N/A	N/A
5.26 (4 mono)	0.85	0.26	1.29	0.7
7.89 (6 mono)	0.88	0.29	0.98	0.39
10.52 (8 mono)	0.82	0.23	0.84	0.25
13.15 (10 mono)	0.80	0.21	0.76	0.17

Note: the energy in the valence band is not shown due to the almost confinement of holes.

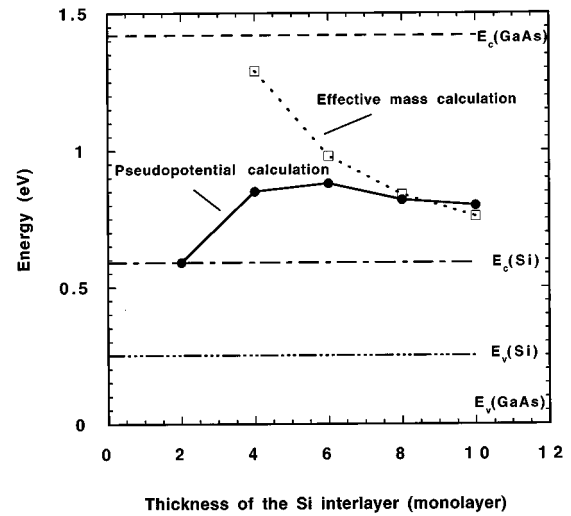


FIG. 6. Energy levels of quantum wells ranging from 2 to 10 ML calculated by both the pseudopotential method and the effective mass calculation.

V. CONCLUSIONS

We have theoretically investigated the band structure of strained Si on (001) GaAs, band lineups of the heterojunction of strained Si/(001) GaAs, and confined energy levels of the $\text{Si}_3\text{N}_4/\text{Si}/\text{GaAs}$ quantum well. We found that in this important structure, strained Si has a very narrow band gap (0.34 eV) at $\Delta_\perp$ point in the Brillouin zone. For the heterojunction of strained Si/(001) GaAs, the conduction band offset from $\Delta_\perp$ valley for Si to Γ valley for GaAs is 0.83 eV and that from $\Delta_\perp$ valley for Si to X valley for GaAs is 1.21 eV, and the valence band offset is 0.25 eV. The 4–10-ML-thick Si, together with Si_3N_4 and GaAs, forms a quantum well. The first confined energy level is 0.22–0.28 eV above the conduction band edge of strained Si or 0.57–0.61 eV below the conduction band edge of GaAs. The confined energy level in the valence band is barely above the valence band of GaAs. Thus the accumulation and inversion all happen in these confined energy levels in the $\text{Al}/\text{Si}_3\text{N}_4/\text{Si}/\text{GaAs}$ metal-insulator-semiconductor structure.

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APPENDIX

In the effective-mass calculation, we assume that the potential barrier with respect to Si_3N_4 is infinite, which is reasonable considering the relatively large band gap of Si_3N_4 .

compared with the band edge discontinuities between Si and GaAs. In the framework of the envelope-function approximation,²⁴

$$\Psi = \sum_{A,B} e^{i\mathbf{k}_\perp \cdot \mathbf{r}_\perp} u_{ck}^{A,B}(\mathbf{r}) \chi(z), \quad (\text{A1})$$

where z is the growth direction. $\mathbf{k}_\perp = (k_x, k_y) = (0,0)$ in this case, which is the transverse electron wave vector. $u_{ck}(\mathbf{r})$ is the Bloch wave function in the A, B materials, and $\chi(z)$ is the envelope wave function determined to a good approximation by the Schrödinger-like equation,²⁴

$$\left[-\frac{\hbar^2}{2m^*(z)} \frac{\partial^2}{\partial z^2} + V_c(z) \right] \chi(z) = E \chi(z),$$

$$V_c(z) = \begin{cases} 0 & \text{for } 0 < z < a \\ \Delta E_c & \text{for } z > a \end{cases}, \quad (\text{A2})$$

where $m^*(z)$ is the electron effective mass of the A or B material, $V_c(z)$ is the potential, and E is the confinement energy of electrons; $a = 5.3\text{--}13.2$ Å. On considering the symmetry characteristics of the Bloch function, ΔE_c is the band edge discontinuity between the $\Delta_\perp$ valley for Si and the X valley for GaAs (not the Γ valley). ΔE_c is 1.21 eV as shown in Figs. 3 and 4.

The continuity conditions at the interfaces are that $\chi(z)$ and $1/m^*(z) \partial\chi(z)/\partial z$ should be continuous,²⁴ rather than the more common continuity condition of the derivative of the wave function.

Due to the assumption that the potential at $z=0$ is infinite, the solution to Eq. (A2) is

$$\chi(z) = \begin{cases} A \sin(kz) & \text{for } 0 < z < a \\ D e^{-k'z} & \text{for } z > a \end{cases}, \quad (\text{A3})$$

$$\text{where } k = \sqrt{\frac{2m_{\text{Si}}^* E}{\hbar^2}} \quad \text{and} \quad k' = \sqrt{\frac{2m_{\text{GaAs}}^* (\Delta E_c - E)}{\hbar^2}} \quad (\text{A4})$$

and we obtain the transcendental relation

$$\cot(ka) = -\frac{1}{\beta} \sqrt{\left(\frac{k_0 a}{ka}\right)^2 - 1}, \quad (\text{A5})$$

where

$$k_0 = \sqrt{\frac{2m_{\text{Si}}^* \Delta E_c}{\hbar^2}} \quad \text{and} \quad \beta^2 = \frac{m_{\text{GaAs}}^*}{m_{\text{Si}}^*}. \quad (\text{A6})$$

ka is in the II or the IV quadrant. Equation (A5) can be numerically or graphically solved to obtain k . Further, from Eqs. (A4) and (A6), we have

$$E = \left(\frac{ka}{k_0 a}\right)^2 \Delta E_c. \quad (\text{A7})$$

The number of the confined energy levels would thus depend on the number of the solutions of Eq. (A5).

In order to calculate the confined energy levels, the effective mass of electrons in strained Si and that of electrons at the X valley for GaAs need to be considered. The effective mass of the electrons in a strained layer is slightly different from that in its bulk counterpart. The crystal structure of

strained Si on GaAs is the same as that of strained Si on Ge. Rieger *et al.*¹² investigated the effective mass of strained $\text{Si}_{1-x}\text{Ge}_x$ alloys on $\text{Si}_{1-x}\text{Ge}_x$ substrates (001). The perpendicular effective mass m_{Si}^* of electrons at $\Delta_\perp$ in strained Si on Ge was found to be $0.854 m_0$ from their formula. The effective mass of electrons at the X valley for GaAs is $1.9 m_0$.²⁵ Using that $m_{\text{Si}}^* = 0.854 m_0$, $m_{\text{GaAs}}^* = 1.9 m_0$, and $\Delta E_c = 1.21$ eV, we obtained one confined energy level. The detailed results are shown in Table IV and Fig. 6.

For the calculation of the confined energy level in the valence band, we may follow the same approach. From the band structure in Fig. 2, it can be found that the effective mass of holes at $\Gamma_{25'a}$ is the heavy hole, and that at $\Gamma_{25'b}$ has both heavy holes and light holes. For the present case, only heavy holes should be available at the valence band maximum. For our calculations, we use the heavy-hole effective mass in the valence band of bulk-Si, because the value for strained Si is not available. For GaAs, there are two effective masses, i.e., $0.35 m_0$ for the heavy hole and $0.10 m_0$ for the light hole which are related to the Luttinger parameters via $m_{\text{hh}}^* = m_0 / (\gamma_1 - 2\gamma_2)$ and $m_{\text{lh}}^* = m_0 / (\gamma_1 + \gamma_2)$. Using that $m_{\text{Si}}^* = 0.29 m_0$, $m_{\text{GaAs}}^* = 0.35 m_0$, and $\Delta E_v = 0.25$ eV, we obtain the confined heavy-hole energy level, $E_{v1} = 0.24\text{--}0.25$ eV, which is almost unconfined. This is similar to the pseudopotential result, i.e., the unconfinement of holes.

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