Band structure of Al/Si/*n*-type GaAs with a strained Si interfacial layer

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The band structure of a coherently strained Si layer (<15 Å) on GaAs has been calculated using the empirical pseudopotential method. The pseudopotential form factor of the strained Si layer is derived by considering that the pseudopotential of the strained layer is slightly modified by a factor which is proportional to the volume change of the unit cell. The band-structure calculation indicates that the band gap of the strained Si layer is 0.7 eV, which is substantially smaller than that of the bulk Si. A revised band-structure model for Al/Si/*n*-type GaAs based on the above calculation is proposed, which agrees very well with the experimental results. This model implies that for the coherently strained Si interfacial layer, the Fermi level is unpinned not only at the Si-GaAs interface but also at the Al-Si interface.

INTRODUCTION

Metal-insulator-semiconductor field-effect transistors (MISFET's) on GaAs have not been successfully realized due to the presence of a high density of interface trap states at the interface between the insulator and GaAs. In recent years, significant progress has been made toward the realization of GaAs MISFET's.[1–4] The key material responsible for this progress is the thin strained Si interfacial layer (10 Å), which is sandwiched between the insulator and GaAs. It is this interfacial layer that greatly reduces the interface states between the insulator and GaAs.

It is well known that the Fermi level is pinned near the midgap at the surface of GaAs due to the large density of the surface states. By incorporating a thin Si interfacial layer between metal and GaAs, it is observed that the Fermi level varies over a wide range in the band gap, which depends on the doping level of the thin Si layer.[5] This unpinning of the Fermi level at the interface between metal and GaAs is an indication of the reduced interface states. Therefore, it is important to investigate the Schottky contacts on GaAs with a thin interfacial Si layer. Waldrop and Grant[5] fabricated Schottky contacts on *n*-GaAs using 15–30-Å Si interfacial layers, which were heavily either *n* or *p* type, and found that the Schottky barrier varies between 0.45 and 1.1 eV depending on doping levels, more specifically, $\phi_b|_{\min}=0.45$ eV for metal/n^+-Si/*n*-GaAs diodes, and $\phi_b|_{\max}=1.1$ eV for metal/p^+-Si/GaAs diodes. Costa *et al.*[6] fabricated Al/*n*-Si/GaAs and Al/*p*-Si/GaAs diodes with 6–100-Å-thick Si layers, and found that the barrier height is in the range of 0.3–1.04 eV for *n*-GaAs and in the range of 0.28–1.01 eV for *p*-GaAs. Miller and Nathan[7] investigated Al/Si/*n*-GaAs Schottky diodes with 100-Å Si layers, and found that the Schottky-barrier height varies between 0.34 and 1.07 eV, depending on the doping level of the Si layer. Cantile *et al.*[8] investigated Al/Si/*n*-GaAs with even submonolayer and monolayer Si. They found that $\phi_b|_{\min}=0.3$–0.4 eV for n^+-Si interfacial layers, and $\phi_b|_{\max}=1.0$–1.1 eV for p^+-Si interfacial layers. It may be noted that all of the above experiments were performed with (100) GaAs. Therefore, our discussions are restricted to *n*-GaAs(100).

Based on the assumption that the Fermi level is pinned at the Al/Si interface, and unpinned at the Si/GaAs interface, Costa *et al.*[9] proposed a band-structure model in the framework of the bulk Si band structure. Figure 1 shows their model for two limiting cases: (a) for the n^+-Si layer, and (b) for the p^+-Si layer. Because most of the experimental data are available for *n*-GaAs, in this paper we only discuss

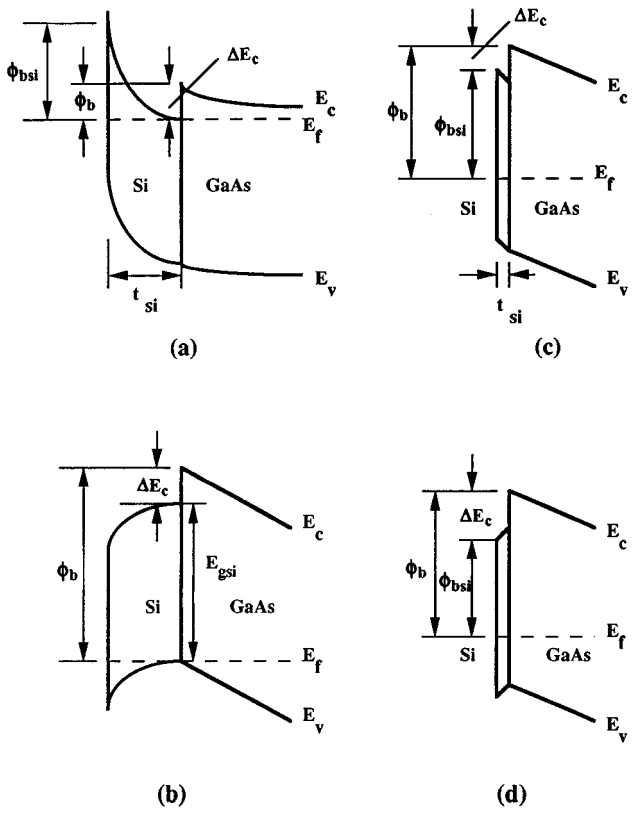

FIG. 1. Band-structure model of Al/Si/*n*-GaAs with $N_d=1\times10^{17}$ cm^{-3} proposed by Costa *et al.*; (a) thick n^+-Si layer, (b) thick p^+-Si layer, (c) very thin n^+-Si layer, and (d) very thin p^+-Si layer.

Schottky contacts on n-GaAs. The usual doping level of n^+-Si and p^+-Si is about 5×10^{19} cm^{-3}, and that of GaAs (Ref. 9) is 1×10^{17} cm^{-3}. The depletion width of Si with the barrier height ϕ_b(Si)=0.7 eV is calculated to be 40 Å, and that of GaAs to be 1000 Å with the same barrier height. From Fig. 1, it is obvious that for Schottky contacts on the n^+-thick Si layer [the thick layer is such that the thickness of Si is larger than its depletion width, and E_c(Si) can reach the Fermi level], $\phi_b|_{\min}=\Delta E_c$(Si-GaAs), because the Al-Si interface is a tunneling barrier; and for Schottky contacts on the p^+-Si thick layer, $\phi_b|_{\max}=E_g$(Si)$+\Delta E_c$ (Si-GaAs). By closely examining this model, we find that there are two aspects of the model which do not agree with the experimental results.

(1) According to this model,[9,7] ΔE_c(Si-GaAs)≈0.3 eV, ΔE_v(Si-GaAs)≈0 eV, and E_g(Si)≈1.1 eV, thus $\phi_b|_{\max}$≈1.4 eV [see Fig. 1(b)]. However, according to the experimental data,[5–8] $\phi_b|_{\max}$=1.0–1.1 eV. Thus there is a discrepancy of at least 0.3 eV between the experimental data and theoretical results.

(2) As the Si layer becomes thinner and thinner, the depletion due to ϕ_b(Si) [~0.7 eV (Ref. 9)] extends into GaAs, leading to $\phi_b|_{\min}=\phi_b$(Si)$+\Delta E_c$=1.0 eV as shown in Fig. 1(c), and $\phi_b|_{\max}=\phi_b$(Si)$+\Delta E_c$=1.0 eV as shown in Fig. 1(d). This indicates that ϕ_b does not depend on the doping level of the Si layer. However, according to Waldrop and Grant,[5] ϕ_b=0.4–1.0 eV for 15–30-Å Si layers. Cantile *et al.*[8] reported that ϕ_b varies between 0.3 and 0.4 eV and 1.0 and 1.1 eV for both 1-ML and submonolayer Si. All these indicate that for the very thin Si layer, ϕ_b still depends heavily on the doping level of the Si.

From the above discussions, it is obvious that the above simple band-structure model does not adequately explain the experimental results at least for a very thin interfacial layer. In an effort to shed some light on this discrepancy, let us first examine the structure of the Si interfacial layer. When the thickness of the Si layer $t_{\rm Si}$ is less than the critical thickness h_c, the lattice mismatch is accomodated by coherent strain, where h_c=10–14 Å for Si on GaAs.[10,11] When the thickness of the Si layer $t_{\rm Si}$ is larger than the critical thickness h_c, the mismatch is accommodated by misfit dislocations at the interface between Si and GaAs. The crystal structure of the strained layer is closer to that of GaAs than of Si, because the in-plane lattice constant of the strained layer remains the same as that of GaAs. Therefore, it may not be appropriate to apply the bulk Si band structure to explain the experimental results for the very thin strained interfacial layers (<15 Å). In this paper, we propose a revised band structure of Al/Si/n-GaAs based on the actual calculation of the band structure of the strained Si interfacial layer (<15 Å) employing the empirical pseudopotential method. Van de Walle and co-workers[12,13] proposed the model-solid theory employing deformation potentials which can predict the band lineups at the interface in the presence of strains. Rieger and Vogl[14] investigated the electronic-band parameters in the strained $Si_{1-x}Ge_x$ alloys on $Si_{1-y}Ge_y$ substrates. They calculated the band structure of the bulk materials employing the empirical pseudopotential method, and determined the band lineups using deformation potentials. We intend to explore an approach by which the overall band structure of a strained semiconductor layer can be calculated directly using the empirical pseudopotential method.

THEORETICAL CONSIDERATIONS FOR THE BAND STRUCTURE CALCULATION OF A STRAINED LAYER

The band structure is numerically calculated by solving the Schrödinger equation.[15–17] The critical problem underlying this calculation is to determine the potential $V(\vec{r})$ which may be expanded in terms of reciprocal lattice vector $\vec{K}_m$:

$$V(\vec{r})=\sum_m V_{\vec{K}_m} e^{i\vec{K}_m\cdot\vec{r}}, \tag{1}$$

where $\vec{r}$ is the lattice vector and m is an integer. $V_{\vec{K}_m}$ may be split into symmetric and antisymmetric parts:

$$V_{\vec{K}_m}=S^s(\vec{K}_m)V^s(\vec{K}_m)+iS^a(\vec{K}_m)V^a(\vec{K}_m), \tag{2}$$

where $S(\vec{K}_m)$ is the structure factor, $V^s(\vec{K}_m)$ is the symmetric pseudopotential form factor, and $V^a(\vec{K}_m)$ is the antisymmetric form factor.

The cubic semiconductors of the diamond or zinc-blende type have a fcc structure with two atoms per unit cell. The origin of the coordinates is taken half way between these two atoms, whose positions are denoted as $\vec{r}_1$ and $\vec{r}_2$, so that $\vec{r}_1=a(\frac{1}{8},\frac{1}{8},\frac{1}{8})=\vec{\tau}$ and $\vec{r}_2=-\vec{\tau}$, where a is the length of the unit cube. In this case,

$$S^s(\vec{K}_m)=\cos(\vec{K}_m\cdot\vec{\tau}) \tag{3a}$$

and

$$S^a(\vec{K}_m)=\sin(\vec{K}_m\cdot\vec{\tau}). \tag{3b}$$

In terms of the atomic potentials,

$$V^s(\vec{K}_m)=\frac{V_1(\vec{K}_m)+V_2(\vec{K}_m)}{2} \tag{4a}$$

and

$$V^a(\vec{K}_m)=\frac{V_1(\vec{K}_m)-V_2(\vec{K}_m)}{2}, \tag{4b}$$

where

$$V_1(\vec{K}_m)=\frac{1}{\Omega}\int V_1(\vec{r})e^{-i\vec{K}_m\cdot\vec{r}}d\vec{r} \tag{5}$$

and

$$V_2(\vec{K}_m)=\frac{1}{\Omega}\int V_2(\vec{r})e^{-i\vec{K}_m\cdot\vec{r}}d\vec{r}. \tag{6}$$

Here $V_1(\vec{r})$ and $V_2(\vec{r})$ are the pseudopotentials due to single atoms in the lattice, and Ω is the volume of the unit cell. For the diamond structure, $V_1(\vec{K}_m)=V_2(\vec{K}_m)$. Thus $V^s(\vec{K}_m)=V_1(\vec{K}_m)=V_2(\vec{K}_m)$, and $V^a(\vec{K}_m)=0$.[15]

The strained Si layer is a tetragonally distorted diamond structure with the in-plane lattice constant $a_\parallel$ equal to the

TABLE I. Pseudopotential form factors and lattice constants of the bulk Si and the strained Si.

Material	$V^s(\sqrt{3})$	$V^s(\sqrt{4})$	$V^s(\sqrt{8})$	$V^s(\sqrt{11})$	$V^a(\sqrt{3})$	$V^a(\sqrt{4})$	$V^a(\sqrt{8})$	$V^a(\sqrt{11})$	a (Å)
Bulk Si[a]	−0.226	0.000	0.057	0.074	0.000	0.000	0.000	0.000	5.43
Strained Si	−0.2054	0.0000	0.0518	0.0673	0.0000	0.0000	0.0000	0.0000	5.52

[a]The form factors of the bulk Si are slightly adjusted in view of those in Ref. 17 to obtain the band gap of 1.15 eV.

lattice constant a of the bulk GaAs,[18] i.e., $a_\parallel$=5.65 Å. The out-of-plane lattice constant $a_\perp$ can be calculated from the following equation:[13]

$$a_\perp = a[1 - D(a_\parallel/a - 1)], \tag{7}$$

where a is the lattice constant of the bulk Si, and D is a constant depending on the elastic constants. For (100) Si, D=0.776.[13] From Eq. (7), the out-of-plane lattice constant $a_\perp$ is calculated to be 5.26 Å. The reciprocal-lattice vector for the strained (100) Si layer may be expressed as

$$\vec{K}_m^* = 2\pi\left(\frac{m_1}{a_\parallel}, \frac{m_2}{a_\parallel}, \frac{m_3}{a_\perp}\right), \tag{8}$$

where m_1, m_2, and m_3 are integers. The band-structure calculation involves $|\vec{K}_m^*|$ with a large number of different $\vec{K}_m^*$ vectors. Therefore, use of the average lattice constant a^* calculated from $(a^*)^3=(a_\parallel)^2(a_\perp)$ should produce a reasonably good approximation, leading to a^*=5.52 Å (see the Appendix).

The structure factors of the strained Si layer as expressed in Eqs. (3a) and (3b) are the same as those of the bulk Si, because any change of the lattice accompanies a corresponding change of the reciprocal lattice, thus canceling each other in Eqs. (3a) and (3b).

Therefore, in addition to the lattice constant, the major factor which affects the band-structure calculation is the form factor. The form factor $V^{s*}(\vec{K}_m^*)$ of the strained Si layer may be expressed as

$$V^{s*}(\vec{K}_m^*) = V_1^*(\vec{K}_m^*) = \frac{1}{\Omega^*}\int V_1^*(\vec{r}) e^{-i\vec{K}_m^*\cdot r} d\vec{r}, \tag{9}$$

where $V_1^*(\vec{r})$ is the pseudopotential associated with the atoms in the strained layer, and Ω^* is the volume of the unit cell in the strained layer.

In the strained layer, the strain energy is induced due to the deformation of the crystal structure, which may cause the increase of the pseudopotential. Therefore,

$$V_1^*(\vec{r}) = V_1(\vec{r}) + \Delta V_1(\vec{r}), \tag{10}$$

where $V_1(\vec{r})$ is the pseudopotential of the bulk Si layer, and $\Delta V_1(\vec{r})(>0)$ is the increment of the pseudopotential due to the strain energy. Equation (10) can be further expressed as

$$V_1^*(\vec{r}) = V_1(\vec{r}) f \tag{11}$$

and

$$f = 1 + \frac{\Delta V_1(\vec{r})}{V_1(\vec{r})}. \tag{12}$$

Because $V_1(\vec{r})<0$ with respect to the vacuum energy level, we have $f<1$. As f is totally caused by strain or deformation, we may assume that f is equal to the ratio of the volume of the strained unit cell to that of the unstrained unit cell, i.e.,

$$f = \begin{cases} \dfrac{\Omega}{\Omega^*} & \text{for } \Omega<\Omega^* \\ \dfrac{\Omega^*}{\Omega} & \text{for } \Omega>\Omega^*. \end{cases} \tag{13}$$

Inserting Eq. (11) into Eq. (9), we obtain

$$V^{s*}(\vec{K}_m^*) = \frac{f}{\Omega^*}\int_{\Omega^*} V_1(\vec{r}) e^{-i\vec{K}_m^*\cdot\vec{r}} d\vec{r}. \tag{14}$$

As Ω^* is slightly larger than Ω for Si, $V_1(\vec{r})$ vanishes rapidly beyond the unit cell, and if we neglect the influence of $\vec{K}_m^*$ on the integral, we obtain

$$V^{s*}(\vec{K}_m^*) \approx \frac{f}{\Omega^*}\int_{\Omega} V_1(\vec{r}) e^{-i\vec{K}_m\cdot\vec{r}} d\vec{r}. \tag{15}$$

Equation (15) is further reduced to

$$V^{s*}(\vec{K}_m^*) \approx \left(\frac{\Omega}{\Omega^*}\right) f V^s(\vec{K}_m). \tag{16}$$

Following the same procedure, for the zinc-blende materials we may obtain

$$V^{a*}(\vec{K}_m^*) \approx \left(\frac{\Omega}{\Omega^*}\right) f V^a(\vec{K}_m). \tag{17}$$

This allows the form factors of the strained layer to be calculated from those of the bulk layer. For the Si strained layer, $\Omega<\Omega^*$. Thus we have $f=\Omega/\Omega^*$. The calculated form factors and the average lattice constant of the strained Si layer as well as those of the bulk Si are listed in Table I.

RESULTS AND DISCUSSIONS

Carrying out the band-structure calculation numerically with the parameters tabulated in Table I, we obtained the band structure of the strained Si layer as shown in Fig. 2. The band structure is calculated with momentum from Γ to X, and the unit of the momentum is arbitrary because we are mainly interested in the energy-band gap. The calculated energy includes a reference level. It may be noted that the band structure of the strained Si layer in the Γ-X direction is very similar to that of the bulk Si calculated by the same method.[15] The major difference between the strained Si and the bulk Si is that the band gap is now decreased. According to our output data, the minimum of the conduction band is 10.905 eV, and the maximum of the valence band is 10.218 eV. Thus the energy-band gap is ~0.7 eV, which is substan-

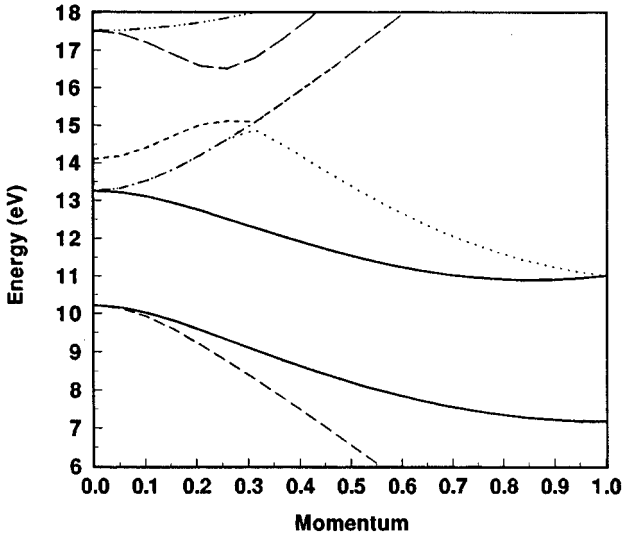

FIG. 2. Band structure (Γ-X) of the strained Si layer (<15 Å) calculated by the empirical pseudopotential method ($E_g=0.7$ eV).

tially smaller than that of the bulk Si (1.1 eV).

Using this band gap and appropriate band offsets, we may construct the band structure of the Al/Si/n-GaAs system. However, the band offsets ΔE_c and ΔE_v may not be calculated using the empirical pseudopotential method, and must be determined by experiments. Bratina *et al.*[19] measured $\Delta E_v=-0.39$ eV for the Si-GaAs structure for which the Si layer is strained. Using this measured $\Delta E_v(-0.39$ eV) and the calculated $E_g(0.7$ eV) we obtain the conduction-band offset $\Delta E_c=0.34$ eV. According to the model of Costa *et al.*, $\Delta E_v=0$ eV, which has a larger discrepancy with the experimental results. Van de Walle's model-solid theory employing deformation potentials predicts that $\Delta E_v=-0.23$ eV and $\Delta E_c=0.7$ eV for the strained Si on GaAs.[13] It seems that the results from the model-solid theory have a smaller discrepancy, but still do not agree very well with the experimental results. As stated by Van de Walle,[13] the model-solid theory does not work very well for interfaces between a group-IV element and a III-V compound, and also not for (001) orientations.

In light of the results obtained above, i.e., $\Delta E_c=0.34$ eV, $\Delta E_v=-0.39$ eV, and $E_g=0.7$ eV, with an assumption that the Fermi level is unpinned at both Si-GaAs and Al-Si interfaces, we may now be in a position to propose a revised model as shown in Fig. 3 for the two limiting cases: (a) n^+-Si and (b) p^+-Si. For Al/n^+-Si/n-GaAs, we obtain $\phi_b|_{\min}=\Delta E_c=0.34$ eV, and for Al/p^+-Si/n-GaAs, $\phi_b|_{\max}=E_g(\mathrm{Si})+\Delta E_c=1.04$ eV. Therefore, our model predicts that ϕ_b is in the range between 0.34 and 1.04 eV, which agrees very well with the experimental results.[8] This result also conforms to the experimental results of the thicker Si layers (15–100 Å),[5–7] suggesting that the thicker layers might not be fully relaxed.

In order to further test this approach, we calculated the band structure of the strained $Si_{1-x}Ge_x$ on the Si substrate. Some of the preliminary results are presented here. The band gap of the strained Ge ($x=1$) on the Si substrate is 0.533 eV, that of the strained $Si_{0.4}Ge_{0.6}$ ($x=0.6$) on the Si substrate is 0.742 eV, and that of the strained $Si_{0.2}Ge_{0.8}$ ($x=0.2$) on the

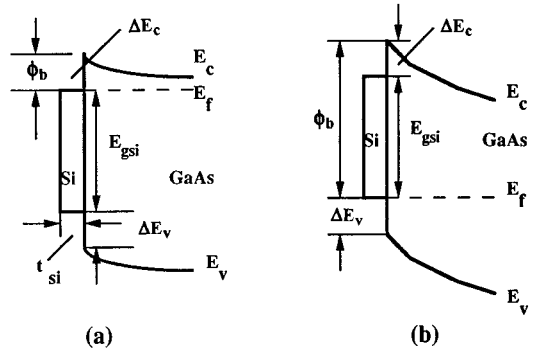

FIG. 3. The proposed band-structure model of Al/Si/n-GaAs with a strained Si interfacial layer: (a) n^+-Si doped with As, and (b) p^+-Si doped by a sufficiently high Al flux.

Si substrate is 1.01 eV. These results agree very well with the experimental results obtained by Lang *et al.*[20] and Noël *et al.*,[21] and also close to the theoretical results of Rieger and Vogl.[14]

We now turn our attention to whether the band-structure calculation using the empirical pseudopotential method is still valid for very thin strained layers. Two key parameters for the band-structure calculation are the structure factor and the form factor. The structure factor is calculated from Eq. (3), which requires the periodicity of the crystal. Actually, the lattice of the strained Si may be considered as an extension of that of the GaAs crystal. If one views the strained Si together with GaAs as a whole crystal, the periodicity of the Si would be just a part of the GaAs crystal. On the other hand, the form factor is calculated from Eq. (9) where $V_1^*(\vec{r})$ is localized in one unit cell. Therefore, we believe that, even for the strained layers, the empirical pseudopotential method is still valid.

CONCLUSIONS

The band structure of the strained Si layer (<15 Å) on GaAs is calculated using the empirical pseudopotential method. The form factor of the strained Si layer is derived by considering that the pseudopotential of the strained layer is slightly modified by a factor which is proportional to the volume change of the unit cell. The band-structure calculation indicates that the band gap of the strained Si layer is 0.7 eV which is substantially smaller than that of the bulk Si. A revised band-structure model for Al/Si/n-GaAs based on the above calculation is proposed, which conforms to the experimental results very well. This model implies that with the strained Si interfacial layers, the Fermi level is unpinned not only at the Si-GaAs interface but also at the Al-Si interface. The striking agreement of our theoretical results with the available experimental data attests to the utility of this approach for the calculation of the band structure of a strained semiconductor layer.

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APPENDIX

The band structure is numerically calculated by solving the following equations which are deduced from the Schrödinger equation employing Fourier transformation:

$$\frac{\hbar^2}{2m^*}|\vec{k}+\vec{K}_l|^2 A_{\vec{K}_l}+\sum_h V_{\vec{K}_l-\vec{K}_h}A_{\vec{K}_h}=E(\vec{k})A_{\vec{K}_l} \quad (l=0,1,\ldots,n) \tag{A1}$$

where $\vec{k}$ is the wave vector, and $E(\vec{k})$ is the corresponding energy. $\vec{K}_l$ and $\vec{K}_h$ are the reciprocal vectors. $A_{\vec{K}_l}$ is the Fourier coefficient of the Bloch function $u_k(\vec{r})$. $V_{\vec{K}_l-\vec{K}_h}$ is the Fourier coefficient of the potential $V(\vec{r})$. These equations can be further expressed in matrix form as

$$[a_{ij}]_{n\times n}[A_{\vec{K}_i}]_{1\times n}=E(\vec{k})[A_{\vec{K}_i}]_{1\times n}, \tag{A2}$$

where

$$a_{ij}=\begin{cases}\dfrac{\hbar^2}{2m^*}|\vec{k}+\vec{K}_i|^2 & \text{if } i=j\\ V_{\vec{K}_i-\vec{K}_j} & \text{otherwise .}\end{cases}$$

Therefore, for a given wave vector $\vec{k}$, we can determine the corresponding set of band-structure energies $E(\vec{k})$ by solving the eigenvalue problem of Eq. (A2). Usually, $n=120$ results in a satisfactory output.

In order to calculate the band structure of a strained semiconductor layer, we may solve the eigenvalue problem in Eq. (A2) with the modified coefficients a_{ij}^* due to the tetragonal distortion:

$$a_{ij}^*=\begin{cases}\dfrac{\hbar^2}{2m^*}|\vec{k}+\vec{K}_i^*|^2 & \text{if } i=j\\ V^*_{\vec{K}_i^*-\vec{K}_j^*} & \text{otherwise.}\end{cases} \tag{A3}$$

In the above expression, $|\vec{k}+\vec{K}_i^*|^2$ can be expressed as $|\vec{k}|^2+2|\vec{k}||\vec{K}_i^*|\cos\theta^*+|\vec{K}_i^*|^2$, where θ^* is the angle between $\vec{k}$ and $\vec{K}_i^*$. $\theta^*\cong\theta$ due to the small change of the crystal structure, where θ is the angle between $\vec{k}$ and K_i. $V^*_{\vec{K}_i^*-\vec{K}_j^*}$ is determined by the structure factors and the form factors. From the above discussions, we find that a_{ij}^* is determined by $|\vec{K}_i^*|$. From Eq. (A2), it can be found that $E(\vec{k})$ is determined by a large number of coefficients a_{ij}^* associated with $|\vec{K}_i^*|$, $i=0,1,2,\ldots,n$ $(n>120)$. Therefore, $E(\vec{k})$ is the average result of the actions produced by $|\vec{K}_i^*|$, $i=0,1,2,\ldots,n$. We can find an average lattice constant a_m^* instead of $a_\parallel$ and $a_\perp$, so that

$$|\vec{K}_m^*|=2\pi\left[\left(\frac{m_1}{a_\parallel}\right)^2+\left(\frac{m_2}{a_\parallel}\right)^2+\left(\frac{m_3}{a_\perp}\right)\right]^{1/2}=\frac{2\pi}{a_m^*}\sqrt{m_1^2+m_2^2+m_3^2}. \tag{A4}$$

Thus we derive

$$a_m^*=\left(\frac{m_1^2+m_2^2+m_3^2}{\left(\frac{m_1}{a_\parallel}\right)^2+\left(\frac{m_2}{a_\parallel}\right)^2+\left(\frac{m_3}{a_\perp}\right)^2}\right)^{1/2}, \quad m_1,m_2,m_3=0,1,\ldots,n. \tag{A5}$$

The average lattice constant can be obtained by

$$a^*=\frac{\sum_m a_m^*}{n} \tag{A6}$$

which is equal to 5.514 Å in our case for $n>125$. Note that this is very close to the value obtained from $a^*=(\sqrt{a_\parallel^2 a_\perp})^{1/3}=5.517$ Å. This demonstrates that it is reasonable to calculate the effect of the tetragonal distortion on band structure using the average lattice constant a^*.

In order to verify the above point, we calculated the band structure without using the average lattice constant a^*, and instead directly using $a_\parallel$ and $a_\perp$ in $|\vec{K}_m^*|$. This yielded the same results as using the average lattice constant. Therefore, we can calculate the band structure of a strained semiconductor layer using the program designed for bulk semiconductors.

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