Calculation of band edge levels of strained Si/(111)$Si_{1-x}Ge_x$ *

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Abstract: Calculations were performed on the band edge levels of (111)-biaxially strained Si on relaxed $Si_{1-x}Ge_x$ alloy using the $k\cdot p$ perturbation method coupled with deformation potential theory. The results show that the conduction band (CB) edge is characterized by six identical valleys, that the valence band (VB) edge degeneracies are partially lifted, and that both the CB and VB edge levels move up in electron energy as the Ge fraction (x) increases. In addition, the dependence of the indirect bandgap and the VB edge splitting energy on x was obtained. Quantitative data from the results supply valuable references for Si-based strained device design.

Key words: strained Si; band edge; $k\cdot p$ method
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1. Introduction

Many applications of devices fabricated using strained Si (s-Si) constitute a considerable enhancement of the presently well-established Si technology[1, 2]. Significant changes in band structure and carrier mobility enhancement of s-Si materials lead to the improvement of s-Si based device performance. In view of the applications and the efficient design of devices fabricated using s-Si, it is of great significance to investigate the band structure of s-Si, especially the band edge levels, which is the theoretical basis of the establishment of carrier scattering models.

(111)-biaxially s-Si on relaxed $Si_{1-x}Ge_x$, or rhombohedral Si (r-Si), is of interest since the (111) plane is one of the common planes used for semiconductor device fabrication. Hence, we calculate the band edge levels in r-Si using the $k\cdot p$ perturbation method coupled with deformation potential theory[3], including the dependence of CB/VB edge levels, bandgap and VB splitting energy on Ge fraction x, which can supply valuable references for Si-based strained device design.

2. Physical model

The band edge levels of r-Si can be obtained using various approaches. The most powerful of all the approaches is the $k\cdot p$ perturbation method coupled with deformation potential theory, since it provides sufficiently high accuracy and gives the analytic E–k relation which is fairly easy to apply. The effect of strain on the electronic system of a semiconductor may be modeled using deformation potential theory. Strain is incorporated into the band structure as a perturbed term in the calculation. The Hamiltonian of this perturbation, H_ε, has matrix elements of the form[4]

$$H_{\varepsilon,ij} = \sum_{\alpha,\,\beta=1}^{3} D_{ij}^{\alpha\beta}\varepsilon_{\alpha\beta}, \tag{1}$$

where $\varepsilon_{\alpha\beta}$ is the element of the strain tensor and $D_{ij}^{\alpha\beta}$ is the deformation potential. The strain tensor for the (111) substrate can be obtained by the following formulae[5].

$$\varepsilon_{||} = \left(a_{Si_{1-x}Ge_x} - a_{Si}\right)/a_{Si}, \tag{2}$$

$$\varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_{zz} = \frac{1}{3}\times\left[2 - 1/\sigma^{(111)}\right]\varepsilon_{||}, \tag{3}$$

$$\varepsilon_{xy} = \varepsilon_{yz} = \varepsilon_{zx} = -\frac{1}{3}\times\left[1 + 1/\sigma^{(111)}\right]\varepsilon_{||}, \tag{4}$$

where the lattice constants $a_{Si_{1-x}Ge_x}$ of $Si_{1-x}Ge_x$ are obtained by linear interpolation. Values of parameters used in calculation are list in Table 1.

First, the perturbed Hamiltonians of the Δ conduction band (CB) are considered. Since the levels of CB are non-degenerate, the $D^{\alpha\beta}$ are diagonal in (i, j) and may be treated as individual deformation potential constants (Ξ_d^Δ, Ξ_u^Δ). So the strain-induced energy shift (δE) in CB and the CB edge level in r-Si may be determined by Eqs. (5) and (6) respectively.

$$H_{\varepsilon,(100)} = H_{\varepsilon,(010)} = H_{\varepsilon,(001)} = \left(\Xi_d^\Delta + \frac{1}{3}\Xi_u^\Delta\right)\left(2 - 1/\sigma^{(111)}\right)\varepsilon_{||}, \tag{5}$$

$$E_c = E_c^0 + \delta E = 1.119 + \left(\Xi_d^\Delta + \frac{1}{3}\Xi_u^\Delta\right)\left(2 - 1/\sigma^{(111)}\right)\varepsilon_{||}, \tag{6}$$

where the value of E_c^0 or the CB edge of unstrained Si, is 1.119 eV.

Analogous to the $k\cdot p$ Hamiltonian matrix of the top of the valence band (VB), the strained Hamiltonian of the VB in $i\alpha$ representation ($i = x, y, z$, $\alpha = \uparrow, \downarrow$)[6] is,

$$H_{\varepsilon,i\alpha} = \begin{bmatrix} H' & 0_{3\times3} \\ 0_{3\times3} & H' \end{bmatrix} \begin{matrix} \uparrow \\ \downarrow \end{matrix}, \tag{7}$$

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Table 1. Values used in the calculation.

Parameter	Symbol (unit)	Value, Reference
Si lattice constant	a_0(Å)	5.431, Ref. [7]
Ge lattice constant	a_0(Å)	5.658, Ref. [7]
Poisson ratio	$\sigma^{(111)}$	2.275, Ref. [8]
Deformation potential	Ξ_d^{Δ}(eV)	1.75, Ref. [9]
Deformation potential	Ξ_u^{Δ}(eV)	9.16, Ref. [9]
Deformation potential	l	– 0.15, Ref. [10]
Deformation potential	m	6.84, Ref. [10]
Deformation potential	n	– 5.89, Ref. [10]

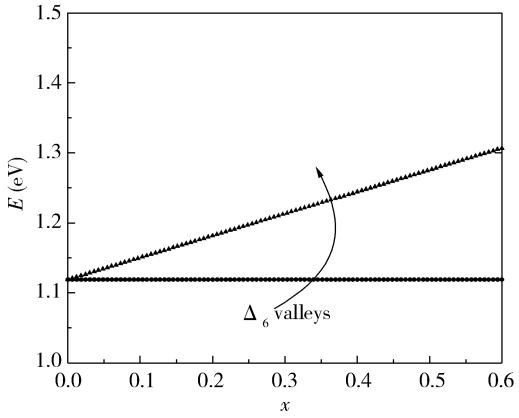

Fig. 1. CB edge versus Ge fraction x in r-Si.

$$H' = \begin{bmatrix} l\varepsilon_{xx}+m(\varepsilon_{yy}+\varepsilon_{zz}) & n\varepsilon_{xy} & n\varepsilon_{zx} \\ n\varepsilon_{xy} & l\varepsilon_{yy}+m(\varepsilon_{xx}+\varepsilon_{zz}) & n\varepsilon_{yz} \\ n\varepsilon_{zx} & n\varepsilon_{yz} & l\varepsilon_{zz}+m(\varepsilon_{yy}+\varepsilon_{xx}) \end{bmatrix}. \quad (8)$$

The notation, x, y, z refer to basis functions with the corresponding rotational symmetry of the $\Gamma_{25}^{'}$ representation of the symmetry group of the top of the VB. The up and down arrows denote spin up and down, respectively.

To get the position of VB near the center of the Brillouin zone, the effect of spin-orbit coupling (H_{so}) and the effects of strain (H_ε) are added to the zero point. The following analytic E–k relations of VB near the zero position in r-Si were obtained.

$$\begin{cases} E_v^1 = 0.073x^2 + 0.4726x - 0.00034, \\ E_v^2 = -0.0225x^2 + 0.1846x + 0.00005, \\ E_v^3 = 0.156 - 0.12\exp(-x/0.7616). \end{cases} \quad (9)$$

3. Results and discussion

The CB edge in r-Si is shown in Fig. 1. It is found that the CB edge is characterized by six identical valleys, which are shifted only slightly upward in energy. The results above can be interpreted from a force diagram of the six Δ valleys. With rhombohedral distortion, arising from growth on a (111) substrate, all Δ valleys are symmetrically equivalent and shift together, as shown in Fig. 2.

The dependence of VB edge on the Ge fraction x in r-Si is plotted in Fig. 3. Figure 3 shows that splitting of the first and second VB occurs and all VB edges move up in electron energy

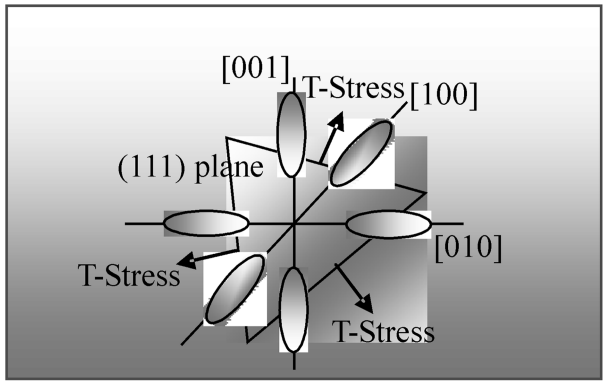

Fig. 2. Schematic equi-energy surfaces of the six valleys in the first CB in r-Si.

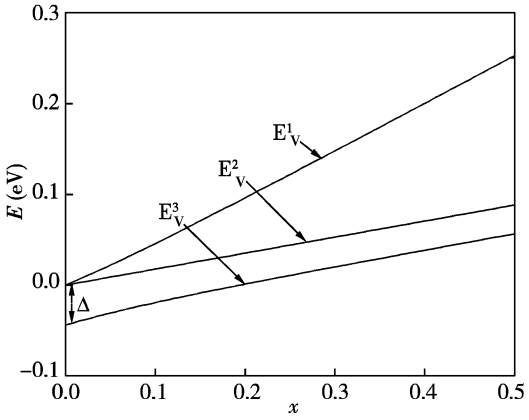

Fig. 3. VB edge levels versus Ge fraction x in r-Si.

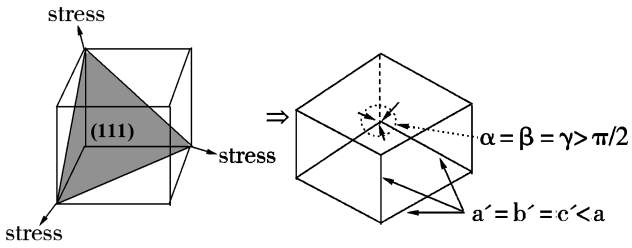

Fig. 4. Schematic cell structure of r-Si, where $a^{'}$, $b^{'}$, $c^{'}$, α, β, γ are lattice constants under strain.

as the Ge fraction x increases. This is attributed to the following fact: under the biaxial tensile stress imposed by the (111) substrate, form transformation of the Si epitaxial layer from cubic to rhombohedral occurs (seen in Fig. 4), which causes lower symmetry, and hence lifts the VB edge degeneracy.

Based on the band edge levels above, the VB edge splitting energy between the first and second bands at $k = 0$ and the bandgap are plotted as a function of x (seen in Figs. 5 and 6). A decrease in the indirect bandgap and an increase in the VB edge splitting energy with increasing x are found. It is noteworthy that the bandgap obtained in our work is in agreement with the one cited in Ref. [11].

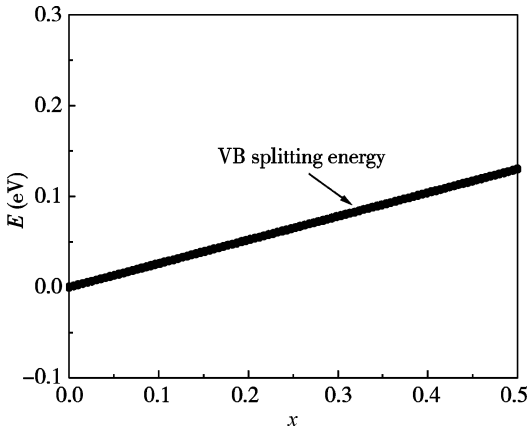

Fig. 5. VB splitting energy versus Ge fraction x in r-Si.

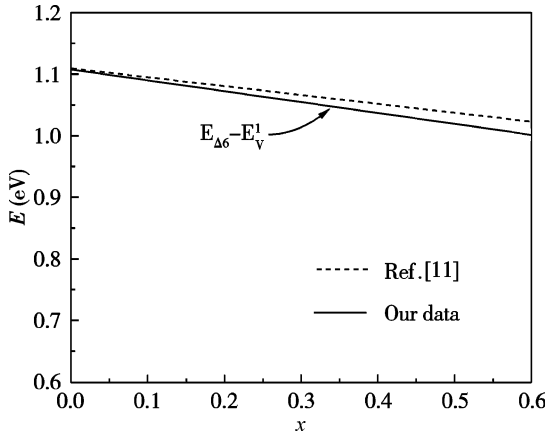

Fig. 6. Indirect bandgap versus Ge fraction x in r-Si.

4. Conclusions

Calculations were performed on the band edge levels in (111)-biaxially strained Si on relaxed $Si_{1-x}Ge_x$ alloy using the $k \cdot p$ perturbation method coupled with deformation potential theory. It is found that both the bottom CB and the top VB edge levels move up in electron energy as the Ge fraction x increases and that, with increasing x, the indirect bandgap decreases while the VB edge splitting energy increases. The band edge model of r-Si obtained can supply valuable references for Si-based device design, including CB/VB edge levels, indirect bandgap and VB splitting energy.

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