A $k \cdot p$ analytical model for valence band of biaxial strained Ge on (001) $Si_{1-x}Ge_x$*

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(Received 16 September 2011; revised manuscript received 19 November 2011)

In this paper, the dispersion relationship is derived by using the $\boldsymbol{k} \cdot \boldsymbol{p}$ method with the help of the perturbation theory, and we obtain the analytical expression in connection with the deformation potential. The calculation of the valence band of the biaxial strained Ge/(001)$Si_{1-x}Ge_x$ is then performed. The results show that the first valence band edge moves up as Ge fraction x decreases, while the second valence band edge moves down. The band structures in the strained Ge/ (001)$Si_{0.4}Ge_{0.6}$ exhibit significant changes with x decreasing in the relaxed Ge along the [0, 0, k] and the [k, 0, 0] directions. Furthermore, we employ a pseudo-potential total energy package (CASTEP) approach to calculate the band structure with the Ge fraction ranging from $x = 0.6$ to 1. Our analytical results of the splitting energy accord with the CASTEP-extracted results. The quantitative results obtained in this work can provide some theoretical references to the understanding of the strained Ge materials and the conduction channel design related to stress and orientation in the strained Ge pMOSFET.

Keywords: strained Ge, valence band, $\boldsymbol{k} \cdot \boldsymbol{p}$ method, dispersion relationship

PACS: 71.20.–b, 73.20.At **DOI:** 10.1088/1674-1056/21/5/057103

1. Introduction

The strain technology has attracted much attention because the performance of the silicon-based metal-oxide semiconductor field-effect transistor (Si-MOSFET) can be enhanced by increasing the carrier mobility in the channel region by applying a controlled strain.[12] Germanium (Ge) has been of special interest in high speed CMOS technology for years. The bulk Ge hole mobility is larger than that in the Si-based semiconductor materials. In recent years, with the strain technology applied to the Si-based CMOS in the industry, the strain effect was also investigated on Ge-MOSFETs[34] The strain is normally achieved by applying $Si_{1-x}Ge_x$ ($x < 1$) substrate underneath the Ge channel, and it is still an interesting topic to study how the strain affects the hole mobility in Ge-pMOSFET.

The strained Ge technology mentioned above stays mainly in experiments,[5−7] and the available theoretical research with the physical insights of the strain effect on the band structure of Ge lags behind the device applications. The effective device design is also ultimately based on the understanding of the correct material parameters and the accurate simulation of the carrier mobility in these devices. The band structure is the basis for fully understanding or appreciating the properties of the material, and the dispersion relation of the valence band in the strained Ge is the theoretical basis for understanding the valence band and calculating the hole mobility. However, to date there is a lack of detailed derivation of the $E(\boldsymbol{k})$–$\boldsymbol{k}$ relationship for the valence band of the strained Ge/(001)$Si_{1-x}Ge_x$. Therefore, the main goal of this paper is to obtain an analytical expression of the $E(\boldsymbol{k})$–$\boldsymbol{k}$ relation for the valence band of the strained Ge/(001)$Si_{1-x}Ge_x$. This work is performed within the framework of the $\boldsymbol{k} \cdot \boldsymbol{p}$ method with the help of the perturbation theory. The parameters of the valence band in the strained Ge/(001)$Si_{1-x}Ge_x$ are calculated from the obtained $E(\boldsymbol{k})$–$\boldsymbol{k}$ relationship. The quantitative results obtained in our work can provide valuable theoretical references to the understanding of the strained Ge materials physics and the channel design related to stress and orientations in the strained

*Project supported by the Fundamental Research Funds for the Central Universities, China (Grant Nos. 72105499 and 72104089) and the Natural Science Basic Research Plan in Shaanxi Province, China (Grant No. 2010JQ8008).

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Ge-pMOSFET.

2. Mathematical modeling

The valence band structure of the strained Ge /(001)$Si_{1-x}Ge_x$ changes under the action of stress, which then is different from that of the relaxed Ge. Based on the dispersion relationship of the valence band of the relaxed Ge, considering the effect of the strain-induced deformation potential[8] and using the $\boldsymbol{k}\cdot\boldsymbol{p}$ perturbation theory,[9] we can establish the $E(\boldsymbol{k})$–$\boldsymbol{k}$ analytical model for the valence band of the strained Ge/(001)$Si_{1-x}Ge_x$ using mathematical tools in this section.

Without the effect of the spin–orbit coupling, in accordance with the relaxed Si, the $\boldsymbol{k}\cdot\boldsymbol{p}$ Hamiltonian of the valence band of the relaxed Ge is expressed as[10]

$$\boldsymbol{H}' = \begin{bmatrix} Lk_x^2 + M(k_y^2 + k_z^2) & Nk_xk_y & Nk_zk_x \\ Nk_xk_y & Lk_y^2 + M(k_z^2 + k_x^2) & Nk_yk_z \\ Nk_zk_x & Nk_yk_z & Lk_z^2 + M(k_x^2 + k_y^2) \end{bmatrix}, \tag{1}$$

where $L = -30.53$ eV, $M = -4.64$ eV, and $N = -33.64$ eV are the Kohn–Luttinger valence band parameters of the relaxed Ge.[11] The energy eigenvalue of $\boldsymbol{H}'$ can be obtained by using the secular equation method, which can lead to the $E(\boldsymbol{k})$–$\boldsymbol{k}$ relationship without considering the spin–orbit coupling.

Similar to the case of the strained Si, the strain induced splitting and the warping of the bands in the strained Ge can be calculated within the $\boldsymbol{k}\cdot\boldsymbol{p}$ method framework by adding the strain-dependent perturbation Hamiltonian $\boldsymbol{H}''$. Since the strain effect is considered as a perturbation, $\boldsymbol{H}''$ should be similar to $\boldsymbol{H}'$ and can reflect the displacement of wave vector $\boldsymbol{k}$ under the action of strain. In the deformation theory, the energy dispersions of the valence bands are obtained from $\boldsymbol{H}' + \boldsymbol{H}''$, and

$$\boldsymbol{H}'' = \begin{bmatrix} l\varepsilon_{xx} + m(\varepsilon_{yy} + \varepsilon_{zz}) & n\varepsilon_{xy} & n\varepsilon_{zx} \\ n\varepsilon_{xy} & l\varepsilon_{yy} + m(\varepsilon_{xx} + \varepsilon_{zz}) & n\varepsilon_{yz} \\ n\varepsilon_{zx} & n\varepsilon_{yz} & l\varepsilon_{zz} + m(\varepsilon_{yy} + \varepsilon_{xx}) \end{bmatrix} \begin{matrix} |e_1\rangle \\ |e_2\rangle \\ |e_3\rangle \end{matrix}, \tag{2}$$

where parameters l, m, and n denote the valence band deformation potentials. For the strained Ge, $l = -2.4$ eV, $m = 4.2$ eV, and $n = -7.62$ eV.[11] In the case of strained Ge on the (001)-oriented $Si_{1-x}Ge_x$ substrate, the Ge fraction-dependent strain tensor has $\varepsilon_{xy} = \varepsilon_{xz} = \varepsilon_{yz} = 0$, $\varepsilon_{xx} = \varepsilon_{yy} = 0.04 \times (1-x)/1.332$, and $\varepsilon_{zz} = 0.04 \times (1-x)$, where x denotes the Ge fraction.

Summing up matrices (1) and (2) is equivalent to adding the strain-induced variation to wave vector $\boldsymbol{k}$ in coordinate (k_x k_y k_z). The eigenvalue of $\boldsymbol{H}'+\boldsymbol{H}''$ is obtained by using the secular equation method, which gives the $E(\boldsymbol{k})$–$\boldsymbol{k}$ relationship of the valence band of the strained Ge/(001)$Si_{1-x}Ge_x$ without considering the effect of the spin–orbit coupling. In basis $|e_i, \sigma\rangle$ where $\sigma = \uparrow\downarrow$, to obtain a more accurate valence band structure, we should take into account the effect of the spin–orbit coupling, which requires first to change the $\boldsymbol{k}\cdot\boldsymbol{p}$ Hamiltonian and the strain-dependent perturbation Hamiltonian from single-group of state into double-group of state

$$\boldsymbol{H}_{\boldsymbol{k}\cdot\boldsymbol{p}} = \begin{bmatrix} \boldsymbol{H}' & \boldsymbol{0}_{3\times3} \\ \boldsymbol{0}_{3\times3} & \boldsymbol{H}' \end{bmatrix} \begin{matrix} |\uparrow\rangle \\ |\downarrow\rangle \end{matrix},$$
$$\boldsymbol{H}_{\text{strain}} = \begin{bmatrix} \boldsymbol{H}'' & 0_{3\times3} \\ \boldsymbol{0}_{3\times3} & \boldsymbol{H}'' \end{bmatrix} \begin{matrix} |\uparrow\rangle \\ |\downarrow\rangle \end{matrix}. \tag{3}$$

The valence band of the relaxed Ge consists of three bands with the energy maximum at the Γ point, i.e., the center of the Brillouin zone. The spin–orbit interaction lifts the three-fold degeneracy and splits the bands by the energy of $\Delta = 0.29$ eV. Hence, the effect of the spin–orbit coupling is taken into account via introducing a spin–orbit interaction term, i.e., $\boldsymbol{H}_{\text{SO}}$. The spin–orbit coupling Hamiltonian is

$$\boldsymbol{H}_{\rm SO}=-\frac{\Delta}{3}\begin{bmatrix} 0 & \mathrm{i} & 0 & 0 & 0 & -1 \\ -\mathrm{i} & 0 & 0 & 0 & 0 & \mathrm{i} \\ 0 & 0 & 0 & 1 & -\mathrm{i} & 0 \\ 0 & 0 & 1 & 0 & -\mathrm{i} & 0 \\ 0 & 0 & \mathrm{i} & \mathrm{i} & 0 & 0 \\ -1 & -\mathrm{i} & 0 & 0 & 0 & 0 \end{bmatrix}. \quad (4)$$

The total Hamitonian of the valence band in the strained Ge in basis $|e_i,\sigma\rangle$ then becomes $\boldsymbol{H}=\boldsymbol{H}_{\boldsymbol{k}\cdot\boldsymbol{p}}+\boldsymbol{H}_{\rm strain}+\boldsymbol{H}_{\rm SO}$. Similarly, by using the secular equation method to obtain the eigenvalues of $\boldsymbol{H}$, the $E(\boldsymbol{k})$–$\boldsymbol{k}$ dispersion relationship of the valence band can be founded.

In particular, it is quite difficult to use the secular equation to obtain the eigenvalues of the 6×6 matrix $\boldsymbol{H}$. It is necessary to reduce its dimensions first. Note that the secular determinant of $\boldsymbol{H}$ is a symmetrical one, its eigenvalues must be three double roots, which is the same conclusion that is obtained by applying the analysis of the group theory. Let E represent the eigenvalue of $\boldsymbol{H}$, proceed as in Ref. [12], the characteristic polynomial of the 6×6 symmetrical determinant $|\boldsymbol{H}|$ can then be reduced to the following cubic characteristic polynomial:

$$E^3+pE^2+qE+r=0, \quad (5)$$

with

$$\begin{aligned} p &= \Delta-(a_{11}+a_{22}+a_{33}),\\ q &= a_{11}a_{22}+a_{22}a_{33}+a_{33}a_{11}-a_{12}^2-a_{13}^2-a_{23}^2\\ &\quad -\frac{2}{3}\Delta(a_{11}+a_{22}+a_{33}),\\ r &= a_{11}a_{23}^2+a_{22}a_{13}^2+a_{33}a_{12}^2-a_{11}a_{22}a_{33}\\ &\quad -2a_{12}a_{23}a_{13}+\frac{1}{3}\Delta(a_{11}a_{22}+a_{22}a_{33}\\ &\quad +a_{33}a_{11}-a_{12}^2-a_{13}^2-a_{23}^2), \end{aligned}$$

where a_{ij} (i, j = 1,2,3) are elements of $\boldsymbol{H}'+\boldsymbol{H}''$, which can be given as

$$a_{ij}=\begin{cases} Lk_x^2+M(k_y^2+k_z^2)+l\varepsilon_{xx}+m(\varepsilon_{yy}+\varepsilon_{zz}), & \text{for } i=j,\\ Nk_xk_y+n\varepsilon_{xy}, & \text{for } i\neq j. \end{cases}$$

Next, in order to facilitate the mathematical modeling, we should process the cubic characteristic polynomial carefully. By making the substitution

$$E'=E+\frac{1}{3}p=z-\frac{1}{3z}\left(q-\frac{1}{3}p^2\right),$$

equation (5) becomes

$$z^6+Az^3+B^3=0, \quad (6)$$

where

$$A=\frac{2}{27}p^3-\frac{1}{3}pq+r,\ B=-\frac{1}{3}\left(q-\frac{p^2}{3}\right).$$

If z is replaced by u, equation (6) can then be treated as a quadratic equation of u^3, and we can obtain

$$u^3=-\frac{1}{2}A+\sqrt{\frac{1}{4}A^2-B^3}. \quad (7)$$

Note that $\omega^3=1$, the three cube roots of Eq. (7) can be written as u, $u\omega^2$, and $u\omega^3$, where

$$\omega=\frac{-1+\mathrm{i}\sqrt{3}}{2},\qquad \omega^2=\frac{-1-\mathrm{i}\sqrt{3}}{2}.$$

With the purpose of using $E'=u+B/u$ mentioned above to find E', B/u should be solved first. After a complex calculation, it is found that B/u is a cube root of

$$-\frac{1}{2}A+\sqrt{\frac{1}{4}A^2-B^3}.$$

We should choose the cube root that multiplied by u equals B, and it will be denoted as v. We then have

$$E_1'=u+\frac{B}{u}=u+v, \quad (8)$$

$$E_2'=u\omega+\frac{B}{u\omega}=u\omega+v\omega^2, \quad (9)$$

$$E_3'=u\omega^2+\frac{B}{u\omega^2}=u\omega^2+v\omega, \quad (10)$$

where u and v are the cube roots of

$$-\frac{1}{2}A\pm\sqrt{\frac{1}{4}A^2-B^3}.$$

The eigenvalue of $\boldsymbol{H}$ must be a real number. Note that $A^2<4B^3$, hence cube roots u and v are both imaginary numbers, and u and v are conjugate complex, since the following equation holds:

$$u\bar{u}=|u|^2=uv.$$

The two cube roots can be consequently rewritten as $u=a+\mathrm{i}b$ and $v=a-\mathrm{i}b$. Equations (8)–(10) are then respectively expressed as

$$E_1'=u+v=2a, \quad (11)$$

$$E_2' = -\frac{1}{2}(u+v) + \mathrm{i}\frac{\sqrt{3}}{2}(u-v) = -a - b\sqrt{3}, \quad (12)$$

$$E_3' = -\frac{1}{2}(u+v) - \mathrm{i}\frac{\sqrt{3}}{2}(u-v) = -a + b\sqrt{3}. \quad (13)$$

Based on the above mathematical procedure, u and v can be obtained by using the CAD tools. In simultaneous Eqs. (8)–(13), the real part a and the imaginary part b can be extracted from

$$\begin{cases} u = a + \mathrm{i}b = |u|\,(\cos\theta + \mathrm{i}\sin\theta), \\ u^n = |u|^n\,(\cos n\theta + \mathrm{i}\sin n\theta), \end{cases} \quad (14)$$

or

$$\begin{cases} v = a - \mathrm{i}b = |v|\,(\cos\theta - \mathrm{i}\sin\theta), \\ v^n = |v|^n\,(\cos n\theta - \mathrm{i}\sin n\theta), \end{cases} \quad (15)$$

where θ is the angle of the amplitude. Then we make the substitution of $E = E' - p/3$, the $E(\boldsymbol{k})$–$\boldsymbol{k}$ relationship of the strained Ge/(001)$Si_{1-x}Ge_x$ is finally given by the following expressions:

$$E_{\mathrm{V}}^1 = 2\left(\frac{p^2-3q}{9}\right)^{1/2}\cos\left(\frac{1}{3}\arccos\left(-\frac{(2p^3-9pq+27r)/54}{((p^2-3q)/9)^{3/2}}\right)\right) - \frac{p}{3}, \quad (16)$$

$$E_{\mathrm{V}}^2 = 2\left(\frac{p^2-3q}{9}\right)^{1/2}\cos\left(\frac{1}{3}\arccos\left(-\frac{(2p^3-9pq+27r)/54}{((p^2-3q)/9)^{3/2}}\right) - \frac{2}{3}\pi\right) - \frac{p}{3}, \quad (17)$$

$$E_{\mathrm{V}}^3 = 2\left(\frac{p^2-3q}{9}\right)^{1/2}\cos\left(\frac{1}{3}\arccos\left(-\frac{(2p^3-9pq+27r)/54}{((p^2-3q)/9)^{3/2}}\right) + \frac{2}{3}\pi\right) - \frac{p}{3}. \quad (18)$$

3. Results and discussion

3.1. CASTEP simulation

In order to certify the accuracy and the applicability, we investigate the band structure of the biaxially strained Ge on (001) $Si_{1-x}Ge_x$ substrate using the Cambride Serial Total Energy Package (CASTEP) approach, where the first-principles simulations from the density functional theory with plane waves and pseudopotentials are involved.[13] In the plane of the strained-Ge/relaxed $Si_{1-x}Ge_x$ interface, the strained Ge film needs to adopt the lattice structure of the $Si_{1-x}Ge_x$ substrate. So the lattice periodicity is preserved under such a strain and the CASTEP calculation on the strained film is valid. The cell structure used for the simulation is shown in Fig. 1, where a, b and c correspond to the modified lattice parameters given by

$$\begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} \frac{0.04(1-x)}{1.332}+1 & 0 & 0 \\ 0 & \frac{0.04(1-x)}{1.332}+1 & 0 \\ 0 & 0 & 0.04(1-x)+1 \end{bmatrix} \times \begin{bmatrix} a_0 \\ a_0 \\ a_0 \end{bmatrix}, \quad (19)$$

and $a = 5.6579$ denotes the lattice constant of the relaxed Ge.

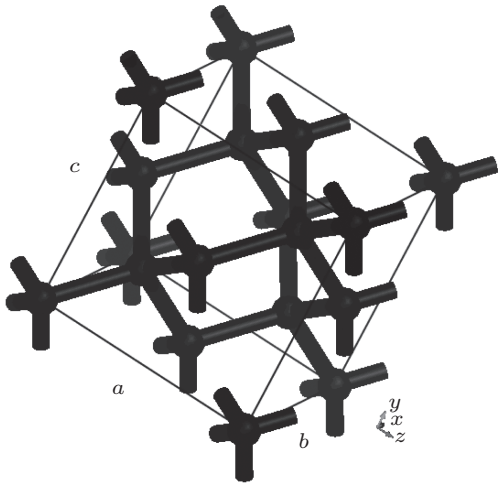


Fig. 1. Modified cell structure of strained Ge in the CASTEP simulation.

The simulation steps are briefly summarized as follows: (i) employ the exchange–correlation potential in the local density approximation (LDA) for the electron–electron interaction, (ii) perform the integration in the Brillouin zone using special $\boldsymbol{k}$ point produced by a 5×5×5 mesh parameter grid, (iii) expand a certain electron valence state in a basis of plane waves with a cutoff energy of 180 eV, (iv) introduce the strained structure determined by such parameters which have been tested to be sufficient for convergence into the energy band calculation. The band structures of the strained Ge on (001) relaxed Si_xGe_{1-x} with the Ge fraction ranging from $x = 0.6$ to 1 are then simulated. Figure 2 exhibits the band structure with $x = 0.6$. We

can see that the first and the second valence bands split at the Γ point.

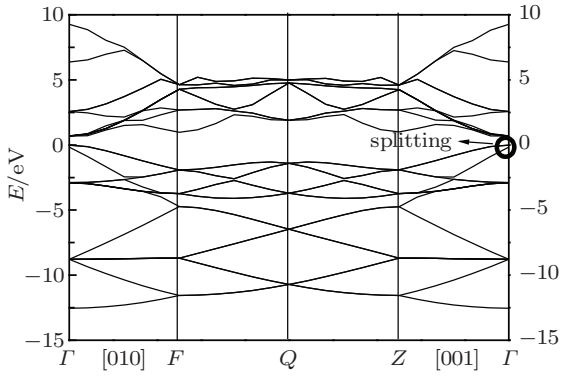


Fig. 2. CASTEP-simulated band structure with $x = 0.6$. The band splitting is found at the Γ point.

In order to compare with the splitting energy between the first and the second bands obtained by the analytical model, we use the same simulation procedure mentioned above to compute the band structures with $x = 0.7$, 0.8, 0.9, 1, and extract the splitting energies. The extracted data are plotted in Fig. 4 for a clear comparison with the calculated ones in our model. The extracted splitting energies between the two bands can be fitted to a function of x as

$$E_{\text{split}}(x) = -0.215x + 0.215. \tag{20}$$

It should be mentioned that the splitting energy extracted from CASTEP is smaller than that obtained from the analytical model. This may be caused by the density functional theory (DFT), which is commonly used in first-principles simulation algorithms. In unstrained (relaxed) semiconductors, the DFT can be fitted well with the band structure simulation, while in the strained Ge, the DFT algorithm does not seem to be modified although the lattice parameters are altered. In any case, the simulated band structure still provides a more reliable comparison with the analytical result, and therefore, the simulation data of the splitting energy can give an indirect certification for the accuracy of our analytical model.

3.2. Model calculation

The valence band of the strained Ge/(001)$Si_{1-x}Ge_x$ can be calculated by using Eqs. (16)–(18). The valence band edges (energy levels at the Γ point) versus Ge fraction x in strained Ge/(001)$Si_{1-x}Ge_x$ are shown in Fig. 3. Note that the splitting between the first and the second valence bands occurs as the Ge fraction decreases. As x decreases, the first band edge E_{V}^1 shifts up, i.e., $E > 0$, while the second band edge E_{V}^2 shifts down ($x = 1$ corresponds to the relaxed Ge), which is attributed to the fact that the crystal symmetry determines the symmetry of the band structure. When the biaxial strain caused by (001) $Si_{1-x}Ge_x$ substrate is applied to the Ge crystal, the crystal symmetry is broken, making the crystal structure of Ge transform from the cubic system to the orthorhombic one, thus the crystal symmetry is lowered, which causes the band shift and splitting.

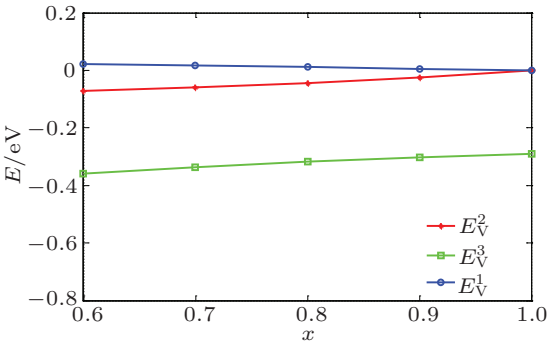


Fig. 3. (colour online) Valence band edges versus Ge fraction x in strained Ge/(001)$Si_{1-x}Ge_x$.

In view of the applications and the efficient design of strained Ge devices, from the above obtained valence band $E(\boldsymbol{k})$–$\boldsymbol{k}$ relationship, we can calculate the strain-induced energy level shift and split at the Γ point. The splitting energy between the first and the second bands at $\boldsymbol{k} = 0$ is plotted as a function of x, which is shown in Fig. 4. It is clearly found that the splitting energy between the two bands increases as Ge fraction x decreases, which is favorable for suppressing the interband scattering. Hence, it can be seen that the biaxial compressive stress is more significant in terms of the reduced scattering and the enhanced hole mobility.

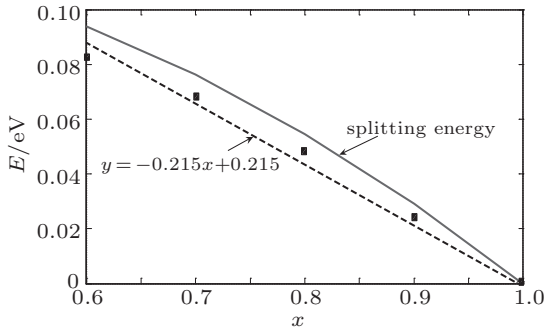


Fig. 4. Valence band splitting energy versus Ge fraction x in strained Ge/(001)$Si_{1-x}Ge_x$.

The valence band structures along the [0, 0, k] and the [k, 0, 0] directions in the strained Ge/(001) $Si_{0.4}Ge_{0.6}$ and the relaxed Ge are shown in Figs. 5 and 6, respectively. Figure 6 shows that the valence band edge at the Γ point (i.e. $k = 0$) is degenerate. Figure 5 shows that the bandedge degeneracies at the Γ point are partially lifted. When the biaxial strain is applied, the splitting between the first and the second valence bands caused by the strain occurs. In addition, the band splitting leads to band warpings along the [0, 0, k] and the [k, 0, 0] directions. Under the biaxial compressive stress imposed by the (001) $Si_{0.4}Ge_{0.6}$ substrate, the crystal structure of the Ge epitaxial layer changes, which also leads to a lower symmetry, and hence lifts the band edge degeneracy.

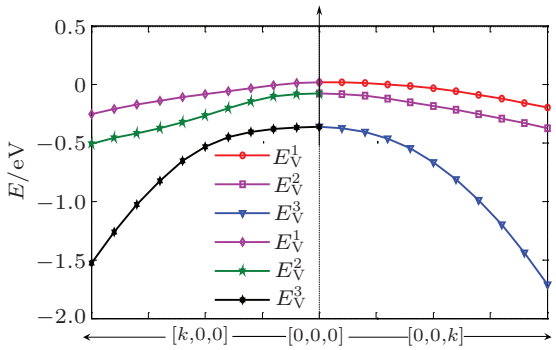


Fig. 5. (colour online) Valence band structures along [k, 0, 0] and [0, 0, k] directions in strained Ge/(001)$Si_{0.4}Ge_{0.6}$.

The three-dimensional (3D) equienergy surface of the valence band provides a straightforward picture for the conductivity effective mass of each band. The effective mass change with the strain can also be seen from the shape change of the equienergy surface. To evidence the modification of the valence band warping, the 40 meV ($\sim 3k_BT/2$) 3D equienergy surfaces of the first and the second bands in the strained Ge/(001) $Si_{1-x}Ge_x$ are shown in Fig. 7. The shape of the 3D equienergy surface of the first band E_V^1 changes more significantly with Ge fraction x decreasing from $x = 0.8$ to $x = 0.6$, which means that the variations of all directional hole effective masses in the strained Ge/(001)$Si_{0.4}Ge_{0.6}$ and the strained Ge/ (001)$Si_{0.2}Ge_{0.8}$ are clearly reflected. It should be noted that the Ge fraction-dependent biaxial strain has little influence on the shape of the second band E_V^2. This may explain why the strained Ge has larger hole mobility.

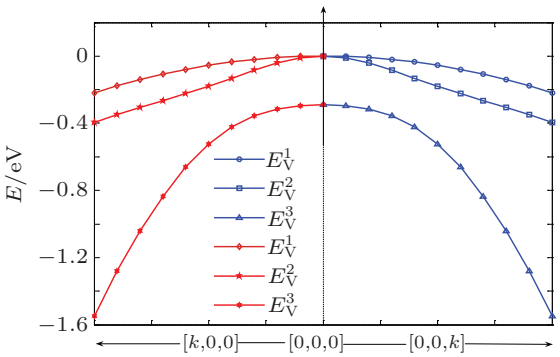


Fig. 6. (colour online) Valence band structures along [k, 0, 0] and [0, 0, k] directions in relaxed Ge.

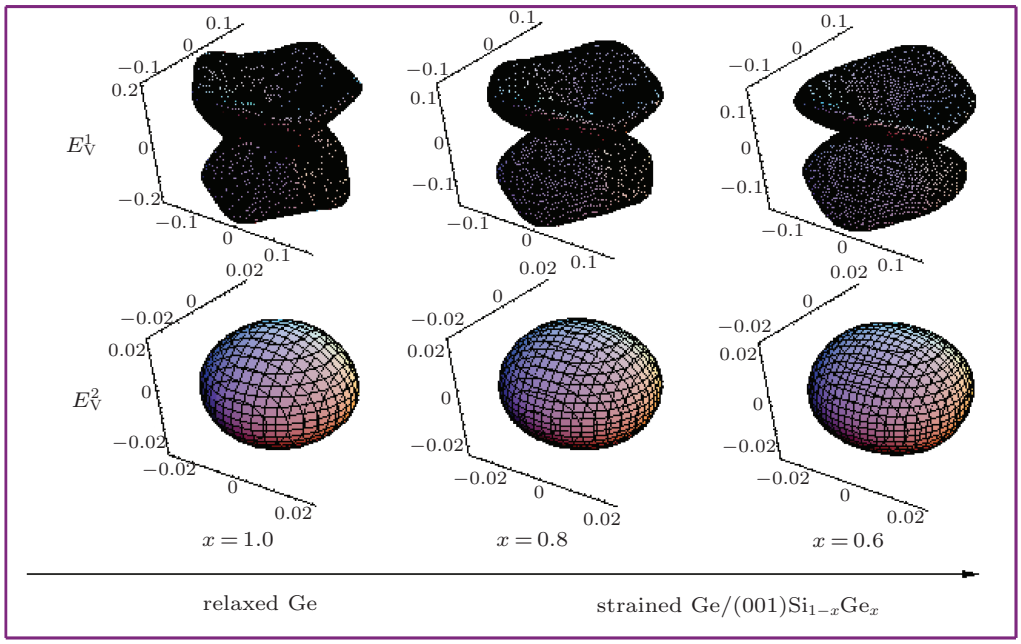


Fig. 7. (colour online) The 40 meV 3D equienergy surfaces of the first and the second bands in relaxed and strained Ge.

4. Summary

The strained Ge is a next-generation MOSFET channel material that has the potential for overcoming the limit of Si-MOSFET performance enhancement. We focus on the analytical modeling of the $E(\boldsymbol{k})$–$\boldsymbol{k}$ relationship for the valence band in the strained Ge/(001) $Si_{1-x}Ge_x$. The $E(\boldsymbol{k})$–$\boldsymbol{k}$ relationship is derived by using the $\boldsymbol{k}\cdot\boldsymbol{p}$ method with the help of the perturbation theory.

The parameters of the valence band in the strained Ge/(001)$Si_{1-x}Ge_x$ are calculated from the obtained $E(\boldsymbol{k})$–$\boldsymbol{k}$ relationship. From the results obtained by our analytical model, it is found that the splitting of the first and the second valences band occurs under the action of strain, and the splitting energy is a nonlinear function of Ge fraction x. The first valence band edge shifts up in electron energy as the Ge fraction decreases, while the second valence band edge shifts down. From a comparison of band structure between the strained Ge/(001)$Si_{0.4}Ge_{0.6}$ and the relaxed Ge, we can deduce the significant changes in the hole effective masses along the [0, 0, k] and the [k, 0, 0] directions. Moreover, our analytical results of the splitting energy accord with the CASTEP-extracted results. The quantitative results obtained in this work can provide valuable theoretical references to the understanding of the strained Ge materials and the conduction channel design related to strain and orientations in the strained pMOSFETs.

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