Valence band structure and density of states effective mass model of biaxial tensile strained silicon based on $k \cdot p$ theory*

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After constructing a stress and strain model, the valence bands of in-plane biaxial tensile strained Si is calculated by $k \cdot p$ method. In the paper we calculate the accurate anisotropy valance bands and the splitting energy between light and heavy hole bands. The results show that the valance bands are highly distorted, and the anisotropy is more obvious. To obtain the density of states (DOS) effective mass, which is a very important parameter for device modeling, a DOS effective mass model of biaxial tensile strained Si is constructed based on the valance band calculation. This model can be directly used in the device model of metal–oxide semiconductor field effect transistor (MOSFET). It also a provides valuable reference for biaxial tensile strained silicon MOSFET design.

Keywords: biaxial tensile strained Si, $k \cdot p$ theory, valance band, density of state effective mass

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1. Introduction

In recent decades, the dimension of metal–oxide semiconductor field effect transistor (MOSFET) has been scaling down constantly to improve device performance and lower device cost, which not only keeps the exponential growth with time in the number of transistors per unit area following Moore's law, but also improves the transistor performance. As complementary metal–oxide semiconductor (CMOS) technology progresses into the nanometer regime, the gate dielectric thickness is gradually reduced down to 1 nm. Physical limits, such as the off-state leakage, the increment of power density and mobility degradation, deteriorate device performance, so scaling technology faces ever more serious challenges. For further scaling, new technology to improve transistor performances is needed. At present, strained silicon technology is widely used.[1−8]

During the last 20 years, the investigation on strained silicon focused mainly on the substrate induced biaxial strain and fabricating silicon layer on the relaxed SiGe buffer layer. The Si elastic deformation occurred due to the lattice mismatch between Si and SiGe. The lattice constant in the direction parallel to the substrate changes and is the same as that of SiGe. The lattice constant of SiGe is larger than that of Si, so the biaxial tensile strain is imposed on Si in the direction parallel to the substrate. The energy band of Si splits up under strain, which reduces the scattering between the energy valley and effective mass, so the carrier mobility is improved. The biaxial stress which can be applied to positive channel metal–oxide semiconductor (PMOS) and N metal–oxide semiconductor (NMOS) is produced, thereby improving the performances of both PMOS and NMOS devices. For modeling and simulating the biaxial tensile strain device, the accurate density of states (DOS) effective mass must be obtained. In order to obtain the accurate result, a lot of work has been done. In Refs. [9]–[11] the effective mass in some typical direction in Brillouin zone was calculated by $k \cdot p$ theory, however the DOS effective mass was not researched there. In Ref. [12] the heavy and the light hole density of states effective masses were calculated, where strain tensor model was different from here and the effective mass is shown as a function of biaxial in-plane strain, furthermore the total density of states effective mass was not researched there either. In the present work, the model of DOS

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effective mass of biaxial tensile strain is established by $k \cdot p$ theory based on the energy band structure calculation of biaxial tensile strained silicon, which can be directly used to model biaxial tensile strained MOS device.

2. Strain tensor model

Strain, a mechanical quantity which is used to describe the degree of deformation at a point, exhibits a strain tensor with three-dimensional coordinates. The constitutive equation of anisotropic elastic material after the generalized Hooke's law is expressed as follows:

$$\begin{aligned}
\sigma_{xx} &= C_{11}\varepsilon_{xx} + C_{12}\varepsilon_{xy} + C_{13}\varepsilon_{zz} \\
&\quad + C_{14}\varepsilon_{yz} + C_{15}\varepsilon_{zx} + C_{16}\varepsilon_{xy}, \\
\sigma_{yy} &= C_{21}\varepsilon_{xx} + C_{22}\varepsilon_{xy} + C_{23}\varepsilon_{zz} \\
&\quad + C_{24}\varepsilon_{yz} + C_{25}\varepsilon_{zx} + C_{26}\varepsilon_{xy}, \\
\sigma_{zz} &= C_{31}\varepsilon_{xx} + C_{32}\varepsilon_{xy} + C_{33}\varepsilon_{zz} \\
&\quad + C_{34}\varepsilon_{yz} + C_{35}\varepsilon_{zx} + C_{36}\varepsilon_{xy}, \\
\sigma_{yz} &= C_{41}\varepsilon_{xx} + C_{42}\varepsilon_{xy} + C_{43}\varepsilon_{zz} \\
&\quad + C_{44}\varepsilon_{yz} + C_{45}\varepsilon_{zx} + C_{46}\varepsilon_{xy}, \\
\sigma_{zx} &= C_{51}\varepsilon_{xx} + C_{52}\varepsilon_{xy} + C_{53}\varepsilon_{zz} \\
&\quad + C_{54}\varepsilon_{yz} + C_{55}\varepsilon_{zx} + C_{56}\varepsilon_{xy}, \\
\sigma_{xy} &= C_{61}\varepsilon_{xx} + C_{62}\varepsilon_{xy} + C_{63}\varepsilon_{zz} \\
&\quad + C_{64}\varepsilon_{yz} + C_{65}\varepsilon_{zx} + C_{66}\varepsilon_{xy}, \qquad (1)
\end{aligned}$$

where factors C_{11} and C_{12} are the elastic constants of the material. Taking the symmetry of silicon into account, the number of coefficients can be reduced to three, which has been proved in detail in Refs. [13] and [14]. The simplified result is shown as follows:

$$\begin{aligned}
&\sigma_{xx} = C_{11}\varepsilon_{xx} + C_{12}\varepsilon_{yy} + C_{12}\varepsilon_{zz}, \\
&\sigma_{yy} = C_{12}\varepsilon_{xx} + C_{22}\varepsilon_{yy} + C_{12}\varepsilon_{zz}, \\
&\sigma_{zz} = C_{12}\varepsilon_{xx} + C_{12}\varepsilon_{yy} + C_{33}\varepsilon_{zz}, \\
&\sigma_{yz} = C_{44}\varepsilon_{yz}, \sigma_{zx} = C_{44}\varepsilon_{zx}, \sigma_{xy} = C_{44}\varepsilon_{xy}. \qquad (2)
\end{aligned}$$

There are only three elastic coefficients namely C_{11}, C_{12}, and C_{44}, owing to the symmetry in silicon. The strain intensity can be expressed by using stress through solving the above equations, as

$$\begin{aligned}
\varepsilon_{xx} &= \frac{C_{11}+C_{12}}{(C_{11}-C_{12})(C_{11}+C_{12})}\sigma_{xx} \\
&\quad - \frac{C_{12}}{(C_{11}-C_{12})(C_{11}+C_{12})}(\sigma_{yy}+\sigma_{zz}), \\
\varepsilon_{yy} &= \frac{C_{11}+C_{12}}{(C_{11}-C_{12})(C_{11}+C_{12})}\sigma_{yy} \\
&\quad - \frac{C_{12}}{(C_{11}-C_{12})(C_{11}+C_{12})}(\sigma_{xx}+\sigma_{zz}), \\
\varepsilon_{zz} &= \frac{C_{11}+C_{12}}{(C_{11}-C_{12})(C_{11}+C_{12})}\sigma_{zz} \\
&\quad - \frac{C_{12}}{(C_{11}-C_{12})(C_{11}+C_{12})}(\sigma_{xx}+\sigma_{yy}), \\
\varepsilon_{xy} &= \frac{1}{C_{44}}\sigma_{xy}, \quad \varepsilon_{zx} = \frac{1}{C_{44}}\sigma_{zx}, \quad \varepsilon_{yz} = \frac{1}{C_{44}}\sigma_{yz}. \qquad (3)
\end{aligned}$$

3. Energy band and density of states effective mass model

The $k \cdot p$ theory is a method of calculating the energy band, developed from perturbation theory, which was proposed first by Shockley and Bardeen.[15] Dresselhaus *et al.*[16] clearly showed the six-band Hamiltonian taking the spin–orbit coupling into account in 1954, and determined the parameters of the Hamiltonian in Si and Ge by cyclotron resonance experiments, which gave the first analytical expression for the valence band peak of silicon through theoretical calculation. It has still been used in recent years. In 1955, Luttinger and Kohn presented the $k \cdot p$ Hamiltonian with other parameters,[17] which is widely cited due to being easy to add various perturbations into it.

The total Hamiltonian in strained silicon is shown as

$$H = H_{k\cdot p} + H_{\text{s.o.}} + H_{\text{strain}}. \qquad (4)$$

In fact, $H_{k\cdot p}$ and $H_{\text{s.o.}}$ are rarely used alone. We mainly use the form of sum after diagonalization, that is, $H'_{k\cdot p} = H_{k\cdot p} + H_{\text{s.o.}}$ Used here in the calculation is the Hamiltonian given by Luttinger and Kohn,[17] as shown in Eq. (5).

$$H'_{k\cdot p} = \begin{bmatrix}
-P-Q & L & -M & 0 & (1/\sqrt{2})L & -\sqrt{2}M \\
L^* & -P+Q & 0 & -M & \sqrt{2}Q & -\sqrt{3/2}L \\
-M^* & 0 & -P+Q & -L & -\sqrt{3/2}L & -\sqrt{2}Q \\
0 & -M^* & -L^* & -P-Q & \sqrt{2}M^* & -(1/\sqrt{2})L^* \\
(1/\sqrt{2})L^* & \sqrt{2}Q^* & -\sqrt{3/2}L & \sqrt{2}M & -P-\Delta & 0 \\
-\sqrt{2}M^* & -\sqrt{3/2}L^* & -\sqrt{2}Q^* & (1/\sqrt{2})L & 0 & -P-\Delta
\end{bmatrix}, \qquad (5)$$

where $p = \dfrac{\hbar^2}{2m_0}\gamma_1(k_x^2+k_y^2+k_z^2)$, $Q = \dfrac{\hbar^2}{2m_0}\gamma_2(k_x^2+k_y^2-2k_z^2)$, $L = \dfrac{\hbar^2}{m_0}\sqrt{3}\gamma_3(k_x - \mathrm{i}\,k_y)k_z$, and

$$M = -\frac{\hbar^2}{2m_0}\sqrt{3}[\gamma_2(k_x^2-k_y^2) - 2\,\mathrm{i}\,\gamma_3 k_x k_y].$$

The Hamiltonian caused by strain is shown in Eq. (6)

$$H_{\text{strain}} = \begin{bmatrix} H'' & 0_{3\times3} \\ 0_{3\times3} & H'' \end{bmatrix} \begin{matrix} x,y,z\uparrow \\ x,y,z\downarrow \end{matrix}, \tag{6}$$

where

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

Based on $k\cdot p$ theory, the biaxial strained silicon valence band structure is obtained by solving the matrix eigenvalues of the total Hamilton. Based on the energy band calculation, the density of states effective masses of heavy and light holes can be obtained respectively using the following equation:

$$\left(\frac{m_p^*}{m_0}\right)^{3/2} = \frac{\hbar^3}{(2\pi m_0 k_{\mathrm{B}}T)^{3/2}}\frac{1}{(2\pi)^3} \times \int \exp\left[-\frac{E(k)}{k_{\mathrm{B}}T}\right]\mathrm{d}k. \tag{7}$$

Because of the splitting of the heavy and the light hole bands, the effective density of states effective mass of the valence band can be expressed as

$$(m_{\text{effective}})^{3/2} = (m_{\text{pH}}^*)^{3/2} + (m_{\text{pL}}^*)^{3/2} \times \exp\left(\frac{\Delta E_{\text{split}}}{k_0 T}\right). \tag{8}$$

Values of parameters used in the energy band calculation are listed in Table 1.

Table 1. Values of parameters in calculation.

	γ_1	γ_2	γ_3	a/eV	b/eV	d/eV
Si	4.22	0.39	1.44	2.46	-2.1	-4.8

4. Results and discussion

Figure 1 shows the energy band diagram along the directions of [001] and [110] at 1-GPa biaxial tensile strained Si. The heavy and light holes split up under biaxial tensile strain—the heavy hole energy band goes up and the light hole energy band comes down. At the same time, the effective mass of strained Si along [001] and [110] changes a lot with energy band distortion, and "heavy hole" loses its original meaning. "Heavy hole" effective mass (m_{HH}) becomes less than "light hole" effective mass (m_{LH}) with stress further increasing.

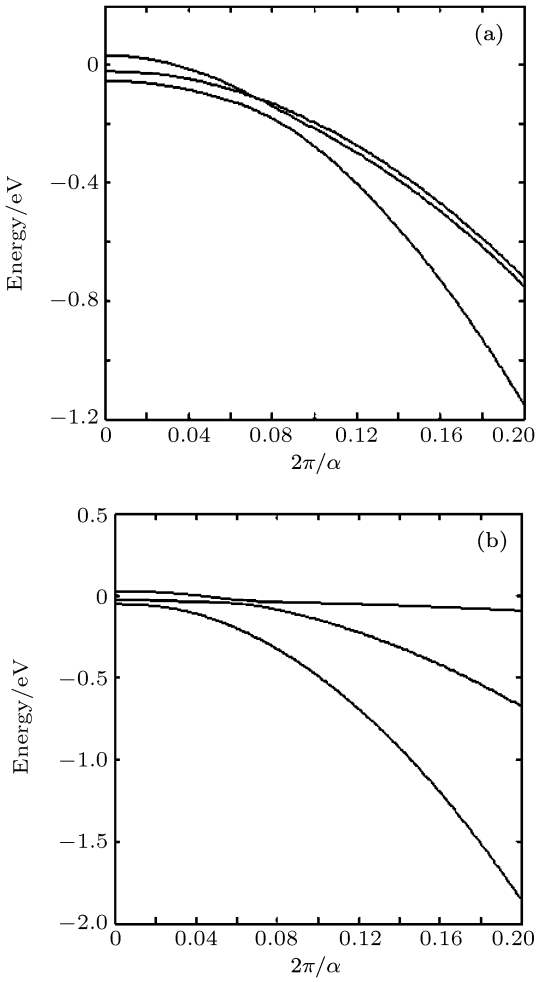


Fig. 1. Energy band diagrams along the directions of (a) [001] and (b) [110] at 1-GPa biaxial tensile strained Si.

The effective masses along [001] are $m_{\rm HH} = 0.1773m_0$, $m_{\rm LH} = 0.2907m_0$, and $m_{\rm Slit} = 0.1540m_0$; the effective masses along [110] are $m_{\rm HH} = 0.2849m_0$, $m_{\rm LH} = 0.2170m_0$, and $m_{\rm Slit} = 0.1097m_0$. Here, $m_{\rm Slit}$ is the effective mass corresponding to the spin–orbit coupling energy level. It can be ignored in the density of states effective mass calculation because the spin–orbit coupling energy of silicon is about 0.04 eV.

The anisotropy in the valence band structure of strained Si under biaxial tensile strain is shown in Fig. 2. We can see that the anisotropy of the energy band structure is still obvious under in-plane biaxial tensile strain. Figure1 also clearly shows that the valence band peak cannot be approximated by a spherical constant energy surface, and density of states effective mass must be calculated by numerical methods. For further understanding the anisotropy of valence band structure, figure 3 shows the calculation result of constant energy surface in k_x–k_y plane and the anisotropy of effective mass.

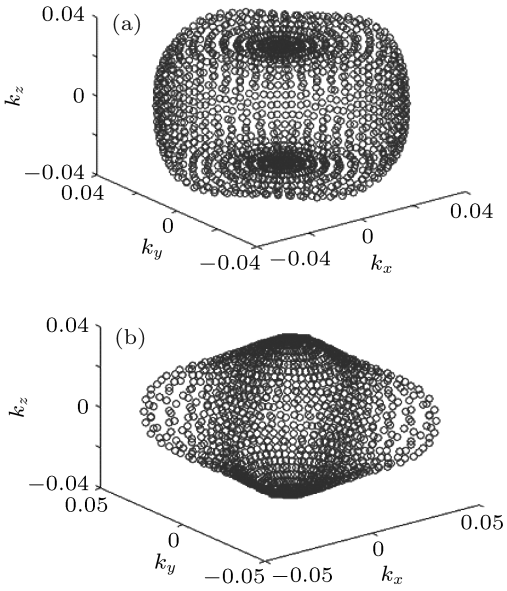


Fig. 2. Energy band structure of strained silicon under 1-GPa in-plane tensile stress, where panel (a) shows the 25-meV heavy hole constant energy surface, and panel (b) the 25-meV light hole constant energy surface.

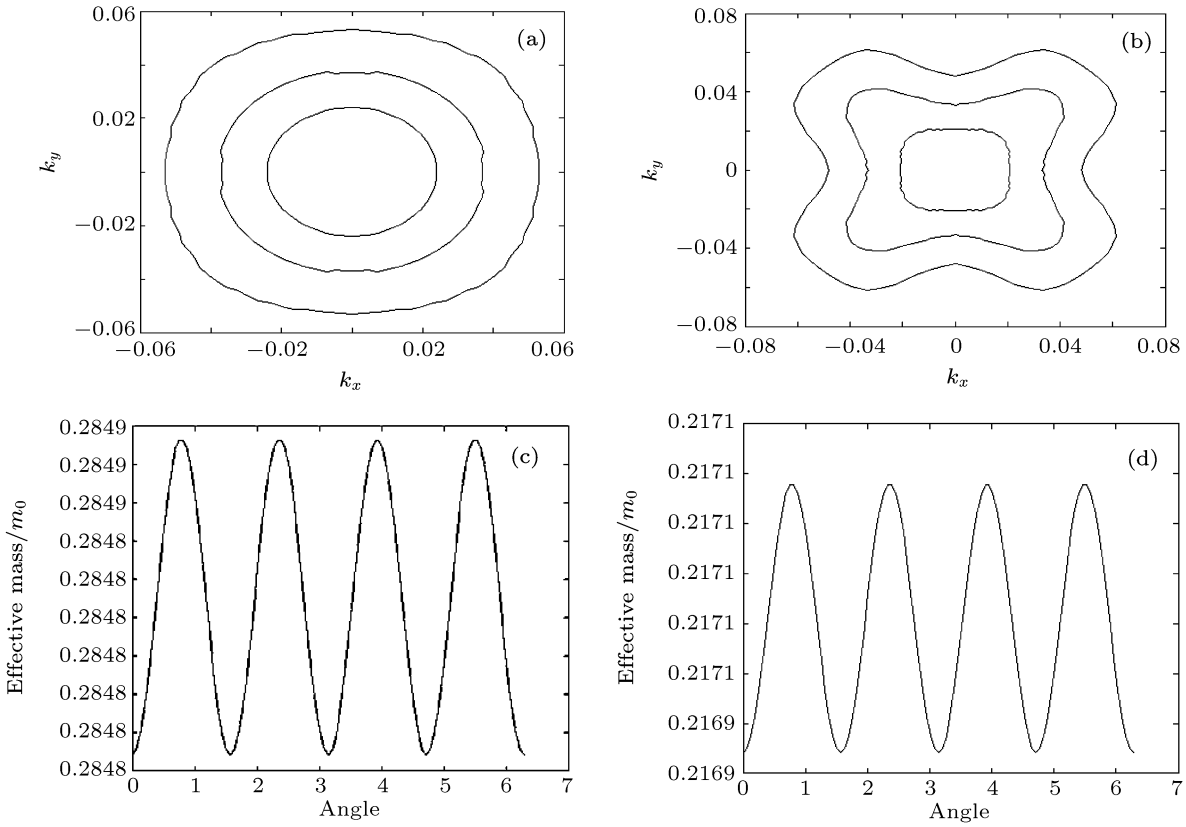


Fig. 3. Energy band structures of strained silicon under 1-GPa in-plane tensile stress, where panel (a) shows the constant energy surface in k_x–k_y plane of heavy hole, and panel (b) the constant energy surface in k_x–k_y plane of light hole, panel (c) the variation of effective mass of heavy hole with angle in k_x–k_y plane, and panel (d) the variation of effective mass of light hole with angle in k_x–k_y plane.

Figure 4 shows the variations of the splitting energy of the heavy and light holes with in-plane biaxial tensile strain. Due to the splitting of heavy and light holes, the calculation of the density of states effective mass becomes more complicated.

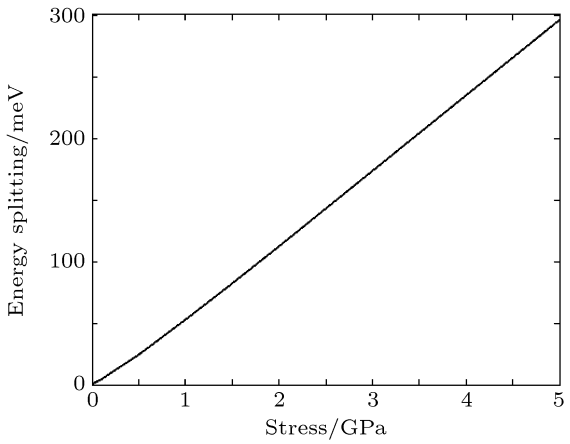


Fig. 4. Variations of the splitting energy of the heavy and light holes with strain.

The energy band calculation shows that the valence band is obviously anisotropic after strain, and the splitting of heavy and light hole bands grows with increasing stress. The complexity of the valence band makes it difficult to obtain the density of states effective mass, and the accuracy of energy band calculation will directly be related to the acquisition of the density of states effective mass. The calculation of effective mass in a typical direction proves that the energy band structure calculated in this paper exactly coincides with that reported in Refs. [9]–[11]. Table 2 and Table 3 show the comparisons of the effective mass in a typical direction and the splitting energy of "heavy hole and light hole" energy levels respectively, which proves that the energy band calculation results in this paper are correct and can be used to calculate the density of states effective mass.

Table 2. Effective mass in typical direction.

	[001] "heavy hole"	[001] "light hole"	[110] "heavy hole"	[110] "light hole"
This paper	$0.1773m_0$	$0.2907m_0$	$0.2849m_0$	$0.2170m_0$
Ref. [12]	$0.18m_0$	$0.29m_0$	$0.28m_0$	$0.23m_0$

Table 3. Splitting energy of heavy hole and light hole energy levels (meV).

Stress/GPa	0.1	0.5	1.0	2.0
This paper	4.3080	24.2876	52.4553	112.0987
Ref. [10]	4.5	24.40	55.60	116.20

Substituting the energy band calculated into Eq. (7), we can obtain the heavy hole and light hole density of states effective masses in the valence band under biaxial tensile strain, which are shown in Fig. 5.

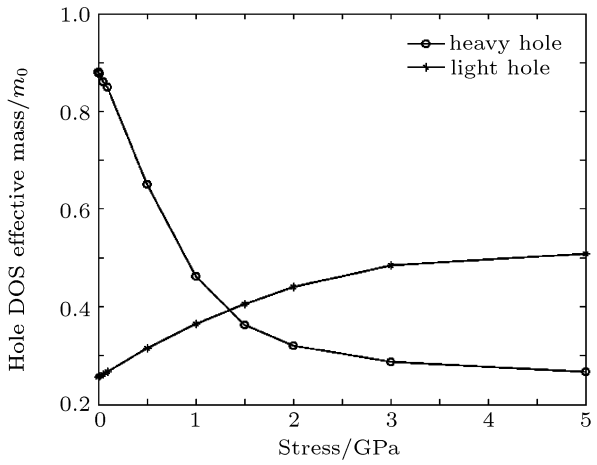


Fig. 5. Variations of hole effective mass for biaxial strained silicon with stress, where the solid symbol represents light hole density of states effective mass, and the open symbol denotes heavy hole density of states effective mass.

The heavy hole density of states effective mass decreases with increasing stress: it is even less than the light hole density of states effective mass when the stress is larger than 1.5 GPa. The light hole density of states effective mass increases with stress, and then tends to a steady value.

To facilitate device modeling, the density of states effective mass is fitted into the form of function

$$m_{\mathrm{DOS}}(s) = 0.0019x^4 - 0.0350x^3 + 0.2099x^2 - 0.4840 + 0.9763 \quad (0 < x < 5\ \mathrm{GPa}). \quad (9)$$

Corresponding changes to the formula can be directly used to device modeling. Figure 6 shows the variation of density of states effective mass with stress. The densities of states effective mass sharply reduces when the stress is 0 GPa–1.5 GPa because the energy band distortion causes a significant change in the density of states effective mass for the stress in this region. The decrease of heavy hole density of states effective mass is more obvious, while the rise of light hole density of states effective mass is smaller than the decline in heavy hole, so is the splitting of heavy and light hole energy levels, which makes the density of states effective mass slightly increase with further increase in stress, and gradually becomes a stable value, which is attributed to the fact that the heavy and the light hole densities of states effective masses tend to stable

values with increasing stress.

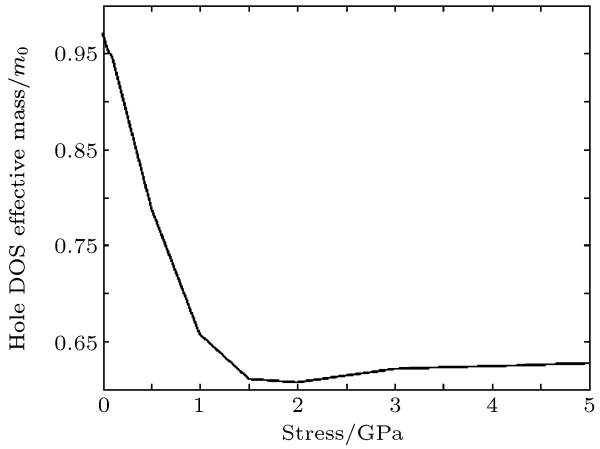


Fig. 6. Variation of density of states effective mass with stress.

5. Conclusion

In this paper, the valence band structure of in-plane biaxial tensile strained silicon is calculated by $k \cdot p$ theory. The heavy and light hole bands split up under strain, and the splitting increases with stress, meanwhile the anisotropy of effective mass is more obvious due to the distortions of heavy and light hole bands. To obtain a very important parameter in device modeling, a density of states effective mass model is established based on the results of accurate energy band calculation. Its accuracy is proved indirectly by comparing energy band structure and "heavy hole and light hole" densities of states effective masses with those reported in the relevant references. The model can be directly used for biaxial tensile strained silicon MOS device modeling.

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