SCIENCE CHINA
Physics, Mechanics & Astronomy

• Research Paper •

March 2010 Vol. 53 No.3: 454–457
doi: 10.1007/s11433-010-0093-2

Valence band structure of strained Si/(111)$Si_{1-x}Ge_x$

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Received June 8, 2009; accepted June18, 2009

The strained Si techique has been widely adopted in the high-speed and high-performance devices and circuits. Based on the valence band *E-k* relations of strained Si/(111)$Si_{1-x}Ge_x$, the valence band and hole effective mass along the [111] and [−110] directions were obtained in this work. In comparison with the relaxed Si, the valence band edge degeneracy was partially lifted, and the significant change was observed band structures along the [111] and [−110] directions, as well as in its corresponding hole effective masses with the increasing Ge fraction. The results obtained can provide valuable references to the investigation concerning the Si-based strained devices enhancement and the conduction channel design related to stress and orientation.

strained Si, KP method, valence band, hole effective mass

PACS: 71.20.–b, 71.70.Fk, 71.18.+y

Aggressive scaling of complementary metal-oxide-semiconductor (CMOS) technology is required so as to meet the International Technology Roadmap of Semiconductors projects in terms of circuit efficiency and device performance. However, to circumvent the downscaling difficulty and extend the lifetime of conventional silicon technology, novel architectures as well as materials are currently explored [1,2]. Engineering the band structure of semiconductor materials is an additional way to improve device performance. Such a material is the strained Si (s-Si) pseudomorphically grown on a relaxed $Si_{1-x}Ge_x$ substrate [3,4]. Many applications of devices fabricated using s-Si constitute a considerable enhancement of the presently well-established Si technology.

Significant change in band structure and carrier mobility enhancement of s-Si materials lead to the improvement of s-Si based devices performance. In particular, it is of great significance to investigate on the valence band structure of s-Si materials and its corresponding hole effective mass for the hole transport enhance understanding and device design. However, in-depth and systematic theoretical research on it lags behind its application. The familiar conclusions, i.e. the valence band edge degeneracy partially lifted and the decreasing hole mass with increasing stress in s-Si materials have been widely reported [5–7]. Although this conclusions appear correct in qualitative analysis on the physical phenomena of the carrier mobility enhancement in s-Si materials, it does not provide, however, valuable accuracy to the investigation in the Si-based strained devices enhancement and the conduction channel design related to stress and orientation.

In fact, the orientation of substrate used to the growth of s-Si materials and the anisotropy of the hole effective mass must be taken into account for the design of devices. Currently, no results for s-Si on (111) orientation were found. And hence, based on the valence band *E-k* relations of strained Si/(111)$Si_{1-x}Ge_x$, the valence band and hole effective mass along [111] and [−110] directions were obtained in this work, which can provide valuable references to the investigation in the Si-based strained devices enhancement and the conduction channel design related to stress and orientation.

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1 Physical model

The valence band structure of strained Si/(111)$Si_{1-x}Ge_x$ can be obtained by solving its corresponding *E-k* relations. The valence band along [111] and [−110] are our interesting in view of device design. Based on the dispersion relation model of valence band in Si-based strained materials (see ref. [8]), the *E-k* relations of valence band of strained Si/(111)$Si_{1-x}Ge_x$ below was obtained [8].

$$\begin{cases} E_V^1 = 2\sqrt{(p^2-3q)/9}\cos\left(\left(\cos^{-1}\left[(-2p^3+9pq-27r)\Big/(54\sqrt{(p^2-3q)^3/729})\right]\right)\Big/3\right)-\dfrac{p}{3}, \\ E_V^2 = 2\sqrt{(p^2-3q)/9}\cos\left(\left(\cos^{-1}\left[(-2p^3+9pq-27r)\Big/(54\sqrt{(p^2-3q)^3/729})\right]-2\pi\right)\Big/3\right)-\dfrac{p}{3}, \\ E_V^3 = 2\sqrt{(p^2-3q)/9}\cos\left(\left(\cos^{-1}\left[(-2p^3+9pq-27r)\Big/(54\sqrt{(p^2-3q)^3/729})\right]+2\pi\right)\Big/3\right)-\dfrac{p}{3}, \end{cases} \tag{1}$$

where E_V^1, E_V^2 and E_V^3 denote the energies of the first, second and third valance band respectively. *p*, *q* and *r* can be written below:

$$\begin{cases} p = 0.044-(a_{11}+a_{22}+a_{33}), \\ q = a_{11}a_{22}+a_{22}a_{33}+a_{33}a_{11}-a_{12}^2-a_{13}^2-a_{23}^2-(0.029)(a_{11}+a_{22}+a_{33}), \\ r = a_{11}a_{23}^2+a_{22}a_{13}^2+a_{33}a_{12}^2-a_{11}a_{22}a_{33}-2a_{12}a_{23}a_{13}+(0.014)\left(a_{11}a_{22}+a_{22}a_{33}+a_{33}a_{11}-a_{12}^2-a_{13}^2-a_{23}^2\right), \end{cases} \tag{2}$$

where $a_{ij}\,(i,j=1,2,3)$ is the element in matrix (3),

$$\begin{bmatrix} -29.4k_x^2-17.5\left(k_y^2+k_z^2\right)+0.154x & -44k_xk_y & -44k_zk_x \\ -44k_xk_y & -29.4k_y^2-17.5\left(k_z^2+k_x^2\right)+0.154x & -44k_yk_z \\ -44k_zk_x & -44k_yk_z & -29.4k_z^2-17.5\left(k_x^2+k_y^2\right)+0.57x \end{bmatrix}, \tag{3}$$

where, *x* is Ge fraction.

The directional dependences of effective masses can be calculated from the energy curvature in the usual manner [9] by

$$\frac{1}{\hbar^2}\left(\frac{\partial^2 E}{\partial k^2}\right)=\frac{1}{m_p^*}, \tag{4}$$

where m_p^* denote hole effective mass.

2 Results and discussion

The valence band structures along [111] and [−110] directions in strained Si/(111)$Si_{1-x}Ge_x$ (Ge fraction range from 0–0.4) were shown in Figures 1(a)–(e). Figure 1(a) shows that the valence band edge at Γ point (i.e. *k*=0) is degenerate. Figures 1(b)–(e) shows that the valence band edge degeneracies at Γ point are partially lifted and that the splitting energy between first and second valence band caused by strain increase with increasing Ge fraction (*x*). In addition, significant change in the hole effective mass along [111] and [−110] directions under strain occurs.

The decrease of hole effective mass plays a significant role in the hole mobility enhancement. And now turn to discuss it. The hole effective masses along [111] and [−110] directions corresponding to the first and second valence band in strained Si/(111)$Si_{1-x}Ge_x$ are respectively shown in Figure 2(a) and (b). As shown in Figure 2(a), when Ge fraction (*x*) is less than 0.2, the hole effective masse of the first valence band along [111] direction decreases significantly with increasing *x*. It is about $0.1m_0$ when *x* is equal to 0.2, which decreases 60% in comparison with the [100]-directional heavy hole effective mass ($0.29m_0$), the lowest heavy hole effective mass in relaxed Si. Note that it does not change nearly when *x* is more than 0.2. If the hole effective mass were merely taken into account, the hole mobility along [111] direction would be enhanced when *x* is more than 0.2. From 0.3 to 0.4 Ge fraction will be taken in device design actually. This can be explained by the fact that the decreased hole interband scattering rate can make the mobility enhanced due to the increasing splitting energy between the first and the second valence bands with the increasing *x*. As shown in Figure 2(a), [−110]-directional hole effective mass of the first valence band does not change so significantly as [111].

Hole mainly occupy the first valence band edge due to the splitting of the first and the second valence band in strained Si/(111)$Si_{1-x}Ge_x$ under strain. The hole effective mass of the second valence band is negligible and the hole effective mass of the first valence band is actually hole mass. So the hole effective mass of the second valence band is not

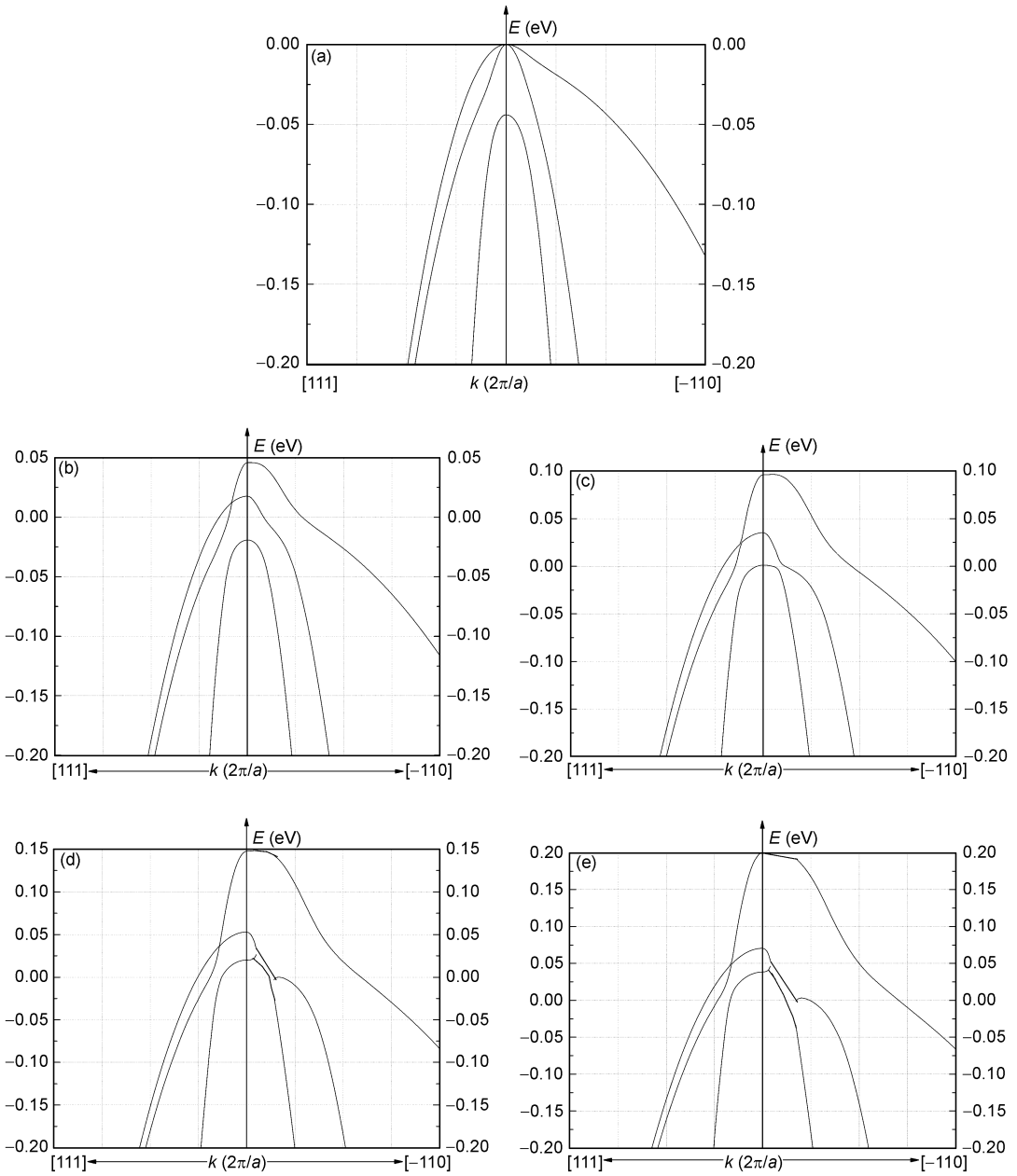

Figure 1 Valence band structure of strained Si/(111)$Si_{1-x}Ge_x$. (a) Relaxed Si; (b) strained Si/(111)$Si_{0.9}Ge_{0.1}$; (c) strained Si/(111)$Si_{0.8}Ge_{0.2}$; (d) strained Si/(111)$Si_{0.7}Ge_{0.3}$; (e) strained Si/(111)$Si_{0.6}Ge_{0.4}$.

stated in detail but shown merely in Figure 2(b).

Strained Si/(111)$Si_{1-x}Ge_x$ has different valence band structure and hole mass from that of relaxed Si. These may be understood by their thin film cell structures. The cell structure of relaxed Si goes triangular due to the tensile stress caused by the growth of Si on (111) relaxed $Si_{1-x}Ge_x$ substrate (shown in Figure 3). The lower symmetry of cell structure lifts the degeneracy of valence band edge and lead to the splitting of the first and the second valence band in strained Si/(111)$Si_{1-x}Ge_x$. And hence, their "mutual coupling force" caused by their splitting and relative moving is different from what is in relaxed Si. For this reason, the significant change in the valence band structures along [111] and [−110] directions and the corresponding hole effective masses with increasing Ge fraction occur.

3 Conclusions

It is of great significance to investigate on the valence band structure of strained Si materials and its corresponding hole effective mass for the hole transport enhance understanding and device design. Based on the valence band *E*-*k* relations of strained Si/(111)$Si_{1-x}Ge_x$, the valence band and hole

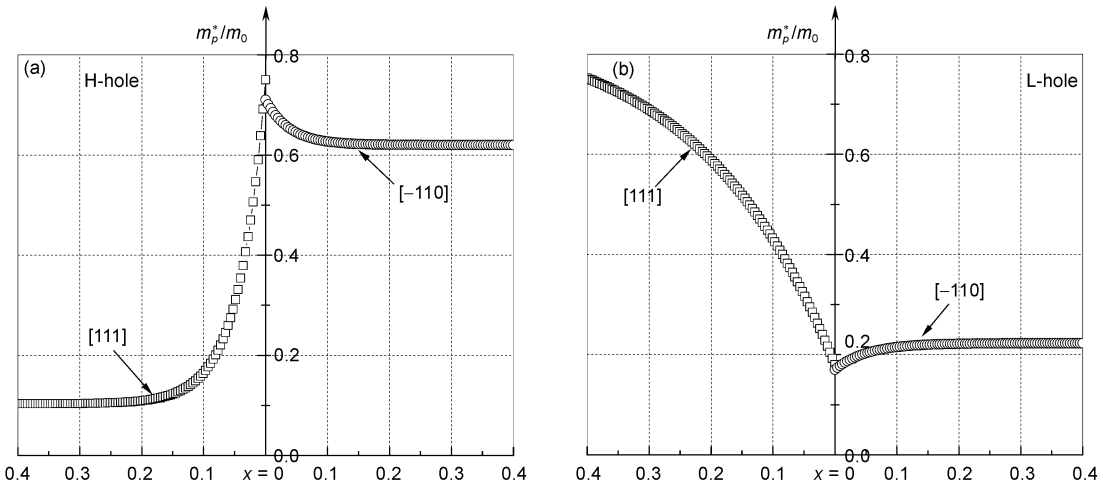

Figure 2 [111] and [−110] directional hole effective masses in strained Si/(111)$Si_{1-x}Ge_x$. (a) Hole effective mass of the first; (b) Hole effective mass of the second valence band (H-hole) valence band (L-hole).

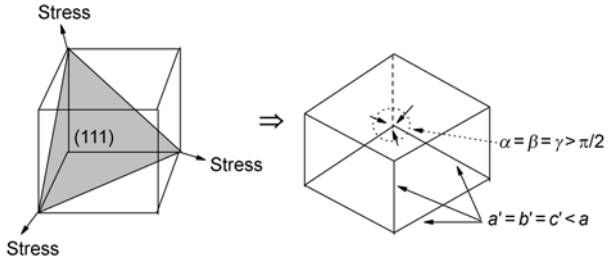

Figure 3 Schematic cell structure of strained Si/(111)$Si_{1-x}Ge_x$, where a', b', c', α, β, γ are lattice constants.

effective mass along [111] and [−110] directions were obtained. It was found that the valence band edge degeneracy is partially lifted, the significant change in the valence band structures along [111] and [−110] directions and the corresponding hole effective masses with increasing Ge fraction occur.

If the hole effective mass were merely taken into account, the hole mobility along the [111] direction would be enhanced when x is more than 0.2. From 0.3 to 0.4 Ge fraction will be taken in device design actually due to the more lower hole interband scattering rate compared to what x is equal to 0.2. The results above can provide valuable references to the investigation in the Si-based strained devices enhancement and the conduction channel design related to stress and orientation.

This work was supported by the National Ministries and Commissions (Grant Nos. 51308040203, 9140A08060407DZ0103, and 6139801).

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