The KP Dispersion Relation Near the Δ^i Valley in Strained $Si_{1-x}Ge_x/Si$ *

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Abstract: Based on an analysis of symmetry, the dispersion relations near the Δ^i valley in strained $Si_{1-x}Ge_x$ ($0 \leqslant x < 0.45$)/(001), (111), (101)Si are derived using the KP method with perturbation theory. These relations demonstrate that Δ^i levels in strained $Si_{1-x}Ge_x$ are different from the Δ_1 level in relaxed $Si_{1-x}Ge_x$, while the longitudinal and transverse masses (m_l^* and m_t^*) are unchanged under strain. The energy shift between the Δ^i levels and the Δ_1 level follows the linear deformation potential theory. Finally, a description of the conduction band (CB) edge in biaxially strained layers is given.

Key words: KP method; conduction band; strained SiGe
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1 Introduction

With each new generation of technology, geometric scaling has become an increasingly complex and expensive task. One way to improve device performance is to enhance the carrier transport by changing the material properties. Strained $Si_{1-x}Ge_x$ alloys are an attractive material for devices in high-speed integrated circuits[1]. Therefore, in order to obtain the proper electrical characteristics of strained $Si_{1-x}Ge_x$/Si devices, correct material parameters, including strain dependence, are required. Currently, there are few detailed theoretical calculations of these parameters, especially the features of the CB edge, most of which were referenced directly in a great amount of research concerning the design of new device structures based on strained $Si_{1-x}Ge_x$.

The goal of this work is to obtain CB edge parameters of strained $Si_{1-x}Ge_x$ such as the minima energy, the number of equivalent CB energy extrema, m_l^*, and m_t^* through the derivation of the dispersion relation near the Δ^i valley under strain. To achieve such a derivation, an analysis of symmetry under strain was performed, and then the dispersion relation was obtained using the KP method with perturbation theory. The parameters extracted are in good accordance with those in Refs. [2,3].

2 Derivation procedure

2.1 Analysis of symmetry under strain

$Si_{1-x}Ge_x$ alloy is a fully miscible solid solution of the Si-like band structure for a range of Ge molar fraction (0～0.85). The CB edge of the unstrained, bulk $Si_{1-x}Ge_x$ ($0 \leqslant x < 0.45$) is modeled as a six-degenerate Δ_1 valley with ellipsoidal energy surfaces[4].

The biaxial stress in $Si_{1-x}Ge_x$ epitaxial layers grown on variously oriented Si substrates by UHV-CVD induces a deformation that causes the change of Δ_1 valleys. Partial symmetry is retained in the lattice of the strained film. Under a tetragonal distortion arising from growth on a (001) substrate, the six Δ_1 valleys are not symmetrically equivalent, with the $[\pm 100]$ and $[0 \pm 10]$ valleys shifting together and splitting from the $[00 \pm 1]$ valleys. Rhombohedral distortion, arising from growth on a (111) substrate, all Δ_1 valleys are symmetrically equivalent and shift together. Growth on a substrate of the third orientation, considered (101) in this work, produces a monoclinic distortion and splits the Δ_1 levels. The $[\pm 100]$ and $[00 \pm 1]$ valleys are symmetrically equivalent, splitting from the $[0 \pm 10]$ valleys.

2.2 KP theoretical[5] derivation

In the single electron approximation, the eigenfunctions of the Schrödinger equation are the Bloch function:

$$\Psi_{nk}(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}} u_{nk}(\boldsymbol{r}) \tag{1}$$

where n is the index of the energy band and the wave vector $\boldsymbol{k}$ changes within the first Brillouin zone.

$$\left\{ -\frac{\hbar^2}{2m_0}\nabla^2 + U'(\boldsymbol{r}) \right\} \Psi(\boldsymbol{r}) = \varepsilon \Psi(\boldsymbol{r}) \tag{2}$$

$$U'(\boldsymbol{r}) = U_{\text{unstrain}}(\boldsymbol{r}) + U_{\text{Deformation}}(\boldsymbol{r}) \tag{3}$$

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where $U_{\text{unstrain}}(\boldsymbol{r})$ is the periodic field of unstrained crystal lattice while an additional field $U_{\text{Deformation}}(\boldsymbol{r})$ is induced by lattice deformation.

Under the biaxial stress imposed by the substrate, in the plane of the interface between the film and its substrate, the film is forced to adopt the lattice structure of its host substrate, and therefore lattice periodicity is preserved under such strain. Moreover, the elastic strain is small enough so as to be treated as a small perturbation. Substituting Eq. (1) into Eq. (2), we get Eq. (4) for the modulating functions $u_{nk}(\boldsymbol{r})$, having the periodicity of the unstrained crystal lattice.

$$\left\{\frac{\hat{\boldsymbol{p}}^2}{2m_0}+\frac{\hbar}{m_0}\boldsymbol{k}\cdot\hat{\boldsymbol{p}}+\frac{\hbar^2k^2}{2m_0}+U'(\boldsymbol{r})\right\}u_{nk}(\boldsymbol{r})=H_k u_{nk}(\boldsymbol{r})=\varepsilon_n(\boldsymbol{k})u_{nk}(\boldsymbol{r}) \tag{4}$$

where $\hat{\boldsymbol{p}}=-\mathrm{i}\hbar\nabla$ is the momentum operator of the electron.

There are six equivalent energy extremal points $\boldsymbol{k}_0^s(s=1,2,3,4,5,6)$ for relaxed $Si_{1-x}Ge_x$ ($0\leqslant x<0.45$), in the vicinity of which the band is non-degenerate. Strain resulting from growth on (001), (101) oriented substrates will partially lead to the degeneracy of K wavevector stars, but not reduce for the (111) case.

We take an arbitrary extremal point $\boldsymbol{k}_0^i$ ($i=1\sim18$) into account. Since for any given $\boldsymbol{k}$, the set u_{nk} forms in the space of functions having the periodicity of the lattice of a complete set, we can expand u_{nk} for any $\boldsymbol{k}$ into functions for $\boldsymbol{k}=\boldsymbol{k}_0^i$.

$$u_{nk}(\boldsymbol{r})=\sum A_{nn'}(\boldsymbol{k}-\boldsymbol{k}_0^i)u_{nk_0^i}(\boldsymbol{r}) \tag{5}$$

This is called the $\boldsymbol{k}_0^i$-representation. By isolating a certain part $H_{k_0^i}$ from the Hamiltonian H_k, Equation (4) may be represented as:

$$(H_{k_0^i}+H_{k\cdot\hat{p}}+H_{\text{strain}})u_{nk}(\boldsymbol{r})=\varepsilon_n^i(\boldsymbol{k})u_{nk}(\boldsymbol{r}) \tag{6}$$

where

$$H_{k_0^i}=\frac{\hat{\boldsymbol{p}}^2}{2m_0}+\frac{\hbar}{m_0}\boldsymbol{k}_0^i\cdot\hat{\boldsymbol{p}}+\frac{\hbar^2k_0^{i2}}{2m_0}+U_{\text{unstrain}}(\boldsymbol{r}) \tag{7}$$

$$H_{k\cdot\hat{p}}=\frac{\hbar}{m_0}[(\boldsymbol{k}-\boldsymbol{k}_0^i)]\cdot\hat{\boldsymbol{p}}+\frac{\hbar^2(k^2-k_0^{i2})}{2m_0} \tag{8}$$

$$H_{\text{strain}}=U_{\text{Deformation}}(\boldsymbol{r}) \tag{9}$$

If $\boldsymbol{k}-\boldsymbol{k}_0^i$ is a sufficiently small quantity, the operator $H_{k\cdot\hat{p}}(\boldsymbol{k}-\boldsymbol{k}_0)+H_{\text{strain}}(\boldsymbol{k}-\boldsymbol{k}_0)$ may be considered to be a small perturbation compared to the operator $H_{k_0^i}$. Particularly, varying $\boldsymbol{k}$ in the vicinity of $\boldsymbol{k}_0^i$, the deformation potential fields are taken as constant and independent of the wavevector. It is convenient to denote $H_{\text{strain}}(\boldsymbol{k}-\boldsymbol{k}_0)$ as $U_{k_0^i}$ for discussion.

Substituting the expansion (5) into (6), multiplying both sides of Eq. (6) by $u^*_{nk_0^i}$, and integrating over the unit cell, we obtain a system of equations that give the eigenvalue:

$$\sum_{n'}\left\{\begin{array}{l}\left[\varepsilon_n^i(\boldsymbol{k}_0^i)+\dfrac{\hbar^2(k^2-k_0^{i2})}{2m_0}+U_{k_0^i}\right]\delta_{nn'}\\ A_{nn'}+\dfrac{\hbar}{m_0}(\boldsymbol{k}-\boldsymbol{k}_0^i)\cdot\boldsymbol{p}_{nn'}(\boldsymbol{k}_0^i)A_{nn'}\end{array}\right\}\times A_{nn'}=\varepsilon_n^i(\boldsymbol{k})A_{nn'} \tag{10}$$

where

$$\boldsymbol{p}_{nn'}(\boldsymbol{k}_0^i)=\langle u_{nk_0^i}\mid\hat{\boldsymbol{p}}\mid u_{n'k_0^i}\rangle=\int_{\Omega_0}u^*_{nk_0^i}\hat{\boldsymbol{p}}u_{n'k_0^i}\,d\boldsymbol{r} \tag{11}$$

is the matrix element of the momentum operator at the point $\boldsymbol{k}=\boldsymbol{k}_0^i$. While deriving Eq. (10), we consider that the functions u are orthonormalized in the unit cell, i.e.

$$\int_{\Omega_0}u^*_{nk_0^i}u_{n'k_0^i}\,d\boldsymbol{r}=\delta_{nn'} \tag{12}$$

The corresponding terms of $H_{k\cdot\hat{p}}+H_{\text{strain}}$ in Eq. (10) may be visualized as small corrections to the energy $\varepsilon_n^i(\boldsymbol{k}_0^i)$. The dependence of energy on the wave vector may be obtained from Eq. (10) by using the ordinary perturbation theory.

$$\varepsilon_n^i(\boldsymbol{k})=\varepsilon_n^i(\boldsymbol{k}_0^i)+\varepsilon_n^{i'}(\boldsymbol{k}_0^i) \tag{13}$$

$$\varepsilon_n^{i'}(\boldsymbol{k}_0^i)=U_{k_0^i}+\frac{\hbar^2(k^2-k_0^{i2})}{2m_0}+\frac{\hbar}{m_0}(\boldsymbol{k}-\boldsymbol{k}_0^i)\cdot\boldsymbol{p}_{nn'}(\boldsymbol{k}_0^i) \tag{14}$$

For the second order, we find,

$$\varepsilon_n^i(\boldsymbol{k})=\varepsilon_n^i(\boldsymbol{k}_0^i)+\varepsilon_n^{i'}(\boldsymbol{k}_0^i)+\varepsilon_n^{i''}(\boldsymbol{k}_0^i)=\varepsilon_n^i(\boldsymbol{k}_0^i)+U_{k_0^i}+\frac{\hbar^2(k^2-k_0^{i2})}{2m_0}+\frac{\hbar}{m_0}(\boldsymbol{k}-\boldsymbol{k}_0^i)\cdot\boldsymbol{p}_{nn'}(\boldsymbol{k}_0^i)+\frac{\hbar^2}{m_0^2}\sum_{n'\neq n}\frac{(\boldsymbol{k}-\boldsymbol{k}_0^i)\cdot\boldsymbol{p}_{nn'}(\boldsymbol{k}_0^i)(\boldsymbol{k}-\boldsymbol{k}_0^i)\cdot\boldsymbol{p}_{n'n}(\boldsymbol{k}_0^i)}{\varepsilon_n^i(\boldsymbol{k}_0^i)-\varepsilon_{n'}^i(\boldsymbol{k}_0^i)} \tag{15}$$

where

$$\varepsilon_n^{i''}(\boldsymbol{k}_0^i)=\sum_{n'\neq n}\left\{\begin{array}{l}\dfrac{\hbar}{m_0}(\boldsymbol{k}-\boldsymbol{k}_0^i)\cdot\boldsymbol{p}_{nn'}(\boldsymbol{k}_0^i)+\\ \left[\dfrac{\hbar^2(\boldsymbol{k}^2-\boldsymbol{k}_0^{i2})}{2m_0}+U_{k_0^i}\right]\delta_{nn'}\end{array}\right\}\times\left\{\begin{array}{l}\dfrac{\hbar}{m_0}(\boldsymbol{k}-\boldsymbol{k}_0^i)\cdot\boldsymbol{p}_{n'n}(\boldsymbol{k}_0^i)+\\ \left[\dfrac{\hbar^2(\boldsymbol{k}^2-\boldsymbol{k}_0^{i2})}{2m_0}+U_{k_0^i}\right]\delta_{n'n}\end{array}\right\}\div\left[\begin{array}{l}\varepsilon_n^i(\boldsymbol{k}_0^i)-\\ \varepsilon_{n'}^i(\boldsymbol{k}_0^i)\end{array}\right]$$

$$=\frac{\hbar^2}{m_0^2}\sum_{n'\neq n}\frac{(\boldsymbol{k}-\boldsymbol{k}_0^i)\cdot\boldsymbol{p}_{nn'}(\boldsymbol{k}_0^i)(\boldsymbol{k}-\boldsymbol{k}_0^i)\cdot\boldsymbol{p}_{n'n}(\boldsymbol{k}_0^i)}{\varepsilon_n^i(\boldsymbol{k}_0^i)-\varepsilon_{n'}^i(\boldsymbol{k}_0^i)} \tag{16}$$

A comparison between Eq. (15) and the expression of relaxed $Si_{1-x}Ge_x$ shows that strained and relaxed $Si_{1-x}Ge_x$ has an identical CB dispersion relation in addition to the added constant term, $U_{k_0^i}$. This means that the Δ^i levels in strained $Si_{1-x}Ge_x$ will be different from the Δ_1 level in relaxed $Si_{1-x}Ge_x$, which is attributed to the two facts: (1) Varying $\boldsymbol{k}$ in the vicinity of $\boldsymbol{k}_0^i$, the deformation potential fields are taken as constant, independent of the K wavevector. To within the same degree of approximation, therefore, all Δ^i valleys

shift rigidly under lattice deformation. That is, all points in the vicinity of a valley minima shift by the same account. Thus, the shape of the valley is preserved and the position of the extremal point $\boldsymbol{k}_0^i$ is unaltered, and they are placed at a distance of $(0.85 \pm 0.03)\ 2\pi/a$ away from the Γ point in the Δ direction; (2) The CB states without strain perturbation, which are degenerate in energy, have significantly different wavevectors, so, for any specific wavevector, no pair of CB states under strain perturbation are degenerate or very close in energy. Therefore, any coupling between them is insignificant and may be neglected. So, the band index n sampling of the term $\varepsilon_n^{i''}(\boldsymbol{k}_0^i)$ in expression (15) has no difference from the one for the relaxed situation.

It is convenient to transform Eq. (15) into a familiar form to understand the strain effect on CB. Because the point $\boldsymbol{k}_0^i$ is extremal, the condition $(\nabla_k \varepsilon_n^i)_{k=\boldsymbol{k}_0^i}$ from Eq. (10) gives

$$\boldsymbol{p}_{nn'}(\boldsymbol{k}_0^i) + \hbar \boldsymbol{k}_0^i = 0 \tag{17}$$

By using this relation, Equation (15) gives the expression for energy in the vicinity of the extremal point $\boldsymbol{k}_0^i$,

$$\varepsilon_n^i(\boldsymbol{k}) = \varepsilon_n^i(\boldsymbol{k}_0^i) + U_{\boldsymbol{k}_0^i} + \frac{\hbar^2}{2}\sum_{\alpha,\beta=1}^{3}\left(\frac{1}{m_{\alpha\beta}^i}\right)_n (k_\alpha^i - k_{0\alpha}^i)(k_\beta^i - k_{0\beta}^i) \tag{18}$$

where the quantities $\left(\frac{1}{m_{\alpha\beta}^i}\right)_n$ are given by the relation:

$$\left(\frac{1}{m_{\alpha\beta}^i}\right)_n = \frac{\delta_{\alpha\beta}}{m_0} + \frac{2}{m_0^2}\sum_{n'\neq n}\frac{p_{nn'}^\alpha(\boldsymbol{k}_0^i)\,p_{n'n}^\beta(\boldsymbol{k}_0^i)}{\varepsilon_n^i(\boldsymbol{k}_0^i) - \varepsilon_{n'}^i(\boldsymbol{k}_0^i)} \tag{19}$$

and $p_{nn'}^\alpha(\boldsymbol{k}_0^i)$ is the α-th component of $\boldsymbol{p}_{nn'}(\boldsymbol{k}_0^i)$ (the indices α and β denote the co-ordinates x, y, z). So, we get the dispersion relation near the Δ^i valley under strain:

$$\varepsilon^i(\boldsymbol{k}) = \varepsilon_c(\boldsymbol{k}_0) + \Delta\varepsilon_c^i + \frac{\hbar^2}{2}\left[\frac{(k_x - k_{0x}^i)^2}{m_x^*} + \frac{(k_x - k_{0y}^i)^2}{m_y^*} + \frac{(k_x - k_{0z}^i)^2}{m_z^*}\right] \tag{20}$$

Finally, taking into account the Ge molar fraction x which slightly affects the parameters ε_c, m^*, Eq. (20) may be represented as:

$$\varepsilon^i(\boldsymbol{k}, x) = \varepsilon_c(\boldsymbol{k}_0, x) + \Delta\varepsilon_c^i + \frac{\hbar^2}{2}\left[\frac{(k_x - k_{0x}^i)^2}{m_x^*(x)} + \frac{(k_x - k_{0y}^i)^2}{m_y^*(x)} + \frac{(k_x - k_{0z}^i)^2}{m_z^*(x)}\right] \tag{21}$$

As noted for Eq. (15), the constant-energy in Eq. (21) is equivalent to that in Eq. (15), showing that only a minima energy shift occurs under strain.

3 Results and discussion

The positions of the Δ_1 levels for the relaxed alloy $\varepsilon_c(\boldsymbol{k}_0, X)$ were obtained from the literature[6]. The dashed lines in Figs. 2, 3, and 4 were fitted using those data. The effective mass components in Eq. (21) are shown in Fig. 1, which can be represented as two significant "effective" masses to describe the shape of the energy ellipsoid——namely, the longitudinal and transverse masses (m_l^* and m_t^*).

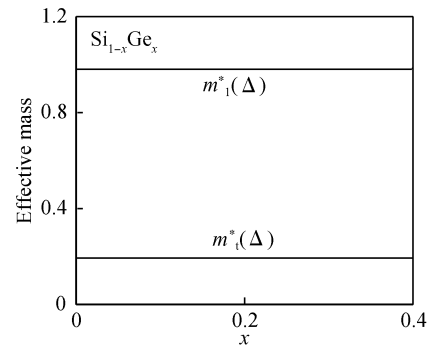

Fig. 1 CB effective mass versus Ge molar fraction x in relaxed $Si_{1-x}Ge_x$

The energy shift $\Delta\varepsilon_c^i$ may be determined by the deformation potential theory. The formulae are as follows[7]. Values of parameters for Si and Ge used in calculation are shown in Table 1. The corresponding parameters for $Si_{1-x}Ge_x$ alloy are obtained by linear interpolation.

$$\varepsilon_{\parallel} = (a_{Si} - a_{Si_{1-x}Ge_x})/a_{Si_{1-x}Ge_x} \tag{22}$$

For the (001) substrate:

$$\varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_{\parallel}$$
$$\varepsilon_{zz} = -\varepsilon_{\parallel}/\sigma^{(001)} \tag{23}$$

For the (111) substrate:

$$\varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_{zz} = \frac{1}{3}\times\left[2 - 1/\sigma_{Si_{1-x}Ge_x}^{(111)}\right]\varepsilon_{\parallel} \tag{24}$$

For the (101) substrate:

$$\varepsilon_{xx} = \varepsilon_{zz} = \frac{1}{2}\times\left[1 - 1/\sigma^{(101)}\right]\varepsilon_{\parallel}$$
$$\varepsilon_{yy} = \varepsilon_{\parallel} \tag{25}$$

Accounting for the six Δ levels:

$$\Delta\varepsilon_c^{(100)} = \Delta\varepsilon_c^{(\bar{1}00)} = \Xi_d^\Delta(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) + \Xi_u^\Delta\varepsilon_{xx}$$
$$\Delta\varepsilon_c^{(010)} = \Delta\varepsilon_c^{(0\bar{1}0)} = \Xi_d^\Delta(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) + \Xi_u^\Delta\varepsilon_{yy}$$
$$\Delta\varepsilon_c^{(001)} = \Delta\varepsilon_c^{(00\bar{1})} = \Xi_d^\Delta(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) + \Xi_u^\Delta\varepsilon_{zz} \tag{26}$$

Substituting this data for any dispersion relation near the Δ^i valleys, Equation (21) in $Si_{1-x}Ge_x$ ($0 \leqslant x < 0.45$)/(001), (111), (101)Si may be determined.

Table 1 Values[6] used in the calculation

Parameter	Si	Ge
a_0/nm	0.54309	0.56579
$\sigma^{(001)}$	1.296	1.332
$\sigma^{(111)}$	2.275	2.691
$\sigma^{(101)}$	1.959	2.222
Ξ_d^Δ/eV	1.75	−0.59
Ξ_u^Δ/eV	9.16	9.42

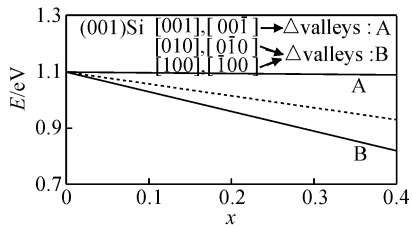

Fig. 2　Δ^i levels versus x in $Si_{1-x}Ge_x/(001)Si$

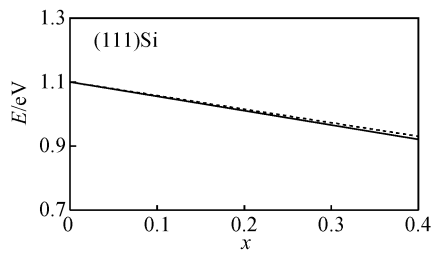

Fig. 3　Δ^i levels versus x in $Si_{1-x}Ge_x/(111)Si$

The dependence of Δ^i valleys under strain resulting from growth on (001), (111), (101) substrates on the Ge molar fraction x are shown in Figs. 2, 3 and 4, respectively. The notation in those figures is as follows: Solid lines: Δ^i levels in strained alloy film; dashed lines: Δ_1 level in bulk alloy. As x increases, the film is under increasing planar isotropic compressive strain. The configuration in Fig. 2 is $Si_{1-x}Ge_x/(001)$ Si, which shows that the strained layer CB edge (B) is characterized by the $[\pm 100]$, $[0 \pm 10]$ valleys, while for the $[00 \pm 1]$ valleys, (A) splits from (B) and shifts to higher energy; The data for the (111) Si substrate are shown in Fig. 3. Primarily, the difference from (001) Si is that the CB valleys are not split. The CB edge is characterized by the same six valleys, which are shifted only slightly downward in energy; As shown in Fig. 4, growth on a (101) Si substrate results in the splitting of CB valleys. The $[\pm 100]$ and $[00 \pm 1]$ valleys (A) rise above the $[0 \pm 10]$ valleys (B), which constitutes the CB edge.

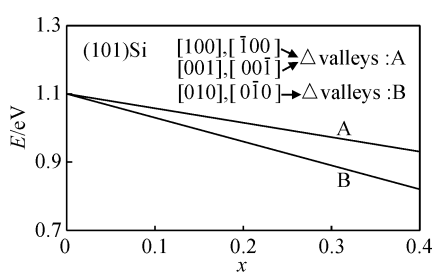

Fig. 4　Δ^i levels versus x in $Si_{1-x}Ge_x/(101)Si$

4 Conclusion

The dispersion relations near Δ^i valleys in strained $Si_{1-x}Ge_x$ ($0 \leqslant x < 0.45$)/(001), (111), (101) Si have been derived. These relations demonstrate that the Δ^i levels in strained $Si_{1-x}Ge_x$ are different from the Δ_1 level in relaxed $Si_{1-x}Ge_x$, while the longitudinal and transverse masses (m_l^* and m_t^*) to describe the shape of the energy ellipsoid are unchanged under strain.

The CB edge in $Si_{1-x}Ge_x$ strained layers has been characterized. The CB edge in $Si_{1-x}Ge_x/(001)$ Si is modeled as four-degenerate Δ valleys ($[\pm 100]$, $[0 \pm 10]$ valleys) that shift to lower energy in comparison with the Δ_1 level. The CB edge in $Si_{1-x}Ge_x/(111)$ Si is characterized by the same six valleys, which are shifted only slightly downward in energy. Growth on a (101) Si substrate results in the splitting of the CB valleys. The $[\pm 100]$ and $[00 \pm 1]$ valleys (A) rise above the $[0 \pm 10]$ valleys (B) and constitute the CB edge.

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应变 $Si_{1-x}Ge_x$/Si Δ^i 能谷附近色散关系的 KP 理论推导*

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摘要：基于对称性分析，应用 KP 微扰理论确定了应变 $Si_{1-x}Ge_x$($0\leqslant x<0.45$)/(001)，(111)，(101)Si 的 Δ^i 能谷附近的色散关系.结果证明：应变 $Si_{1-x}Ge_x$ 中的 Δ^i 能级大小不同于弛豫 $Si_{1-x}Ge_x$ 的 Δ_1 能级，而二者的横向、纵向有效质量(m_l^*，m_t^*)相同.Δ^i 和 Δ_1 能级之差由形变势理论确定.最后，描述了双轴应变下外延层材料的导带带边特征.

关键词：KP 法；导带；应变硅锗

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