Energy-Band Structure of Strained Indirect Gap Semiconductor: A k . p Method

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ABSTRACT

A strain Hamiltonian H_{st}, associated with a *sps** **k** . **p** Hamiltonian H_{kp}, is used to describe the valence band and the first two conduction bands of a strained indirect semiconductor. H_{st} takes into account the Bir-Pikus parameters (a, b) used up to now to describe only the Brillouin zone center. The H_{kp}+H_{st} Hamiltonian allows one to calculate the energy dispersion all over the Brillouin zone. The method is applied to Si strained on $Si_{1-x}Ge_x$ alloy. We do not use the local (in k space) deformation potentials Ξ_u and Ξ_d conventionally used in indirect gap semiconductor to describe the conduction band. The energy band gap, the conduction bands split into the four equivalent in-plane valleys Δ_4 and the two valleys along the growth direction Δ_2 which result from the above H_{kp}+H_{st} Hamiltonian are in very good agreement with other publications.

Keywords: **k** . **p** theory, strain, SiGe.

1 INTRODUCTION

The application of an external stress on semiconductor has a strong influence on the band structure. Hydrostatic stress causes a forbidden band gap energy shift while a uniaxial stress produces an additional splitting of the degenerate levels by lowering the lattice symmetry. The deformation potential parameters a_c, a_v and b [1], which are applied at Γ-point (k = 0) of the Brillouin zone, connect the shift and the splitting with the strain tensor. a_c is related to the conduction band (CB) and (a_v, b) are linked to the valence band (VB). For a direct gap semiconductor, the bands of interest near the band gap are Γ_{1c} and Γ_{5v}. The parameters a_c and a_v give the hydrostatic shift of Γ_{1c} and Γ_{5v}, whereas b gives the splitting of the triply degenerated Γ_{5v} band under [001]-stress. But in an indirect gap semiconductor, the minimum of the CB is not at k = 0 ; this minimum stems from the Γ_{5c} CB in silicon where the minimum is at Δ point (in [001] direction). It is then necessary to use two parameters, Ξ_u and Ξ_d to describe the shift and the splitting at this minimum [1]. These two parameters do not allow one to calculate the band dispersion all over the Brillouin zone because they are defined only at the Δ point for the CB minima. However the knowledge of the $Si/Si_{1-x}Ge_x$ band structure is of prime importance since the Si/SiGe heterostructure is very promising for the new generation of high-mobility Si devices. For an accurate modeling of these devices the complete dispersion relation of the electrons in strained Si is needed. Furthermore, in these devices, the high density of hot carriers involves a "full-band" simulation of transport phenomena, and an overall description of the carrier's dispersion relation is crucial.

In the present paper we show that the use of a **k** . **p** Hamiltonian, taking into account the strain via only (a_c, b_c, a_v, b) parameters, allows one to calculate the band energy all over the Brillouin zone. The starting point of this method is a twenty-band *sps** **k** . **p** Hamiltonian [2] used to describe the VB and the first two CBs all over the Brillouin zone; the accuracy is adequate for transport calculation (particularly the effective masses). We apply this method to strained Si on $Si_{1-x}Ge_x$ with a biaxial [001]-strain.

In this paper we first present the both *sps** **k** . **p** and strain Hamiltonian. In second section we propose the results of our approach compared with other works.

2 HAMILTONIAN

2.1 *The sps** k . p Hamiltonian

In the present approach, the initial step is the band-structures calculation of the bulk semiconductors using the **k** . **p** theory. In this goal we use an original *sps** **k** . **p** Hamiltonian H_{kp} which is a twenty-band **k** . **p** Hamiltonian taking into account the spin-orbit coupling. H_{kp} was shown to be valid for both direct and indirect band gap semiconductors [2]. The basis functions are *sps** -like functions used in linear combination of atomic orbitals theory [3]. To get the right dispersion up to the Brillouin zone edge, the influence of other bands (d bands) is mimiced via Luttinger-like parameters in the VB and in the CB.

The Si bulk band-structure obtained with this approach is shown Fig. 1. Note the equality of the bands (CB and

VB) in [100] and [001] directions. On the other hand one can note that the [100]-valleys Δ_4 and the two [001]-valleys Δ_2 stems from the Γ_{5c} CB.

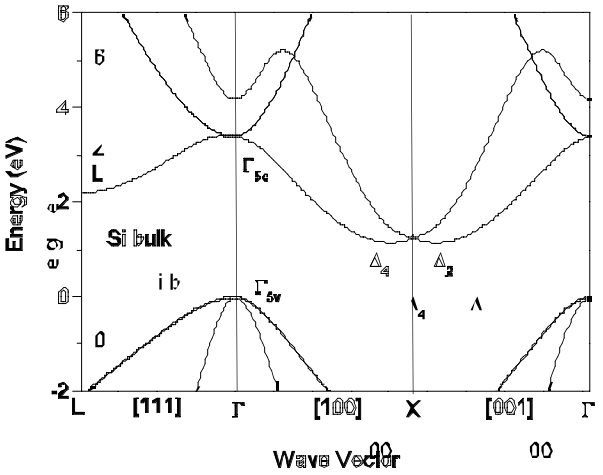

Figure 1: Calculated band-structure of Si bulk. Note the triply degenerate Γ_5 valence and conduction bands and the Δ valley (Δ_2 and Δ_4) in conduction band.

2.2 The Strain Hamiltonian

Schematically, to solve the Schrödinger equation in semiconductor with a biaxial [001]-strain, we use the total Hamiltonian $H = H_{kp} + H_{st}$ where H_{st} is a strain Hamiltonian. Now we describe this strain Hamiltonian. The biaxial [001]-strain is due to the difference between the bulk Si and the bulk $Si_{1-x}Ge_x$ alloy lattice constants. The deformed system investigated in this work is schematically described in Fig. 2.

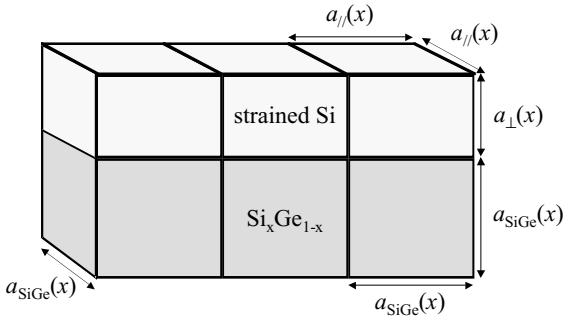

Figure 2: The deformed system investigated in this work.

The lattice constant for bulk $Si_{1-x}Ge_x$ alloy can be represented by the expression

$$a_0(Si_{1-x}Ge_x) = a_0(Si) + 0.200326 \times (1-x) + [a_0(Ge) - a_0(Si)]x^2 \quad (1)$$

where $a_0(\ )$ is the lattice constant of the bulk considered material. The Si lateral lattice constant $a_{//}(x)$ is equal to the bulk lattice constant $a_0(Si_{1-x}Ge_x)$. The lattice constant $a_{\perp}(x)$ of the strained layer in the direction perpendicular to the interface is adapted so as to minimized the elastic energy

$$a_{\perp}(x) = a_0(Si)\left[1 - 2\frac{C_{12}}{C_{11}} \times \frac{a_{//}(x) - a_0(Si)}{a_0(Si)}\right] \quad (2)$$

where C_{11} and C_{12} are the elastic constants of Si. From this lattice deformation we can define the symmetric strain tensor whose the elements take the form

$$\begin{aligned} \varepsilon_{xx} &= \varepsilon_{yy} = \varepsilon_{//} = (a_{//} - a_0(Si)) / a_0(Si) \\ \varepsilon_{zz} &= \varepsilon_{\perp} = (a_{\perp} - a_0(Si)) / a_0(Si) \\ \varepsilon_{xy} &= \varepsilon_{xz} = \varepsilon_{yz} = 0 \end{aligned} \quad (3)$$

The biaxial strain is seen as two contributions on the Si band-structure. A hydrostatic stress, which causes a forbidden band-gap energy shift, and a uniaxial stress that produces an additional splitting of the degenerate levels by lowering the lattice symmetry. The result of the biaxial strain Hamiltonian on the band-structure is qualitatively describe in Fig. 3.

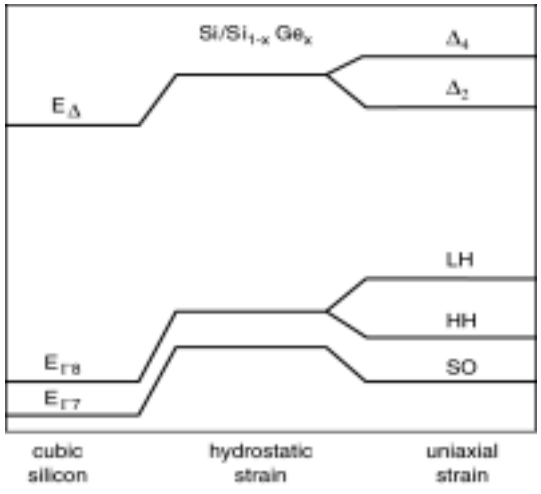

Figure 3. Qualitative description of the hydrostatic and uniaxial components contribution on the conduction band minimum (in Δ direction) and on the valence band maximum (Γ point) resulting from the biaxial stress experienced by a pseudomorphic silicon on a cubic $Si_{1-x}Ge_x$. The wave functions of HH level are well defined while the wave functions of LH and SO are mixed.

For the triply degenerate $\Gamma_{5v,c}$ band ($\Gamma_{8v,c}^{1/2}$, $\Gamma_{8v,c}^{3/2}$ and $\Gamma_{7v,c}$) as well VB as CB, the strain Hamiltonian matrix takes the form [1]

$$\begin{array}{c} \begin{matrix} \Gamma_{8v,c}^{3/2} & \Gamma_{8v,c}^{1/2} & \Gamma_{7v,c} \end{matrix} \\ \begin{bmatrix} a_{v,c}\varepsilon + b_{v,c}\varepsilon_{//\perp} & 0 & 0 \\ 0 & a_{v,c}\varepsilon - b_{v,c}\varepsilon_{//\perp} & \sqrt{2}b_{v,c}\varepsilon_{//\perp} \\ 0 & \sqrt{2}b_{v,c}\varepsilon_{//\perp} & a_{v,c}\varepsilon \end{bmatrix} \end{array} \qquad (4)$$

where $\varepsilon = 2\varepsilon_{//} + \varepsilon_{\perp}$ and $\varepsilon_{//\perp} = \varepsilon_{\perp} + \varepsilon_{//}$ and $a_{v,c}$ and $b_{v,c}$ are respectively the hydrostatic and the splitting deformation potentials. For the CB this Hamiltonian split the four equivalent in-plane valleys Δ_4 and the two valleys along the growth direction Δ_2. This split is directly linked to the splitting deformation potentials b_c. For the VB the strain Hamiltonian split the light hole (LH or $\Gamma_{8v}^{1/2}$) and the heavy hole (HH or $\Gamma_{8v}^{3/2}$). On the other hand, due to the non-diagonal term in matrix of Eq. 4, the wave functions of LH and SO (Γ_{7v}) are mixed. Then in strain semiconductor the concept of light and heavy hole band is not usable because the band are mixed and the light or heavy character of a band (linked to the band curvature) is direction-dependent.

3 RESULTS AND DISCUSSION

3.1 The Deformation Potentials

The hydrostatic deformation potentials used in our model have been calculated by Blacha *et al.* [4] with a pseudopotential theory. Note that the absolute values of these deformation potentials may differ by an identical additive constant. This does not affect the hydrostatic dependence of the energy bands on the strain since the difference between two hydrostatic parameters remains constant. The splitting parameter b_v is also given in Ref. [4]. Note that these deformation potentials can be measured experimentally and their values are well-know in silicon.

This does not apply to b_c which is, in our model, the only adjustable parameter. Its value is estimated by fitting the published results on the CB splitting $\Delta_{2\text{-}4}$ into the four equivalent in-plane valleys Δ_4 and the two valleys along the growth direction Δ_2, extract from our calculation results. In other words we adjust b_c to reproduce $\Delta_{2\text{-}4}$ versus the germanium content x of the $Si_{1-x}Ge_x$ buffer, given by the usual local parameters Ξ_u.

3.2 Band Structure Results

The band structure of Si grown on relaxed $Si_{0.7}Ge_{0.3}$ calculated following our model is shown in Fig. 4. Numerical results are given in Table 1 for the most usual germanium content x of the $Si_{1-x}Ge_x$ buffer.

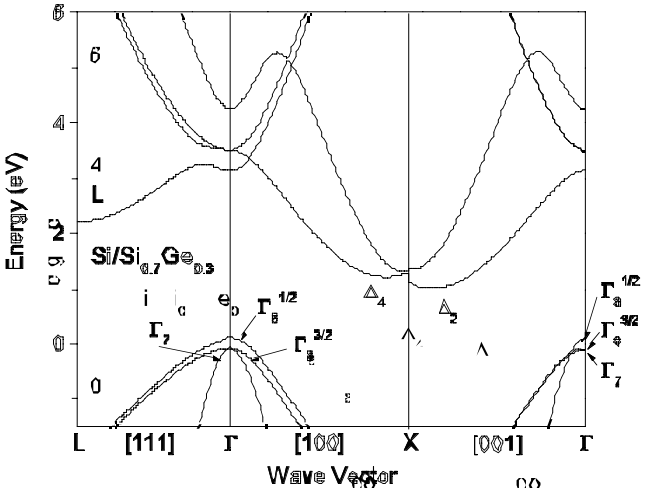

Figure 3: Calculated band-structure of Si grown on an unstrained [001] $Si_{0.7}Ge_{0.3}$ surface. The biaxial [001]-strain lifts the degeneracy in conduction band Δ valley (Δ_2 and Δ_4) and in the valence band Γ_8 ($\Gamma_8^{1/2}$ and $\Gamma_8^{3/2}$). The fundamental energy band-gap is defined by the energy between Δ_2 and $\Gamma_8^{1/2}$ because of the tensile strain.

	This Work		Previous Work	
x	$\Delta_{2\text{-}4}$	E_g	$\Delta_{2\text{-}4}$	E_g
0.1	0.063	1.096	0.07[a], 0.06[b]	1.07[a], 1.04[b]
0.2	0.128	1.014	0.15[a], 0.13[b]	0.99[a], 0.98[b]
0.3	0.194	0.928	0.22[a], 0.19[b]	0.92[a], 0.90[b]
0.4	0.262	0.839	0.29[a], 0.26[b]	0.85[a], 0.83[b]

[a]Ref. [5]
[b]Ref. [6]

Table 1. Comparison of the energies gap E_g and of the energies splitting $\Delta_{2\text{-}4}$, for several germanium content x of the buffer, obtained in the present work at 0 K with the ones of Refs. [5, 6]. All energies are given from the top of the valence band ($\Gamma_8^{1/2}$). The results in Refs. [5, 6] are given at 300 K. To show their results at 0 K, we have used:
$E_g(T) = E_g(0) - \alpha T^2 / (T + T_0)$
with $\alpha = 4.73 \times 10^{-4}$ (eV / K) and $T_0 = 636$ K.

The CB energy splitting $\Delta_{2\text{-}4}$ and the band gap energy E_g, which are a crucial test for the quality of our model, are in good agreement with calculation results obtained by use of Ξ_u and Ξ_d in Ref. [5] and [6]. The small discrepancy between the $\Delta_{2\text{-}4}$ values presented here and those published elsewhere are mainly due to a significant uncertainty on published parameters that were used in the calculation as

the elastic constants of Si. Moreover the temperature dependence of all parameters is not well known.

This uncertainty on published parameters is particularly significant for the value of the CB splitting deformation potential b_c. The value of b_c has been published only once in Ref. [4] and to our knowledge no experimental results are available. We have used in our calculation $b_c = 5.5$ eV. In Ref. [4], b_c is equal to 0.5 eV, but if we take this value in our method, we get $\Delta_{2\text{-}4} = 0.02$ eV for Si strain on $Si_{0.7}Ge_{0.3}$ which corresponds to an underestimation of this value. With $b_c = 5.5$ eV we obtain a CB splitting $\Delta_{2\text{-}4}$ in agreement with the splitting reported in figure 5 of Ref. [5] and with Ref [6].

4 CONCLUSION

In conclusion, we have reported the energy band structure of strained Si on $Si_{1-x}Ge_x$ alloys. The method, which accounts for a strain Hamiltonian and a *sps** **k** . **p** Hamiltonian, gives the energy gap E_g and the conduction band splitting $\Delta_{2\text{-}4}$ versus the strain and more generally allows to calculate the band dispersion versus **k** of strained indirect band gap semiconductors. These results confirm that the *sps** **k** . **p** model [2] is efficient to calculate the band structures all over the Brillouin zone for energies of interest for the study of transport in strain heterosystems like those used in high-mobility devices.

In addition we propose a new value of the deformation potential b_c in Si which is used instead of the local parameter Ξ_u. To our knowledge, this is the second value published of this deformation potential. Note that the factor between these two published values is equal to 11. Thus, the strain effect in semiconductor and particularly in Si technology, with the very large prospects both in optoelectronic and electronic, seems to be a good field for experimenters.

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