Transport properties of p-type metal-oxide-semiconductor inversion layer in
(110) and (111) silicon channel under uniaxial stress

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Abstract

Valence subband and transport properties of p-type metal-oxide-semiconductor
(PMOS) inversion layer in uniaxially strained (110) and (111) Si channel have been
studied theoretically in this work. Equal energy lines, carrier concentration effective
mass, conductivity effective mass, and mobility are calculated based on
Luttinger-Kohn Hamiltonian [16]. Three compact expressions of scattering rate are
derived in this paper. PMOS channel direction is chosen as 45° in x-y plane, namely,
\([-1, 1, -\sqrt{2}]\) in (110) system and \([1-\sqrt{3}, 1+\sqrt{3}, -2]\) in (111) system and z
direction is chosen to be the quantization direction. The direction of applied uniaxial
stresses considered is in either parallel or perpendicular to channel. My results show
mobility is very sensitive to effective mass under different stresses. The favorable
mobility directions are found in (110) system with -3 GPa stress parallel to channel
and +3 GPa stress perpendicular to channel.

keywords: inversion layer ; transport ; (110) Si ; (111) Si ; scattering ; uniaxial stress ;
effective mass ; mobility

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1. Introduction

It has been shown strain technology in complementary metal–oxide–semiconductor (CMOS) results in favorable transport properties [3-4]. Recently, researchers are trying to develop various novel structures, such as fin field-effect transistor (FinFET) or multiple gate field-effect transistor (MuGFET), for next generation devices. However, strain technology remains an effective and economical manipulation to produce higher carrier mobility for electronic devices [5]. In general, strains can be created to channel by lattice mismatch between channel and substrate or through the external mechanical stresses, or combinations of these two methods. Biaxial strains produced by lattice mismatching has been proven effective of lowering carrier effective masses but uniaxial stress applied to the channel in some specific substrate orientations can also create favorable transport properties in the experiments [6-13]. In this work, I theoretically calculated the equal energy lines, carrier concentration effective mass \( m_c \), conductivity effective mass \( m_\sigma \), and hole mobility \( \mu_h \) under uniaxial stresses \(-3, -2, -1, 0, 1, 2, 3 \) GPa etc. of (110) and (111) Si channel, respectively. Channel direction is chosen as 45° direction in x-y plane, namely, \([-1, 1, -\sqrt{2}]\) in (110) system and \([1-\sqrt{3}, 1+\sqrt{3}, -2]\) in (111) system. The z direction is chosen to be the quantization direction. The direction of the applied stress considered is either parallel or perpendicular to channel and unaxial stresses can be realized by doping carbon or germanium into the opposite sides of the Si channel.

2. Physics Methods

2.1. Luttinger-Kohn Hamiltonian

On the basis of \( k \cdot p \) theory, the valence energy subband structures of diamond structures under strain can be found through diagonalizing a 6×6 Luttinger-Kohn
Hamiltonian [16]. The electric field produced by the gate bias, which gives rise to the quantum confinement effects, is assumed to be a constant and quantizes the z-component of momentum $\hbar k_z$ along the z-direction. Consequently $\hbar k_z$ is expressed as $\hbar \frac{\partial}{i \partial z}$. I discretize the linear potential energy into $N$ equal height steps such that the Hamiltonian matrix for the inversion layer is constructed as $H_{FEM}$ [7],

\[
H_{FEM} = \begin{bmatrix}
\ddots & \ddots & \ddots & \ddots & \ddots \\
\cdots & D_{-} & D_{n-1} & D_{+} & 0 & 0 & \cdots \\
\cdots & 0 & D_{-} & D_{n} & D_{+} & 0 & \cdots \\
\cdots & 0 & 0 & D_{-} & D_{n+1} & D_{+} & \cdots \\
\ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots
\end{bmatrix},
\]

(1)

\[H_{IK} = H_0 + H_1 k_z + H_2 k_z^2\]

\[D_n = H_0 + 2 \frac{H_2}{(\Delta z)^2} + V_n\]

with

\[D_+ = \frac{H_1}{2i\Delta z} - \frac{H_2}{(\Delta z)^2}\]

\[D_- = \frac{H_1}{2i\Delta z} - \frac{H_2}{(\Delta z)^2}\]

where $V_n$ is the potential energy value of the $n^{th}$ step, and $\Delta z = 0.2$ nm gives the width of each step. We take the total number of step $N=50$ for the calculations. Due to the strain effect each valence subband splits into a set of two very close subbands, which correspond to spin up and down, respectively. The three sets of lowest energy valence subbands, in increasing order of energy, are labeled as the 1$^{st}$ subband, the 2$^{nd}$ subband, and the 3$^{rd}$ subband. The strain tensors used in our work are adopted from Ma et al [17]. So far we have all the details of Energy-Momentum dispersions of 2D carriers with strains.

2.2. Scattering Formulas

Instead of the conventional scattering formulas [18-22], three compact expressions
of scattering rate including acoustic phonon, optic phonon, and, surface roughness scatterings have been derived in this work, which are following Harrison’s [1] and Lundstrom’s [2] formulas.

The $n^{th}$ acoustic phonon scattering rate in the inversion layer is derived as

$$\frac{1}{\tau_n(E)} = \frac{D_A^2 m_c k_B T}{\hbar^3 \rho \nu_s^2 (2\pi)^2} \times \theta \left( k_n^2(E) - \frac{2m_c \Delta}{\hbar^2} \right) \pi \int_0^\infty G^2(K_z) dK_z,$$

(2)

where $G(K_z) = \int \psi_f^*(z) e^{-iK_z z} \psi_i(z) dz$, in which $K_z$ is the acoustic phonon wave number in the $z$ direction, and $\theta \left( k_n^2(E) - \frac{2m_c \Delta}{\hbar^2} \right)$ is the unit step function, in which $\Delta \equiv E_{zf} - E_{zi}$, $E_{zf}$ and $E_{zi}$ give the final and initial quantization energy in the $z$ direction, respectively. $D_A$ is acoustic phonon deformation potential energy, $\rho$ is Si mass density, $m_c$ is carrier concentration effective mass, $k_B$ is Boltzmann’s constant, and $v_g$ is acoustic phonon group velocity. The subscript $n$ represents the $n^{th}$ subband in the whole place of this paper.

The $n^{th}$ optic phonon scattering rate is derived as

$$\frac{1}{\tau_n(E)} = \frac{D_o^2 m_c}{\hbar \omega_o (2\pi)^3} \left( N_o + \frac{1}{2} \pm \frac{1}{2} \right) \times \theta \left( k_n^2(E) - \frac{2m_o \Delta}{\hbar^2} \right) \pi \int_0^\infty G^2(K_z) dK_z,$$

(3)

where $G(K_z) = \int \psi_f^*(z) e^{-iK_z z} \psi_i(z) dz$, in which $K_z$ is the acoustic phonon wave number in the $z$ direction, and $\theta \left( k_n^2(E) - \frac{2m_o \Delta}{\hbar^2} \right)$ is the unit step function, in which $\Delta \equiv E_{zf} - E_{zi} \mp \hbar \omega_o$, $E_{zf}$ and $E_{zi}$ give the final and initial quantization energy in the $z$ direction, respectively. $\hbar \omega_o$ gives hole optic phonon energy and $D_o$ is optic phonon deformation potential. $N_o$ is the Bose-Einstein’s function, because the phonons are bosons.

The $n^{th}$ surface roughness scattering rate is derived as
\[ \frac{1}{\tau_n(E)} = \frac{\pi n_e (eFAL)^2}{h^3} \int_0^\infty \frac{G^2(K_z)}{1 + \frac{L^2 k_n^2}{2}} dK_z, \quad (4) \]

where \( L \) and \( A \) are surface roughness parameters. Furthermore, \( A \) is root-mean-square amplitude of fluctuations and \( L \) is their correlation length, which is roughly the distance between fluctuations. \( F \) is electric field strength which is chosen as 1 MV/cm in all stress cases in this paper.

2.3. Carrier Concentration Effective Mass

Carrier concentration effective mass \( (m_c) \), is calculated according to ref. [7]. \( m_c \) is also a parameter for calculating mobility.

\[ m_{c,n} = \frac{\pi h^2 \int_{E_0}^\infty D_n(E) f(E) dE}{\int_{E_0}^\infty f(E) dE}, \quad (5) \]

where \( D_n(E) \) is density of states of holes and \( f(E) \) is Boltzmann’s function, because the Fermi’s level is canceled [7].

2.4. Conductivity Effective Mass

Conductivity effective mass \( (m_\sigma) \), is calculated according to ref. [7].

\[ m_{\sigma,j} = \frac{\int_{E_0}^\infty D_n(E) f(E) dE}{\int_{E_0}^\infty D_n(E) v_j^2(E) \left( -\frac{\partial f(E)}{\partial E} \right) dE}, \quad (6) \]

where \( v_j \) is the \( j^{th} \) component of hole group velocity, \( \tau(E) \) is hole scattering time. Similar to the case of carrier concentration effective mass, Fermi’s level is also canceled.

2.5. Mobility

Carrier mobility \( (\mu_j) \), is also calculated according to ref. [7].
\[
\mu_y = \frac{e \int \sum_{E_n}^3 D_n(E) v_j^2(E) \tau(E) \left( - \frac{\partial f(E)}{\partial E} \right) dE}{\int \sum_{E_n}^3 D_n(E) f(E) dE},
\]

where \( e \) is carrier charge of a hole. The results of \( m_c, m_\sigma, \) and \( \mu_y \), in (110) and (111) systems are all under applied electric field strength 1 MV/cm with external stresses from -3 GPa to +3 GPa either parallel or perpendicular to channel. All calculations are performed by Luttinger-Kohn parameters of Si [14-17] and scattering parameters of Si shown in TABLE I [2].

3. Results and Discussions

3.1. Equal Energy Lines

For (110) Si channel system, Fig. 1, 2, and 3 show the 25 meV equal energy lines of the three lowest energy valence subbands (only one spin state with internal strain are shown) of the inversion layer with different uniaxial stresses of -3, -2, -1, 0, 1, 2, 3 GPa, respectively. Fig. 4, 5, and 6 show the same thing as in Fig. 1, 2, and 3 for (111) Si channel system. The choice of 25 meV as a demonstrated energy for plotting the equal energy lines in Fig. 1 to 6 is because the thermal energy is 25 meV and is also because I follow the Fishetti’s choice [18]. We can see equal energy lines in (110) Si channel are elliptic and when the external stress getting large the major axes of the ellipse lie on different directions for the 1\textsuperscript{st} and the 2\textsuperscript{nd} subband while the 3\textsuperscript{rd} subband become more wrap than the other subbands. When compress stresses are added in the (110) system equal energy lines turn the major axes of the ellipse into negative degree and tensile stresses cause opposite effects to compress stresses. The symmetry of the equal energy lines in (111) system are not elliptic but hexagonal. As the external stress are increasing in the (111) system, equal energy lines are become ellipse from hexagon and the major axes lie also on the negative degree when the applied stress are
compress for the 1\textsuperscript{st}, 2\textsuperscript{nd} and 3\textsuperscript{rd} subband and tensile stresses cause the opposite effects to the major axes of the 1\textsuperscript{st}, 2\textsuperscript{nd} and 3\textsuperscript{rd} subband.

3.2. Carrier Concentration Effective Mass

Fig. 7 and 8 show $m_c$ of the three lowest valence subbands as a function of external stresses in (110) and (111) Si channel, respectively. Comparing Fig. 7 and 8 we find generally speaking at a given external stress, $m_c$ for each subband in (111) system is larger than in (110) system except for the 3\textsuperscript{rd} subband in the cases of large compressive and tensile stresses. The trends of the $m_c$ variations are different in (110) and (111) Si systems when external stresses are added. In (110) system, $m_c$ of the 1\textsuperscript{st} and 2\textsuperscript{nd} subband increase slightly when external stresses are enhanced in both compressive and tensile cases but $m_c$ of the 3\textsuperscript{rd} subband increases monotonically from -3 GPa to +3 GPa. In (111) system, $m_c$ of the 1\textsuperscript{st} and 3\textsuperscript{rd} subband decrease when external stresses are enhanced in both compressive and tensile stresses but $m_c$ of the 2\textsuperscript{nd} subband behaves oppositely. The reason of the difference is due to the 1\textsuperscript{st} and 2\textsuperscript{nd} subband are both heavy hole like but the 3\textsuperscript{rd} subband is light hole like in (110) Si channel and the 1\textsuperscript{st} and 3\textsuperscript{rd} subband in (111) channel are heavy hole like but the 2\textsuperscript{nd} subband is light hole like.

3.3. Conductivity Effective Mass

Fig. 9 and 10 show conductivity effective mass ($\sigma_m$) in both (110) and (111) channels. It can be seen $\sigma_m$ of the three lowest subbands in (110) system are generally speaking smaller than (111) system, but in either (110) or (111) system, it is lowered by compressive stresses applied in the direction parallel to channel and tensile stresses applied perpendicular to channel. The channel direction is chosen as along the 45° direction in the x-y plane, namely, $[-1 \ 1 \ -\sqrt{2}]$ in the (110) system and $[1-\sqrt{3} \ 1+\sqrt{3} \ -2]$ in the (111) system.
3.4. Mobility

Results of the mobility ($\mu_y$) in (110) and (111) channels under external electric field strength 1 MV/cm with external stresses applied either parallel or perpendicular to channel are shown in Fig. 11. The external stress conditions of $\mu_y$ are all same as the conditions of $m_\sigma$. We can see $\mu_y$ in (110) system is in general larger than (111) system, but in either (110) or (111) system, it is arisen by compressive stresses applied in the direction parallel to channel and tensile stresses applied perpendicular to channel. After comparing the behaviors of $m_\sigma$ and $\mu_y$, my results show mobility is very sensitive to effective mass under different stresses.

4. Conclusions

In this work I reported theoretical analysis of valence energy subband properties including the hole mobility of p-type metal-oxide-semiconductor (PMOS) inversion layer with both compressive and tensile external stresses in both (110) and (111) Si channels. Three compact expressions of scattering rate are also derived in this paper. Channel direction is chosen as along the 45° direction in the x-y plane, namely, $[-1 \ 1 \ -1/\sqrt{2}]$ in (110) system and $[1-\sqrt{3} \ 1+\sqrt{3} \ -2]$ in (111) system. Uniaxial stresses are considered in the directions both parallel and perpendicular to channel. Compressive and tensile stresses considered in this paper can be realized by doping carbon or germanium into the opposite sides of Si channel. Equal energy lines, carrier concentration effective mass ($m_\epsilon$), conductivity effective mass ($m_\sigma$), and hole mobility ($\mu_y$) under uniaxial stresses -3, -2, -1, 0, 1, 2, 3 GPa etc. of (110) and (111) Si channels are all calculated and discussed.
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Scattering parameters of Si are shown in TABLE I [2].

| Parameter                                           | Symbol | Value  |
|-----------------------------------------------------|--------|--------|
| Mass density (g/cm$^3$)                             | $\rho$ | 2.329  |
| Hole acoustic phonon group velocity (m/s)           | $v_g$  | 9040   |
| Hole acoustic phonon deformation potential energy (eV) | $D_A$  | 5.0    |
| Hole optic phonon deformation potential ($\times 10^8$eV/cm) | $D_o$  | 6.00   |
| Hole optic phonon energy (eV)                       | $\hbar \omega_o$ | 0.063  |
| Root-mean-square amplitude of fluctuations (nm)     | $A$    | 0.4    |
| Correlation length (nm)                             | $L$    | 3      |
Figure Captions

Fig. 1 The 25 meV equal energy lines of the 1st valence subband at gate electric field 1 MV/cm as a function of different stresses in (110) Si channel.

Fig. 2 The 25 meV equal energy lines of the 2nd valence subband at gate electric field 1 MV/cm as a function of different stresses in (110) Si channel.

Fig. 3 The 25 meV equal energy lines of the 3rd valence subband at gate electric field 1 MV/cm as a function of different stresses in (110) Si channel.

Fig. 4 The 25 meV equal energy lines of the 1st valence subband at gate electric field 1 MV/cm as a function of different stresses in (111) Si channel.

Fig. 5 The 25 meV equal energy lines of the 2nd valence subband at gate electric field 1 MV/cm as a function of different stresses in (111) Si channel.

Fig. 6 The 25 meV equal energy lines of the 3rd valence subband at gate electric field 1 MV/cm as a function of different stresses in (111) Si channel.

Fig. 7 The carrier concentration effective mass ($m_c$) of the three lowest valence subbands at gate electric field 1 MV/cm as a function of compressive and tensile stresses in (110) Si channel.

Fig. 8 The carrier concentration effective mass ($m_c$) of the three lowest valence subbands at gate electric field 1 MV/cm as a function of compressive and tensile stresses in (111) Si channel.

Fig. 9 The conductivity effective mass ($m_\sigma$) of the three lowest valence subbands at gate electric field 1 MV/cm as a function of compressive and tensile stresses in (110) Si channel.

Fig. 10 The conductivity effective mass ($m_\sigma$) of the three lowest valence subbands at gate electric field 1 MV/cm as a function of compressive and tensile stresses in (111) Si channel.
Fig. 11 The mobility in parallel and perpendicular directions relative to channel direction at gate electric field 1 MV/cm as a function of compressive and tensile stresses in (110) and (111) Si channels, respectively.
Fig. 1

- $k_x$ (1/nm)
- $k_y$ (1/nm)

1st band

(110)
Fig. 2

![Graph showing 2nd band (110) at different stresses]
Fig. 3

3rd band
(110)
Fig. 4

The diagram shows the dispersion relation for the first band (111) in a material, with the energy levels indicated at different pressures: 0 GPa, 1 GPa, 2 GPa, 3 GPa, -1 GPa, -2 GPa, -3 GPa.
Fig. 6

![Graph showing the 3rd band (111) on a 2D Brillouin zone with contours for different pressures: 0 GPa, 1 GPa, 2 GPa, and 3 GPa. The contours are labeled with their corresponding pressure values, and the Brillouin zone axes are marked as $k_x$ (1/nm) and $k_y$ (1/nm).]
Fig. 7

Stress (GPa)

1st Band
2nd Band
3rd Band

\( m_c \) (\( m_o \))

\( \text{(110)} \)

-3 -2 -1 0 1 2 3

Stress (GPa)
Fig. 9

$F = 1 \text{ MV/cm}$  (110)
Fig. 10

$F = 1 \text{ MV/cm} \quad (111)$

$\sigma(m_o)$

$\text{Stress (GPa)}$

$1^{st}$ Band (Parallel)

$2^{nd}$ Band (Parallel)

$3^{rd}$ Band (Parallel)

$1^{st}$ Band (Perpendicular)

$2^{nd}$ Band (Perpendicular)

$3^{rd}$ Band (Perpendicular)
Fig. 11

-3 -2 -1 0 1 2 3

Mobility (cm²/V s)

Stress (GPa)

(110) Parallel
(110) Perpendicular
(111) Parallel
(111) Perpendicular