Hole Mobility in Strained Ge and III-V P-channel Inversion Layers with Self-consistent Valence Subband Structure and High-k Insulators

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HOLE MOBILITY IN STRAINED GE
AND III-V P-CHANNEL INVERSION LAYERS WITH
SELF-CONSISTENT VALENCE SUBBAND STRUCTURE
AND HIGH-κ INSULATORS

A Dissertation Presented

by

YAN ZHANG

Submitted to the Graduate School of the
University of Massachusetts Amherst in partial fulfillment
of the requirements for the degree of

DOCTOR OF PHILOSOPHY

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Department of Electrical and Computer Engineering
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AND III-V P-CHANNEL INVERSION LAYERS WITH
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To my family.
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ABSTRACT

HOLE MOBILITY IN STRAINED GE AND III-V P-CHANNEL INVERSION LAYERS WITH SELF-CONSISTENT VALENCE SUBBAND STRUCTURE AND HIGH-κ INSULATORS

SEPTEMBER 2010

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We present a comprehensive investigation of the low-field hole mobility in strained Ge and III-V (GaAs, GaSb, InSb and In_{1-x}Ga_{x}As) p-channel inversion layers with both SiO\textsubscript{2} and high-κ insulators. The valence (sub)band structure of Ge and III-V channels, relaxed and under strain (tensile and compressive) is calculated using an efficient self-consistent method based on the six-band \textbf{k} \cdot \textbf{p} perturbation theory. The hole mobility is then computed using the Kubo-Greenwood formalism accounting for non-polar hole-phonon scattering (acoustic and optical), surface roughness scattering, polar phonon scattering (III-Vs only), alloy scattering (alloys only) and remote phonon scattering, accounting for multi-subband dielectric screening. As expected, we find that Ge and III-V semiconductors exhibit a mobility significantly larger than the “universal” Si mobility. This is true for MOS systems with either SiO\textsubscript{2} or high-κ

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insulators, although the latter ones are found to degrade the hole mobility compared to SiO$_2$ due to scattering with interfacial optical phonons. In addition, III-Vs are more sensitive to the interfacial optical phonons than Ge due to the existence of the substrate polar phonons. Strain – especially biaxial tensile stress for Ge and biaxial compressive stress for III-Vs (except for GaAs) – is found to have a significant beneficial effect with both SiO$_2$ and HfO$_2$. Among strained p-channels, we find a large enhancement (up to a factor of 10 with respect to Si) of the mobility in the case of uniaxial compressive stress added on a Ge p-channel similarly to the well-known case of Si. InSb exhibits the largest mobility enhancement. In$_{0.7}$Ga$_{0.3}$As also exhibits an increased hole mobility compared to Si, although the enhancement is not as large. Finally, our theoretical results are favorably compared with available experimental data for a relaxed Ge p-channel with a HfO$_2$ insulator.
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CHAPTER 1
INTRODUCTION

Continued scaling of the physical size of conventional VLSI devices causes significant degradation of channel mobility (mainly because of Coulomb interactions [10–12] and increased scattering with interfacial roughness) as well as severe gate leakage problem. Several ideas aimed at retaining the much-needed device performance (e.g., replacing Si with high-mobility channel materials, straining the channel, employing high dielectric-constant insulators) are either already in production or at an exploratory stage. In particular, attention has been paid to Ge and III-Vs as possible alternative channel materials: Their intrinsic carrier mobility significantly higher than Si (for either electrons or holes) [13] promises high performance, while the advent of new gate-insulator technologies – such as SiO$_2$ on a thin Si cap, GeO$_x$N$_y$ and HfO$_2$ – has rendered the prospect of a Ge or III-V technology more realistic [2, 4, 5, 7].

Previous work has mainly focused either on electron mobility in Ge and III-V nMOS devices [14] or on hole mobility, but limited to Si p-channel inversion layers [1, 3, 15–17]. Not so in the cases of Ge and III-Vs. Indeed, a detailed review of the experimental research on high-mobility biaxially strained Si, SiGe and Ge channel MOSFETs has been given by Lee et al. [18] only recently, with theoretical investigations being limited to the work on Ge by Sun and coworkers [3]. A large hole mobility enhancement in uniaxially compressively strained Ge p-channel has been shown in Ref. [3]. However, these commendable first efforts are based on simplified physical models for various scattering mechanisms and make use of the triangular-well approximation to calculate the valence subband structure [3]. Here we intend to provide a comprehensive
and rigorous approach to study the strain-dependent hole mobility in Ge and III-V p-channels employing a self-consistent subband structure.

Hole mobility studies are complicated by the nonparabolic, warped, and anisotropic nature of the valence subband structure. Two are the main problems we need to face: Obtain efficiently an accurate valence subband structure and employ physically accurate models to calculate the relaxation rates due to the various scattering processes which affect hole transport.

The first problem is complicated by the nonparabolic, warped, and anisotropic nature of the subband structure. Brute force requires inordinate computational efforts. Thus conventional approximations based on the use of the effective masses [16] or of the triangular-well approximation [1] have been embraced. However, the complicated subband structure mentioned above renders the former inaccurate at all densities, while the latter has been shown to become questionable under strong inversion [16]. This impasse has been broken by using methods either based on simplifying expansions of the wavefunctions into suitable basis-functions [19] or resorting to brute force and paying a hefty computational price [15]. In order to retain the efficiency and accuracy in the valence subband structure calculation, we first propose a hybrid self-consistent method, in which a two-stage procedure is employed: First, for a specific surface field, we calculate the density-of-state (DOS) of the three lowest-energy subbands ($hh, lh$ and $so$) using a triangular-well approximation and by removing crossing points among these subbands. Then the DOS are stored in a look-up table for the application in the next stage. In the second stage, we solve Schrödinger-like equation using the six-band $\mathbf{k} \cdot \mathbf{p}$ method using some suitable form for the initial potential (usually the classical solution). Then, according to the solutions of the $\mathbf{k} \cdot \mathbf{p}$ equation, the hole density distribution is calculated by shifting the tabulated DOS to the corresponding energy level. Finally, the Poisson equation is solved using a finite difference algorithm, and the new potential is employed as the update input.
for the next iteration until the desired convergence criterion is met. Since the time-
consuming DOS calculation in each iteration is overcome by shifting the tabulated
ones with a triangular-well approximation, this method retains the high efficiency of
the triangular-well approximation. For some semiconductor materials (e.g. Si), the
accuracy of the hybrid method is satisfactory due to the analogy of the subbands.
However, when the subbands are different too much, the DOS in the second stage
can not be obtained via simply shifting the tabulated ones. Under this circumstance,
the hybrid self-consistent method is not suitable any more.

Recently, an encouraging breakthrough has been provided by the fast $k \cdot p$ solver
proposed in Ref. [20]: The space of two-dimensional $K$-vectors on the plane of the
interface (the space of the “in-plane” vectors $K$, here denoted by capital letters) is
discretized by building a mesh in polar coordinates. The subband energy and proba-
bility density function for wavevectors of a given magnitude $K$ are expanded in series
of trigonometric functions of the polar angle $\phi$ while a cubic spline interpolation is
employed along the radial direction. However, since the number of required har-
monic (trigonometric) interpolation functions is determined by the anisotropy of the
subband structure, materials with a severely anisotropic subband structure require a
large number of them, and therefore more grid points along the angular direction. As
a result, the efficiency of this method varies depending on the material considered.
Ge and III-Vs are indeed these “unlucky” semiconductors requiring a large number of
harmonic functions. Thus, we consider here an alternative self-consistent method: We
first discretize the two-dimensional (2D) $K$-space with a coarse mesh as in Ref. [20]
and tabulate the subband energies and squared wavefunctions on this mesh and rely
on a cubic-spline interpolation to obtain these quantities at an arbitrary $K$. The time
required to perform the additional interpolation step is more than compensated by
the fact that we do not require to determine the number of harmonic-interpolation
functions and do not have to perform expansions over a large number of them.
The second problem we must face consists in calculating in a physically accurate way the various scattering mechanisms affecting hole transport in inversion layers. For non-polar phonon (NP) scattering, we employ the very same model of Ref. [1, 17, 21, 22] assuming once more equipartition, elastic scattering with non-polar phonons, and making use of the isotropic approximation. Regarding scattering with surface roughness, we employ the full Ando’s model for which a thorough discussion can be found in Ref. [1, 21, 23–25]. For III-V materials considered in this paper, the longitudinal Fröhlich polar optical (LO) phonon scattering [26, 27] is taken into account. Furthermore, scattering due to the remote phonon or surface optical (SO) phonon originating from the dipole field of insulators as well as Landau damping is also included to account for the effect of high-$\kappa$ dielectrics [28–30]. Γ-point wavefunction approximation has been widely used in momentum relaxation rate calculation. However, in our calculation we found the failure of the approximation in the cases of biaxially tensily strained GaSb and InSb p-channels. Thus, we used the wavefunction at the extreme point of each subband, which is named as the ground-state wavefunction approximation. Dielectric screening of surface roughness potential, usually either neglected or treated in a simplified way using a simple scalar screening wavevector [31], has been included employing a static, wavevector-dependent multi-subband screening model [1, 32–34]. Due to the dynamic property of LO phonon scattering potential, the dielectric screening should be treated in its full dynamic formulation [34]. Usually, however, simpler models are used: Either a static approximation [34] or the even more drastic use of an “effective screening parameter” [35], strictly valid only in the electric quantum limit for a $\delta$-function sheet charge distribution. In our calculation, we treat the dielectric screening for LO phonon scattering in the similar way as for SR scattering. Discussion of the effect of the various screening models will be given in the later section. NP scattering with acoustic and optical phonons is left intentionally unscreened, for the reasons discussed in Ref. [34]. Coulomb scattering with
interface traps, oxide charges, or ionized impurities (dopants) is neglected here since it only plays an important role in weak inversion case and we are interested in the best-scenario “intrinsic” mobility.
CHAPTER 2

VALENCE SUBBAND STRUCTURE CALCULATION WITH SELF-CONSISTENT METHODS

2.1 Six-Band $k \cdot p$ Method

In this section we present the methods we have followed to calculate the self-consistent valence subband structure. We start with the six-band $k \cdot p$ eigenvalue problem which provides a sufficiently accurate hole dispersion for wavevectors close to the $\Gamma$ symmetry point, namely, $k < 0.3(2\pi/a_0)$, where $a_0$ is the lattice constant [17, ?]

$$\left[\hat{H}_{k \cdot p} + \hat{H}_{so} + \hat{H}_{strain} + \hat{I}eV(z)\right] \Psi_K(z) = E(K)\Psi_K(z).$$ (2.1)

Here $\hat{H}_{k \cdot p}$, $\hat{H}_{so}$, and $\hat{H}_{strain}$ are the $k \cdot p$, the spin-orbit, and strain Hamiltonian, respectively. $e$ is the magnitude of the electron charge and $I$ is the six-order Identity matrix. $V(z)$ is the external potential (assuming the $z$-axis is perpendicular to the insulator/substrate interface), for which in bulk semiconductor $V(z) = 0$ while in inverted channels, $V(z)$ has three terms: An image-term, $V_{im}(z)$, which, in the limit of an infinitely thick channel layer, has the form $e^2\tilde{\varepsilon}/(16\pi\varepsilon z)$, and $\tilde{\varepsilon} = (\varepsilon_s - \varepsilon_{ox})/(\varepsilon_s + \varepsilon_{ox})$, $\varepsilon_s$ being permittivity of substrate, $\varepsilon_{ox}$ of the insulator. The second term, the exchange and correlation potential, $V_{ac}(z)$ [1] and the Hartree term, $V_{H}(z)$, which is the solution of the Poisson equation Eq. (2.2) and we only consider this term in our self-consistent calculation as done in [1]. The Poisson equation is given by [1, 21]

$$\frac{d^2V(z)}{dz^2} = -\frac{e}{\varepsilon_s} [\rho(z) - n(z) + N_D],$$ (2.2)
where \( N_D \) is uniform doping density, \( n(z) \) is the classical electron density given by

\[
n(z) = N_C \int_0^\infty \frac{x^{1/2}}{1+e^{x}} dx = N_C F_{1/2}(\eta),
\]

(2.3)

where \( N_C \) is the effective density-of-state and \( F_{1/2}(\eta) \) is the well-known Fermi-Dirac integral of order 1/2. \( \rho(z) \) is the hole concentration given by

\[
\rho(z) = \sum_\nu \int dK f(E_K - E_F) \|\psi_K(z)\|^2,
\]

(2.4)

where \( E_F \) is the Fermi level calculated by the bisection method with pre-set hole sheet density \( n_s \) according to the equation

\[
n_s = \sum_\nu \int dK f(E_K - E_F)
= \sum_\nu \int_0^\infty dE \frac{\rho_\nu(E)}{1 + e^{(E + E^{(0)}_\nu - E_F)/k_B T}},
\]

(2.5)

where \( k_B \) is the Boltzmann constant, \( T \) is the temperature and \( \rho_\nu(E) \) is the density-of-state in subband \( \nu \) at energy \( E \) given by

\[
\rho_\nu(E) = \theta[E - E^{(0)}_\nu] \frac{1}{(2\pi)^2} \int_0^{2\pi} d\phi \frac{K_\nu(E, \phi)}{\partial E_\nu / \partial K_\nu |_{K_\nu(E, \phi)}}.
\]

(2.6)

As given in Ref. [1], the expression for \( \hat{H}_{k_p} \) is

\[
\hat{H}_{k_p} = \begin{pmatrix}
H_{k_p} & \hat{0} \\
\hat{0} & H_{k_p}
\end{pmatrix},
\]

(2.7)
where \( \hat{0} \) is three order zero matrix and

\[
\mathbf{H}_{kp} = \begin{pmatrix}
Lk_x^2 + M(k_y^2 + k_z^2) & Nk_xk_y & Nk_xk_z \\
Nk_xk_y & Lk_y^2 + M(k_x^2 + k_z^2) & Nk_yk_z \\
Nk_xk_z & Nk_yk_z & Lk_z^2 + M(k_x^2 + k_y^2)
\end{pmatrix},
\]

(2.8)

where \( L, M, N \) are the Kohn-Luttinger parameters for \( \mathbf{k} \cdot \mathbf{p} \). The spin-orbit Hamiltonian \( \hat{H}_\text{so} \) has the following expression

\[
\mathbf{H}_\text{so} = \frac{\Delta_{so}}{3} \begin{pmatrix}
0 & -i & 0 & 0 & 0 & 1 \\
i & 0 & 0 & 0 & 0 & -i \\
0 & 0 & 0 & 0 & -1 & i \\
0 & 0 & -1 & 0 & i & 0 \\
0 & 0 & -i & -i & 0 & 0 \\
1 & i & 0 & 0 & 0 & 0
\end{pmatrix},
\]

(2.9)

where \( i \) is the imaginary units and \( \Delta_{so} \) is the spin-orbit split-off energy. The Hamiltonian associated with strain for the (001)—surface orientation, \( \hat{H}_\text{strain} \), is given by [1, 36]

\[
\hat{H}_\text{strain} = \begin{pmatrix}
\mathbf{H}_\text{strain} & \hat{0} \\
\hat{0} & \mathbf{H}_\text{strain}
\end{pmatrix},
\]

(2.10)

where

\[
\mathbf{H}_\text{strain} = \begin{pmatrix}
le_{xx} + m(e_{yy} + e_{zz}) & ne_{xy} & ne_{xz} \\
ne_{xy} & lk_{yy} + m(e_{xx} + e_{zz}) & ne_{yz} \\
ne_{xz} & ne_{yz} & le_{zz} + m(e_{xx} + e_{yy})
\end{pmatrix},
\]

(2.11)

where \( l, m \) and \( n \) are deformation potentials related to the deformation potentials \( a, b \) and \( d \) via \( l = a - 2b \), \( m = a - b \) and \( n = \sqrt{3}d \). The strain tensor \( \hat{\varepsilon} \) has components
Depending on which direction the stress is added, the strain tensor has different elements. In this thesis, we only consider stress added on (001) surface and along [110] direction, which are corresponding to a biaxial strain and uniaxial strain, respectively. For a biaxial strain on (001) surface, the only nonzero components of the strain tensor are [1, 37]

\[ e_{xx} = e_{yy} = e_{\parallel}, \]
\[ e_{zz} = -\frac{c_{12}}{c_{11}} e_{\parallel}. \] (2.13)

While for strain along [110] direction, the nonzero components of the strain tensor are

\[ e_{xx} = e_{yy} = 2c_{44} - \frac{c_{12}}{c_{11} + c_{12} + 2c_{44}} e_{\parallel}, \] (2.14)
\[ e_{xy} = -\frac{c_{11} + 2c_{12}}{c_{11} + c_{12} + 2c_{44}} e_{\parallel}, \] (2.15)
\[ e_{zz} = e_{\parallel}. \] (2.16)

In the above equations, \( e_{\parallel} = \frac{a_{\text{substrate}}}{a_{\text{channel}}} - 1 \) is the strain component parallel to the surface plane, and \( c_{11}, c_{12}, c_{44} \) are the elastic constants. All of the above band structure parameters are obtained from Refs. [1, 38].

As an example, we have plotted the equienergy surfaces as well as contours for bulk Si on the \( xy \) plane (25 meV above the ground state), which are shown in Fig. 2.1 and 2.3. The in-plane ([100] direction) and out-of-plane ([110] direction) energy dispersions for relaxed and biaxially tensilly and compressively strained bulk Ge on (001) surface are also illustrated in Fig. 2.4 - 2.6.

### 2.2 Self-Consistent Methods

Due to the confinement of surface field closing to the interface, the band structure of the holes in the channel are quantized into subbands and can be considered as
Figure 2.1. 3D equienergy surface (25meV) above ground state energy in relaxed bulk Si.

a 2D hole gas (2DHG). The quantization effect causes the shift of the hole density in the channel, due to which the classical approximation underestimates the gate capacity [16, 39]. Taking into account the quantization effect, the term $k_z$ in $H_{k,p}$ (Eq. (2.1)) needs to be replaced with the operator $-i\frac{d}{dz}$. A finite difference algorithm with uniform and non-uniform meshes is employed to numerically solve Eq. (2.1). In addition, the computation of hole density (Eq. (2.4)) requires the energy and gradient for a given wavevector in the 2D $K$-space, which are the solution of Eq. (2.1). Therefore, the Schrödinger-like equation (Eq. (2.1)) is coupled with the Poisson equation (Eq. (2.2)) and we have to solve them iteratively at each wavevector $K$ in the 2D $K$-space. Consequently, it results in a huge computational cost as mentioned.
Figure 2.2. 3D equienergy surface (25meV) above ground state energy in bulk Si with 1GPa tensile stress along [001] direction.
Figure 2.3. 3D equienergy surface (25 meV) above ground state energy in bulk Si with 1GPa tensile stress along [110] direction.
Figure 2.4. Energy dispersion in relaxed bulk Ge.
Figure 2.5. Energy dispersion in 2% biaxially compressively strained bulk Ge.
Figure 2.6. Energy dispersion in 2% biaxially tensile strained bulk Ge.
in Chap. 1. Therefore, in order to increase the efficiency as well as keep an acceptable accuracy, we propose two self-consistent methods to calculate the valence subband structure: The hybrid self-consistent method and the efficient self-consistent method.

2.2.1 Hybrid Self-Consistent Method

Our first proposed method is the hybrid self-consistent method. This method has the efficiency of the triangular-well approximation and its accuracy is dependent on which semiconductor material is in use. In this section, we first introduce the detailed techniques of this method and validate its accuracy via comparing the computed hole density using this method and the conventional self-consistent method.

2.2.1.1 Techniques

As mentioned before, there are two stages in this method. In the first stage, there are two steps: The first step is extracting the three ground-state subbands, $hh$, $lh$ and $so$ by removing crossing points among them, and the second step is calculating the DOS of the extracted three ground-state subbands and storing them in a look-up table. In the second stage, the self-consistent calculation is performed by shifting the tabulated DOS in the first stage.

In order to explain the whole procedure about how to remove crossing points to extract the pure first three subbands, we use the subband structure along [100] direction in a relaxed Si p-channel as an example. The nature of each subband can be established by looking at the “shape” of the equienergy lines in the 2D $K$-space and “counting the nodes” of the wavefunctions [1]. From the Fig. 2.7(a), we can see that the first two subbands are the pure first $hh$ and $lh$ subbands and no crossing points with other subbands. For the third subband, $so$ subband, within some region ($K < 0.12\pi/a_0$), the $so$ is pure. However, beyond this region, the $so$ crosses with the higher energy ladders of the $hh$ and $lh$ by observing the wavefunctions of these subbands. Therefore, we define these two positions as crossing points and intend
to extract the pure $so$ by removing them. The removing can be done in this way: Identify various energy ladders at $\Gamma$ point by solving the Eq. (2.1) and shift the energy dispersion of the first $hh$ to the energy position of the second $hh$ at $\Gamma$ point. Then, compare the shift energy dispersion with all of the subbands at each $K$ point, the subband which has smallest energy difference with the shift $hh$ is set as the second $hh$. By this way, one of the crossing point can be removed and the $so$ is partially extracted as shown in Fig.2.7(b). Figure 2.7(c) shows the result of removing another crossing point by repeating the similar procedure to the first $lh$. In the end, we obtain the pure $so$ as illustrated in Fig. 2.7(d). Finally, we store the energy dispersion of the extracted $hh$, $lh$ and $so$ in the first look-up table.

In the second step, we compute the DOS using a triangular-well potential. According to Eq. (2.6), we need to know the wavevector $K_\nu$ and gradient $\frac{\partial E_\nu}{\partial K}|_{K_\nu(E,\phi)}$ for a given subband $\nu$, energy $E$ and direction $\phi$ in the 2D $K$-space, for which the general energy eigenvalue problem (Eq. 2.1) needs to be transformed into a wavevector eigenvalue problem, or inverse eigenvalue problem [1]. The detailed derivation for this procedure is as follows. After discretizing in the real space along $z$-direction with uniform meshes and the boundary condition is set as $\psi_K(z=0) = \psi_K(z \rightarrow \infty) = 0$, Eq. (2.1) becomes

\[
\begin{pmatrix}
\ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\
\hat{D}_- & \hat{D}_{\ell-1} & \hat{D}_{\ell} & \hat{D}_+ & 0 & 0 & \ddots & \ddots \\
0 & \hat{D}_- & \hat{D}_{\ell} & \hat{D}_+ & 0 & \ddots & \ddots & \ddots \\
0 & 0 & \hat{D}_- & \hat{D}_{\ell+1} & \hat{D}_+ & \ddots & \ddots & \ddots \\
\ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\
\end{pmatrix}
\begin{pmatrix}
\psi_{K,\ell-1} \\
\psi_{K,\ell} \\
\psi_{K,\ell+1} \\
\vdots
\end{pmatrix}
= E(K)
\begin{pmatrix}
\psi_{K,\ell-1} \\
\psi_{K,\ell} \\
\psi_{K,\ell+1} \\
\vdots
\end{pmatrix},
\tag{2.17}
\]

where each $\psi_{K,\ell} = \psi(z_\ell)K$ is a 6-component column-vector $\psi_i(z_\ell)$, the index $i$ running over the $k \cdot p$ basis. For the particular case of (001) surfaces, the discretized differential operators are give by
\[
\hat{D}(K)_{\ell} = \begin{pmatrix} D(K)_{\ell} & 0 \\ 0 & D(K)_{\ell} \end{pmatrix} + \hat{H}_{so} + IV(z_{\ell}),
\] (2.18)

where

\[
D(K)_{\ell} = \begin{pmatrix} \frac{Lk^2_z + Mk^2_y + \frac{2M}{\Delta^2}}{Nk_xk_y} & Nk_xk_y \\ Nk_xk_y & \frac{Lk^2_y + Mk^2_x + \frac{2M}{\Delta^2}}{0} \\ 0 & 0 & M(k^2_x + k^2_y) + \frac{2L}{\Delta^2} \end{pmatrix},
\] (2.19)

\[
\hat{D}(K)_{-} = \begin{pmatrix} D(K)_{-} & 0 \\ 0 & D(K)_{-} \end{pmatrix},
\] (2.20)

and

\[
D(K)_{-} = \begin{pmatrix} -\frac{M}{\Delta^2} & 0 & i\frac{Nk_x}{2\Delta} \\ 0 & -\frac{M}{\Delta^2} & i\frac{Nk_y}{2\Delta} \\ i\frac{Nk_x}{2\Delta} & i\frac{Nk_y}{2\Delta} & -\frac{L}{\Delta^2} \end{pmatrix},
\] (2.21)

and \(\hat{D}(K)_{+} = \hat{D}(K)_{-}^\dagger\). Because of the quadratic dependence in \(K\), the total Hamiltonian \(\hat{H}(K, K_z)\), writing \(K\) as \((K \cos \phi, K \sin \phi)\), Eq. (2.1) can be rewritten as

\[
[K^2\hat{D}_2(\phi, K_z) + K\hat{D}_1(\phi, K_z) + \hat{D}_0(\phi, z, K_z)] \cdot \psi_K(z) = E(K) \cdot \psi_K(z).
\] (2.22)

Introducing the column vector \(\psi_K^{(1)} = K\psi_K\), the above equation can be recast in the form of the following eigenvalue problem in \(K\) of rank twice as large as the original problem

\[
\begin{pmatrix} 0 & \mathbf{I} \\ -\hat{D}_2^{-1}(\phi, K_z) \cdot [\hat{D}_0(\phi, K_z) - IE] & -\hat{D}_2^{-1}(\phi, k_z) \cdot \hat{D}_0(\phi, k_z) \end{pmatrix} \begin{pmatrix} \psi_K(z) \\ \psi_K^{(1)}(z) \end{pmatrix}
\]
Thus, setting $\phi = \phi_m$, $E = E_n$, and solving the eigenvalue problem defined by Eq. (2.23), one obtains the desired “equienergy lines” $K_{m,n} = K(E_n, \phi_m)$. The gradients $\nabla K E$ at the same points $(E_n, \phi_m)$ can also be computed. Finally, the DOS (Eq. (2.6)) for the first three subbands, $hh, lh$ and so, are calculated and stored in the second look-up table. Figure 2.8 shows the calculated DOS in a relaxed Ge p-channel.

In the second stage, the self-consistent calculation is performed using the stored DOS of the first $hh, lh$ and so in the 1st stage. The iteration starts from a guess channel potential, which is the solution of the Poisson equation (Eq. (2.2)) with the classical model for the density of both electrons and holes. Then with the obtained potential, we solve the $k \cdot p$ equation (Eq. (2.1)) at $\Gamma$ point using finite difference method with uniform grids. The obtained eigen-energy determines the positions of different energy ladders. The tabulated DOS in the first stage is shifted to these positions of the corresponding energy ladder, and thus we can evaluated the Fermi level $E_F$ using Eq. (2.5). For the hole density (Eq. 2.4), we use the wavefunction at $\Gamma$ point to approximate the wavefunctions of other $K$ value in the same subband, which is the so-called $\Gamma$-point wavefunction approximation. Thus, Eq. (2.4) can be expressed as

$$\rho (z) = \sum_{\nu} \psi_{\nu}^{\Gamma} (z) \int_{0}^{\infty} dE \frac{\rho_{\nu} (E)}{1 + e^{(E + E_{\nu}^{(0)} - E_F) / K_B T}},$$

(2.24)

The goodness of this $\Gamma$-point wavefunction approximation can be evaluated by the mean square error (MSE) by the following equation

$$MSE = |\psi_{\mathbf{K}} - \psi_{\Gamma}|^2,$$

(2.25)
which is shown in Fig. 2.9. The obtained hole density is then input in the Poisson 
equation (Eq. (2.2)) and solve it with Newton-Raphson method to get an update 
potential $V(z)$, which will be used as the input of the next iteration. This stage will 
be repeated until the potential $V(z)$ converges to some pre-set threshold. A flowchart 
for the hybrid self-consistent method is shown in Fig. 2.10.

2.2.1.2 Accuracy Validation

Since we have employed the tabulated DOS with triangular-well potential in the 
second stage, this method retains the efficiency of the triangular-well approximation. 
In order to validate the accuracy of the hybrid method, we compare the hole density 
calculated through this method and the conventional self-consistent method. Good 
agreement can be found from Fig. 2.11. One thing needs to be clarified is the way 
to calculate the hole density by conventional self-consist method. After the hybrid 
self-consistent calculation, we input the obtained potential into the Schrödinger-like 
equation (Eq. (2.1)) again and compute the DOS in the exact way using Eq. (2.6). 
Then, re-evaluate the Fermi level and hole density using Eq. (2.4) instead of Eq. (2.24). 
From Fig. 2.11, we can also see that the accuracy of the hybrid self-consistent method 
depends on which semiconductor is in use. For instance, the error can be 1.86% for 
Si while 9.6% for Ge. Thus, this method can not provide the maximum generality 
for application. Under this circumstance, another efficient self-consistent method is 
proposed.

2.2.2 Efficient Self-Consistent Method

As mentioned before, the efficient self-consistent method is motivated by [15] and 
the fast $k \cdot p$ solver proposed by A.T.Phma et al. in [20]. As done for introducing the 
hybrid self-consistent method, we first describe techniques for this method and then 
show its validity by comparing the hole density, energy dispersion and equienergy 
contour.
Figure 2.7. The 1st step in the 1st stage of the hybrid self-consistent method: removing crossing points and extract the first three subbands. The subband structure is along [100] direction in a relaxed Si p-channel with surface field $F_S = 1.0$ MV/cm.
2.2.2.1 Techniques

A nonuniform finite difference method is employed to numerically solve the eigenvalue problem (Eq. (2.1)). In order to preserve its Hermitian form, we follow the method proposed in Ref. [21, 40] and recast Eq. (2.1) as

$$
\left[ \hat{H}^{(2)} \frac{d^2}{dz^2} + \hat{H}^{(1)} \frac{d}{dz} + \hat{H}^{(0)} \right] \Psi_K(z) = E(K)\Psi_K(z), \tag{2.26}
$$

where $\hat{H}^{(2)}$, $\hat{H}^{(1)}$ and $\hat{H}^{(0)}$ are the matrices obtained from Eq. (2.1) when isolating the terms quadratic, linear, and homogeneous in $k_z$. Their form is given by

$$
\hat{H}^{(2)} = \begin{pmatrix}
\hat{h}^{(2)} & \hat{0} \\
\hat{0} & \hat{h}^{(2)}
\end{pmatrix}, \tag{2.27}
$$

with

$$
\hat{h}^{(2)} = \begin{pmatrix}
-M & 0 & 0 \\
0 & -M & 0 \\
0 & 0 & -L
\end{pmatrix}, \tag{2.28}
$$

$$
\hat{H}^{(1)} = \begin{pmatrix}
\hat{h}^{(1)} & \hat{0} \\
\hat{0} & \hat{h}^{(1)}
\end{pmatrix}, \tag{2.29}
$$

with

$$
\hat{h}^{(1)} = \begin{pmatrix}
0 & 0 & -iNk_x \\
0 & 0 & -iNk_y \\
-iNk_x & -iNk_y & 0
\end{pmatrix}, \tag{2.30}
$$
and

\[
\hat{H}^{(0)} = \begin{pmatrix}
\hat{h}^{(0)} & \hat{0} \\
\hat{0} & \hat{h}^{(0)}
\end{pmatrix} + \hat{H}_{so} + \hat{H}_{strain} + \hat{IV}(z) ,
\]

with

\[
\hat{h}^{(0)} = \begin{pmatrix}
Lk^2 + Mk_y^2 & Nk_xk_y & 0 \\
Nk_xk_y & Lk_y^2 + Mk_x^2 & 0 \\
0 & 0 & M(k_x^2 + k_y^2)
\end{pmatrix},
\]

where \( \hat{0} \) is the \( 3 \times 3 \) null matrix. The final eigenvalue problem discretized over a nonuniform mesh takes the form

\[
\hat{A}\Psi = E\Psi ,
\]

where the \( 6 \times 6 \) matrix element \( \hat{A}_{mn} \) is given by

\[
\hat{A}_{mn} = \begin{cases}
-\frac{2\hat{f}^{(2)}}{\Delta_m(\Delta_m + \Delta_{m-1})} - \frac{i\hat{f}^{(1)}}{\Delta_m + \Delta_{m-1}}, & m = n + 1 \\
\frac{2\hat{f}^{(2)}}{\Delta_m(\Delta_m + \Delta_{m-1})} + \frac{i\hat{f}^{(1)}}{\Delta_m + \Delta_{m-1}}, & m = n - 1 \\
-\hat{A}_{m,m+1} - \hat{A}_{m,m-1} + \hat{H}^{(0)}, & m = n \\
0, & \text{otherwise}
\end{cases}
\]

As given in Ref. [40, ?], we introduce a transformation matrix \( \hat{M} = \hat{L} \times \hat{L} \) where \( \hat{L} \) is a diagonal matrix with diagonal element \( L_{mm} = \sqrt{\frac{\Delta_m + \Delta_{m-1}}{2}} \). Equation (2.33) can be rewritten as

\[
\hat{A}\Psi = E\Psi \implies \hat{A}\hat{L}^{-1}\hat{L}\Psi = E\hat{L}^{-1}\hat{L}\Psi
\]
\[(\hat{L}\hat{A}\hat{L}^{-1})\hat{L}\Psi = E\hat{L}\Psi \implies \hat{B}\Omega = E\Omega.\] (2.35)

By defining another matrix \(\hat{B} = \hat{L}\hat{A}\hat{L}^{-1}\) and wavevector \(\Omega = \hat{L}\Psi\), this matrix is still Hermitian, but having employed a nonuniform mesh size we are able to reduce the size of the eigenvalue problem, Eq. (2.1), and thus reduce the computational effort required to solve the original problem [40].

As mentioned before, the computation of the hole density requires the knowledge of the hole energy and of its gradient for a given wavevector in 2D \(\mathbf{K}\)-space. Therefore, we need to discretize the 2D \(\mathbf{K}\)-space and at each \(\mathbf{K}\)-point we must solve Eq. (2.1). This is the major numerical effort required to solve the self-consistent problem. Here we first discretize \(\mathbf{K}\)-space into \(N_K \times N_\phi\) equally spaced mesh points along the radial and the angular directions. We then solve Eq. (2.1) at each mesh point using the nonuniform finite difference method discussed above and store the energy and wave functions in a look-up table. The energy dispersion at arbitrary \(\mathbf{K}\) can be interpolated from this table using a 1D cubic-spline method [41] along both the radial and the angular directions. One segment of the cubic-spline function \(S^\nu(K)\) for the \(\nu^{th}\) subband along the radial direction is given by

\[S_j^\nu(K) = a_j(K - K^j)^3 + b_j(K - K^j)^2 + c_j(K - K^j) + E^\nu_{K^j,\phi^j},\] (2.36)

for which \(K \in [K^j, K^{j+1}], j = 0, \cdots, n\), where \(E^\nu_{K^j,\phi^j}\) are the tabulated values and \(a_j, b_j, c_j\) are the cubic-spline interpolation coefficients. These are obtained by imposing the following conditions

\[
\begin{cases}
S'_{j-1}(K_j) = S'_{j}(K_j), j = 1, \cdots, n - 1 \\
S'_{j-1}(K_j) = S''_{j-1}(K_j), j = 1, \cdots, n - 1 \\
S'_0(K_0) = 0 \\
S''_{n-1}(K_n) = 0
\end{cases}
\] (2.37)
Having obtained the energy at an arbitrary wavevector along the given direction, we repeat the same procedure now along the angular direction. This 2D interpolation is used exactly as just described when dealing with Eq. (2.4). On the contrary, when solving for the Fermi level, Eq. (2.5), we employ a finer mesh in $\mathbf{K}$-space to evaluate the density-of-state, $\rho_\nu(E)$ in each subband. This finer mesh is constructed by tabulating the dispersion obtained via the interpolation from the coarser mesh, as just described. Once the Fermi level has been determined using a bisection method from Eq. (2.5), the hole density in each subband $\nu$, $\rho_{K,\phi}^\nu(z)$, (we have employed up to 30 subbands) at the $N_K \times N_\phi$ mesh points is calculated from Eq. (2.4) and inserted into the Poisson equation, Eq. (2.2), to obtain an updated potential. The calculation is performed iteratively using Broyden second method [42, 43] until convergence is reached. The flowchart for the whole procedure is shown in Fig. 2.14.

In order to show the convergence of Broyden second method, we make a comparison for the norm of residual vector $V^{(m+1)} - V^{(m)}$ computed by the linear mixing ($\beta = 0.25$) and Broyden second method as shown in Fig. 2.12.

2.2.2.2 Accuracy Validation

The validity of the efficient self-consistent method is proved by comparing our simulated energy dispersion, the equienergy contour, the hole density and channel potential with the results from the conventional self-consistent method [15] in a relaxed GaAs p-channel with surface field $F_s = 1.0$ MV/cm. Good agreement can be found.
Figure 2.8. Density-of-state for the hh, lh and so subbands extracted in the first stage of the hybrid self-consistent method.
Figure 2.9. Evaluation of the Γ-point wavefunction approximation.
1. Get ground–state subbands by removing crossing in triangular–well potential approximation

2. Tabulate DOS of the first three subbands (\(hh\), \(lh\) and so) in step 1

3. Solve Schrödinger equation with some guess channel potential \(V_0\)

4. Calculate hole density distribution by shifting the tabulated DOS to the energy level given in step 3 and applying \(\Gamma\) point wavefunction approximation

Solve Poisson equation to get the new channel potential \(V_n\)

Replace \(V_0\) with \(V_n\) in step 3

Stop

**Figure 2.10.** Flowchart for hybrid self-consistent method.

(a) Relaxed Si p-channel inversion layer

(b) Relaxed Ge p-channel inversion layer

**Figure 2.11.** Validation of the hybrid self-consistent method by comparing its hole density with the one calculated by the conventional self-consistent (labeled by exact in the figure).
Figure 2.12. Comparison of the convergence of linear mixing and Broyden second method.
Figure 2.13. Comparison of hole density calculated by different iteration algorithms: the linear mixing and Broyden second method.
Put the obtained hole density into Poisson equation and compute the potential $V(z)$

Compute the hole density using the obtained $E_F$ and results in the 1\textsuperscript{st} table, then repeat the 1D cubic–spline interpolation to get hole density at arbitrary k-point

Compute the Fermi energy $E_F$ for a given hole sheet density with the results stored in the 2\textsuperscript{nd} table

Compute the energy along the radial and angular directions using 1D cubic–spline interpolation and store results in the 2\textsuperscript{nd} table

Solve the 6–band $k$-$p$ Schrodinger equation at $N_k \times N_\phi$ mesh grids in the 2D $k$–space and store results in the 1\textsuperscript{st} table

Initial guess $V_0$ for the potential

$|V-V_0|<\varepsilon$

\[\text{end}\]

\textbf{Figure 2.14.} Flowchart of the efficient self-consistent method.
Figure 2.15. Energy dispersion in a relaxed GaAs p-channel with surface field $F_s = 1.0$ MV/cm calculated by the efficient self-consistent method and conventional self-consistent method.
Figure 2.16. Equienergy contours in a relaxed GaAs p-channel with surface field $F_s = 1.0$ MV/cm calculated by the efficient self-consistent method and conventional self-consistent method.
Figure 2.17. Hole density in a relaxed GaAs p-channel with surface field $F_s = 1.0$ MV/cm calculated by the efficient self-consistent method and conventional self-consistent method.
CHAPTER 3
PHYSICAL MODELS FOR LOW-FIELD HOLE MOBILITY IN AN INVERSION LAYER

The low-field hole mobility is computed by solving the linearized Boltzmann transport equation. Following the discussion in Ref. [1], the $xx$-component of the mobility tensor, $\mu_{ij}$, can be written as

$$
\mu_{xx} = \frac{e}{4h^2 \pi^2 k_B T n_s} \sum_\nu \int_0^{2\pi} d\phi \int_{E_{\nu(0)}}^{\infty} dE \frac{K_{\nu}(E, \phi)}{\left| \frac{\partial E_{\nu}}{\partial K} \right|} \cdot \left( \frac{\partial E_{\nu}}{\partial K} \right)^2 \tau_x^{(\nu)} [K_{\nu}(E, \phi), \phi] f_0(E)[1 - f_0(E)], \quad (3.1)
$$

where $n_s = \sum_\nu n_\nu$ and $n_\nu$ is the population of subband $\nu^{th}$. $\tau_x^{(\nu)}(K, \phi)$ is the relaxation time for $x$-component of the momentum in subband $\nu$ and given by

$$
\frac{1}{\tau_x^{(\nu)}} = \frac{1}{\tau_{x,NP}^{(\nu)}} + \frac{1}{\tau_{x,SR}^{(\nu)}} + \frac{1}{\tau_{x,LO}^{(\nu)}} + \frac{1}{\tau_{x,SO}^{(\nu)}} + \frac{1}{\tau_{x,AL}^{(\nu)}}, \quad (3.2)
$$

where $\tau_{x,NP}$, $\tau_{x,SR}$, $\tau_{x,SO}$, $\tau_{x,LO}$, $\tau_{x,AL}$ are the momentum relaxation time for non-polar acoustic/optical phonon scattering, surface roughness scattering, remote phonon scattering, longitudinal optical phonon scattering which only exists in polar materials and alloy scattering (for alloy only), respectively.

According to Ref. [1, 33], the momentum relaxation rate is defined as

$$
\frac{1}{\tau_{\mu \nu}(K)} = \frac{2\pi}{\hbar} \int \frac{dK'}{(2\pi)^2} |M_{\mu \nu}(k')|^2 \delta[E_\mu(K) - E_\nu(K')]
$$

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\[ \pm \hbar \omega_{\mathbf{K}'-\mathbf{K}} \times \frac{1-f(E')}{1-f(E)} \times \left\{ 1 - \frac{v_x^{(\nu)(\mathbf{K}')_z}}{v_x^{(\nu)(\mathbf{K})_z}} \frac{f^{(\nu)(\mathbf{K}')}}{f^{(\nu)(\mathbf{K})}} \right\}, \]  

(3.3)

where \( E' \) is the energy of the final state \( \mathbf{K}' \) and \( v_x^{(\mu)}(\mathbf{K}) \) is \( x \)-component of the hole group velocity at the wavevector \( \mathbf{K} \) and \( M_{\mu\mathbf{K}',\nu\mathbf{K}} \) is the scattering potential \( \Phi(\mathbf{R}, z) \) associated matrix element defined by

\[
M_{\mu\mathbf{K}',\nu\mathbf{K}} = \int \frac{d\mathbf{R}}{(2\pi)^2} e^{-i(\mathbf{K}'-\mathbf{K}) \cdot \mathbf{R}} \times \int_0^\infty dz \Psi_{\mathbf{K}'}^\dagger(\nu)(z) \cdot \Psi_{\mathbf{K}}^{(\mu)}(z) \Phi(\mathbf{R}, z). \tag{3.4}
\]

The implicit expression given by Eq. (3.3) requires a self-consistent solution since the total relaxation rate appears inside the integral, rendering the problem equivalent to finding the solution of a nonlinear integral equation. For the isotropic and elastic NP scattering, the term in curly brackets in Eq. (3.3) reduces to unity and thus it is unnecessary to do the time-consuming self-consistent calculation. For other scattering processes, we simplify the term in curly brackets to \( 1 - \cos \theta \) as done in Refs. [1, 17, 21, 22]. Another significant complication is caused by the fact that the matrix element defined in Eq. (3.4) depends on the initial and final wavevectors \( \mathbf{K} \) and \( \mathbf{K}' \) also via the \( \mathbf{K} \)-dependence of the wavefunctions. This renders futile any attempt to perform analytically at least one of the integrations and also requires the tabulation of all wavefunctions \( \Psi_{\mathbf{K}}^{(\mu)} \). Thus, when dealing with thermal carriers (as in our case) populating only a small region of the 2D \( \mathbf{K} \)-space, it is reasonable to assume that the wavefunctions change weakly with \( \mathbf{K} \) and replace \( \Psi_{\mathbf{K}}^{(\mu)} \) with the wavefunction calculated at the zone-center, \( \Psi_{\Gamma}^{(\mu)} \) (\( \Gamma \)-point approximation). While this approximation has been employed before [1, 17, 22], we found at least two cases, in which it fails quite dramatically: Considering biaxially tensile strained GaSb and InSb p-channels, we found that the two lowest-energy subbands, a heavy- and a light-hole subband, cross near the \( \Gamma \) point as the hole sheet density increases. This
happens when the symmetry-breaking due to the confining field results in subband minima away from the symmetry-point $\Gamma$. It implies that, except in a very small region around the zone center, the $\Gamma$-point approximation would mix the heavy- and light-hole wavefunctions, which results in a significant discontinued mobility, an artifact, with the increased hole sheet density. A better approximation which we have embraced consists in assuming $\Psi_K^{(\mu)} \approx \Psi_g^{(\mu)}$, instead of $\Psi_K^{(\mu)} \approx \Psi_{\Gamma}^{(\mu)}$, where $\Psi_g^{(\mu)}$ is the wavefunction calculated at the extreme point of the $\mu$-th subband (ground-state wavefunction approximation), in general away from the zone center.

Coulomb scattering with interface traps, oxide charges, or ionized impurities (dopants) is neglected here since it only plays an important role in weak inversion case and we are interested in the best-scenario “intrinsic” mobility.

### 3.1 Momentum Relaxation Rate for AL Scattering

For AL scattering, we use the model given by Ref. [35]

$$\frac{1}{\tau_{AL}^{(\mu)}(k)} = \frac{2\pi(\Delta E)^2 \times (1 - x) a^3 \rho_{\nu} [E_{\mu}(k)]}{\hbar} F_{\mu\nu},$$

(3.5)

where $\Delta E$ is the alloy scattering potential which takes the value of 0.267 eV for In$_{1-x}$Ga$_x$As [35], $x$ is the indium mole fraction and $a$ is the lattice constant and the “form factor” $F_{\mu\nu}$ is given by

$$F_{\mu\nu} = \int_0^W dz |\Psi_{(\mu)}^{(g)}(z) \cdot \Psi_{(\nu)}^{(g)}(z)|^2.$$

(3.6)

Here $\Psi_{(\mu)}^{(g)}$ represents the ground-state envelope function of the $\mu$th subband which usually (but not always) coincides with the wavefunction at the $\Gamma$ point.
### 3.2 Momentum Relaxation Rate for NP Phonon Scattering

Following Ref. [1], we adopt the equipartition, elastic, and isotropic approximation for acoustic and optical phonon scattering and ignore the dependence on $\mathbf{K}$ of the wave functions assuming $\psi^{(\mu)}_K(z) \approx \psi^{(\mu)}_g(z)$. Thus, accounting for both emission and absorption processes, the momentum relaxation rate for non-polar acoustic phonon scattering is given by

\[
\frac{1}{\tau^{(\mu)}_{x,ac}(\mathbf{K})} \approx \frac{2\pi k_BT\Xi_{eff}^2}{\hbar \rho v_f^2} \sum_\nu \mathcal{F}_{\mu\nu} \rho_\nu \left[ E_\mu(\mathbf{K}) \right], \quad (3.7)
\]

where $\Xi_{eff}$ is the acoustic deformation potential averaged over angles. Similarly, the momentum relaxation rate due to nonpolar scattering with optical phonon scattering can be expressed as

\[
\frac{1}{\tau^{(\mu)}_{x,op}(\mathbf{K})} \approx \frac{\pi (DK)_{op}^2}{\rho \omega_{op}} \sum_\nu \mathcal{F}_{\mu\nu} \rho_\nu \left[ E_\mu(\mathbf{K}) \mp \hbar \omega_{op} \right] \times \frac{1-f_0[E_\mu(\mathbf{K})\mp \hbar \omega_{op}]}{1-f_0[E_\mu(\mathbf{K})]} \left( n_{op} + \frac{1}{2} \pm \frac{1}{2} \right), \quad (3.8)
\]

where $(DK)_{op}$ is the average optical deformation potential. The “form factor” $\mathcal{F}_{\mu\nu}$ is given by the usual expression

\[
\mathcal{F}_{\mu\nu} = \int_0^\infty dz \left| \psi^{(\mu)}_g(z) \psi^{(\nu)}_g(z) \right|^2. \quad (3.9)
\]

### 3.3 Momentum Relaxation Rate for SR Scattering

we have treated scattering with surface roughness accounting both for the Prange-Nee as well as for Ando’s Coulomb terms. Thus, the corresponding momentum relaxation rate can be written as

\[
\frac{1}{\tau^{(\mu)}_{x,SR}(\mathbf{K})} \approx \frac{2\pi}{\hbar} \sum_\nu \frac{1}{4\pi^2} \int_0^{2\pi} d\phi \frac{K_\nu(E,\phi)}{|\partial E_\nu/\partial K|_{E_\nu(\mathbf{K})}} \left| V^{(SR)}_{\nu\mu}(\mathbf{K}) \right|^2.
\]

38
\[ [1 - \cos \theta_{K,K'}] \theta \left[ E_\mu(K) - E_\nu^{(g)} \right]. \] (3.10)

In this expression \( \theta_{K,K'} \) is the angle between the initial and final states and \( \theta(E) \) is the step function. The matrix element \( V^{(SR)}_{\nu K',\mu K} \) is given by

\[ V^{(SR)}_{\nu K',\mu K} = S(K - K') \times \left\{ \Gamma^{(SR)}_{\nu K',\mu K} + \frac{e^2}{\epsilon_s (\Delta + \epsilon_{ox})} \left[ -H^{(1)}_{\nu K',\mu K} + \tilde{\epsilon}H^{(2)}_{\nu K',\mu K} \right] \right\}, \] (3.11)

where \( \tilde{\epsilon} = \frac{\epsilon_{ox} - \epsilon_{vc}}{\epsilon_s + \epsilon_{ox}} \) and the roughness power spectrum \( |S(Q)|^2 \) is given by

\[ |S(Q)|^2 = \frac{\pi \Delta^2 \Lambda^2}{(1 + Q^2 \Lambda^2/2)^3}, \] (3.12)

where \( Q = |K - K'| \). As usual, the two empirical parameters \( \Lambda \) and \( \Delta \) are correlation length and average step-height of the surface roughness, respectively. Here, given the lack of experimental information regarding the interfacial roughness and its dependence on strain, we choose the value of \( \Lambda = 2.6 \) nm and \( \Delta = 0.59 \) nm, similar to the values previously employed in Ref. [1]. The effect of these two parameters are shown in Fig. 3.1 and 3.2.

The first term on the right-hand side of Eq. (3.11), \( \Gamma^{(SR)}_{\nu K',\mu K} \) is the customary Prange-Nee term

\[ \Gamma^{(SR)}_{\nu K',\mu K} \approx \hat{T}_{k-p} \left( \frac{d\psi^{(\nu)}_g}{dz}, \frac{d\psi^{(\mu)}_g}{dz} \right), \] (3.13)

where, for (001) surfaces, \( \hat{T}_{k-p}(a,b) = -M(a_1^*b_1 + a_2^*b_2 + a_4^*b_4 + a_5^*b_5) - L(a_3^*b_3 + a_6^*b_6) \) with \( M, L \) being the Kohn-Luttinger parameters given by [32, 38]. The additional Coulomb terms we have alluded to above are due to the shift along the \( z \) direction of the hole inversion charge at a step

\[ H^{(1)}_{\nu K',\mu K} = \int_0^\infty d\psi^{(\nu)}_g(z) \cdot \psi^{(\mu)}_g(z) \]
\[ \times \int_0^\infty dz' G_Q(z, z') \frac{\partial \rho(z')}{\partial z}, \]  

(3.14)

where \( G_Q(z, z') \) is the Poisson Green’s function for the geometry of interest

\[ G_Q(z, z') = \frac{1}{2Q} \left[ e^{-Q|z-z'|} + e^{-Q|z+z'|} \right]. \]  

(3.15)

and to the potential associated to the interfacial dipoles

\[ H_{\nu K',\mu K}^{(2)} = \int_0^\infty dz \psi_{g}^{\dagger}(\nu) \cdot \psi_{g}^{(\mu)}(z) \times \left\{ (n_s + n_d) e^{-Qz} + \frac{Q^2}{16\pi} \left[ \frac{K_1(Qz)}{Qz} - \frac{1}{2} K_0(Qz) \right] \right\}, \]  

(3.16)

where \( n_d \) is the density of depletion charge and \( K_1 \) and \( K_0 \) are the modified Bessel functions of the second kind.

### 3.4 Momentum Relaxation Rate for LO Phonon Scattering

Regarding the LO phonon associated momentum relaxation rate, we have adapted to our case the results of Ref. [26] and obtained the following expression

\[
\frac{1}{\tau_{\mu\nu}(K)} = \frac{e^2 \omega_{LO}^2}{4\pi} \times \frac{1-f(E')}{1-f(E)} \times \left( \frac{1}{\varepsilon^2} - \frac{1}{\varepsilon_s^2} \right) \times \left\{ \begin{array}{c} n_{LO} \\ 1 + n_{LO} \end{array} \right\} \times \int_0^{2\pi} d\phi \int_{-\infty}^{\infty} \frac{dq_z}{2\pi} |M_{Q,\mu,\nu,q_z}^{(ex)}|^2 \times (1 - \cos \theta) \]  

(3.17)

using the approximated “relaxation” factor \( 1 - \cos \theta \), where \( \theta \) is the angle between initial and final states \( K \) and \( K' \) and \( n_{LO} \) is the Bose function. The matrix element above is given by

\[ M_{Q,\mu,\nu,q_z}^{(ex)} = \frac{\mathcal{F}_{\mu,\nu}(q_z)}{\sqrt{Q^2 + q_z^2}}, \]  

(3.18)

with \( Q = |K - K'| \) and the overlap factor

\[ F_{\mu\nu}(q_z) = \int_0^{\infty} \Psi_{g}^{(\mu)}(z) \Psi_{g}^{\dagger}(\nu) e^{iq_z z} dz, \]  

(3.19)
Figure 3.1. Study of the parameter Λ in surface-roughness scattering potential model by setting $\Delta = 2.6\text{nm}$ in a 2% biaxially compressively strained Ge p-channel.
Figure 3.2. Study of the parameter $\Delta$ in surface-roughness scattering potential model by setting $\Lambda = 0.56$ nm in a 2% biaxially compressively strained Ge p-channel.
where we use ground-state wavefunction approximation indicated by the subscript \( g \).

For unscreened matrix element (dielectric screening will be discussed in the following section), we can get a close form expression for the integral over \( q_z \) in Eq. (3.17) using the Fourier transform

\[
\int_{-\infty}^{\infty} \frac{dq_z}{2\pi} \left| M_{Q,\mu,\nu,q_z}^{(ex)} \right|^2 = \int_0^\infty \int_0^\infty \phi_\mu(z_1) \phi_\nu^*(z_2) \phi_\mu(z_2) \phi_\nu^*(z_1) \frac{1}{2Q} \left[ \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{Q}{\pi Q^2 + q_z^2} e^{-iq_z(z_1 - z_2)} dq_z \right] dz_1 \, dz_2 = \frac{1}{2} H_{\mu\nu}(Q),
\]

where the “form factor” \( H_{\mu\nu}(Q) \) is

\[
H_{\mu\nu}(Q) = \int_0^\infty \int_0^\infty \psi_\mu(z_1) \psi_\nu^*(z_2) \phi_\nu(z_2) \phi_\mu(z_1) e^{-Q|z_1 - z_2|} dz_1 \, dz_2.
\]

Therefore, Eq. (3.17) becomes

\[
\frac{1}{\tau_{\mu\nu}(K_\parallel)} = \frac{\epsilon^2 \omega_{LO}}{4\pi} \times \frac{1 - f(E')}{1 - f(E)} \times \left( \frac{1}{r_x^2} - \frac{1}{r_y^2} \right) \times \left\{ \begin{array}{c} n_{LO} \\ 1 + n_{LO} \end{array} \right\} \int_0^{2\pi} d\phi' \frac{K' \frac{\partial E}{\partial K'}}{2Q(\phi')} H_{\mu\nu}(Q(\phi)) \biggr|_{\phi'}.
\]

### 3.5 Momentum Relaxation Rate for SO Phonon Scattering

When considering the interfacial optical modes arising from the coupling between the insulator optical phonons and the surface plasmons, dealing with the III-V polar channel materials considered here requires an extension of the picture presented in Refs. [28, 29], and [30], because of the additional presence of the LO phonons in the substrate. Following Refs. [28, 29], and [30], we proceed in three steps to obtain the scattering strength for the SO phonon scattering. First, we calculate the dispersion of
the coupled modes by solving Maxwell’s equations at the insulator/substrate bound-
ary (assuming an infinitely thick insulator and no interfacial layers here and in the
following) obtaining the following secular equation

$$\epsilon_{ox}(\omega) + \epsilon_{sub}(\omega, Q) = 0,$$

where $\epsilon_{ox}$ is the dielectric function in the insulator given by

$$\epsilon_{ox}(\omega) = \epsilon_{\infty}^{ox}(\omega_{TO1}^2 - \omega^2)(\omega_{TO2}^2 - \omega^2),$$

and $\epsilon_{sub}$ is the dielectric function in the substrate

$$\epsilon_{sub}(Q, \omega) = \epsilon_{\infty}^{s} \left[ 1 - \frac{\omega_{p,s}^2(Q)}{\omega^2} \right] + (\epsilon_{\infty}^{0} - \epsilon_{\infty}^{s}) \frac{\omega_{TO3}^2}{\omega_{TO3}^2 - \omega^2},$$

expression in which the last term expressing the ionic dielectric response applies only
to III-V compound semiconductors. In Eq. (3.25) $\epsilon_{\infty}^{0}$ is the static permittivity of substrate, $\epsilon_{\infty}^{\infty}$ and $\epsilon_{\infty}^{s}$ are the optical permittivity for insulator and substrate, respectively, $\omega_{TO1}$ and $\omega_{TO2}$ are the angular frequencies of the two transverse optical phonon modes of the insulator and the relation between the longitudinal and transverse modes is
given by generalized Lyddane-Sachs-Teller relation as discussed in Ref. [28]. Also, $\omega_{TO3}$ is the frequency of substrate optical phonons, $\omega_{p,s} = [\Sigma_{\nu} e^2 n_{\nu} Q/(2\epsilon_{\infty}^{s} m_{\nu})]^{1/2}$ is the plasma frequency of the 2D hole gas (2DHG), $n_{\nu}$ and $m_{\nu}$ being the hole den-
sity and density-of-state effective mass for subband $\nu$. Equation (3.23) has multiple
solutions. Each one of them represents excitations coupling both the electronic (at
the insulator/substrate interface) and the ionic (of the two insulator TO-modes we
consider one substrate TO-mode) oscillations [28]. Therefore, in order to consider
only excitations able to subtract momentum from the hole gas, we must separate the
phonon content from the substrate-plasmon content of each mode. This leads us to the second step, consisting in extracting the relative phonon content for each branch, following Ref. [44]. Finally, in the final step, the scattering strength for each SO mode is calculated and the momentum relaxation rate for SO phonon scattering can be calculated as following

\[
\frac{1}{\tau_{\mu\nu}(K)} = \frac{\hbar^2}{2\pi^2} \int_0^{2\pi} d\phi \left| b_{Q,\omega} \right|^2 \left| F_{\mu\nu} \right|^2 \frac{K'}{\partial E/\partial K'} \times \left\{ \begin{array}{c} n_Q \\ n_Q + 1 \end{array} \right\} \times \frac{1-f(E_\mu)}{1-f(E_\nu)} \times (1 - \cos \theta), \quad (3.26)
\]

where the expressions for scattering strength \( b_{Q,\omega} \) and overlap factor \( F_{\mu\nu} \) can be found in Ref. [34]. In this expression \( n_Q \) is the Bose function and \( K' \) is determined by

\[
Q = |K - K'|
\]
\[
E_\mu \pm E_\nu = \hbar \omega_Q. \quad (3.28)
\]

These two equations constitute a non-linear problem which is solved iteratively[28].

When the collective substrate-plasmon like excitations enter the single-particle continuum in the substrate, plasmons cease to be proper excitation because of their short lifetime leading to a decay into single-particle excitations. (Landau damping). This happens as soon as the plasmon wavevector allows conservation of energy and momentum for decay into a single-particle excitation, that is when

\[
\hbar \omega_{LD}' = E'_{\nu}[K_F + Q] - E'_{\nu}[K_F]
\]

where \( K_F \) is the carrier wavevector at the Fermi energy at absolute zero and \( \omega_{LD} \) is the subband-dependent Landau damping frequency. In terms of the complicated valence subband structure, we approximate \( \omega_{LD} \) by the weighted average

45
\[ \omega_{LD} = \sum_\nu \frac{n_\nu}{n_s} \omega_{LD} \]  

(3.30)

where the weight-factor \( \frac{n_\nu}{n_s} \) is the occupation of \( \nu \)th subband. When \( \omega_{p,s} \) is within this region, the physical model of SO phonon scattering coincides with the Wang-Mahan model[45], in which the coupling between SO phonons and substrate plasmons is effectively suppressed.

A discussion of the dispersion of the interfacial modes, of their phonon and plasmon content, of the scattering strength for each mode and of the effect of Landau damping will be presented in the following section.

### 3.6 Dielectric Screening

Following the discussion in Refs. [1, 21] and [25], for an arbitrary scattering potential \( V \) the screened inter-subband (\( \mu \neq \nu \)) matrix elements \( V_{Q,\mu\nu} \) is given by

\[ V_{Q,\mu\nu} = V_{Q,\mu\nu}^{(ex)} - \sum_\lambda \epsilon_{\mu\nu,\lambda\lambda} V_{Q,\lambda\lambda}, \]  

(3.31)

where \( V_{Q,\mu\nu}^{(ex)} \) is the unscreened scattering matrix element. The diagonal (intrasubband) matrix elements entering the equation above can be obtained by inverting the linear problem

\[ \sum_\lambda \epsilon_{\mu\mu,\lambda\lambda}(Q, \omega) V_{Q,\lambda\lambda} = V_{Q,\mu\mu}^{(ex)}, \]  

(3.32)

with the dielectric matrix

\[ \epsilon_{\mu\nu,\lambda\lambda}(Q, \omega) = \delta_{\mu\nu} \delta_{\lambda\lambda} + \frac{\beta_{\lambda\lambda}}{Q} \Omega_{Q,\mu\nu,\lambda\lambda}, \]  

(3.33)

in which \( \Omega \) is the form factor

\[ \Omega_{Q,\mu\nu,\lambda\lambda} = 2 \int_0^\infty dz \Psi^{(\mu)}_g(z) \Psi^{(\nu)}_g(z). \]
\[ \times \int_0^\infty dz' \tilde{G}_Q(z, z') \Psi_g^{(\mu)}(z') \Psi_g^{(\nu)}(z') , \]

and again we use the ground-state wavefunction approximation. The quantity \( \tilde{G} \) is the reduced Green’s function \( \tilde{G} = 2QG \), and \( \beta_{\lambda\lambda} \) is the \( 2D \) screening wavevector. For time-dependent scattering potentials we must employ the dynamic screening wavevector which, in the nondegenerate, high-temperature limit is given by \([34, 44]\)

\[ \Re \left[ \beta_{\lambda\lambda}^{(2D)} \right] = \beta_{DH} \frac{\pi}{Q\ell_{\lambda}} \left\{ \Phi \left( \frac{m_{\lambda}}{2k_BT} \right)^{1/2} \left( \frac{\omega}{Q} + \frac{hQ}{2m_{\lambda}} \right) \right. \\

\left. - \Phi \left( \frac{m_{\lambda}}{2k_BT} \right)^{1/2} \left( \frac{\omega}{Q} - \frac{hQ}{2m_{\lambda}} \right) \right\}, \]  

and

\[ \Im \left[ \beta_{\lambda\lambda}^{(2D)} \right] = \beta_{DH} \frac{\pi h\omega}{Q\ell_{\lambda}k_BT} \times \exp \left( \frac{-m_{\lambda} \omega^2}{2k_BTQ^2} - \frac{h^2 Q^2}{8\pi^2 m_{\lambda} k_BT} \right) \sinh \left( \frac{h\omega}{2k_BT} \right), \]  

where \( \beta_{DH}^{(\lambda)} = \left( \frac{e^2 n_{\lambda}}{2\pi k_BT} \right)^{1/2} \) is the two-dimensional Debye-Hückel limit of the dynamic screening wavevector, and \( \ell_{\lambda} = \left[ \frac{2m_{\lambda} k_BT}{2\pi^2} \right]^{1/2} \) is the thermal wavelength of free carriers in the \( \lambda^{th} \) subband, and \( \phi(y) = 2e^{-y^2} \int_0^y e^{t^2} dt \) is the Plasma Dispersion function. \( m_{\lambda} \) is the density-of-state effective mass for the \( \lambda^{th} \) subband.

In static limit \( (\omega = 0) \), only the real part of the screening wavevector is nonzero and it is given by\([1, 21, 25]\)

\[ \beta_{\lambda\lambda}^{(2D)} = \Re \left[ \beta_{\lambda\lambda}^{(2D)} \right] = \beta_{DH} \frac{2\pi^{1/2}}{Q\ell_{\lambda}} \Phi \left[ \frac{Q\ell_{\lambda}}{4\pi^{1/2}} \right] . \]  

Screening, either dynamic or static, makes the computation of scattering potential more complicated and time-consuming. One way previously widely used to simplify
the above screening models is the effective screening model, for which the complex expression for 2D wavevector is replaced by a scalar given by[46]

\[
q_s = \sum_{\lambda} \text{Re}(\beta^{(2D)}_{\lambda\lambda}).
\]  

(3.38)

The effect of different screening models will be shown in the following section.
CHAPTER 4
DISCUSSIONS AND SIMULATION RESULTS

The structure considered in our simulation is a uniformly doped inversion layer on the (001) interface with an infinite thick insulator. We assume an infinite barrier at the substrate-insulator interface and consider the mobility along the [110] direction at room temperature. A variety of semiconductor materials (Ge, GaAs, In$_{1-x}$Ga$_x$As, GaSb, InSb) and insulating dielectrics (SiO$_2$, HfO$_2$, ZrO$_2$, Al$_2$O$_3$ and ZrSiO$_4$) are considered. In addition, biaxial and uniaxial, either tensile or compressive, stress is applied on the channel and related mobility is also investigated. We have assumed an InP substrate for In$_{1-x}$Ga$_x$As p-channel due to the lattice match when $x = 0.53$ which corresponds to the relaxed case. While $x = 0.7$ and $x = 0.3$ are for biaxial tensile and biaxial compressive strain cases, respectively.

4.1 Ge P-Channel Inversion Layer

4.1.1 Subband Structure

In this section, we present our results regarding the self-consistent subband structure of the inversion layer. We have employed $N_\phi=10$ and $N_K=49$ points (20 points for interpolation along both angular and radial direction) to discretize K-space.

Figures 4.1 and 4.2 illustrate the energy of first two subbands at the Γ-point – with the corresponding Fermi levels – as functions of the surface field for different stress conditions. We can see that the subband splitting due to the biaxial tensile stress counters the confinement-induced splitting by enhancing intersubband scattering and thus decreasing the hole mobility, however, at the same time the biaxial tensile stress
pushes the \( lh \) subband to the ground-state subband and therefore results a smaller effective-mass which increases the mobility. A comprehensive effect of biaxial tensile stress on hole mobility will be shown and discussed in the next section. Contrary to the biaxial tensile stress case, the uniaxial stress, either tensile or compressive, pushes the \( lh \) subband to higher energy and the second \( hh \) subband becomes the first excited state, which is indicated as \( hh2 \) while the first \( hh \) subband is \( hh1 \) in Fig. 4.2.

Figure 4.3 shows the complicated coupled nature of the subband dispersion along [110] direction in relaxed and biaxially and uniaxially (compressively and tensilily) strained Ge p-channel with a hole sheet density \( n_s = 7.12 \times 10^{12} \text{ cm}^{-2} \). Unlike the much simpler situation found in Si inversion layers[1] we see several subband ‘crossings’. The larger spin-orbit interaction, as thus the large splitting of subbands corresponding to different spin states, is largely responsible for this behavior. Thus, once more unlike Si, spin degeneracy must be fully accounted for, especially when noticing that about 70% of the holes occupy the two spin states of the first subband.

Figure 4.4 shows the equienergy contour plot which is a helpful guide to judge the conductivity effective mass, another important factor affecting hole transport. In this figure we show the equienergy contour plots of the first two spin-state subbands for the cases of biaxially and uniaxially strained Ge. The energy interval between contours is 30 meV. A strong anisotropy is evident. Although biaxial tensile stress pushes the \( lh \) subband to lower energies, rendering it the ground-state subband, and uniaxial stress pushes away the \( lh \) subband and the second \( hh \) becomes the first excited state (Fig. 4.2), uniaxial stress affects subband warping much more than biaxial stress. Especially along [110] direction uniaxial compressive stress causes a more significant reduction of the conductivity effective mass than other stress conditions. So uniaxial compressive stress and biaxial tensile stress both show great potential to enhance hole mobility in Ge p-channel inversion layers. In the next section we will validate these expectations with calculations of the hole mobility. Furthermore, looking at
the occupation of the subbands (Fig. 4.5-4.6), we can see that biaxial tensile strain modifies the warping to such an extent as to “swapping” the light hole ($lh$) and the heavy hole ($hh$) subbands.

![Subband Energy Graph](image)

**Figure 4.1.** Ground energy versus surface field in relaxed Ge p-channel with SiO$_2$ insulator.

### 4.1.2 Low-Field Hole Mobility with SiO$_2$ and High-$\kappa$ Insulators

In this section we present results of the calculation of the hole mobility in Ge p-channel inversion layer with SiO$_2$ or HfO$_2$ insulator. We first discuss the effect of different ways to treat SR scattering and dielectric screening. Then our results for various stress configurations and insulators are presented.

As discussed in previous sections, Jin and coworkers [25] have shown the importance of accounting for scattering caused by the full image- and dipole-induced
Figure 4.2. Ground energy versus various surface fields for (a) biaxial compressive (b) biaxial tensile (c) uniaxial compressive and (d) uniaxial tensile cases in Ge p-channels with SiO₂ insulator.
Figure 4.3. Energy dispersion along [110] direction in Ge p-channels with SiO$_2$ insulator (a) relaxed or under 2% (b) (001) biaxial compressive, (c) (001) biaxial tensile, (d) [110] uniaxial compressive, and (e) [110] uniaxial tensile stress at a hole sheet density $n_s = 7.12 \times 10^{12}$ cm$^{-2}$. 
Figure 4.4. Equienergy contour plots for the first two spin states in Ge p-channels with SiO$_2$ insulator under 2.81 GPa (a) (001) biaxial compressive, (b) (001) biaxial tensile, (c) [110] uniaxial compressive, and (d) [110] uniaxial tensile stress corresponding to 2% strain. The energy interval between contours is 30 meV and the hole sheet density is $n_s = 7.12 \times 10^{12}$ cm$^{-2}$. 
Figure 4.5. Subband occupation versus surface field in relaxed Ge p-channel with SiO$_2$ insulator.
Subband occupation plots for the first four spin states in Ge p-channels with SiO\textsubscript{2} insulator under 2% (a) (001) biaxial compressive, (b) (001) biaxial tensile, (c) [110] uniaxial compressive, and (d) [110] uniaxial tensile stress corresponding to 2% strain.

Figure 4.6.
roughness potential modeled by Ando [23, 24]. We demonstrate in Fig. 4.7 the validity of this conclusion also in the case of hole-SR scattering. The SR-limited and the total hole mobility in a relaxed Ge p-channel along the [100] direction without static screening are calculated accounting or neglecting Ando’s Coulomb effects, showing how using the simple Prange-Nee term results in a substantial overestimation of the hole mobility. In Fig. 4.8 we compare results obtained employing the full Ando model both neglecting and accounting for static multi-subband screening: As expected, dielectric screening depresses hole-SR scattering and thus boosts the mobility.

In Fig. 4.9 we illustrate the effect of the individual scattering processes on the hole mobility as a function of surface field in a relaxed Ge p-channel along the [100] and [110] directions. Static screening is included in all cases. A larger hole mobility is seen along [100] direction, thanks to the smaller conductivity effective mass.

Figure 4.10 demonstrates the strain-dependent hole mobility. Uniaxial tensile stress results in a small ‘longitudinal’ (i.e., along the [110] stress direction) mobility enhancement compared to the relaxed case. Biaxial compressive stress is even found to degrade the in-plane (i.e. on the stress plane) [110] mobility in strong inversion. Indeed in this case a larger fraction of holes populates the $lh$ subband in the relaxed case resulting in a higher mobility. Uniaxial compressive and biaxial tensile stress yield a higher (longitudinal and in-plane, respectively) [110] mobility enhancement than all other cases, as discussed above. Note that in weak inversion uniaxial compressive stress has the effect of enhancing the mobility more than biaxial tensile stress, but in strong inversion this enhancement weakens. This results from the nontrivial interplay between the variations with confinement of the effective masses and occupations of the $lh$ and $lh$ subbands, and of their energetic separation, the latter determining the strength of inter-subband transitions. Note also that, comparing with the Si/SiO$_2$ ‘universal mobility’ curve also shown in the same figure, a significant mobility enhancement can be found: Relaxed Ge p-channels exhibit a 3× higher mobility than
Si and uniaxially compressed strained Ge p-channels result in a mobility up to 10× larger than relaxed Si p-channels.

In Fig. 4.11 we show the calculated Ge hole mobility as a function of stress level at a sheet density of \( n_s = 7.16 \times 10^{12} \text{ cm}^{-2} \) for the cases of uniaxial compressive and biaxial tensile stress compared to available theoretical data from Ref. [3]. The Ge hole mobility increases monotonically with increasing uniaxial compressive stress (although we can not reproduce the large enhancement factor calculated in Ref. [3]), while for biaxial tensile stress, a mobility degradation is seen in the low stress range. This is mainly due to the fact that increasing stress reduces the energetic splitting between the first two subbands and thus causes enhanced intersubband scattering. As the stress increases further, the energies of these two subbands eventually merge and split in the opposite way, so that the hole mobility begins to increase. A similar behavior was found in Si p-channels under biaxial stress both theoretically and experimentally in Refs. [3] and [47], respectively, although the calculations by Oberhuber et al. [15] and the experimental results by Leitz et al. [48] do not exhibit any mobility degradation at small stress. We have no explanation for this inconsistency. However, contrary to the expectations expressed in Ref. [3], our calculations still predict a degradation of the hole mobility in the case of Ge p-channels under small tensile biaxial stress.

Finally, we conclude by showing in Figs. 4.13 and 4.12 a comparison between experimental data and our calculated hole mobility in the relaxed and biaxial compressive case. In relaxed Ge p-channel (Fig. 4.13) our theoretical results with HfO\(_2\) insulator show good agreement with the experimentally observed value [2, 7–9]. While our results with SiO\(_2\) yield a mobility much larger than the experimental data due to the effect of SO phonon scattering. When looking at our calculated results for 2% biaxial compressive stress in Fig. 4.12, as noted above, we see clearly that we underestimate severely the mobility enhancement measured by the MIT group [4, 6]
in structures under 1.3% and 2% stress with a thin Si capping layer, while we overestimate the results by Ritenour [5] in 1.3%-stressed structures with a high-\(\kappa\) insulator. While it is ‘easy’ to attribute the latter disagreement to the different level of strain and to high-\(\kappa\) effects, we can only speculate that the different channel structure employed by Gomez et al. [6] and by Lee et al. [4] may be responsible for the much larger mobility enhancement: The presence of the Si capping layer may reduce interface scattering and, more notably, may weaken the confinement of the wavefunctions allowing to ‘spill’ into the capping layer (see Fig. 11 of Ref. [49]), thus depressing the form factors appearing in Eqns. (3.7)-(3.9), (3.14), and (3.16), reducing the momentum relaxation rate, and thus boosting the mobility beyond the value we calculate.

Figure 4.14 present the results of hole mobility in relaxed, 2% biaxially compressively and tensily stained Ge p-channel inversion layers with HfO\(_2\) and SiO\(_2\) insulators. It has been shown that the effect of SO phonon scattering on electron mobility in a n-channel with a SiO\(_2\) insulator is insignificant [28]. However, it is not clear yet what is the effect on hole mobility in a p-channel with SiO\(_2\). Therefore, in our calculations two cases have been taken into account for SiO\(_2\) systems: Including and excluding SO phonon scattering. From the figures, we can see that: First, the application of high-\(\kappa\) insulators degrades the channel mobility compared with the application of SiO\(_2\) insulators for the reasons explained before. Second, adding stress is always a promising way to enhance channel mobility with either SiO\(_2\) or HfO\(_2\) insulators. Moreover, biaxial tensile strain improves channel mobility than the other two cases in a Ge p-channel with both SiO\(_2\) and HfO\(_2\) insulators.

In Fig. 4.15, insulator-dependent hole mobility in a relaxed Ge p-channel is illustrated. Among the investigated materials, HfO\(_2\) and ZrO\(_2\) appear to be the worst while Al\(_2\)O\(_3\) and ZrSiO\(_4\) show some promise, which is consistent with the result given by Ref. [28].
Figure 4.7. Effect of different surface-roughness (SR) models on the hole mobility in relaxed Ge p-channels with SiO$_2$ insulator. PN represents the first Prange-Nee term, Eq. 3.13, while the full Ando’s model is treated as in Ref. [1] accounting for Eqns. 3.14 and 3.16. $n_s$ is the hole sheet density.
Figure 4.8. Effect of static dielectric screening on the hole mobility in relaxed Ge p-channels with SiO$_2$ insulator. $n_s$ is the hole sheet density. SR indicates the surface-roughness scattering.
Figure 4.9. Individual mobility components and total hole mobility in relaxed Ge p-channels with SiO$_2$ insulator along the [100] and [110] directions. $n_s$ is the hole sheet density. SR indicates the surface-roughness scattering. NP represents the non-polar phonon scattering.
Figure 4.10. Comparison of the calculated hole mobility in relaxed and strained Ge p-channels with SiO$_2$ insulator with a stress of 2.81 GPa (corresponding to approximately 2% strain). Comparison is also made with the Si/SiO$_2$ universal curve from Joshi et al. [2]. $n_s$ is the hole sheet density.
Figure 4.11. Calculated stress-dependent hole mobility in Ge p-channel under uniaxial compressive (square) and biaxial tensile (triangle) stress (lines connecting the calculated data are only a guide to the eye) compared with theoretical data for Ge p-channel under [110] uniaxial compressive stress from Sun et al. [3] (circle).
Figure 4.12. Comparison of calculated hole mobility (squares) on the (001) plane along the [110] direction for Ge p-channels under (001) biaxial compressive stress with experimental data: Lee et al. [4] (dashed line), Ritenour et al. [5] (solid line) Gomez et al. [6] (dot-dashed line) and relaxed-Si universal curve (dotted line) from Joshi et al. [2]. The solid line connecting the calculated data is only a guide to the eye. The data of Ref. [4] are for ‘ring’ devices, thus averaged over all in-plane directions. In parentheses are the corresponding strain values. The gate different gate insulators are also indicated. $F_{eff}$ is the effective surface field.
Figure 4.13. Calculated hole mobility (symbol) on the (001) plane and along the [110] direction in relaxed Ge p-channels compared to experimental data by Shang et al. [7] (dotted line), Joshi et al. [2] (solid line), Clavelier et al. [8] (dashed line), Martens et al. [9] (dot-dashed line) and the Si universal curve (solid line) from Ref. [2]. $F_{eff}$ is the effective surface field. Good agreement can be found between experimental data and our simulated results for HfO$_2$/Ge system.
Figure 4.14. Strain-dependent hole mobility in relaxed (solid lines), 2% biaxially compressively (dotted lines) and tensilily (dashed lines) strained Ge p-channels with SiO$_2$ excluding (squares) and including (open circles) SO phonon scattering and HfO$_2$ (solid circles) insulators. Stress is added on (001) surface.
Figure 4.15. Insulator-dependent hole mobility in relaxed Ge p-channels. Results show that high-κ dielectrics decrease channel hole mobility compared with SiO₂ due to the effect of remote phonons. In addition, ZrO₂ and HfO₂ degrade hole mobility more than Al₂O₃ and ZrSiO₄.
4.2 III-V P-Channel Inversion Layers

III-V nMOSFET shows extremely large electron mobility, and it has been studied for decades theoretically and experimentally. However, there is no comprehensively theoretical study for hole mobilities in III-V pMOSFETs yet. In this section, the hole mobility in GaAs, InGaAs, GaSb and InSb p-channel inversion layers with SiO$_2$ and HfO$_2$ insulators are investigated. Both relaxed and biaxially strained cases (2% strain on (001) surface) are studied.

4.2.1 Discussions

The matrix element defined in Eq. (3.4) depends on the initial and final wavevectors $\mathbf{K}$ and $\mathbf{K}'$ also via the $\mathbf{K}$-dependence of the wavefunctions. This renders futile any attempt to perform analytically at least one of the integrations and also requires the tabulation of all wavefunctions $\Psi^{(\mu)}_\mathbf{K}$. Thus, when dealing with thermal carriers (as in our case) populating only a small region of the 2D $\mathbf{K}$-space, it is reasonable to assume that the wavefunctions change weakly with $\mathbf{K}$ and replace $\Psi^{(\mu)}_\mathbf{K}$ with the wavefunction calculated at the zone-center, $\Psi^{(\mu)}_\Gamma$ (Γ-point approximation). While this approximation has been employed before[1, 17, 22], we found at least two cases, in which it fails quite dramatically: Considering biaxially tensily strained GaSb and InSb p-channels, we found that the two lowest-energy subbands, a heavy- and a light-hole subband, cross near the Γ point as the hole sheet density increases. This happens when the symmetry-breaking due to the confining field results in subband minima away from the symmetry-point Γ. It implies that, except in a very small region around the zone center, the Γ-point approximation would mix the heavy- and light-hole wavefunctions, which results in a significant discontinued mobility, an artifact, with the increased hole sheet density. A better approximation which we have embraced consists in assuming $\Psi^{(\mu)}_\mathbf{K} \approx \Psi^{(\mu)}_g$, instead of $\Psi^{(\mu)}_\mathbf{K} \approx \Psi^{(\mu)}_\Gamma$, where $\Psi^{(\mu)}_g$ is
the wavefunction calculated at the extreme point of the $\mu$-th subband (ground-state wavefunction approximation), in general away from the zone center.

Figure 4.16. Failure of $\Gamma$-point wavefunction approximation in hole mobility calculation. Ground-states need to be identified and the corresponding wavefunctions can be used in hole mobility calculation. An example is shown in a 2% biaxially tensilly strained InSb p-channel with SiO$_2$ insulator.

Figure 4.17 shows the calculated results for SO phonon dispersion, phonon content, plasmon content and scattering strength in a relaxed GaAs p-channel inversion layer with HfO$_2$ at a hole density $n_s = 1.4 \times 10^{13}$ cm$^{-2}$. The four solutions of Eq. (3.23) are denoted by $\omega_1$, $\omega_2$, $\omega_3$ and $\omega_4$ from low to high frequency. Landau damping has been excluded in these results. However, the curve labeled $\omega_{LD}$ indicates the strong damping region of the substrate plasmons and the curve labeled $\omega_{p,s}$ represents the
substrate-plasmon frequency. Strong coupling between remote optical phonons and substrate plasmons can be seen from the modes dispersion, total phonon and plasmon content from Fig. 4.17(a-c): At small wavevector $Q$, $\omega_1$ is almost substrate-plasmon like then converges to the low-energy insulator optical phonon mode $\omega_{TO1}$ at large $Q$. Oppositely, at large $Q$, $\omega_4$ is substrate-plasmon like while at small $Q$ it becomes the high-energy insulator optical phonon mode $\omega_{TO2}$. $\omega_2$ originates from $\omega_{TO1}$ and converges to the substrate optical phonon mode labeled $\omega_{TO3}$ quickly. Its intermediate part is substrate-plasmon like. $\omega_3$ has almost the same dispersion as $\omega_2$ except that it begins at $\omega_{TO3}$ and ends at $\omega_{TO2}$. Total phonon content (Fig. 4.17(b)) and plasmon content (Fig. 4.17(c)) also illustrate this strong coupling between substrate plasmons and SO phonons. The strong coupling between substrate-plasmon and SO phonons enhances scattering strength which can be seen from Fig. 4.17(d). One thing has to be noticed is that the SO-limited hole mobility is not only determined by scattering strength of each mode, but also the energy of each mode: If energy is too large, holes can not emit such a large energy while Bose population will be too small to induce any significant absorption at room temperature as discussed in Ref. [28].

Figure 4.18 illustrates the effect of Landau damping on SO-limited hole mobility for a relaxed GaAs p-channel inversion layer with SiO$_2$ and HfO$_2$ insulators. As we can see excluding Landau damping significantly overestimates the SO-limited hole mobility especially in the situation of large sheet density, for which the strong dielectric screening due to the substrate plasmons reduce the scattering potential and thereby increase channel mobility. In Fig. 4.19, we make a comparison of LO-limited hole mobility in a relaxed GaAs channel with SiO$_2$ insulator calculated by various dielectric screening models discussed in Sec. 3.6. One can clearly see that the use of an effective screening parameter underestimates dielectric screening effects, while leaving the interaction unscreened would result in a severely underestimated mobility. Somewhat surprisingly, the difference between static screening and screening is
almost negligible, mainly because at the large sheet densities we have considered the 2D hole plasma has a frequency large enough to follow the LO-phonon oscillations. It is thus reasonable to restrict our calculations to the use of a static screening model also in dealing with LO phonon scattering.

4.2.2 Low-Field Hole Mobility with SiO$_2$ and HfO$_2$ Insulators

In Fig. 4.20 we show the various components of the mobility (i.e., limited by a single scattering process, NP, LO, SO and SR) in a relaxed GaAs p-channel with SiO$_2$ and HfO$_2$ insulators: The interface phonons originating from the high-$\kappa$ TO modes exhibit a much stronger scattering strength in the case of HfO$_2$ than SiO$_2$, as expected, resulting in a smaller SO-limited hole mobility. However the presence of a high-$\kappa$ dielectric improves the SR-limited mobility. This effect stems from the sign of the surface polarization charge induced by the roughness. This charge is proportional to \( \frac{\epsilon_s - \epsilon_{ox}}{\epsilon_s + \epsilon_{ox}} \), where \( \epsilon_s \) and \( \epsilon_{ox} \) are static dielectric constants of the substrate and insulator, respectively. Thus, in the case of SiO$_2$ the polarization charge increases the amplitude of the SR scattering potential, while in the case of HfO$_2$ the polarization acts as a screening charge. Consequently, the reduced SR scattering potential compensates for the enhanced SO-scattering potential in high-$\kappa$ systems.

Figures 4.21 to 4.9 present our results regarding the hole mobility in relaxed, 2% biaxially strained (both compressive and tensile) InSb, GaAs, GaSb, In$_{1-x}$Ga$_x$As and Ge p-channels with HfO$_2$ and SiO$_2$ insulators. For the latter, we show results obtained by ignoring or accounting for SO-phonon scattering: Indeed, while the effect of Si/SiO$_2$ SO-phonon scattering on the electron mobility has been found to be small [28], we still need to verify that the same is true for the hole mobility in more general situations.

From these figures we can draw the following conclusions: First, the presence of a high-$\kappa$ insulator degrades the mobility compared with the case of SiO$_2$, as explained...
before. Second, the application of stress enhances the mobility with either SiO$_2$ or HfO$_2$. In particular, in the case of Ge channels, biaxial tensile strain boosts the mobility by a larger extent than compressive strain, the opposite being true for III-V channels. One exception is the case of GaAs channels which exhibit the largest mobility under compressive stress in SiO$_2$ systems, under tensile stress in HfO$_2$ systems. Especially noteworthy is the fact that for systems with HfO$_2$ insulator the mobility seen under the application of biaxial tensile strain is larger than when applying biaxial compressive strain. This might be due to the subband structure dependent Landau damping frequency (Eq. (3.29)) which renders the biaxial tensile strain case is less sensitive to the high-κ insulator. Third, in relaxed and strained Ge channels with a SiO$_2$ insulating layer, the effect of SO-phonon scattering on the mobility is consistent with previous observations [28]. However, in III-V p-channels the presence of the substrate LO mode – obviously absent in Ge – results in a slightly different behavior: At low sheet densities the additional interfacial mode originating from the coupling of the substrate LO-phonon with the interfacial plasmons and high-κ modes results in an additional scattering process which, in turn, yields a hole mobility which is very strongly affected by the presence of the high-κ insulator. At higher hole sheet densities, instead, dielectric screening weakens this scattering potential and the difference between the hole mobility in channels with an SiO$_2$ gate insulator or in channels with a high-κ insulator is reduced. We should also note that, in general, materials with higher hole mobility exhibit a higher sensitivity to SO-phonon scattering than others, which can also be seen from Fig. 4.25.

In drawing Fig. 4.25, we have selected for each material the stress condition resulting in the largest mobility enhancement in a SiO$_2$ system (namely: biaxial compressive strain for III-Vs and biaxial tensile strain for Ge) with (solid lines) and without (dashed lines) SO phonon scattering and have assembled an overall birds-eye comparison. While Fig. 4.26 presents the comparison for a HfO$_2$ system, in which biaxial
compressive strain is for some III-Vs (GaSb, InSb and In_{1−x}Ga_{x}As) and biaxial tensile strain is for GaAs and Ge p-channels. Most notably, while in all cases we see an improvement over the Si universal curve [2], the biaxially compressively strained InSb p-channel yields the best overall result.

![Graphs showing mode dispersion, total phonon content, plasmon content, and scattering strength.](image)

**Figure 4.17.** Results for SO phonon scattering in a relaxed GaAs p-channel with HfO_{2}: (a) mode dispersion (b) total phonon content (TO1+TO2+TO3) (c) plasmon content and (d) scattering strength. In (a), ω_{LD} indicates the Landau damping frequency and ω_{p,s} represents the substrate-plasmon frequency. ω_{TO1,TO2} are frequencies for the two insulator optical phonon modes. ω_{TO3} is the frequency of the substrate optical phonon mode.
Figure 4.18. Effect of Landau damping on SO-limited hole mobility in relaxed GaAs p-channels with SiO$_2$ (lines) and HfO$_2$ (lines with symbols).
Figure 4.19. Effect of various screening models (effective, static and dynamic) on the LO-limited hole mobility in a relaxed GaAs p-channel with SiO$_2$ insulator. Effective screening underestimates the hole mobility while static screening shows a modest overestimation of LO-limited mobility.
Figure 4.20. Comparison for single scattering process limited hole mobility in relaxed GaAs p-channels with SiO\(_2\) (lines) and HfO\(_2\) (lines with symbols) insulators.
Figure 4.21. Strain-dependent hole mobility in relaxed (solid lines), 2% biaxially compressively (dotted lines) and tensilly (dashed lines) strained InSb p-channels with SiO$_2$ excluding (squares) and including (open circles) SO phonon scattering and HfO$_2$ (solid circles) insulators. Stress is added on (001) surface.
Figure 4.22. As in Fig. 4.21, but for GaAs channels.
Figure 4.23. As in Fig. 4.21, but for GaSb channels.
Figure 4.24. As in Fig. 4.21, but for \(\text{In}_{1-x}\text{Ga}_x\text{As}\) channels lattice-matched to InP.
Figure 4.25. Calculated hole mobility in 2% biaxially compressively strained GaAs, GaSb, InSb, In$_{0.7}$Ga$_{0.3}$As and biaxially tensilly strained Ge p-channels with SiO$_2$ insulators including (solid lines) and excluding (dashed lines) the SO phonon scattering. The Si universal curve is from Ref. [2]. Biaxial stress is added on (001) surface.
Figure 4.26. Calculated hole mobility in 2% biaxially compressively strained GaSb, InSb, In\textsubscript{0.7}Ga\textsubscript{0.3}As and biaxially tensilly strained Ge and GaAs p-channels with HfO\textsubscript{2} insulators. The Si universal curve is from Ref. [2]. Biaxial stress is added on (001) surface.
CHAPTER 5
CONCLUSIONS AND FUTURE WORK

5.1 Conclusions

In this paper we have presented a comprehensive theoretical study of the hole mobility in the inversion layers of both relaxed and strained Ge and III-V p-channels with a variety of insulators. Two self-consistent methods, hybrid and efficient self-consistent methods, are first introduced in the framework of six-band $k \cdot p$ method. Then our calculations have been performed using a six-band $k \cdot p$/Poisson self-consistent valence subband structure obtained using an efficient numerical scheme. Employing physically accurate models to describe non-polar scattering with acoustic and optical phonons, statically-screened surface roughness and polar Fröhlich phonon scattering, remote optical phonon scattering and alloy scattering, we have presented results for several cases of biaxial and uniaxial stress, both compressive and tensile. Our main result consists in the observation that in a Ge p-channel, uniaxial compressive stress exhibits the largest mobility enhancement, up to a factor of 10 compared to the universal Si-SiO$_2$ hole mobility. Furthermore, biaxial tensile stress degrades hole mobility in low stress region while uniaxial compressive stress increases mobility monotonically as in Si p-channels. Furthermore, both Ge and III-V materials exhibit a hole mobility larger than the universal relaxed-Si value with either SiO$_2$ or HfO$_2$ insulators. We also found that the III-Vs are more sensitive to the SO phonon scattering than Ge. In addition, biaxially compressively strained InSb can provide largest hole mobility, but also In$_{0.7}$Ga$_{0.3}$As lattice-matched to InP (and so biaxially compressively stressed as well) yields a promising mobility enhancement.
5.2 Future Work

The possible future works could be

1. Study the validity of ground-state wavefunction approximation in mobility calculation. Applying the exact wavefunction in mobility calculation. Utilizing the full model for non-polar phonon scattering to replace the isotropic model.

2. Extending current work to more realistic structure (e.g. heterostructure with finite insulator).
BIBLIOGRAPHY


