INVESTIGATION OF THEORETICAL LIMITATIONS OF RECOMBINATION DCIV METHODOLOGY FOR CHARACTERIZATION OF MOS TRANSISTORS

By

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This dissertation investigates the accuracy of using the recombination direct-current current voltage (R-DCIV) method to measure the interface traps and spatial variations or profiles of impurities and oxides in silicon MOS transistors. The Boltzmann electron-hole distribution and ionized impurity approximations (Boltzmann ionization or BI) are much faster than the Fermi-Deionized (FD) model. The accuracy of using the BI approximation to extract the device and material parameters of an MOS transistor is investigated by comparing with the time-consuming and complicated FD model. The accuracies or confident levels on the extractable device and material parameters are analyzed, such as dopant impurity concentration $P_{AA}$, oxide thickness $X_{OX}$, interface trap concentration $N_{IT}$, injected minority carrier concentration at SiO$_2$/Si interface represented by the p/n junction $V_{PN}$, energy level of interface traps distribution in silicon gap $E_{IT}$ and temperature $T$. From R-DCIV lineshape analyses, it is shown that the BI approximation gives a small (1%~5%) deviation when matching 90% of the experimental DCIV curve.
to theory. These results indicate that the simple and time-saving BI approximations are sufficiently accurate to extract from experimental data the spatial profiles of the dopant impurity concentration, and interface trap concentration at the SiO2/Si interface, and oxide thickness in modern MOS transistors.

Effects of energy distribution of the interface traps on the R-DCIV lineshape are also investigated. Comparison are made among three density of state (DOS) distributions of interface traps (1) a U-shaped DOS, (2) a constant DOS, and (3) a discrete interface trap energy level at mid-gap. These comparison shows that the experimental broadened R-DCIV lineshapes may also be accounted partially for the spatial variation of surface dopant impurity concentration but also by the energy distribution of interface traps in silicon gap. Slater’s perturbation theory is employed to suggest that a U-shaped DOS is the most probable distribution in silicon gap. Thus, the extractions of parameter spatial profiles, from experimental, should use a U-shaped density of interface traps, instead of the commonly assumed trap level at mid-gap $E_{TI}=0$ in the silicon energy gap.

For both the continuous energy distribution of interface traps and a discrete interface trap energy level at midgap, the peak R-DCIV current has large temperature dependence. However, the thermal activation energy, the lineshape, reciprocal slope, and peak gate voltage all have negligible temperature dependence. The analyses of impurity deionization effect show that deionization has a negligible effect on the R-DCIV lineshape when using Fermi ionization approximation (FI) to match experimental data from peak current down to 10% of the peak. The errors of FI approximation are nearly identical to the confident level of BI for all device and material parameters in practical range, for both metal gate and silicon gate MOS transistors.
CHAPTER 1
INTRODUCTION

Today, the metal-oxide-semiconductor (MOS) transistor has become the most important building block of ultra-large-scale-integrated (ULSI) circuits. The dimension of MOS transistors has narrowed from 25um in 1962 [1] to 90nm in 2002 [2]. The scaling trend, propelled by the rapid advancement of VLSI technology, is expected to continue [3] and the MOS transistor in production may shrink to 50nm in 2012 [4] as projected by the 1999 International Technology Roadmap for Semiconductors (ITRS).

The success of today’s semiconductor industry can be partially if not dominantly attributed to the extremely low density of electron-hole recombination, generation and trapping centers or traps at the SiO₂/Si interface (interface traps). Routine manufacturing processes have reduced the interface trap concentration N_it to $10^{10}$ cm⁻² by slow cooling after the final high temperature oxidation step and by post-oxidation annealing in hydrogen. The traditional small-signal measurement techniques such as the MOS capacitance voltage method can only resolve interface trap density higher than about $10^{11}$ cm⁻² and not its spatial variation and can not detect the very low density manufacturing residual interface traps in the state-of-the-art MOS transistors. Recombination Direct Current Current-Voltage (R-DCIV) methodology is a simple and sensitive tool to extract spatial variation or profile of dopant impurity concentration and interface trap concentration profiles and oxide thickness. The high sensitivity is attained by forward-biasing one or more p/n junctions ($V_{PN}$) in a MOS transistor to exponentially raise the injected minority carrier concentration, exp($qV_{PN}/kT$). In this dissertation, the
differences among BI, BD, FI, and FD solutions will be analyzed to determine the accuracy of the BI approximation which is computational the fastest. Here, BI stands for Boltzmann distribution of electrons and holes in energy and impurity full ionization. BD stands for Boltzmann distribution and impurity Deionization. FI stands for Fermi distribution of electrons and holes and impurity full ionization. FD stands for Fermi distribution and impurity deionization. We will evaluate the accuracy of simple and computational time-saving BI approximation solutions by comparison with the exact, complicated and time-consuming FD theory. One of the novelties is that R-DCIV lineshape is very sensitive to the device and material properties but rather insensitive to multi-dimensional effects inherent in the very small transistors.

In chapter 2, the current in the base terminal of the MOS transistor IB, as a function of gate voltage VGB, due to electron-hole recombination at the SiO2/Si interface traps in the basewell channel region, is analyzed theoretically using the Shockley-Read-Hall steady state recombination kinetics which has been applied by us [5-21]. Families of theoretical IB -VGB curves are presented to illustrate their dependencies on the variations of dopant impurity concentration, oxide thickness, injected minority carrier concentration, interface trap energy level and temperature. The percentage deviation as a function of gate voltage and %RMS deviation over a range gate voltage covering the peak current are used to evaluate the accuracy of simple and time-saving BI approximation, by comparing with the exact, complicated and time-consuming FD theory. According to these accuracy or confidence levels, it is shown that extracted value from experimental data would have only a small error from using BI approximation when matching 90% of the experimental R-DCIV curve from peak current IB-peak down to
10% of the peak. The comparison of BI, BD, FI and FD solutions indicates that BI and FI solutions are respectively nearly as good as the BD and FD solutions, and the deionization only has effect on DCIV lineshape in accumulation region for n-MOS transistors. This R-DCIV lineshape analysis gives a comprehensive baseline that can be used to guide the analysis when extracting the spatial profiles of the impurity concentration, interface trap concentration and oxide thickness from the experimental data. This simple and nondestructive R-DCIV methodology provides a powerful capability for routine monitoring and feedback during transistor fabrication.

In chapter 3, the effect on R-DCIV lineshape of electron and hole capture rates at mid-gap is analyzed. It shows that the ratio assumption with $0.01 < \text{cns/cps} < 100$ at mid-gap has a small effect on the lineshape. Family of curves are computed to illustrate the effects on R-DCIV lineshapes from the three distributed energy level of interface traps in silicon gap: (1) a U-shaped DOS, (2) a constant DOS, and (3) a discrete interface trap energy level at mid-gap. Comparisons among these distributions indicate that the broadened lineshape in experiments can also be accounted for partially by the energy distribution of interface traps in silicon gap, not just the spatial variation of surface dopant impurity concentration. Based on Slater’s perturbation theory, we conclude that the most probable density distribution of the interface traps in the silicon energy gap is U-Shaped. This is from the random variations of bond length and bond angle of the Si::O4. Thus, the theory to extract impurity concentration and interface concentration profiles should be modified from the traditional assumption of interface energy level at mid-gap $\text{ETI}=0$, to a U-Shaped density distribution of interface traps throughout the energy silicon gap.
The forward bias VPN dependence of peak gate voltage $V_{GB\text{-peak}}$, thermal activation energy $E_A$ and peak current peak current $I_{B\text{-peak}}$ can provide a determination of the effective interface trap energy level $E_{TI^*}$ for discrete interface trap levels. For both discrete and continuous interface trap level, $E_A$, $I_{B\text{-peak}}$, $V_{GB\text{-peak}}$, $n$, and $I_{B\text{-peak}}-V_{GB\text{-peak}}$ lineshape have negligible temperature dependence, while $I_{B\text{-peak}}$ has large temperature dependence.

In chapter 4, impurity deionization dependence of dopant concentration and oxide thickness on $R_{DCIV}$ lineshape will be analyzed. The percentage deviation and $\%RMS$ deviation of Fermi ionization approximation (FI) show that there is a negligible impurity deionization near the SiO2/Si interface in MOS transistors when matching 90% of experimental data from peak current down to 10% of the peak. We can expect that the errors of FI approximation are nearly identical to the confident level of BI for other device and material parameters in practical range, such as injected minority concentration, interface trap energy level and temperature, for both metal gate and silicon gate MOS transistors. The analyses of impurity deionization confirms that the time-saving and simple BI is a good approximation to extract the spatial profiles from experiment data, such as the dopant impurity concentration, interface trap concentration, oxide thickness since it has a good physical basis at around the recombination peak current.

Chapter 5 gives the summaries and concludes this dissertation.
CHAPTER 2
THEORETICAL CONFIDENT LEVEL OF BI APPROXIMATION COMPARED WITH THE EXACT FD SOLUTIONS

2.1 Introduction

Recombination-DCIV (R-DCIV) methodology is a reliable and powerful tool for diagnosing interface properties as well as for characterizing transistor design. It is the only method which can extract profiles of the channel impurity concentration and oxide thickness with high resolutions in nanometer dimension range. However, its accuracy has not been evaluated. As we already know, the BI approximation solution is time saving and simple compared with the time consuming and complicated FD solution. There are some possible sources of errors using BI approximation in extracting parameters from experimental R-DCIV data such as impurity and interface trap concentration profiles and oxide thickness profiles. In this chapter, we will evaluate these errors and present the confident level of BI approximation by comparing the BI and BD results with those of FD.

The principle of R-DCIV is the use of a surface-potential-controlling gate terminal voltage, $V_{GB}$, to modulate the base-terminal DC current, $I_B$, from electron-hole recombination at the SiO$_2$/Si interface traps. The lineshape, linewidth, peak gate voltage and peak amplitude of the recombination currents from electron-hole recombination at the interface traps in the channel space charge region are analyzed using Shockley-Read-Hall steady-state recombination kinetics. The material physics used in this thesis are
based on the textbook of Sah [5, 6] and references cited therein, including previous work on R-DCIV [7-21].

Compared with the widely used differential C-V profiling method, the R-DCIV profiling technique provides several advantages: (1) low sensitivity to gate area variation; (2) no special test structures required to perform the test – all production MOS transistors can be used with sufficient sensitivity and resolution; (3) direct-current (DC) measurements allowing long-time average to reduce noise and increasing sensitivity using simple computer-controlled digital data collection; and (4) the test is nondestructive. Its high sensitivity is derived from forward-biasing one of the p/n junctions to greatly increase the minority carrier concentration and recombination rate. In MOS transistor structures, it gains further sensitivity from the common-emitter and common-base current gain of the BJT which is present in all MOS transistor structures.

Sah [7, 8] measured the R-DCIV characteristics of MOS-gated silicon bipolar transistors in 1961 to investigate the effects of surface recombination and channel on p/n junction and transistor characteristics. The R-DCIV method was reactivated 35 years later by Neugroschel et al. [9] in 1995 as a sensitive monitor for transistor reliability. They investigated the generation kinetics of the interface traps and the degradation kinetics of electrically stressed transistors from electrical-stress-created oxide and interface traps.

In the past several years, many R-DCIV applications were reported which included the delineation of interface trap generation/annealing kinetics on electrically-stressed transistors by hot carriers and high current densities, and diagnosis and evaluation of transistor design and manufacturing processes on pre-stress transistors [10-25].
In this chapter, the characteristics of the surface electron-hole recombination current in the channel region are studied theoretically and the confident levels of Boltzmann Ionized approximation solutions are computed in order to provide a comprehensive baseline that can be used to guide the analyses of experimental data in the applications. These results can help quantify the applications of the simple and time-saving BI solutions for the extraction of fundamental and application-specific properties of transistors and their materials, such as the physical (spatial location and density) and electronic (quantum density of states) properties of the residual and stress-generated interface and oxide traps, and the dopant impurity concentration profiles. The formulation includes high injection level in the quasi-neutral basewell and electrical non-equilibrium from the forward applied p/n junction voltage which gives NP \( > n_i^2 \). Analytical solutions and their physical models are presented to illustrate the effects of material parameters on the \( I_B-V_{GB} \) lineshape, the amplitude of peak current \( I_{B-peak} \), and peak gate voltage \( V_{GB-peak} \) at the \( I_{B-peak} \).

Families of base current versus gate/base voltage (\( I_B-V_{GB} \)) are computed to illustrate the effects of the bulk impurity concentration and interface trap properties on the lineshape and the \( (I_{Bpk}, V_{GBpk}) \) location and \( I_B \) magnitude. The systematic computation begins with the ideal transistor structure in which there is no spatial variation of the basewell impurity concentration and a discrete energy distribution of interface traps is at mid-gap \( E_{TI}=0 \). The simple ideal model can allow us to extrapolate the BI confident levels when extending to include spatial variations of dopant impurity interface trap concentrations, injected minority carrier concentration, and a U-shaped density distribution of interface traps in silicon gap.
2.2 Configurations of the R-DCIV method

One of the most important DCIV applications is to extract the surface dopant impurity profile at the interface of SiO₂/Si. As the transistor dimensions decrease, the conventional optical and traditional electrical methods are increasingly inaccurate to monitor and measure the impurity profiles. The major difficulty lies in having as accurate a measurement to monitor impurity profiles in order to provide the feedback necessary for iterative fabrication processing to attain the optimum impurity profile and transistor characteristics to maintain or improve the high-performance electrical functions of the million-transistor circuit chips.

The discussion in this analytical theory chapter will follow the schematic cross-sectional view of modern n-channel MOS transistor shown in Figure 2.1. The important physical features of the nMOS include the n-type heavily doped high-conductivity polysilicon gate (n++G), the refractory metal silicide gate on n++G and the heavily doped very-high-conductivity n-type drain and source extension (n++D and n++S), the medium-highly doped high-conductivity n-type drain and source extension regions (n+SER and n+DER), the p-type basewell channel region (p-BCR), the drain and source oxide spacers, and the shallow-trench oxide isolation.

Electron-hole recombination can occur at the SiO₂/Si interface traps located in the five regions along surface channel: (1) the basewell-surface channel region (BCR), (2) the source-junction space-charge region (SJR), (3) the drain-junction space-charge region (DJR), (4) source extension region (DER) and (5) drain extension region (DER). This study will focus on basewell-surface channel region and the results are also applicable to the other regions.
Figure 2.1 Schematic device cross section of modern n-channel MOS transistor. It is comprised of a gate dielectric, a doped polysilicon gate electrode and titanium silicide over-layer, frequently called a shunt. (adapted from Chih-Tang Sah[26])

Only the $I_B$ component from recombination at the interface space charge layer at interface traps will vary with $V_{GB}$ since the recombination rate at the interface is controlled by the interface or surface electron and hole concentration which are only modulated or varied by $V_{GB}$ under the gate electrode. Other $I_B$ components are from the injected minority carriers (such as electrons), which are from forward biased n++Drain/p-Basewell (n+D/p-B) or/and n++Source/p-Basewell (n+S/p-B). These injected minority carriers recombine with majority carriers (such as holes) at the bulk-traps in the bulk p-basewell and space charge regions of the n+D/p-B and n+S/p-B junctions, at the bulk traps in the p-substrate and at the interface traps at ohmic contact. These regions are not
covered by the gate-conductor. Thus, the recombination rate or current don’t vary with the gate voltage. It is the $I_B$ baseline.

Recombination DCIV measurement on MOS transistors can use four different bias configurations to inject minority carriers to the SiO$_2$/Si interface [8, 15-17, 26], as illustrated in Figure 2.2. These four configurations can be grouped in accordance with the two traditional BJT geometries, the vertical BJT (VBJT) and lateral BJT (LBJT). For the LBJT, given in Figures 2.2 (a) and (b), they are called the Drain-Emitter configuration (DE-DCIV) and Source-Emitter configuration (SE-DCIV). For the VBJT, given in Figures 2.2 (c) and (d), the drain and source p/n or n/p junctions are simultaneously forward DC biased to the same terminal voltage, which is known as the Top Emitter configuration or TE-DCIV. The other VBJT configuration is to forward bias the bottom p/n junction of the p/n-junction basewell, which is known as the Bottom Emitter configuration or BE-DCIV. The p/n junctions not forward biased are zero-biased, though they can also be reverse-biased or even forward-biased at a lower voltage in each of the bias configurations.

These four DC-bias configurations can provide high sensitivity and resolution to monitor the dopant-impurity and interface trap concentration profiles and as well as the electrical length of the five regions (SER, SJR, BCR, DJR and DER) and other transistor design parameters, such as the gate/source, gate/base, and gate/drain oxide thickness, and the series drain and source resistances [15-17]. All of these are increasingly difficult to measure accurately and with confidence by traditional MOS transistor and metallurgical-optical methods as the transistor shrinks due to the fundamental microscopic limitations.
Each of the configurations, in Figures 2.2 (a)-(d), provides a different and desired BJT injection pathway and spatial distribution of minority at the SiO₂/Si interface to help further delineate the spatial distribution of the impurities and interface traps.

The boron acceptor has a liquid/solid segregation coefficient of 0.8, which gives only about 20% variation of boron-concentration over the crystal length, while phosphorus donor segregation coefficient is 0.35 and phosphorus sources have very high vapor pressures to make the continuous-dopant during growth difficult to control. Thus, all silicon integrated circuits start with a p-type high-resistance, 50 to 100 Ω cm p-type 8" or 12" diameter silicon wafer for high-yield reason since 8" –by-several-foot silicon single crystals can be grown nearly defect-free, dopant-impurity-free and oxygen-free (using float-zone in vacuum chamber). Therefore, only the pMOST in digital circuits manufactured on high-resistivity p-Si wafers has an n-base/p-collector-substrate n/p junction basewell for transistor isolation which can be used in the BE-DCIV methodology. The n-B/p-C (p-collector) junction well is formed by ion-implantation.

It is not available for the digital nMOST which has a boron ion-implanted p-B/p-C high/low junction basewell. However, both nMOST and pMOST can be measured in the BE-DCIV bias configuration on analog test transistor wafers since the higher-gain or high-transconductance nMOST requires a p-B/n-C junction basewell for electrical isolation.

For the two lateral BJT or LBJT configurations, the DE-DCIV is the most commonly used due to the ganged base pad and source pad. These ganged pads come from test transistor patterns with many channel lengths and widths. Due to large real
estate requirements, few test transistors have isolated source, drain, gate and baswell contact pads.

Figure 2.2 Four DCIV bias configurations for a pMOS transistor: (a) Drain-Emitter (DE), (b) Source-Emitter (SE), Top-Emitter (TE), and (d) Bottom-Emitter (BE). (adapted from Yih Wang, PH.D thesis, December, 2000)

Sah proposed this classification of the four DCIV bias configurations [15-17, 26] in order to simplify and systemize the many possible DCIV measurements that are needed to give unique diagnostic solutions of test transistors for optimizing advanced manufacturing transistor-designs and processes development. In this thesis on the determination of the distribution of interface trap level, the TE-DCIV is exploited to the fullest in order to provide reliable and accurate diagnoses. Future accuracy analysis will include the DE-DCIV (and SE-DCIV) and additional geometric effect.
2.3 Theory of R-DCIV Methodology

The dimensions of Metal-Oxide-Silicon (MOS) field-effect transistors have continued to decrease, projected by SIA [4] in 1999 to drop below 100nm around the end of decade and has done so [2]. The width to length ration, W/L, could be unity or even smaller, making the width effect as important as the length effect on the transistor electrical characteristics. In this case, the transistor is three-dimensional (3D). If a MOS transistor is much wider than its length, the structure is nearly two-dimensional (2D) as indicated by the cross-sectional view shown in Figure 2.1.

The traditional industrial practice to design a transistor has been the use of supercomputers to obtain the DC steady-state numerical solutions of the three-dimensional (3D) structure via the finite-different method. The 3D electrical characteristic solutions are tedious and complicated since they include the five simultaneous nonlinear partial Shockley equations, which govern the diffusion, drift and generation-recombination-trapping of electrons and holes [6, pp. 268, Eqs (350.1)-(350.6)]. As a diagnostic methodology, it is untenable to experimentally verify the transistor design during the engineering phase and manufacturing since the numerical solution takes a huge amount of time to reach an optimum transistor design. The dependence of the nonlinear coefficients (mobility, diffusivity, generation-recombination-trapping rates) on the solutions (the electric field and potential, and the electron and hole concentrations) is not precisely known and can only be approximated by highly simplified quantum and statistical mechanical theory to give tractable analytical formulas.

The further simplified empirical formulas have been used in common engineering practice for the fundamental parameters, which make the model and methodology inapplicable as an extrapolation scheme. Here, we use the partitioning methodology to
divide the three-dimensional (3D) transistor structure into one-dimension (1D), disregarding the coupling effects of the other two dimensions (such as lateral diffusion and drift of the electrons and holes), because the salient feature of the DCIV methodology is that some of the 1D features in the DCIV characteristics are strictly independent of the lateral (or y-axis) variation.

Compared with the channel length (y-axis), the thickness of surface space-charge layer and gate oxide is very thin. Thus, the variation of electric potential and field is small in the y-axis compared their x-variation, i.e., \( E_y(x,y) \ll E_x(x,y) \), which allows us to solve the 1D x-variations exactly using 1D MOS Capacitor (MOSC) and to sum these adjacent (in y-direction) to give the 2D solution such as the DC current of the basewell terminal.

In the R-DCIV measurements, excess minority carriers are injected by a forward-biased p/n junction into the SiO\(_2\)/Si interface which covers channel region between the source and drain of MOS transistors: the basewell channel region (BCR) and the drain and source junction and extension regions (DJR, SJR, DER and SER). The peaked-components in a \( I_B-V_{GB} \) plot arise from electron-hole recombination at the SiO\(_2\)/Si interface traps, \( N_{IT} \) (No./cm\(^2\)), in the five gate-covered regions along the interface channel. The surface recombination rate and current of each region reach their maximum when the gate voltage is varied to make the local surface concentration of electrons and holes nearly equal. When the bias configurations contain one or more forward-biased p/n junctions, the device structure becomes a lateral or vertical bipolar junction transistor (LBJT and VBJT). Since LBJT is always available in a MOS transistor, the R-DCIV
measurement method can be applicable to actual small MOS transistors used in the integrated circuit [16].

Figure 2.3 is the energy band diagram of the metal-oxide-silicon structure. The E-x energy band diagram is on a plane normal to the SiO₂/Si interfacial plane and designated as the x-direction. It passes through the p-basewell underneath the gate oxide. It is labeled in detail to help describe the approximations of the analyses as follows. All voltages are normalized to the Boltzmann thermal voltage, k_BT/q, where k_B is the Boltzmann constant, T is the local lattice temperature and the q is the magnitude of the electron charge. The forward bias is U_PN while the DC voltage applied to the gate relative to the p-Si base is U_GB. U_N and U_P are electron and hole quasi-Fermi potentials in p-Si and their difference, known as the quasi-Fermi-potential split, is U_PN=U_P-U_N. According to the charge neutrality condition and the electrical non-equilibrium from forward bias which gives N*P = n_i^2*exp(U_PN) > n_i^2, the quasi-Fermi-potentials in the quasi-neutral region of p-Si base are

\[
U_P = \log_e \left\{ N_{IM} + 4n_i^2 \exp(U_{PN})^{1/2} - N_{IM} \right\} / 2n_i \]  
(2.1a)

\[
= \log_e \left\{ P_{AA} + 4n_i^2 \exp(U_{PN})^{1/2} - P_{AA} \right\} / 2n_i \]  
(2.1b)

\[
= \log_e \left\{ 0.5 \exp(U_P) \left\{ \left(\exp(-2U_F) - 1\right)^2 + 4 \exp(-2U_F) + U_{PN}\right\}^{1/2} - \left(\exp(-2U_F) - 1\right) \right\} \]  
(2.1c)

\[
U_N = \log_e \left\{ N_{IM} + 4n_i^2 \exp(U_{PN})^{1/2} + N_{IM} \right\} / 2n_i \]  
(2.2a)

\[
= -\log_e \left\{ P_{AA} + 4n_i^2 \exp(U_{PN})^{1/2} - P_{AA} \right\} / 2n_i \]  
(2.2b)

\[
= \log_e \left\{ 2 \exp(U_F) \left\{ \left(\exp(2U_F) - 1\right)^2 + 4 \exp(-2U_F) + U_{PN}\right\}^{1/2} + \left(1 - \exp(2U_F)\right) \right\} \]  
(2.2c)

Here, N_{IM}=N_{DD}-P_{AA} is the net impurity concentration in base. Using

\[
U_F = \log_e \left( P_{AA} / n_i \right) \text{ and } U_F = -\log_e \left( N_{DD} / n_i \right), \text{ we get (2.1c) and (2.2c)}.\]
The total energy band bending is denoted by the surface potential $U_S$. The electron and hole concentrations at the SiO$_2$/Si interface ($N_S$ and $P_S$) are modulated by the gate voltage via bending the Si energy band:

$$P_S = P(x = 0, y) = n_i \exp(U_p - U_S)$$  \hspace{1cm} (2.3)$$

$$N_S = N(x = 0, y) = n_i \exp(U_S - U_N)$$  \hspace{1cm} (2.4)$$

In our analysis, the surface potential normalized to the thermal voltage, $kT/q$, is the intrinsic position of the Fermi Potential Level at the surface or SiO$_2$/Si interface.

$$U_t(x = 0, y) \equiv U_S = qV_s / kT$$  \hspace{1cm} (2.5)$$

Four fundamental electron-hole transition processes, between the continuous band states of silicon crystal and the localized trap states with an energy level $E_T$ in the silicon gap, can be illustrated using the energy band diagram as shown in figure 2.4. The rate (event/second-cm$^3$) of the four processes can be conveniently described by: (a) electron capture from the conduction band at $c_n(N_{TT-nT})$, (b) electron emission to the conduction band at $e_nN_{TT}$, (c) hole capture from the valence band at $c_pN_T$, and (d) hole emission to the valence band at $e_p(N_{TT-nT})$. Here, $n$ and $p$ are electron and hole concentrations in the conduction band and valence band respectively, $N_{TT}$ is the total density (#/cm$^3$) and $n_T$ is the electron-occupied density of the trap states (#/cm$^3$), and $e$’s (sec$^{-1}$) and $c$’s (cm$^3$sec$^{-1}$) are emission and capture rate coefficients of the four processes which depend on the energy levels of both the trap state and the band state.
Figure 2.3  Energy band diagram and cross sectional view of a gated n+Si/SiO2/p-Si structure in the basewell channel region along x direction. UP and UN are respectively the electron and hole quasi-Fermi potential normalized to the thermal voltage (kT/q). (adapted from Yih Wang, PH.D thesis, December, 2000)
These four transition processes are mostly thermal involving emission and capture of phonons. The thermal capture and emission processes could involve about ten phonons for mid-gap trap levels since the maximum optical phonon energy is only about 62meV in silicon [27]. Huang and Rhys [28] did the first theoretical calculation of multi-phonon process and Huang [29] refined it later. The first-principles calculation of the capture cross-sections in a multi-phonon process is rather laborious. For the purpose of developing a theory for the DCIV methodology, Shockley and Read, and Hall in 1952 [30] treated the fundamental capture and emission rates as constants independent of kinetic energies of band electrons and holes in order to develop the phenomenological kinetic theory.

Figure 2.4 A transition energy band diagram showing the four fundamental transition processes between a conduction or valence band state and an electron trap state in the silicon energy gap: (a) capture of a conduction band electron by the trap, (b) emission a trapped electron to conduction band, (c) capture a valence hole by the trap, and (d) emission a trapped hole to valence band. The volume density of band electrons, band holes, electron-occupied traps and total traps are \( n \), \( p \), \( n_T \), and \( N_{TT} \) respectively. The rates of the four processes are shown in terms of e’s and c’s. Purely thermal emission and capture processes involve multiple phonons. (adapted from Chih-Tang Sah [6,31].)
In a R-DCIV measurement, the base terminal current, \( I_B \), is measured as a function of gate-basewell voltage, \( V_{GB} \), which modulates the electron-hole concentrations and recombination rate at the traps located at the gated SiO\(_2\)/Si interface. The excess minority carriers are injected into the MOS-gated Si/SiO\(_2\) interface by one or more forward biased p/n junctions in the MOS transistor structure, but also remote p/n junctions not part of the MOS transistor structure. The steady-state areal rate, \( R_{SS} \), of electron-hole recombination at a discrete-energy-level of interface trap, with a interface trap density of \( N_{IT} \), is given by the Shockley-Read-Hall formula:

\[
R_{SS} = \frac{c_{ns} e_{ps} N_S P_s - e_{ns} e_{ps}}{c_{ns} N_S + e_{ns} + c_{ps} P_s + e_{ps}} N_{IT} \equiv R_{SS1} \times N_{IT} \quad (2.6)
\]

Here, \( R_{SS1} \) is the steady-state recombination rate at \( N_{IT}(y)dy=W=1 \) or the unit steady-state recombination rate \([26]\). \( c_{ns} \), \( e_{ps} \), \( e_{ns} \) and \( e_{ps} \) are the electron-hole capture-emission rate coefficients at the interface traps, first introduced by Shockley and Read. From detailed balance near thermal equilibrium, \( c \)’s and \( e \)’s are related by \( e_{ns} = c_{ns} n_i \exp(U_{TI}) \) and \( e_{ps} = c_{ps} n_i \exp(-U_{TI}) \). Using the Boltzmann representation for \( N_S \) and \( P_S \) given by (2.3) and (2.4), \( R_{SS1} \) can be expressed by the more convenient forms as follow:

\[
R_{SS1} = \frac{c_{ns} e_{ps} N_S P_s - e_{ns} e_{ps}}{c_{ns} N_S + e_{ns} + c_{ps} P_s + e_{ps}} \left( \frac{N_{IT}}{\exp(U_{PN}/2) \cosh(U_{SI}^*) + \cosh(U_{TI}^*)} \right) \quad (2.7a)
\]

\[
= \left( \frac{c_{ns} e_{ps}}{c_{ns} N_S + e_{ns} + c_{ps} P_s + e_{ps}} \right)^{1/2} n_i \left[ \exp(U_{PN}) - 1 \right] \left( \frac{\exp(U_{PN}/2) \cosh(U_{SI}^*) + \cosh(U_{TI}^*)}{2} \right) \quad (2.7b)
\]

Here, \( U_{SI}^* \) and \( U_{TI}^* \) are the effective surface potential and interface trap energy, respectively.

\[
U_{SI}^* = U_s + \log_e \left( \frac{c_{ns}}{c_{ps}} \right)^{1/2} - \left( U_p + U_n \right) / 2 \quad (2.8a)
\]

\[
\equiv U_s + \log_e \left( \frac{c_{ns}}{c_{ps}} \right)^{1/2} - U_F + U_{PN} / 2 \quad \text{for } p-Si \quad (2.8b)
\]

\[
\equiv U_s + \log_e \left( \frac{c_{ns}}{c_{ps}} \right)^{1/2} - U_F - U_{PN} / 2 \quad \text{for } n-Si \quad (2.8c)
\]
Here, $U_{TI}$ is the interface trap energy level, measured from the intrinsic Fermi level $E_i$, defined by $U_{TI} = -(E_T - E_i)/q$. $U_S(y) = U_I(x=0,y)$, commonly known as the surface energy band bending in the basewell channel region, is the total change of the electric potential along the x-axis at a particular y-position from the SiO$_2$/Si interface (x=0) to the interior. $U_I(x=\infty, y) = 0$ is taken as the reference). The expression of (2.7) is exact with no approximations other than the thermal Boltzmann distribution with lattice temperature $T$. It immediately shows the presence of a peak at $U_S^*=0$ or $c_{ns}N_S = c_{ps}P_S$ when the surface potential, $U_S$, or the gate voltage $V_{GB}$ is varied.

$$R_{SS1-peak} = \frac{\left(c_{ms}c_{ps}\right)^{1/2}n_i}{2} \frac{[\exp(U_{PN}) - 1]}{\exp(U_{PN}/2) + \cosh(U_{TI}^*)}$$  \hspace{1cm} (2.10a)$$
$$= \frac{\left(c_{ms}c_{ps}\right)^{1/2}n_i}{2} [\exp(U_{PN}/2) - 1]$$  \hspace{1cm} (2.10b)$$

For an interface trap energy level at around mid-gap with $U_{TI}^*=0$, we will have the classic $I_B \propto \exp(qV/2kT)$ dependence, shown in (2.10b). This dependence suggests that many of the observed n=2 non-ideal IV characteristics of p/n junctions [1, 7, 8, 31] could be due to interface traps at the surface perimeter of the p/n junction rather than residual bulk traps in the bulk space-charge-layer of the p/n junction.

$R_{SS1}$ has a peak when the steady-state capture rate of electrons and holes are equal. It is expected from the equality of the four transitions, electron and hole capture and emission transitions at the trap. But more important, it is an immensely useful result that provides the simplest basis for qualitative interpretation and understanding of experimental data. The peak amplitude increases exponentially with forward bias, $U_{PN}$,
which gives the tremendous sensitivity and hence spatial resolution that are unique features of the DCIV method. The surface potential at the peak current ($U_s^*=0$) is

$$U_{S_{-peak}} = -\log_e\left(\frac{c_{ns}}{c_{ps}}\right)^{1/2} + \frac{(U_p + U_n)}{2} \quad (2.11a)$$

$$\equiv -\log_e\left(\frac{c_{ns}}{c_{ps}}\right)^{1/2} + \frac{U_f - U_{PN}}{2} \quad \text{for p-Si} \quad (2.11b)$$

$$\equiv -\log_e\left(\frac{c_{ns}}{c_{ps}}\right)^{1/2} + \frac{U_f + U_{PN}}{2} \quad \text{for n-Si} \quad (2.11c)$$

The peak formula (2.11a) was derived by Sah-Noyce-Shockley in 1957 [31] and used by Cai and Sah in 2000 for DCIV theory [20].

The basewell recombination current ($I_{B_{-BCR}}$) [7, 8, 20, 26] is obtained by integrating the SRH steady-state electron-hole recombination rate at the interface over the channel area $dydz$:

$$I_B(V_{GB}) = q\int\int R_{SS1}(V_{GB}, y)N_{IT}(y)dydz \quad (2.12a)$$

$$= \frac{q(c_{ns}c_{ps})^{1/2}}{2}\int n_iW \frac{[\exp(U_{PN}(y)) - 1]}{\exp(U_{PN}(y)/2) \cosh(U_s^*(y)) + \cosh(U_{IT}^*)} N_{IT}(y)dy \quad (2.12b)$$

For low injection levels, traditionally defined as $N < P_{AA}/10$ in p-Si, we have $U_F > 0$ for p-Si and $U_N < U_F < 0$ for n-Si, where $U_F$ is the majority carrier Fermi potential. This is the common application range of the DCIV methodology. According to (2.11b) and (2.11c), the $R_{SS1}$ peak lies in the flat-band to the intrinsic gate voltage range ($0 < U_s < U_F$, for p-Si). Using the Sah’s exact formula [5, pp.129]:

$$V_S = V_{GB} - V_{FB} - 2\cdot\text{sign}(V_S)\cdot V_{AA}\left\{1 + (V_{GB} - V_{FB} - kT\Delta_m/q)/V_{AA}\right\}^{1/2} - 1 \quad (2.13)$$

We have an approximation in this flat-band/intrinsic range,

$$V_{GB} = V_{FB} + V_S + (V_{AA})^{1/2}(V_S)^{1/2} \quad (2.14a)$$

$$= V_{FB} + V_S + 0.053(X_{OX}/1nm)(P_{AA}/10^{17}\text{cm}^{-3})^{1/2} \quad (2.14b)$$

Then, the gate voltage at peak current $I_{B_{-peak}}$ is
$$V_{GB-peak} = V_{FB} + V_{S-peak} + 0.053 \left( \frac{X_{OX}}{1 \text{nm}} \right) \left( \frac{P_{AA}}{10^{17} \text{ cm}^{-3}} \right)^{1/2} (V_{S-peak})^{1/2} \quad (2.15)$$

Here, $V_{AA} = \varepsilon_S q P_{AA} / 2C_{OX}^2 = 0.695 \times 10^{-3} \times (X_{OX}/1 \text{nm}) (P_{AA}/10^{17} \text{ cm}^{-3})^{1/2}$. $V_{FB}$ is the flat-band voltage which contains Si-Gate/SiO$_2$/Si work function difference and the oxide charge from the charged electron and hole traps inside the thin oxide film, $Q_{OX}/C_{OX}$, where $C_{OX} = \varepsilon_S / X_{OX}$ is the oxide capacitance per unit area. The last term in (2.13), (2.14) and (2.15) is the voltage drop across the oxide layer.

The gate voltage at peak current $V_{GB-peak}$ is determined by the three terms: $V_{FB}$, $V_{S-peak}$ and $V_{AA}$, as indicated by (2.15) and (2.11). The dependencies on the transistor design parameters are (1) the substrate dopant concentration, (2) gate oxide thickness through $V_{AA}$, (3) the ratio of electron and hole capture rates, (4) the flat-band voltage $V_{FB}$ and (5) the emitter junction forward bias $V_{PN}$. As a result, the $I_{B-peak}$ will shift toward a more positive $V_{GB}$ for a higher substrate impurity concentration or a thicker oxide thickness at a given forward-bias-voltage $V_{PN}$ in an nMOS transistor.

The theoretical variation of $R_{SS1-V_{GB}}$ lineshape due to device parameters is examined below, using the formula of half-width at half maximum (HWHM) at low injection levels [20]:

$$\Delta V_{GB+} = \Delta V_S + 2 \sqrt{V_{AA}} \left[ \sqrt{V_{S-peak}} - \sqrt{\left( V_{S-peak} - \Delta V_S \right)} \right] \quad \text{(flatband – side)} \quad (2.16a)$$

$$\Delta V_{GB-} = \Delta V_S + 2 \sqrt{V_{AA}} \left[ \sqrt{V_{S-peak}} + \Delta V_S - \sqrt{\left( V_{S-peak} \right)} \right] \quad \text{(int rinsic – side)} \quad (2.16b)$$

As indicated in (2.16a) and (2.16b), the half-width on the flat-band accumulation side of the peak is always larger and broader than that on the intrinsic-inversion side of the peak. Thus, the recombination current lineshape is fundamentally asymmetric. A higher surface
impurity concentration and thicker oxide will each give a larger HWHM or broader lineshape.

For low injection levels, injected minority concentration has negligible effect on surface band bending, since $V_S - V_{GB}$ curve is mainly determined by the concentration of the majority carriers and ionized impurity atoms in the substrate. Therefore, effect of forward bias $V_{PN}$ at low injection level will have a negligible effect on DCIV lineshape. At high injection levels with $N > 10 \times P_{AA}$, we have $U_P \approx U_N$ or the electron and hole concentrations in the channel region are nearly equal, and the maximum surface recombination rate is near the flat-band. The exact result is $U_{S\text{-peak}} = \log_2(c_{ps}/c_{ns})^{1/2}$ which can be derived from (2.11a).

As shown in (2.12b), the $I_B$ versus $V_{GB}$ lineshape is affected by $U_S^*$ via the $\cosh(U_S^*)$ term in the denominator, assuming a single-level interface trap at the mid-gap, $E_{TI}^* = 0$. Interface trap concentration $N_{IT}$ in the numerator of (2.12) only alters the peak amplitude but not the lineshape. Consequently, lineshape of $I_B-V_{GB}$ curve will be determined by the dopant impurity concentration and oxide thickness.

### 2.4 Theoretical Computations for Confident Level

Before an attempt can be made to obtain the confident level of $BI$ by comparing with the FD exact solutions when using the R-DCIV methodology, a phenomenological model must be created and its analytical solutions derived. It is well known that the more exact the model is, the more accurate the derived solution will be. However, the solution will become complex with the advantage of model exactness, which will become quite clear in this thesis.
In a semiconductor, temperature has an enormous influence on the electrical properties, especially the conductivity. The dielectric constants of silicon and silicon oxide have slight temperature dependence. A formula for SiO$_2$/Si is not available since structural effects may begin to play an important role for thin oxides, and the formula would become a function of temperature and thickness. In this thesis, $\varepsilon_{\text{SiO}_2} = 3.90$. For thin oxides transistors, the effective dielectric constant may be different due to interfacial layers. In fact, the concept of dielectric constants becomes debatable when only a few layers of atoms are involved.

Increasing temperatures are associated with a narrowing of the energy gap. A second-order polynomial by Bludau, Onton and Heinke [32] has been modeled to cover temperature range from 0 to 300K from the data on the absorption coefficient of highly pure p-type silicon. Sah, McNutt and Chan [33] gave the formula when temperature is above 300K and less than 500K. Since the intrinsic carrier concentration is an exponential-like function of the energy gap, it is important to have an accurate value for the energy gap. Otherwise, the result will be substantially inaccurate.

The calculated values of the energy gap and measures values of the intrinsic carrier concentration by Sah, McNutt and Chan [33], can use to compute the $m_e m_h$ product. One remaining problem is the requirement of the individual effective masses to calculate $N_C$ and $N_V$. Since there is no way to unequivocally separate the effective masses at temperatures significantly above 4.2K, this thesis uses the 4.2K data, obtained from cyclotron resonance measurements, which gave $m_e/m_0 = 1.065$ and $m_h/m_e = 0.647$, for an $m_e/m_h$ ratio of 1.646.
The Boltzmann distribution (exponential) is a well-known method used in the non-degenerate case, i.e. low carrier concentration \( \ll 10^{18} \text{ cm}^{-3} \), best approximating the Fermi statistics integral at low temperatures and/or low impurity doping, when \( (E_C-E_F)/kT>4 \) or \( E_F>E_C-4kT \). Degeneracy or Fermi statistics is used to deal with high carrier concentrations. Degeneracy is always important when the carrier concentration is high (and not just the dopant), such as in the presence of a highly forward biased p/n junction or under a bright light. In particular, degeneracy is important in the inversion and accumulation regions along the SiO2/Si interface channel of MOS transistors.

Nevertheless, degeneracy is still generally not taken into account due to the complexity. There is no analytical solution for the Fermi statistics integral, so either full-range analytical approximations must be used, such as those shown in Blackemore’s paper on the subject of F-D integrals [34], or iterative solutions must be employed, such as the rational Chebyshev approximations [35] used in this thesis.

It is reasonably accurate to assume that all dopant impurities are ionized in most conditions. As long as shallow-level dopants are used, which is equivalent to saying that the binding energy for electron (n-type) or hole (p-type) is small, so that almost complete ionization is expected. In p-type material, this can be easily rationalized by considering the Fermi level with respect to the dopant impurity level: as long as the Fermi level is above the acceptor level, the level should be filled with an electron and unoccupied by a hole, and hence the acceptors will be completely ionized. Similarly, as long as the Fermi level lies below the donor level in an n-type sample, the probability of the level being filled is low, and hence, the donor is likely ionized. When temperature is very low and the material is heavily doped, and/or the impurity level is deep, the impurity may not
ionize completely, which is what is called deionization. This can be made sense physically at low temperatures: if there is not enough thermal energy to release the electrons or holes, then the impurities will not be ionized, or an electron will be trapped at the donor and hole will be trapped at the acceptor. For high doping concentrations, the Fermi level can go above donor level or below the acceptor level, and the fraction of ionized impurities will be consequently decrease. For electron-hole recombination current at the SiO₂/Si interface traps, gate voltage would attract electrons to interface and push holes away from interface in accumulation region. Thus, some donor impurities atoms near the SiO₂/Si interface are occupied by the electrons and are deionized. The acceptor impurities are still ionized. In inversion region, gate voltage will push electrons away from interface and attract holes to interface. Thus, donor impurities are still ionized and acceptor impurities trap the holes at interface and are deionized. In this thesis, we only consider non-compensated materials, i.e. Pₐₐ=0 in n-Base and Nₜₜ=0 in p-Base. Thus deionization is entirely negligible except in the strong accumulation range.

For modern ULSI technology, polysilicon gates are universally used on MOS devices. Gate depletion is possible and potentially non-negligible for lowly doped gates (<5×10²⁰ cm⁻³). Polysilicon gates have some tremendous processing and transistor density benefits over metal gates, and can withstand high temperature steps that would cause most deposited metal gates to evaporate, particularly the source/drain drive-in step. As oxide thickness continues to decrease, polysilicon depletion becomes a more important problem. The addition of the polysilicon depletion increases calculation complexity substantially since it introduces a second surface potential for the polysilicon gate. Yaron and Frohman-Bentchkowsky [36], as well as Sah [5] have shown how to include the
polysilicon depletion effect in CV theory. In this thesis, the confidence levels are computed for both metal and silicon gates.

The most important effects are included in modeling R-DCIV characteristics of a MOS transistor. However, there are many factors which are to be assumed negligible, but we should mention them for completeness. The transition layer between Si and SiO₂ is not abrupt and on the order of about one or two atomic layers (~6Å) in thin oxide [37-39]. The transitional layer of SiOₓ has a different dielectric constant. The dielectric change in this very thin region should not be drastic enough to effect DCIV curves significantly, thus this effect was not included in this thesis. Energy gap narrowing was ignored for very high impurity concentrations. There is much debate about the modeling of the energy gap narrowing as a function of doping, and it is questionable whether the formulae are independent of deionization and especially impurity banding. Fringe field effects as well as frequency dependency of the dielectrics were not included. Series resistance, which is simple to include, was omitted since the R-DCIV current density is low. Also, impurity banding was ignored in the analysis.

The charge density in the semiconductor is given the equation

$$\rho = q(-N + P - N_A + P_D - n_T)$$  \hspace{1cm} (2.4.1)

Here, N and P are electron and hole concentrations, respectively. The n_T terms represents the contribution from trapped charge. N_A and P_D are respectively the ionized acceptors and donors [6,30].

$$N_A = \frac{P_A}{1 + g_A \exp((E_A - E_F)/kT)}$$  \hspace{1cm} (2.4.2a)

$$N_D = \frac{N_D}{1 + g_A \exp((E_F - E_D)/kT)}$$  \hspace{1cm} (2.4.2b)
(2.4.2a) and (2.4.2b) take deionization into account. Generally, it is assumed that all of the impurities are completely ionized in doped silicon when shallow level impurities are used. This is a good approximation when \( T \) is large or \( E_F \gg E_A \).

Incomplete impurity ionization occurs at low temperature and/or high doping \((10^{18}\text{cm}^{-3})\). For deep level impurities, deionization will become significant even at moderate doping and room temperature. In this thesis, we assume that MOS transistor has negligible trap charge.

Using Poisson’s equation, we can find the electric field \( E_S \) in semiconductor. Starting from the d.c. steady-state equation in one dimension, we have

\[
\varepsilon_s \frac{dE}{dx} / dx = \rho \quad (2.4.3)
\]

Where, \( \varepsilon_S \) is the dielectric constant of silicon, \( E \) is the electric field in x direction, and \( \rho \) is the charge density given in (2.4.1). Since \( E=-(dV/dx) \), we have

\[
\varepsilon_s \frac{dE}{dx} = -\varepsilon_s \left( \frac{d}{dx} \right) \left( \frac{dV}{dx} \right) = -\varepsilon_s \left[ \left( \frac{dV}{dx} \right) \left( \frac{d}{dx} \right) \left( \frac{dV}{dx} \right) \right] = -\left( \varepsilon_s / 2 \right) \left( \frac{d}{dx} \right) \left( \frac{dV}{dx} \right)^2 = -\left( \varepsilon_s / 2 \right) \left( \frac{dE^2}{dx} \right) \quad (2.4.4)
\]

Thus, from (2.4.3) and (2.4.4)

\[
dE^2 = \left( 2 / \varepsilon_s \right) \rho dV = \left( 2q / \varepsilon_s \right) \left( -P + N - N_A + P_D \right) dV \quad (2.4.5)
\]

In (2.4.5), electric field can be integrated from \( E_S(x=0) \) to \( E(x=\infty)=0 \) and surface potential can be integrate from \( U_S(x=0) \) to \( U(x=\infty)=0 \) for charge density term. Then electric field is
The surface potential, $U_S$, represents the amount of band bending of the silicon band at the SiO$_2$/Si interface caused by the applied electric field or gate voltage. In this thesis, we only discuss the non-compensated region, i.e., either donor or acceptor is the dopant in substrate of MOS transistor.

### 2.4.1 BI, BD and FI Approximations Compared with FD Exact Theory

Before finding the confident level of on % deviation the BI approximation, we first compare BI, BD and FI approximations with FD exact theory using R-DCIV methodology. Here, BI stands for Boltzmann distribution of electrons and holes in energy and impurity full ionization. BD stands for Boltzmann distribution and impurity Deionization. FI stands for Fermi distribution of electrons and holes and impurity full ionization. FD stands for Fermi distribution and impurity deionization.

For modeling R-DCIV curves, the BI approximation is the fastest solution. There are two ways to derive the BI solution. One would be to build a BI model from the start using the Boltzmann (exponential) distribution for the carrier concentration while ignoring the effects of deionization completely. This is the typical textbook approach. A somewhat more instructive method is to present one complete derivation for the exact case (the degenerate and deionized model) and then reduce to a simper case. The later approach will be used in this thesis.
The Boltzmann ionized solution is most useful just after the onset of accumulation or inversion at temperatures higher than 250K and doping less than $10^{18}$ cm$^{-3}$. When in the strong accumulation or inversion ranges, Fermi statistical distribution are required. At low temperatures and/or high doping, the effect of deionization becomes non-negligible and should be included. However, temperature at around 300K and impurity concentration lower than $10^{18}$ cm$^{-3}$ are in the practical ranges. In addition, BI approximation solution is simple and time-saving. These were the right reasons we used BI approximation when using DCIV methodology to extrapolate the profile of impurity concentration, interface trap concentration and oxide thickness [26, 40].

The exact FD solution for a p-doped semiconductor is given by [5, pp.129]:

$$V_{GB} = V_{FB} + V_S + \text{sign}(V_S)\varepsilon_S E_S / C_{OX}$$  \hspace{1cm} (2.4.7)

According to (2.4.6), the electric field at the surface p-Si, which includes the electrical non-equilibrium from the forward applied p/n junction voltage $V_{PN}$, is given by

$$E_S = \frac{2kT}{\varepsilon_S} \left\{ N_V [ F_{3/2} (-U_S - U_V + U_F) - F_{3/2} (-U_V + U_F) ] \\
+ N_C [ F_{3/2} (U_S + U_C - U_F + U_{PN}) - F_{3/2} (U_C - U_F + U_{PN}) ] \\
+ P_{AA} (U_S + \log \left[ \frac{1 + g_A \exp(U_F - U_A - U_S)}{1 + g_A \exp(U_F - U_A)} \right] ) \right\}$$

for FD  \hspace{1cm} (2.4.8)

Once we assume that all the dopant impurities are fully ionized, the logarithmic term of (2.4.8) is dropped, we have the electric field of FI

$$E_S = \frac{2kT}{\varepsilon_S} \left\{ N_V [ F_{3/2} (-U_S - U_V + U_F) - F_{3/2} (-U_V + U_F) ] \\
+ N_C [ F_{3/2} (U_S + U_C - U_F + U_{PN}) - F_{3/2} (U_C - U_F + U_{PN}) ] \\
+ P_{AA} U_S \right\}$$

for FI  \hspace{1cm} (2.4.9)

Reducing this result to BD solution is straightforward. All the FD integrate are simply replaced by exponentials, which is valid when Fermi energy less than about -4 [69].
\[ E_s^2 = \frac{2kT}{e_s} \{ N_v \left[ \exp(-U_s - U_v + U_f) - \exp(-U_v + U_f) \right] \\
+ N_c \left[ \exp(U_s + U_c - U_f + U_{PN}) - \exp(U_c - U_f + U_{PN}) \right] \\
+ P_{AA} (U_s + \log_e \left[ \frac{1 + g_A \exp(U_f - U_A) - U_s}{1 + g_A \exp(U_f - U_A)} \right] \} \]  
for BD  
(2.4.10)

In order to remove the deionization effect, we assume the trap level is far away from the Fermi level \( \exp(U_F - U_A) \ll 1 \), which causes the logarithmic term of (2.4.8) to approach zero. Thus, the electric field of BI is

\[ E_s^2 = \frac{2kT}{e_s} \{ N_v \left[ \exp(-U_s - U_v + U_f) - \exp(-U_v + U_f) \right] \\
+ N_c \left[ \exp(U_s + U_c - U_f + U_{PN}) - \exp(U_c - U_f + U_{PN}) \right] \\
+ P_{AA} U_s \} \]  
for BI  
(2.4.11)

The different electric field form (BI, BD, FI and FD) give different surface potential \( U_s \), which would affect the lineshape of DCIV curves.

The four recombination DCIV curves are shown in Figure 2.5. The Lineshape of the three approximations are almost the same as the exact Fermi-Deionization solution, the difference between Fermi and Boltzmann statistics appears only when IB is around eight decades smaller than peak current \( I_{B\text{-peak}} \). The difference between using fully ionization and deionization models, such as BI and BD or FI and FD, is very small as shown in Figure 2.5(a). From Figure 2.5(a), the 90 percent of the peak current covers a gate voltage range from -0.10V to +0.10V. Figure 2.5(b) shows the % deviation is less than 0.1% for all three approximations in this gate voltage range for peak current \( I_{B\text{-peak}} \) down to the 10% peak.

As shown in Figure 2.5, the switch from full ionization to deionization generally results in very little gain by comparing with the increase in accuracy gained by switching from Boltzmann to Fermi statistics. However, in situations where the temperature is very
low and/or the dopant concentration is quite high, deionization effects are non-negligible. Also, if the dopant produces a deep-level trap, deionization will become significant factor regardless of the doping concentration or temperature. According to Figure 2.5, we can conclude that BI and FI solutions are respectively nearly as good as BD and FD solutions, especially in accumulation region since deionization occurs only in this region.

The non-degenerate, fully-ionized solution is simplest when we assume that the minority carrier terms are negligible and the majority surface concentration is much larger than the bulk concentration, and the deionization term is dropped. This assumption would invalidate the Boltzmann assumption in some case, such as in strong accumulation region. But it allows us to find an analytical solution. For Fermi-Deionization case, the final solution will be iterative, which is the main disadvantage of including degeneracy. An exactly accurate numerical theoretical solution is impossible because of the approximation the formulae used for the normal and inverse Fermi integrals.

The effects of deionization in the application range are generally so small that the error from using Boltzmann statistics instead of Fermi will swamp any gain from including deionization, except at the extremes, such as high doping and/or low temperature at the onset of inversion or accumulation, or for deep level traps. The inclusion of deionization also makes the Boltzmann case non-analytical. More important, BI solution is simple and time-saving. For these reasons, we will compute the confident level or percentage deviation of the BI solution by comparing with the exact FD theory.
Figure 2.5  (a) Comparison of the theoretical R-DCIV curves between BI, BD, FI, and FD solutions. (b) Normalized percentage deviation with respect to the exact or real FD theory. %Deviation = %[(IB-BI/BD/FI-peak)/(IB-FD-peak)-1]*100. The three points are for flat-band (US=0), subthreshold voltage (US=UF), threshold voltage (US=2UF). Temperature T=296.15K. Metal gate MOS transistor.
Five important factors that affect $I_R-V_{GB}$ lineshape are analyzed. These are expected to be dominant in conventional or production MOS transistors. They are:

- Dopant Impurity Concentration Dependence
- Oxide Thickness Dependence
- Injected Minority Carrier Concentration Dependence
- Energy Position of Discrete Energy Level Interface Traps
- Temperature Dependence

A mid-gap symmetrical interface trap is assumed $E_T-E_i=0$ with $c_{ns}=c_{pu}=10^{-8}\text{cm}^{-3}/s$, and $N_{IT}=10^{10}\text{cm}^{-3}$. The effect of ratio of electron and hole capture rates at the mid-gap on the DCIV lineshape is small, which will be discussed in the chapter 3. $n_i=10^{10}\text{cm}^{-3}$ corresponding to $T=296.57\text{K}=23.42\text{C}=74.156\text{F}$. The length and width of MOS transistors are 10um and 1um, respectively. These results are the new applications that provide the feedbacks for optimization of the design and fabrication of increasing smaller transistor when using the simple and time-saving Boltzmann approximation with impurity full-ionized solution of R-DCIV methodology.

2.4.2 Dopant Impurity Concentration Dependence

When the channel length of modern MOS transistor is scaled to 0.25um and below, a much higher dopant impurity concentration is necessary to reduce the thickness of the surface space charge region $X_{SS}$ and the reverse-biased p/n junction space-charge layer $Y_{pn}$, as shown in Figure 2.1, in order to maintain the desired transistor characteristics. The high impurity concentration limit the worsening of the transistor characteristics from short channel and channel length modulated by the thickening of drain junction space charge region from the reverse voltage applied to the drain [41-45]. If a spatially constant impurity concentration is used to limit the drain junction space charge thickness and thickness modulation by the drain voltage, the gate voltage required to turn on the MOS
conduction channel would be excessive in order to overcome this high impurity concentration. In order to avoid this, two-dimension impurity profile, such as the halo concentration contour by low-angle ion implantation or the “pocket”, are designed into modern short channel transistors.

The unavoidable impurity redistribution from diffusion and segregation disturbs the designed impurity profile during thermal oxidation [46-47]. The impurity concentration profile is further complicated by defect annealing after ion implantation [48-51] for a self-aligned source and drain to reduce overlap capacitances and shallow dopant at the Si/SiO₂ interface for threshold voltage adjustment. In this section, constant dopant impurity profile is used to find the confident level of BI solution using DCIV methodology, but it still allows us to extrapolate the confident level of U-shaped or inverted U-shaped impurity profiles since the confident level depends on the impurity concentration.

The effect of impurity concentration 10^16 to 10^19 per cubic centimeters on the error analysis using Boltzmann-Ionization approximation is compared with the exact Fermi-Deionization results. Figures 2.6 and 2.7 show a family of normalized theoretical recombination DCIV curves using BI approximation solution in dash line and the FD exact theory in solid line for metal gate case and silicon gate transistors, respectively.

For short channel and small area transistors, the DCIV current is in the Femtoampere range. So only the current near the peak can be measured because of noise. Thus, the lineshape and error on percentage deviation are presented in the linear scale as shown in Figure 2.6(a) and 2.7(a). For large area and long channel transistors, the recombination DCIV current can be in the nano-ampere range and the noise is three or more decades
smaller. The lineshape and errors on percentage deviation are presented in semilog scale as shown in Figure 2.6 (b) and (c), and Figure 2.7(b) and (c), respectively.

In both Figure 2.6(a) and 2.7(a), the 10% peak current, which means 100% $I_{B\text{-peak}}$ down to 10% $I_{B\text{-peak}}$, is covered by a gate voltage range from -0.2V to +0.2V. We can see that the error or % deviation of the Boltzmann ionization approximation less than 8% for $10^{19}$ impurity concentration for both metal gate and silicon gate cases as shown in Figure 2.6(c) and 2.7 (c). When impurity concentration is $5 \times 10^{17}$, which is in practical range, % deviation is less than 1% for metal gate case, while it is less than 2% for silicon gate devices.

Figure 2.6(d) and 2.7(d) give the %RMS deviation when matching 10% to 90% of the theoretical curve to the experimental data. We can see that the Boltzmann approximation gives less than 4% RMS deviation at $10^{19}$ impurity concentration for both metal gate and silicon gate cases. For $10^{18}$ impurity concentration, the %RMS deviation is less than 1% for metal gate case and 2% for silicon gate case, when matching 90% of the theoretical curve to the experimental data.

As already proved by Yih Wang and Sah [40], the distortion of $I_B$ vs. $V_{\text{GB}}$ lineshape is from the spatial variation of dopant impurity concentration which can be further distorted by the spatial variation of interface trap concentration $N_{\text{IT}}$, but not by $N_{\text{IT}}$ alone at the interface of SiO$_2$/Si with a constant impurity concentration. This allows us to extrapolate the percentage deviation and %RMS for non-constant dopant impurity concentration at the interface of a MOS transistor. For U-shaped impurity concentration along channel with $P_{\text{AA}} = 10^{17}$ cm$^{-3}$ in the middle of the channel $P_{\text{AA}} = 10^{18}$ cm$^{-3}$ at the end of the channel, the percentage deviation and %RMS error are all no more than 1% for
Figure 2.6 Effect of dopant impurity concentration on the DCIV on the normalized $I_B$ vs. $V_{GB}$ lineshape. (a) $I_B$ vs. $V_{GB}$ in linear scale, (b) $I_B$ vs. $V_{GB}$ in semilog scale. The substrate impurity. (c) percentage deviation and (d) %RMS deviation. RMS90, RMS75(FWQM), RMS50(FWHM), RMS25 and RMS10 represent the lineshape for peak current $I_{B\text{-peak}}$ down to 90%, 75%, 50%, 25% and 10% of $I_{B\text{-peak}}$, respectively. Metal gate nMOS transistors.
Figure 2.6 Continued

(c) %DEV of $(I_B/I_{BPK})$

(d) %RMSdev of $(I_B/I_{BPK})$

n-MOST
$X_{ox}=3.5\text{nm}$
$V_{PP}=200\text{mV}$

$P_{AA}/(\text{cm}^{-3})$

$V_{GB}-V_{GBPK}/(1\text{V})$
Figure 2.7 Effect of dopant impurity concentration on the DCIV on the normalized $I_B$ vs. $V_{GB}$ lineshape. (a) $I_B$ vs. $V_{GB}$ in linear scale, (b) $I_B$ vs. $V_{GB}$ in semilog scale, (c) percentage deviation and (d) %RMS deviation. Silicon gate nMOS transistors.
Figure 2.7 Continued
metal gate cases, and they are respective not more than 6% and 2% for silicon gate cases when matching 90% of the curve, since we can assume a constant \( P_{AA} = 10^{18} \text{ cm}^{-3} \) along the channel, and the percentage deviation and %RMS are monotone increasing with impurity concentration as shown in Figure 2.6(c) and (d), Figure 2.7(c) and (d).

Similarly, we can obtain the same results for inverted U-shaped impurity concentration along channel with \( P_{AA} = 10^{18} \text{ cm}^{-3} \) in the middle of the channel \( P_{AA} = 10^{17} \text{ cm}^{-3} \) at the end of the channel, since the distortion of DCIV lineshape is in accumulation region or negative \( V_{GB} \) side for inverted U-shape \( P_{AA} \) while the distortion is in inversion region or positive \( V_{GB} \) side for a U-shape \( P_{AA} \) in a nMOS transistor.

2.4.3 Oxide Thickness Dependence

Boltzmann approximation solutions are reasonable for thick oxide MOS transistors. For thin oxides, neglecting degeneracy in inversion or accumulation is less accurate because accumulation and inversion give high carrier concentrations, which compromise the assumption of the Boltzmann distribution. Degeneracy can be included because there are several approximations which can be used [34, 35, 52-55], although the Fermi integrals used in solid-state applications have no analytical solutions. In the last ten years, the more accurate FD approximations have been available by the high-speed computers, such those by Cody and Thacher [35], and Van Halen and Pulfrey [54]. Thus, degeneracy can be included for a more accurate solution. However, the error or percentage deviation is still so small enough for the simple and time-saving BI approximation solution in practical range, such as \( P_{AA} = 5 \times 10^{17} \text{ cm}^{-3} \) for p-Si and \( X_{OX} = 35 \text{A} \) as shown in Figure 2.6 and 2.7, which is what we shall continue to use.
Figures 2.8 and 2.9 respectively give one family of normalized I_B vs. V_GB to show the lineshape dependence on the one of the most basic MOS transistor design parameters, the oxide thickness (another is dopant impurity concentration), in the transistor spatial regions where the gate voltage is designed to control the electrical characteristics of the transistor, for metal gate and silicon gate case. Oxide thickness varies from 10Å to 300Å, which covers all practical range. The lineshape broadens, and the linewidth (ΔV_{GB+} and ΔV_{GB-}) increases as the oxide thickness and dopant impurity concentration increases as shown in Figure 2.6 and 2.7, and Figure 2.8 and 2.9, respectively. The peak gate voltage (V_{GB-peak}) shifts toward the more positive gate voltage, i.e. towards increasing hole-accumulation range in the SiO_2/Si interface for a p type doped substrate.

These dependencies are anticipated by (2.15) and (2.16). They are also expected by simple device and material physics. For instance, a higher gate voltage or electric field is required to change the amount of surface potential or surface energy band bending in order to reach the peak recombination rate condition, c_{nS}N_S=c_{pS}P_S, as indicated by (2.6). It is evident that these curves are equally applicable to the p-Base of nMOS transistor and the p-DER and p-SER of pMOS transistors.

The linear DCIV curves in Figure 2.8(a) and Figure 2.9(a) are application to short channel application and semi-log curves in Figure 2.8 (b) and Figure 2.9(b) are for application to long channel application of MOS transistors. The oxide thickness varies from 13 angstroms from 300 angstroms.
Figure 2.8  Effect of oxide thickness on the DCIV on the normalized $I_B$ vs. $V_{GB}$ lineshape. (a) $I_B$ vs. $V_{GB}$ in linear scale, (b) $I_B$ vs. $V_{GB}$ in semi-log scale (c) percentage deviation and (d) %RMS deviation. Metal gate nMOS transistors.
Figure 2.8  Continued
Figure 2.9  Effect of oxide thickness on the DCIV on the normalized $I_B$ vs. $V_{GB}$ lineshape. (a) $I_B$ vs. $V_{GB}$ in linear scale, (b) $I_B$ vs. $V_{GB}$ in semilog scale. (c) percentage deviation and (d) %RMS deviation. Silicon gate nMOS transistors.
Figure 2.9  Continued

For thin oxide MOS transistors, gate voltage covers from -0.1V to +0.1V for peak current down to 10 percent of the peak. While for metal and silicon gate thick oxide, gate voltage widen to the range of -0.4V to +0.4V for peak current down to 10 percent of peak.
Figure 2.8(c) and 2.9(c) show the %deviation using the Boltzmann approximation and full ionization of impurity for metal gate and silicon transistors. Again, it is compared with the exact Fermi distribution and impurity deionization. We see that the deviation is about 2% or less for metal gate devices and 4% for silicon gate MOS transistors covering the curve above 10% \( I_{B\text{-peak}} \). The %RMS deviation for \( 10^{18} \) impurity concentration is given in Figure 2.8(d). The error is less than 2% if we use only 90% of the measured DCIV curve down from \( I_{B\text{-peak}} \) and it is less if we use less of the DCIV for both metal and silicon gate MOS transistors.

In this section, constant oxide thickness profile is assumed to find the confident level of BI solution using DCIV methodology, but it still allows us to extrapolate the confident level of U-shaped or inverted U-shaped oxide thickness profiles at the interface of a MOS transistor since the confident level depends on oxide thickness.

From the confidence levels of BI, we can conclude that the errors are small enough by using the BI model to extract oxide thickness from experiments over entire practical range. Thus, the simple and time-saving BI approximation solutions can used to extract the oxide thickness profile in MOS transistors.

### 2.4.4 Injected Minority Carrier Concentration Dependence

At low injection levels in an p-Si with \( P_{AA} = 10^{17} \text{cm}^{-3} \), defined as

\[
N < P_{AA}/10 = 10^{16} = [n_i^2 P_{AA}] \exp(U_{PN})
\]

or \( V_{PN} = (kT/q)U_{PN} < -760 \text{mV} \), \( V_{PN} \) has only minor effect on DCIV lineshape. In this case, we have \( U_p = U_f > 0 \) for p-Si and \( U_n = U_f < 0 \) for n-Si. According to (2.11) and (2.15),

\[
V_{GB\text{-peak}} \propto -\log_e \left( \frac{c_{ns}}{c_{ps}} \right)^{1/2} + U_f - U_{PN} / 2 \propto V_{PN} / 2 \quad \text{for p-Si}
\]

\[
V_{GB\text{-peak}} \propto -\log_e \left( \frac{c_{ns}}{c_{ps}} \right)^{1/2} + U_f + U_{PN} / 2 \propto V_{PN} / 2 \quad \text{for n-Si}
\]
Thus, gate voltage at the peak current $V_{\text{GB-peak}}$ would increase with forward bias $V_{\text{PN}}$ in the n-Base of pMOST and decrease with $V_{\text{PN}}$ in the p-Base of nMOST. Low injection level is the common application range of the DCIV methodology.

At high injection levels with $V_{\text{PN}} \gtrsim 800\text{mV}$, the linewidth has the $\exp(U_{\text{PN}}/4)$ dependence on forward bias $V_{\text{PN}}$ [20]. Thus, at low injection levels, the $I_B-V_{\text{GB}}$ linewidth can be large which is determined by the effective trap energy level, $E_{\text{TI}}^*$. The linewidth then decreases with increasing $V_{\text{PN}}$ until the onset of high injection level condition, beyond which it increases exponentially with $V_{\text{PN}}$.

The broadening of DCIV lineshape from high injection levels could occur at lower $V_{\text{PN}}$ in real transistors due to voltage-drop or $V_{\text{PN}}$ drop from high current density through the lateral base resistance and series drain and source resistances, and due to gate voltage lowering of the forward biased drain and source p/n junction barrier heights, and reduced majority carrier concentration at surface channel from surface band bending in the sub-threshold region. Another important source of lineshape modification comes from the diffusion and drift current limitation on the emitter junction injection efficiency due to built-in electric field from graded vertical (x-direction) impurity concentration profile $P_{\text{AA}}(x,y)$, which is from the designed ion implantation in the bottom-emitter configuration as shown in Figure 2.2(d). Since the diffusion-drift current is in series with the recombination current at the interface traps, the smaller one would dominate. The importance of the diffusion-drift limitation of the injection current has been demonstrated using experimental data [26].

The applications of short channel and long channel of MOS transistors are given in the linear Figure 2.10(a) and Figure 2.11(a), in the semi-log curves in Figure 2.10(b) and
2.11(b). The figures for metal gate and silicon gate MOS transistors are respectively shown in Figure 2.10 and 2.11. The injected minority carrier concentration is increased from forward bias of 100mV from 800mV. For small injection minority carrier concentration, gate voltage covers from -0.1V to +0.1V for peak current down to 10 percent of the peak. While, gate voltage should change from -0.25V to +0.25V for peak current down to 10 percent of peak for high injection MOS transistors.

Figure 2.10(c) and 2.11(c) show the %deviation using the Boltzmann approximation and full ionization of impurity for metal gate and silicon gate transistors. Again, it is compared with the exact Fermi distribution and impurity deionization. We see that the deviations are respectively about 6% and 10% for metal gate and silicon gate devices when matching 90% of experimental data from peak current $I_{B\text{-peak}}$ down to 10% of the peak using Boltzmann full ionization approximation solution.

The %RMS deviation for $10^{18}$ impurity concentration is given in Figure 2.10(d) and 2.11(d). The error is around less than 3% for forward bias $V_{PN}$ smaller than 600mV and 6% for $V_{PN}$ smaller than 800mV if we use only 90% of the measured DCIV curve for metal gate transistors. While in silicon gate devices, these two values are respectively 4% and 8%. The %RMS deviation is less than 0.4% if we match only 10% of DCIV curves to experiments for both metal gate and silicon gate cases.

These values of % deviation and %RMS deviation indicate that the Boltzmann full ionization approximation solution is good enough to extract the parameters of MOS transistors when forward bias $V_{PN}$ is in practical range.
Figure 2.10 Effect of injection carrier concentration on the DCIV on the normalized IB vs. VGB lineshape. (a) IB vs. VGB in linear scale, (b) IB vs. VGB in semilog scale. (c) percentage deviation and (d) %RMS deviation. Metal gate nMOS transistors.
Figure 2.10 Continued
Figure 2.11 Effect of injection carrier concentration on the DCIV on the normalized IB vs. VGB lineshape. (a) IB vs. VGB in linear scale, (b) IB vs. VGB in semilog scale, (c) percentage deviation and (d) %RMS deviation. Silicon gate nMOS transistors.
2.4.5 Energy Position of Discrete Energy Level Interface Traps

If a semiconductor is doped with a shallow-level impurity, the impurity is expected to be fully ionized at room temperature. However, if the dopant produces a deep-level
trap, deionization will become a significant factor regardless of the doping concentration or temperature.

According to (2.7) and (2.12), the interface trap energy level $E_{TI}$ determines the DCVI linewidth. As shown in Figure 2.10 and 2.11, the lineshape changes with increasing forward biases, $V_{PN}$, applied to an n/p junction in p-Si with an acceptor impurity concentration $P_{AA}=10^{18}\text{cm}^{-3}$, an oxide thickness of 3.5nm, and a discrete interface trap at mid-gap ($E_{TI}=0$). Figures 2.12(a) and 2.13(a) give the effect of the interface trap energy level position on the recombination DCIV lineshape for metal gate and silicon gate transistors, respectively. These figures are for 1-discrete interface trap level. The reference of interface trap level is intrinsic Fermi level or mid-gap. If forward bias is less than interface trap energy, i.e., $V_{PN}<E_{TI}/q$, there is a flat-top region around the peak current $I_{B\text{-peak}}$ and the lineshape is symmetrically broadened by shallower energy level traps, such as 0.2eV and 0.3eV traps. Note, the broad top is the distinct signature of a shallow interface trap energy level. The application on large area and long channel transistors is given in Figure 2.12(b) and 2.13(b). The %deviations for Boltzmann ionization approximation are given in Figure 2.12(c) and 2.13(c). Since gate voltage varies from -0.5V to +0.5V for peak current down to 10 percent of the peak for shallow trap levels, such as $E_{TI}=300\text{mV}$. The %deviation is about 8% for metal gate devices and 15% for silicon gate transistors when matching 90% of experiment DCIV curve to theory using Boltzmann ionization approximation solutions. At mid-gap level, which is the commonest assumption for interface trap level during computations using DCIV mythology, the %deviation are less than 2% for metal gate devices and 5% for silicon
gate transistors. Figure 2.12(d) and 2.13(d) show the %RMS deviation using 10% to 90% of the theoretical

Figure 2.12  Effect of energy position of discrete interface trap energy level on the DCIV on the normalized IB vs. VGB lineshape. (a) IB vs. VGB in linear scale, (b) IB vs. VGB in semi-log scale. (c) percentage deviation and (d) %RMS deviation. Metal gate nMOS transistors.
Figure 2.12 Continued

(c) Increasing $E_T$ from $0$ meV to $300$ meV

(d) $n$-MOST parameters:
- $X_{OX}=3.5\text{nm}$
- $V_{PN}=200\text{mV}$
- $P_{AA}=10^{18}\text{cm}^{-3}$

Graphs showing the effects of $E_T$ on the characteristics of $n$-MOST devices.
Figure 2.13  Effect of energy position of discrete interface trap energy level on the DCIV on the normalized IB vs. VGB lineshape. (a) IB vs. VGB in linear scale, (b) IB vs. VGB in semi-log scale. (c) percentage deviation and (d) %RMS deviation. Silicon gate nMOS transistors.
Figure 2.13  Continued

curve to compare with experimental data. Again the error is less than 2% for metal gate case and 5% for silicon gate case even for the shallowest level.
The percentage deviation in accumulation region is greater than that in inversion region, as shown in the percentage curves from Figure 2.6 to 2.13, which is clearer by comparing the DCIV curves using BI approximation solutions with the exact FD theory in the semi-log figures. In accumulation region, gate voltage attracts electrons to interface. Thus, electrons are trapped at the donor impurities near the SiO₂/Si interface. While the donor impurities at interface are still ionized since gate voltage push electron away for p-type substrate. Therefore, deionization occurs only in accumulation region for p-Si.

The above discussion of energy position of discrete energy level interface traps has been based on the physics-based assumptions that the ratio of electron and hole capture rates is a constant and the interface trap density is also a constant in the silicon gap. The detail discussion of interface trap energy profile on DCIV lineshape will be given in the next chapter.

2.4.6 Temperature Dependence

When the interface of SiO₂/Si of a MOS device is in the strong accumulation or inversion ranges, degeneracy comes into play with respect to device modeling. Thus, Fermi statistics are required. At low temperature and/or high doping, the effect of deionization becomes non-negligible, and should be included. The Boltzmann ionized approximation solution is most useful around the onset of accumulation or inversion at temperatures higher than 250K and doping less than \(10^{18}\, \text{cm}^{-3}\). The practical temperature varies from 293K to 333K for a MOS transistor. In this section, we will try to find the confident levels in this range of temperature of BI approximation solution by comparing the exact FD theory using DCIV methodology.
Figure 2.14 Effect of temperature on the DCIV on the normalized IB vs. VGB lineshape. (a) IB vs. VGB in linear scale, (b) IB vs. VGB in semi-log scale, (c) percentage deviation and (d) %RMS deviation. Metal gate nMOS transistors.
Figure 2.14  Continued

(c) Decreasing T

- nMOST
- $X_{ox}=35\text{A}$
- $V_{PN}=200\text{mV}$
- $P_{AA}=10^{18}\text{cm}^{-3}$
- $T=293-333K$

(d) $V_{GB}-V_{GBpk}/(1V)$

- nMOST
- $X_{ox}=35\text{A}$
- $V_{PN}=200\text{mV}$
- $P_{AA}=10^{18}\text{cm}^{-3}$
- $T=293-333K$

- RMS90
- RMS75
- RMS50
- RMS25
- RMS10

- %DEV of $(I_B/I_{Bpk})$
- %RMSdev of $(I_B/I_{Bpk})$

- $T/(1K)$

Figure 2.14  Continued
Figure 2.15 Effect of temperature on the DCIV on the normalized IB vs. VGB lineshape. (a) IB vs. VGB in linear scale, (b) IB vs. VGB in semi-log scale, (c) percentage deviation and (d) %RMS deviation. Silicon gate nMOS transistors.
The temperature dependence of surface recombination current in the basewell channel region is mainly determined by the temperature dependence of intrinsic carrier concentration $n_i$, in which, the effective density state in conduction band $N_C$ and in
valence band $N_V$ and silicon energy gap $E_G$ are functions of temperature. Thus, the transistor characteristics are temperature dependent.

The linear DCIV curves in Figure 2.14(a) and 2.15(a) are for short channel application and semilog curves in Figure 2.14(b) and 2.15(b) for the application of long channel and large area MOS transistors. In this temperature range, gate voltage covers from -0.15V to +0.15V for peak current $I_{B\text{-peak}}$ down to 10 percent of the peak for both metal gate and silicon gate transistors.

Figure 2.14(c) and 2.15(c) show the \%deviation using the Boltzmann approximation and full ionization of impurity by comparing with the exact Fermi distribution and impurity deionization. We see that the deviation is about 2\% or less for metal gate case and 5\% for silicon gate case when marching peak current $I_{B\text{-peak}}$ down to 10\% of the peak. The \%RMS deviations are given in Figure 2.14(d) and 2.15(d). The error is less than 1\% for metal gate transistors and 2\% for silicon gate devices if we use only 90\% of the measured DCIV curve and it is less if we use less of the DCIV.

These confidence levels indicate that temperature fluctuation gives negligible errors when using BI approximation solutions to extract the parameters such as surface dopant impurity concentration and interface trap concentration profiles and oxide thickness profile in a MOS transistor.

A detail discussion about temperature effect on DCIV lineshape, peak current amplitude $I_{B\text{-peak}}$, peak gate voltage $V_{GB}$ and thermal active energy $E_A$ at different interface trap energy levels $E_{TI}$ will be described in the next chapter.
2.5 Summary

Effects from variation at the SiO₂/Si interface of the dopant impurity concentration $P_{AA}$, oxide thickness $X_{OX}$, the injected minority carriers $V_{PN}$, energy position of interface trap level $E_{TI}$ and temperature $T$ on the lineshape of the DCIV $I_B-V_{GB}$ curves are analyzed. The confident level or deviation from using the Boltzmann ionization approximation instead of the exact Fermi Deionization theory is computed. It is illustrated by a family curves that BI and FI solutions are respectively found to be nearly as good as BD and FD solutions, particularly in inversion region where deionization is less a factor. For a practical MOS transistor with $V_{PN}=200\text{mV}$, $X_{OX}=35\text{Å}$, $P_{AA}=10^{18}\text{cm}^{-3}$, $E_{TI}=0.0\text{eV}$ and $T=296.57\text{K}$, the percentage deviation and %RMS deviation are respectively no more than 2% and 1% for metal gate devices, and 4% and 2% for silicon gate transistors when matching 90% of DCIV curves from peak current to experimental data using Boltzmann ionized approximation solutions. These results indicate that the simple and time-saving BI approximation solutions of R-DCIV methodology are good enough to extract the spatial concentration profiles of the dopant impurity and interface trap at the SiO₂/Si interface and the oxide thickness profile in modern MOS transistors.
CHAPTER 3
R-DCIV LINESHAPES FROM DISTRIBUTED ENERGY LEVELS OF INTERFACE TRAPS IN SILICON GAP

3.1 Introduction

In this chapter, we analyze the effect of the energy level distribution of interface trap on the R-DCIV lineshape. First, we give a review. Interface properties along the channel have dominated the electrical characteristics and performance, and reliability of MOS transistors. Due to the technological importance, extensive research efforts have been undertaken to study interfacial electronic traps at the SiO2/Si interface and to delineate their microscopic origin [56, 57]. First, we will review the history of interface traps or surface states at the interface of SiO2/Si in a MOS transistor.

For a Schottky diode, the current formula is \( I(M/S) = I_0 \exp(qV/kT) \), where \( I_0 = A \exp(-\Phi_B/kT) \) is dark current or saturation current. The reverse current is dependent on the work function difference between metal and semiconductor. It should be different values when using different metals. However, Mayerhof [58] in 1946 observed metal-independent Schottky barrier height. In 1947, John Bardeen [59] presented two models of interface trap level distribution to account for Mayerhof’s results. One proposed distribution of density of interface state was U-Shaped that rises towards the two band edges. This is from random variations of Si-O bond length and bond angles as explained by Sah [56, 57]. The second was the two-level interface traps [59]. Two-level interface traps are from periodic dangling silicon bond [57].
In 1948, Shockley-Pearson [60] used thin film FET (Field Effect Transistor) to find a solid-state replacement of a vacuum tube. But they found no conductivity modulation in the FET. The null result was attributed to high density of interface states. High density of interface traps will pin or lock the position of the Fermi level at the surface of the thin Silicon film [56, 57, 59, 61] since band bending from the metal/semiconductor work function difference is negligible compared with that due to the high density of interface traps. So the voltage applied to the metal gate over air-gap will not modulate the conductance or resistance of the thin silicon film on glass. The pinning or locking of the Fermi level to the neutral Fermi level position at the metal/semiconductor interface not only causes the experimental Schottky barrier height to differ from that calculated using the vacuum work function value of the metal but also makes the Si surface band bending or barrier height nearly independent of the type of metal or conductor used for the metal/Si Schottky diodes [61].

There was another experimental uncertainty of experimental level determined by the thermal activation (or temperature dependence) of a device current. In 1957, Sah-Noyce-Shockey [31] used theory to fit experimental data in order to obtain the bulk trap energy level. What they found was that the trap energy levels were always near the mid-gap over a small energy range for many different p/n junctions. These values are not unique since different matching points will give different energy level. In addition, what was measured was (2.9), \( ETI^* = ETI + kT \ln(cns/cps) \), not ETI.

Another historical example was reported on the uncertainty of the interface trap energy levels in 1962. Sah [8] observed two discrete energy levels using recombination R-DCIV methodology. However, the two levels may come from the same interface trap
energy level because in a very thick oxide transistor, a non-uniform impurity concentration would shift peaked base current versus gate voltage from one into two locations.

In 1971, Nishi [62] obtained discrete interface trap energy levels on large area and thick oxide using EPR (Electron Paramagnetic or Spin Resonance). The area is around one square centimeter and the oxide thickness is around one micrometer. For modern transistors, the area is much smaller than one square centimeter (~1um2) and oxide thickness is much less than one micrometer (~10-3 micrometer or 1nm). Therefore, the discrete energy level obtained from EPR is not likely the interface trap in modern MOS transistors. One limitation using EPR is its lack of sensitivity, needing 1013-1014 spins per square centimeter to detect the signal. For modern MOS transistors with 1018cm-3 impurity concentrations, 250nm of channel length and width, there are only 60 traps at 1011cm-2 or 6000 traps at 1013cm-2. Therefore, it is impossible to observe the EPR signal even on the state-of-the-art transistors.

The R-DCIV methodology has been proposed to extract device properties of deep submicron MOS transistor with spatial nanometer resolutions (or 10 atomic layers) which can not be obtained by conventional metallurgical-optical techniques. In this novel method, the d.c. current voltage characteristics are measured and then analyzed by device-physics-based analytical theory to give the device and material properties. The novelty is the selection of the particular electrical characteristics which are very sensitive to the material properties in these devices, but also insensitive to multi-dimensional effects.
The d.c. recombination current at basewell terminal, $I_B$, is modulated by the applied gate/base voltage, $V_{GB}$, in a MOS transistor. This method was used to monitor electric-field-stress generated interface traps as a transistor reliability monitor [11, 15, 26, 57] and to serve as pre-stress diagnostic monitor for transistor design and processing [26]. The $I_B$ modulated by gate voltage $V_{GB}$ arises from recombination of the majority carrier at the SiO$_2$/Si interface traps under the gate oxide with the injected minority carriers by one or more forward biased p/n junctions (Drain/Base, Source/Base, and Substrate/Basewell) into the basewell. The R-DCIV peak current $I_{B\text{-peak}}$ and its lineshape are highly sensitivity to the transistor design, such as channel $L$ and width $W$, the spatially variation of the dopant impurity and interface trap concentrations along the SiO$_2$/Si interface, and the profile of interface trap energy level over the silicon gap in MOS transistors. A detailed theoretical analysis on R-DCIV methodology was presented in the chapter 2 for basewell channel region (BCR). The recombination at the interface traps in space charge region of source junction (SJR) and drain extension region (DER) becomes increasingly important in unstressed transistors as the channel length is scaled down and it is well-known that recombination in SJR dominates in stressed transistors [15,10,21] regardless of the channel length [15,18].

In this chapter, Slater’s perturbation theory [63] is used to explain the two models of interface trap energy distributions described by Sah [57] as shown in Figure 3.1. The energy band diagram in Fig 3.1(a) is for ideal case, zero traps at interface and in the bulk. The band diagrams in Fig 3.1(b) and Fig 3.1(c) are for bulk traps from perturbation in the silicon bulk. All the localized energy level with symmetry wave function will be pushed up when the localized perturbation from the trap potential $\Delta$ is positive (such as P type
Figure 3.1 Energy distribution of Interface traps: (a) ideal case without traps, (b) traps distributed in the silicon bulk with trap potential $\Delta$ is positive, (c) traps distributed in the silicon bulk with trap potential $\Delta$ is negative, and (d) 2 traps at 2 interface locations. N traps at N interface locations give U-Shaped DOS.

Similarly, all the localized energy level with symmetry wave function will be pushed down when the localized perturbation from the trap potential $\Delta$ is negative (such as N type impurity). The energy bands for anti-symmetry wave function stay the same positions since the perturbation effect is cancelled after integration in space. The band diagram in Fig 3.1(d) is energy distribution for many traps at different interface locations. 2 traps at 2 interface locations give two discrete interface trap levels. N traps at N interface locations give U-Shaped DOS. In this model, the energy level below conduction band is acceptor-like and energy level above valence band is donor-like.
The lineshape of R-DCIV is primarily determined by the dopant impurity concentration and its areal profile at the SiO2/Si interface, and only secondarily determined by the areal variation of the interface trap concentration provided the impurity concentration is not a constant. The injected minority concentration at the interface gives only a small change of the lineshape for the usually encountered dopant impurity concentration profiles. However, energy distribution of interface traps is assumed at the mid-gap (ETI=0) in these cases. There is negligible lineshape change between the three distributions of density of interface traps: a discrete level at the mid-gap, a constant density of traps over the entire silicon gap, and a U-shape density of traps if we assume that the electron capture rates is equal to hole capture rate in silicon energy gap.

A U-shaped density of traps in silicon gap with a U-shaped ratio of electron and hole-capture rates for a constant impurity concentration profile over the channel can still broaden the lineshape, which will be shown in this chapter. Thus, lineshape, peak current \( I_{B\text{-peak}} \) and peak gate voltage \( V_{GB\text{-peak}} \) of R-DCIV curves may give the energy distribution of interface traps. Families of base current versus gate/base voltage (\( I_B-V_{GB} \)) are computed to illustrate the effects of energy level of interface traps which could extract a possible energy distribution in the silicon gap from experimental R-DCIV lineshape. The potential applications from the analysis are proposed.

3.2 Effect of ratio of electron and hole capture rates at mid-gap trap

The analytical formula were derived and described in chapter 2 for the Shockley-Read-Hall (SRH) steady-state recombination rate RSS at interface traps in the basewell channel region (BCR). We first examine the effect of the \( cns \) and \( cps \) on the R-DCIV lineshape. In (2.7), the electron capture rate is assumed to equal to hole capture rate, i.e., \( cns=cps=10^{-8}\text{cm}^3/\text{s} \), generally the capture cross section, effective mass and thermal-
velocity of electrons are different from those of holes. In addition, the capture cross section may vary with the velocity or kinetic energy. Thus, the cns value should be different from cps. According to (2.10) and (2.12), the peak position occurs at (2.11), ETI* = ETI + kT * ln(cns/cps). The ratio of cns/cps not only change peak current IB-peak but also shift the gate voltage at the peak VGB-peak. According to (2.11), VGB-peak is proportional to the log of the ratio of cns/cps by the term -0.5*ln(cns/cps). The VGB-peak shifts 0.059V towards the accumulation region or negative VGB side and 0.059V towards the inversion region or positive VGB side when cns=100*cps and cns=0.01cps, respectively.

The peak of recombination current is proportional to the product of cns and cps and inversely proportional to the ratio of cns and cps as shown in (3.1)

\[
I_{B-\text{peak}} \propto (c_{ns}c_{ps})^{1/2} \frac{[\exp(U_{PN}) - 1]}{\exp(U_{PN}/2) + \cosh(U_{TI} + \frac{1}{2} \ln(c_{ns}/c_{ps}))}
\]

\[
\propto (c_{ns}c_{ps})^{1/2} [\exp(U_{PN}/2) - 1]
\text{ for } E_{-TI} = 0, \text{ and } c_{ns} = c_{ps}
\]

As indicated by the formulas, the ratio of cns/cps can seriously affect the peak current IB-peak. However, this is not important because we always compare the normalized R-DCIV curves with experimental data, i.e. the lineshape is what we need to care about when using R-DCIV methodology.

For a single interface energy level at mid-gap, the effect of c_{ns}/c_{ps} ratio on the R-DCIV lineshape is shown in Fig 3.1(a) and (b). The 90% peak current, which means 100% I_{B-peak} down to 10% I_{B-peak}, is covered by a gate voltage range from -0.1V to +0.1V in Figure 3.1(a). Using the R-DCIV curve at c_{ns}=c_{ps} as reference, we can see in Figure 3.1(c) that the error or % deviation is less than 4% for C_{PN}=10 or c_{ns}/c_{ps}=0.1, and 15% for
Figure 3.2  Effect of ratio of electron and hole-capture rates on normalized IB-VGB lineshape: (a) IB vs. VGB in linear scale, (b) IB vs. VGB in semilog scale. CPN=cps/cns varies from 100 to 0.01. (c) percentage deviation and (d) %RMS deviation. Interface trap level is at mid-gap.

\[ \frac{I_B}{I_B^{pk}} \]

\[ V_{GB} - V_{GBpk} / (1V) \]
Figure 3.2  Continued

$C_{PN}=0.01$ or $c_{ns}/c_{ps}=100$. The %RMS deviation is around 8% for $c_{ns}/c_{ps}=100$ as shown in Figure 3.1(d). While the percentage deviation and %RMS error are respectively smaller than 10% and 6% for $C_{PN}=0.1$ or $c_{ns}/c_{ps}=10$. In practice, since the effective electron mass
is smaller than the effective mass of hole, the $c_{ns}$ value may be greater than $c_{ps}$. Thus, the ratio of $c_{ns}/c_{ps}$ only gives a small change of lineshape for a single interface level at mid-gap.

The ratio of $c_{ns}/c_{ps}$ at the mid-gap energy level could vary in a range from 0.01 to 100. According to this family figure, the ratio of $c_{ns}/c_{ps}$ at the mid-gap has only a minor effect on R-DCIV lineshape for a single interface energy level right at the mid-gap.

3.3 Effect of Distribution of Interface Trap Energy Level on R-DCIV Lineshape

In the preceding sections, we have already tested the effect of $c_{ns}/c_{ps}$ ratio on R-DCIV lineshape for single interface energy level at mid-gap. There are several possible combinations of energy dependence between density of interface traps and the ratio of $c_{ns}/c_{ps}$ over the silicon gap: (1) a constant density of interface traps with a constant $c_{ns}/c_{ps}$, (2) a constant density of interface traps with a U-shaped $c_{ns}/c_{ps}$, (3) a U-shaped density of interface traps with a constant $c_{ns}/c_{ps}$, (4) a U-shaped density of interface traps with a U-shaped $c_{ns}/c_{ps}$. Since capture rate is a function of energy position in silicon gap, $c_{ns}$ could be several orders greater than $c_{ps}$ when interface energy level is close to conduction band. Similarly, $c_{ps}$ could be several orders greater than $c_{ns}$ when interface energy level is close to valence band. According to Slater’s perturbation theory, interface trap levels are those localized energy levels with symmetry wave function in conduction and valence bands, shifted into silicon gap by localized perturbation potential. Thus, the density of interface traps near the conduction and valence bands should be greater than those at around mid-gap. Therefore, the combinations of energy level distribution of interface trap in (1), (2) and (3) may not be possible. The most probable combination is the last one, i.e., a U-shaped density of interface traps and a U-shaped ratio of $c_{ns}/c_{ps}$ over the silicon gap. In this section, we then investigate the distribution of
interface trap level ETI with a U-shaped cns/cps ratio in silicon gap on the R-DCIV or IB-VGB lineshape. Since the cns/cps ratio is a function of interface trap level, we will not study the case for a constant cns/cps ratio over the silicon gap.

Before we look into the effect of energy position of interface traps, we should first give the definition of U-shaped distribution in silicon gap. For density of interface traps, a U-shape distribution has a minimum interface state density (NIT=10^{10} cm^{-2}) at mid-gap (or ETI=0) and rises towards the two band edges (conduction and valence bands). Similarly, a U-shaped distribution for the ratio of electron and hole capture rates cns/cps has cns=cps=10^{-8}cm^{3}/s at mid-gap and rises towards the two band edges, and cns is several orders greater than cps at the edge of conduction band and cps is several orders greater than cns. Both density of interface trap states and cns/cps ratio are functions of energy position of interface traps, i.e., NIT=f(ETI) and cns/cps =f(ETI) . For simplicity, we will not include the temperature effect on the two distributions in silicon gap and a normalized energy level of interface traps ETIN is introduced for this purpose. The formulae of density of interface traps, electron and hole capture rates are given

\[ N_{IT} = 10^{10} \times \cosh\left(\frac{ETI}{ETIN}\right) \]

\[ c_{ns} = 10^{-8} \times \exp\left(\frac{ETI}{ETIN}\right), \quad c_{ps} = 10^{-8} \times \exp\left(-\frac{ETI}{ETIN}\right) \]

In our computations, the value of ETIN equals to 0.0625eV so that density of interface states at the two band edge is around \( NIT \approx 5.0 \times 10^{13} \text{cm}^{-2} \) and the electron and hole capture rates are respectively \( 2.5 \times 10^{6} \) or around seven orders greater than hole and electron capture rates respectively at the edge of conduction and valence bands.

In an R-DCIV measurement, the contribution of each of interface trap energy level can be added to give the total contribution to recombination current I_B. Computed
examples are given to show the effects on the R-DCIV lineshape using the following formula.

\[
I_B = \frac{q}{2} n_s \int \frac{[\exp(U_{PN}) - 1]N_{IT}(E_{TI})}{\exp(U_{PN}/2) \cosh(U_s') + \cosh(U_{TT}^+)} \, dE_{TI} \, dy
\]  

(3.2)

The interface traps are each characterized by its electron and hole capture rate coefficients, \(c_{ns}\) and \(c_{ps}\), and its energy level in the silicon energy gap, \(E_{TI}\), which is measured from the intrinsic Fermi position near the silicon mid-gap. These three properties define the star interface trap energy level,

\[E_{TI}^* = E_{TI} + kT \ln\left(\frac{c_{ns}}{c_{ps}}\right)^{1/2} = U_{TI}^* (kT/q),\]

at which the steady-state recombination rate peaks and begins to decrease due to the increase of the electron or hole surface concentration by the applied gate voltage, \(V_{GB}\).

Since we don’t know if the interface trap level in silicon gap is only 1 level at the mid-gap, it is necessary to investigate the effect of \(c_{ns}/c_{ps}\) ratio on the lineshape for multi-interface trap levels. The effect of \(c_{ns}/c_{ps}\) ratio on the R-DCIV lineshape is shown in Fig 3.2(a) and (b) for a U-shaped density of interface traps and a U-shaped \(c_{ns}/c_{ps}\) ratio over the silicon gap. The ratio of CPN labeled in the figures 3.2(a) and (b) is for the mid-gap level. For instance, the formulas of \(c_{ns}\) and \(c_{ps}\) are changed into \(c_{ns}=10^{-10} \times \exp(E_{TI}/E_{TIN})\) and \(c_{ps}=10^{-8} \times \exp(E_{TI}/E_{TIN})\) for CPN=\(c_{ps}/c_{ns}=100\), the CPN ratio at other trap levels are computed using these two formulas. The 10% peak current is covered by a gate voltage range from -0.15V to +0.15V in Figure 3.2(a). Again, using the R-DCIV curve from the mid-gap level with \(c_{ns}=c_{ps}\) as reference, we can see in Figure 3.2(c) that percentage deviation is less than 30% for CPN=0.01 or \(c_{ns}/c_{ps} = 100\). The %RMS deviation is around 8% for \(c_{ns}/c_{ps} = 100\) as shown in Figure 3.2(d). The
percentage deviation and %RMS error are respectively smaller than 10% and 4% for CPN=0.1 or cns/cps =10. Thus, the cns/cps ratio only gives a small change of lineshape for a U-shaped density of interface trap and a U-shaped cns/cps over the silicon energy gap.

According to figures 3.1 and 3.2, the ratio of cns/cps has only a minor effect on R-DCIV lineshape for both a single interface energy level right at the mid-gap and a U-shaped distribution of density of interface trap with a U-shaped cns/cps over the silicon gap. Thus, for the analysis convenience, we can assume the ratio of cns/cps equals to 1 or cns=cps at the mid-gap in the followings for the discussion of energy distribution of interface traps.

For interface trap level at the edge of conduction band, electron capture and emission rates are respectively much greater than hole capture and emission rates. From (2.6), we have

\[
R_{SS} = \frac{c_{ns}c_{ps}N_sP_s - e_{ns}e_{ps}}{c_{ns}N_s + e_{ns} + c_{ps}P_s + e_{ps}} N_{IT}
\]

(2.6)

\[
= \frac{c_{ns}c_{ps}(N_s P_s - n_i^2)}{c_{ns}(N_s + n_i) + c_{ps}(P_s + p_i)} N_{IT}
\]

(3.3a)

\[
\approx \frac{c_{ps}n_i^2 \exp(U_{PN})}{N_s + n_i} N_{IT}, \quad \text{at the edge of CB}
\]

(3.3b)

\[
R_{SS-peak} \approx e_{ps} N_{IT} \exp(U_{PN}), \quad \text{at the edge of CB}
\]

(3.3c)

\[
R_{SS-peak} \approx e_{ns} N_{IT} \exp(U_{PN}), \quad \text{at the edge of VB}
\]

(3.3d)
Figure 3.3  Effect of ratio of electron and hole-capture rates on normalized IB-VGB lineshape: (a) IB vs. VGB in linear scale, (b) IB vs. VGB in semilog scale. (c) percentage deviation and (d) %RMS deviation. Density of interface traps is U-shaped and the ratio of cps/cns = CPN.
In (3.3a) and (3.3b), $n_1$ and $p_1$ are respectively electron and hole concentrations when Fermi level $E_F$ coincides interface trap level $E_T$. At the edge of conduction band, the product of surface electron and hole concentration is much greater than intrinsic
carrier concentration, i.e., \( \text{NSPS} = n_i \exp(UPN) >> n_i \), and \( \text{cns} >> \text{cps} \), \( \text{ens} >> \text{eps} \), and \( n_1 >> p_1 \). Thus, we can ignore the term \( n_i \) in numerator and \( \text{cps} \) in denominator of eq. (3.3a), and eq. (3.3a) can be simplified into (3.3b). Since \( n_1 \) is much greater than \( \text{NS} \), \( \text{NS} \) can dropped in (3.3b) near the peak recombination current, \( I_{\text{B-peak}} \). Using \( \text{eps} = \text{cps} n_1 \), we have a formula of steady-state recombination rate near the peak at the edge of conduction band as shown in (3.3c). From this formula, it is obviously that the emission rate of holes dominates RSS recombination rate because it is the lowest among the four transitions as shown in Figure 2.4. Similarly, a formula RSS recombination rate near the peak at the edge of valence band can be obtained in (3.3d) using the same procedures. In this case, the emission rate of electrons dominates RSS since it is the lowest among the four transitions.

According to (3.3c) and (3.3d), for a constant forward bias \( \text{VPN} \), the contribution from a interface trap level above or below mid-gap may give a recombination current with sharp peak, which is dependent on the product of electron or hole emission rate (\( \text{eps} \) or \( \text{ens} \)) and density of interface states \( \text{NIT} \) at the level. Normally, the contribution from an interface level at the edge of conduction or valence bands give a R-DCIV curve with a maximum flat-top since the hole or electron emission rate is around seven orders smaller than that at the mid-gap, while the density of interface states is only three orders greater than that at the mid-gap. Thus, interface trap levels that can contribute a sharp peak R-DCIV curve are those trap levels at around the silicon mid-gap. This result confirms that the most effective recombination centers are those interface traps with energy close to the mid-gap [31].
Figure 3.4 Effect of discrete and asymmetrical interface trap energy distribution on IB-VGB lineshape: (a) Two interface trap energy levels $E_{TI}=0, 0.2\,\text{eV}$. (b) Three interface trap energy levels $E_{TI}=0, 0.1, 0.2\,\text{eV}$. (c) Eleven $E_{TI}$ varies from 0 to 0.5eV with a step of $E_{TI}=0.05\,\text{eV}$. (d) Eleven $E_{TI}$ varies from 0 to -0.5eV with a step of $E_{TI}=-0.05\,\text{eV}$. NIT=$f(E_{TI})$ and cns/cps=$f(E_{TI})$. 
Figure 3.4  Continued

Figures 3.3 (a) to (d) show the effect of many energy levels on the IB-VGB lineshape. According to equations in (2.11) and (2.15), gate voltage at the peak current VGB-peak is proportional to the log of electron and hole capture rate ratio, cns/cps, i.e.,
VGB-peak = \loge(\text{cns cps}). Since cns/cps ratio is a function of interface trap level, different energy position of interface traps can give different peak gate voltage as shown in Figures 3.3(a)-(d). For those cns/cps ratio greater than 1 at the energy positions of interface traps above the mid-gap, the peak gate voltage VGB-peak will shift towards accumulation region or negative VGB side. Thus, the contribution from interface trap energy levels distributed above mid-gap broadens the shoulder of peak current IB-peak in accumulation side as shown in Figure 3.3(a), (b) and (c). Similarly, VGB-peak will shift towards inversion region or positive VGB side for those energy positions of interface traps below the mid-gap, and the contribution for each ETI broadens the shoulder of IB-peak in inversion side as shown in Figure 3.3(d). However, the shoulder broadening on both sides of peak current IB-peak is not exactly symmetrical as indicated by (2.16a) and (2.16b). R-DCIV IB-VGB lineshape is asymmetric and slightly wider on the accumulation side of the peak than on the inversion side. The difference is on the order of 0.5(VAAVS-peak)\(1/2(\Delta V S/V S\text{-peak})^2\), which is more pronounced in MOST with thick oxide and high surface impurity concentration since VAA = \(\varepsilon S q \text{PAA}/(2COX^2) = \varepsilon S q \text{PAAXOX}^2/(2\varepsilon O X^2)\).

Figure 3.4 gives the effect of symmetrical interface trap energy distribution (without mid-gap level) on R-DCIV lineshape. The effect from two discrete interface trap levels is shown in Figure 3.4(a), (b), (c) and (d), and the effect from four discrete trap levels is given in Figure 3.4(e) and (f). These symmetric interface trap energy levels symmetrically broaden the R-DCIV lineshape. Once the value of normalized interface energy \(E_{\text{ITN}}\) becomes half, or the density of interface trap \(N_{\text{IT}}\) and \(c_{\text{ns}}/c_{\text{ps}}\) ratio are functions of two times of interface trap level (i.e., \(c_{\text{ns}}/c_{\text{ps}} = f(2E_{\text{TI}})\) and \(N_{\text{IT}} = f(2E_{\text{TI}})\)), then
there is a double peak $I_B$-$V_{GB}$ curve contributed from two interface trap levels $E_{TI}=\pm 0.05\text{eV}$ as shown in Figure 3.4(b). At $E_{TI}=\pm 0.05\text{eV}$, the values of $N_{IT}$, $c_{ns}$ and $c_{ps}$ are given by

$$N_{IT}=10^{10}\cosh(2\times 0.05/0.0625)=4.95\times 10^{10},$$

$$c_{ns}=10^{-8}\exp(2\times 0.05/0.0625)=4.95\times 10^{-8},$$

$$c_{ps}=10^{-8}\exp(-2\times 0.05/0.0625)=2.02\times 10^{-9}.$$  Thus, we have the ratio of $c_{ns}/c_{ps}=24.53$.

Since the density of interface traps $N_{IT}$ is from the localized energy levels by the perturbation of localized potential, which is from the random variation of bond length and bond angle, $N_{IT}$ could be as much as five times of that at the mid-gap. For the $c_{ns}/c_{ps}$ ratio, the electron and hole capture rates could have 20 times of difference at $E_{TI}=\pm 0.05\text{eV}$.

Therefore, it is possible to observe a double peak R-DCIV curve during experimental measurements if two discrete interface trap levels are presented one above and one below the mid-gap as shown in Figure 3.4(b).

If the density and ratio are large, of $N_{IT}=f(2E_{TI})$ and $c_{ns}/c_{ps}=f(2E_{TI})$, for the two interface trap levels $E_{TI}=\pm 0.1\text{eV}$, we would have a flat top R-DCIV curve as shown in Figure 3.4(d). If there are four discrete levels of interface traps in silicon energy gap, such as $\pm 0.05\text{eV}$ and $\pm 0.1\text{eV}$ interface trap levels, the contribution from each trap will give a double peak R-DCIV curve with symmetric broadening both in accumulation and inversion regions as shown in Figure 3.4(f). These two peaks and broadening of both shoulders signify discrete interface trap energy levels with different $c_{ns}/c_{ps}$ ratio in silicon energy gap. However, we have not observed an R-DCIV curve with a double peak in our comprehensive experimental measurements. Jin Cai [64] did observe a double peak R-DCIV curve in a pMOS transistor using top-emitter (TE) configuration.
Figure 3.5 Effect of two discrete symmetrical interface traps at ETI =±0.05eV on IB-VGB lineshape: (a) NIT=f(ETI) and cns/cps =f(ETI), (b) NIT=f(2ETI) and cns/cps=f(2ETI). (c) NIT=f(ETI) and cns/cps=f(ETI), (d) NIT=f(2ETI) and cns/cps=f(2ETI). (e) NIT=f(ETI) and cns/cps=f(ETI), (f) NIT=f(2ETI) and cns/cps=f(2ETI). Temperature T=296.57K.
Figure 3.5  Continued
But the double peak curve cannot indicate two discrete interface trap energy levels in silicon gap since one of the peaks in the double peak curve is from increased interface trap concentration near the drain extension region (DER) of a stressed MOS transistor.
[26]. As indicated in (2.12b), the spatial interface trap concentration could greatly increase the shoulder amplitude to form a double peak curve for a MOS transistor with U-shaped dopant impurity concentration.

Figure 3.5 shows the effect of discrete and mid-gap symmetrical interface trap energy distribution (with mid-gap) on R-DCIV lineshape. As predicted by the theory in chapter 2, the peak current $I_{B-peak}$ occurs at the gate voltage $V_{GB-peak}$ or the interface or surface concentrations of electrons and holes, $N_S$ and $P_S$, when $c_{ns}N_S$ and $c_{ps}P_S$ are equal. From the unit steady-state recombination rate (2.7a), it is evident that the lineshape is strongly affected by the emission rates of electrons and holes which in turn are dependent on the energy level position of the interface traps in the silicon gap. A more direct representations is given in (2.7b) which explicitly shows the effect of the energy level position as indicated by the term $\cosh(U_{TI}^*)$. It is not just the energy level position but also the electron and hole capture rate ratio as indicated by the definition of $U_{TI}^*$,

$$E_{TI}^* = U_{TI}^* k_B T = [(E_i - E_f) + \frac{1}{2} k_B T \ln(c_{ns} / c_{ps})]$$

From the base recombination current equation in (3.2), it is immediately obvious that there is a plateau in the $I_B-V_{GB}$ curves centered at the maximum whose width is proportional to $ETI^*$ as shown in Figure 3.5, such as the curves with interface trap energy level $ETI=\pm0.45, \pm0.40, \pm0.35$ and $\pm0.30eV$ in Fig 3.5(c). Only when the surface energy band bending or the gate voltage is sufficiently large to make $PS>(ens+eps)/cps$ or $NS>(ens+eps)/cns$ that the unit steady-state recombination rate RSS1 or the basewell recombination current $I_B$ will start to decrease. For a interface trap level at mid-gap, $(ens+eps)/(cps+cns)$ is about equal to intrinsic carrier concentration $n_i$. Therefore, this corresponds to the sharp lineshape centered at the intrinsic surface condition or the
subthreshold voltage. But for a shallow interface trap energy level, such as \( \text{ETI}=\pm 0.4, \)
\( 0.50 \text{eV} \), either \( \text{ens} \) or \( \text{eps} \) will be very large since they are assumed to be proportional to \( \exp(\text{ETI}) \). Therefore, a much larger gate voltage \( \text{VGB} \) is necessary to increase electron or hole concentration at surface in order to reduce recombination current \( \text{IB} \).

In Figure 3.5 (a), the interface trap energy level \( \text{ETI}=\pm 0.1 \text{eV} \) symmetrically broadens the R-DCIV lineshape. While \( \text{ETI}=\pm 0.2 \text{eV} \) give a broadening shoulder on both side of peak as shown in Figure 3.5(b). Figure 3.5(c) gives the contribution to total recombination recurrent \( \text{IB} \) from each interface trap energy level varying from \(-0.5 \text{eV}\) to \(+0.5 \text{eV}\) with a \( 0.05 \text{eV} \) step. The effect of energy level number of interface traps \( \text{NETIN} \) is given in Figure 3.5(d).

The contribution from less than about 11 levels of interface traps, except \( \text{NETI}=1 \) at mid-gap \( \text{ETI}=0 \), gives an R-DCIV lineshape with a hump on both shoulders as shown by these curves labeled \( \text{NETI}=7, 9 \) and 11 in Figure 3.5(d). Once \( \text{NETIN} \) is greater than 21 for the interface traps with symmetrically distributed density in Si-gap, the humps disappear on the shoulders and the total contribution will give a smooth \( \text{IB-VGB} \) curve, (curves labeled \( \text{NETI}=21, 101 \) and 999).

Figure 3.6 shows the comparison among three distributions of interface traps in silicon gap: (1) a U-shaped DOS with \( N_{IT}=10^{10} \times \cosh(E_{TI}/E_{TIN}) \text{cm}^{-2} \), (2) a constant DOS \( N_{IT}=10^{10} \text{cm}^{-2} \), and (3) a discrete interface trap energy level at mid-gap \( E_{TI}=0 \). The normalized R-DCIV curves are given in Figure 3.6(a) and (b) for linear scale and semilog scale. The percentage deviations using the curve with interface trap energy \( E_{TI}=0\) as reference is shown in Figure 3.6(c), while %deviations using a constant density of interface traps as the reference is given in Figure 3.6(d).
Figure 3.6  Effect of two discrete and one mid-gap interface traps on IB-VGB lineshape: (a) ETI = 0.0, ±0.1eV, (b) ETI = 0.0, ±0.2eV. Density of interface traps \( N_{IT} = f(E_{TI}) \) and \( c_{ns}/c_{ps} = f(E_{TI}) \) over the silicon gap. (c) ETI varies from -0.5eV to +0.5eV with a step of 0.05eV. The curves with \( E_{TI} = ±0.5\text{ ev} \) are not included in the figures due to software limitation on curve number that can be plotted in on figure. (d) Number of ETI in Si-gap varies from 1 to 999. \( N_{IT} = f(E_{TI}) \) and \( c_{ns}/c_{ps} = f(E_{TI}) \). Temperature \( T=296.57\text{K} \).
Figure 3.6 Continued
Figure 3.7 Comparison for three distribution of density of interface traps in Si-gap: a U-shaped DOS, a constant DOS and a discrete interface trap energy level at mid-gap ETI=0. (a) Normalized IB vs. VGB in linear scale, (b) Normalized IB vs. VGB in semilog scale. (c) Using the curve with ETI=0 as reference. (d) Using the curve with a constant DOS as reference. Temperature T=296.57K.
Two salient features are immediately evident: (1) The lineshape is symmetrically broadened for a constant or U-shaped density distribution of interface traps compared with the lineshape from a single level interface trap energy at mid-gap, and (2) The
broadening for a U-shaped density distribution of interface traps is greater than a constant distribution of DOS. These indicated that the lineshape is strongly affected by density of states for continues density distribution of traps. Thus, the broadened lineshape observed in experiment R-DCIV data can not only be accounted for by the spatial variation of the surface concentration of the dopant impurity concentration at the Si-surface under the SiO2/Si interface, but also by the density distribution of interface traps in silicon gap.

The equation of effective interface trap energy level, 
\[ E_{TI^*} = E_{TI} + kT \log_2(c_{nS}/c_{pS})^{1/2}, \]
is completely independent of the surface energy band bending and other material properties, such as surface impurity concentrations, oxide thickness, and carrier capture rates. In modern Si integrated circuit manufacturing technology, ion implantation has become the principal method for introducing energetic, charged atoms into a substrate to modify surface properties of materials in order to accuracy control the electrical characteristics of MOS transistors. According to Slater’s perturbation theory, the interface trap energy levels are those shifted from the ideal positions of energy level in both conduction and valence bands into the energy gap, by localized perturbation of trap potential. The localized perturbations are from the random variation of bond angle and bond length at the SiO2/Si interface, therefore stain-distorted Si-Si and Si-O bond can give a perturbation. The beam incident angle, energy, and dose of ion implantation, HALO implantation step designed to suppress the short channel effect, and post-implantation high temperature processing step, can also contribute to perturbations. The larger perturbations or larger changes of bond length and angles, give deeper trap energy levels, and smaller perturbations are more numerous. Thus, the energy
distribution of interface trap density is most likely U-shaped and symmetrically arises towards to the edge of two energy bands from the mid-gap.

The above analysis on IB-VGB lineshape provides the basis for calculating the dependence of energy position of interface traps. This study can allow us to extract the energy distribution of interface traps in silicon gap from the experimental R-DCIV IB-VGB curves. If energy distribution of interface traps is a single level, we would see R-DCIV curves with a flat-top in experimental data once the interface trap level is not right at the midgap. If the energy distribution of interface traps contains several discrete levels, then DCIV curves with multiple peaks or broad shoulders would appear in the experimental measurements, which can be analyzed to extract the energy position and distribution of energy levels. However, all the R-DCIV lineshape so far observed has a sharp peak in our comprehensively experimental measurements, and we have not observed any R-DCIV curves with flat-top or double peaks and/or broad shoulders. This indicates that the contribution from each interface trap energy level, if some discrete level is present, is washed out by a continue distribution of interface trap levels due to random bond lengths and angles of Si:Si and Si:O4. The R-DCIV experiment data confirm that the energy distribution of interface traps is not several discrete energy levels and a most probable distribution is a U-shaped one in silicon energy gap for modern MOS transistors. Thus, we should use a U-shaped energy distribution of interface traps to extract the spatial profiles of the dopant impurity concentration, interface trap concentration and oxide thickness, instead of using a trap level at mid-gap ETI=0 which is commonly used or a constant energy distribution of interface traps over the entire silicon gap.
3.4 Temperature Dependence

The MOS-gated structure [7, 8] described here [9, 10, 26] eliminates the uncertainties during the earlier experiments which attempted to analyze the electrical characteristics of the field-effect in the p/n junction diode and transistors [65-66], since the surface potential is exactly known at the surface recombination current peak.

Theoretical analysis shows that the lineshape of R-DCIV curves can be characterized by three parameters: peak current amplitude $I_{B_{\text{peak}}}$, gate voltage at the peak $V_{G\text{B}_{\text{peak}}}$, and the half-width at half-maximum (HWHM). The three parameters are highly sensitive to the transistor design, such as channel length $L$ and width $W$, and the spatial variation of the dopant impurity and interface trap concentrations. Method for extracting dopant impurity concentration at mid-gap interface trap was demonstrated by Yih Wang [40]. However, the accuracy of the extraction of transistor parameters may be sensitively dependent on the transistor temperature, which may vary during the experiment measurements. In the section, we shall investigate the temperature dependence to ascertain its limitation on the accuracy and resolution of R-DCIV methodology.

It is well-known that the transistor characteristics are temperatures dependent, some with a power law $T^n$ from the dependence of the electron or hole mobility and diffusivity, and from other parameters with much stronger temperature dependences due to thermally activated mechanism, such as the electron and hole emission from a bound state in the silicon energy gap, with a thermal activation energy as high as $E_G/2$. There are two reasons to ascertain the temperature dependence of the $I_{B}-V_{G\text{B}}$ curves: (1) the transistor temperature could be controlled to 0.1°C accuracy in controlled laboratory experiments on small chips bonded to a small (~1/8 to 1/4 inch diameter) metal headers in which the error or uncertainty on the extraction of dopant impurity profile from experimental
lineshape data is the prime concern, and (2) in manufacturing applications of R-DCIV method for profiling, processing, design and reliability monitoring [26] in which, the sample is an 8-inch to 12-inch diameter silicon disks where temperature cannot be easily controlled to such precision.

Bludau et al. [32], has modeled the effect of energy gap narrowing with increasing temperatures for temperature below than 300K as given in (3.6a) and (3.6b). Sah, McNutt and Chan [5, 6, 33] gave an additional formula for temperatures above 300K, which can be simplified for temperatures less than 500K as given in (3.6c).

\[
\begin{align*}
  n_i(T) &= 2.5100 \times 10^{19} (m_N m_p / m^2)^{3/4} (T / 300)^{3/2} \exp(E_g / 2k_B T) \\
  E_g(T) &= 1.1700 - 1.059 \times 10^{-5} T - 6.05 \times 10^{-7} T^2 \quad (0 < T < 150K) \\
  E_g(T) &= 1.1785 - 9.025 \times 10^{-5} T - 3.05 \times 10^{-7} T^2 \quad (150K < T < 300K) \\
  E_g(T) &= 1.2080 - 2.800 \times 10^{-4} T \quad (300K < T) \\
  (m_N m_p / m^2) &= 0.81577 + 3.4353 \times 10^{-3} T \times \\
                & \left[ 1 - (T / 437.64) + (T / 814.2)^2 + (T / 1356)^3 \right]^2
\end{align*}
\]

The temperature dependence of the intrinsic carrier concentration $n_i$ is obtained by Sah, McNutt and Chan in 1974 [5, 6, 33]. Using the above expressions, they fitted the theory to extensive data reported in the literature from Boltzmann distribution at low concentrations or low temperatures, up to the melting point of silicon. We shall use these formulas.

3.4.1. Temperature Dependence of the Peak Current $I_{B\text{-}peak}$

Temperature dependence of electron-hole recombination at interfacial electronic traps under the MOS-gated surface channel in the basewell channel region is mainly determined by the temperature dependence of intrinsic carrier concentration $n_i$ in (2.12). For a single energy level SRH recombination rate at ET-EI from the intrinsic Fermi level EI, the temperature dependence of peak current $I_{B\text{-}peak}$ can be evaluated using the
temperature dependence of intrinsic carrier concentration $n_i$ and the SRH steady-state electron-hole recombination rate at the peak, RSS-peak, given by (2.6) and (2.10). For multi-interface trap levels or U-shaped density of interface traps, the total of RSS-peak is summed over all the recombination rates from each interface trap level in the silicon gap.

\[ R_{SS-peak} = \frac{(c_{ns}c_{ps})^{1/2} n_i}{2} \frac{[\exp(U_{PN}) - 1]}{\exp(U_{PN} / 2) + \cosh(U_{TI}^{*})} N_{IT} \]  

(3.8a)

\[ \propto \sum_{E_T = E_G} E^{1.5} \exp[(qV_{PN} - E_G / 2)/k_BT] \exp(U_{PN} / 2) + \cosh(U_{TI}^{*}) N_{IT} \]  

(3.8b)

Where, $U_{PN} = V_{PN}/kT$ is the normalized forward bias. The effective interface trap level $ETI^{*}$ or $UTI^{*}$ is given by (2.9). The dependence of RSS-peak on the trap energy level is contained in the hyperbolic cosine term, $\cosh(UTI^{*})$ in (3.8). This term is symmetric around the minimum at $UTI^{*} = 0$ or $UT-UI = 0.5*\ln(cns/cps)$ at which the denominator reaches its minimum value. Thus, RSS-peak is at its maximum. The equation is completely independent of the surface energy band bending and other material properties, such as surface impurity concentrations, oxide thickness. The recombination peak current $IB$-peak is given by $\int R_{SS-peak} dydz$ integrated through the channel length, from $y=0$ to $y=L_{CH}$, between the source and drain junction-space-charge regions, and the channel width from $Z=0$ to $W$. In the denominator of SRH recombination rate, (3.8a) and (3.8b) there are two terms. One is $\exp(U_{PN}/2)$ which is from forward bias at one or more p/n junctions, the other is $\cosh(UTI^{*})$ which is from effective interface trap energy level. In the limiting cases, when $\exp(U_{PN}/2)$ is much greater than $\cosh(UTI^{*})$ or $\cosh(UTI^{*})$ is much greater than $\exp(U_{PN}/2)$, RSS-peak can be simplified to
Figure 3.8  Forward bias VPN dependence of recombination peak current $I_{B-PK}$ for an interface trap with discrete interface energy level: (a) density of interface traps is a constant; (b) density of interface traps is a function of interface trap energy level. Temperature $T=296.57K$
Figure 3.9 Forward bias VPN dependence of recombination peak current $I_{BPK}$ for continuous distribution of interface energy level in silicon gap: (a) density of interface traps is a constant; (b) density of interface traps is a function of interface trap energy level. Temperature $T=296.57K$. 

\[ N_{It}=\text{Constant} \]
\[ C_{nu}/C_{ps}=f(E_{It}) \]

\[ N_{ET}=999 \]

\[ N_{ET}=1 \]

\[ 10^{-15} \]

\[ 10^{-10} \]

\[ 10^{-5} \]

\[ 10^{-1} \]

\[ V_{PN}/(1V) \]

\[ I_{BPK}/(1A) \]
Figure 3.10 Temperature T dependence of recombination peak current IB-peak for: (a) a discrete interface energy level with density of interface traps N_{IT}=f(E_{TI}) or N_{IT}≠f(E_{TI}); (b) continuous distribution of interface energy level with density of interface traps N_{IT}=f(E_{TI}) or N_{IT}≠f(E_{TI}). Temperature T varies from 293K to 333K.
Figure 3.11  Forward bias VPN dependence of thermal activation energy $E_A$ for an interface trap with discrete interface energy level: (a) density of interface traps is a constant; (b) density of interface traps is a function of interface trap energy level. Temperature $T=296.57K$
Figure 3.12 Temperature T dependence of recombination peak current $I_{B\text{-peak}}$ for a discrete interface energy level $E_{TI}=0, \pm 0.5\text{eV}$, with density of interface traps $N_{IT}=f(E_{TI})$ or $N_{IT}\neq f(E_{TI})$. Temperature T varies from 293K to 333K.

For simplicity, we will not consider the temperature effect on density of interface traps $N_{IT}$, which is a function of interface trap energy level over silicon gap, i.e., $N_{IT}=10^{10} \times \cosh(ETI/ETIN)$. Here, ETIN is a normalized interface energy value.
Equations (3.9a) and (3.9b) show that recombination rate RSS-peak strongly depends on the temperature due to the large activation energies. Since the ratio of electron and hole capture rates cns/cps is a function of interface trap energy level ETI, i.e., cns/cps = \( f(ETI) \), we can use the relation to characterize the ETI dependence of RSS-peak. The forward bias VPN dependence of the activation energy EA of RSS-peak in (3.9a) and (3.9b) gives several important consequences.

For a discrete and deep interface trap energy level ETI at around the silicon mid-gap or ETI varying from -0.1eV to +0.1eV, recombination peak current IB-peak and activation energy EA are essentially proportional to VPN/2 for entire range of forward bias VPN as shown in Figure 3.7(a) and 3.10(a), at which density of interface traps is a constant at each interface trap level, and in Figure 3.7(b), and 3.10(b), at which density of interface traps is a function of interface trap energy level, since \( \exp(UPN/2) \) is much greater than \( \cosh(UTI^*) \) in this case.

For an interface trap with a shallow and discrete trap energy level at the near of conduction and valence bands or ETI varying from ±0.3eV to the edge of two energy bands, recombination peak current IB-peak and activation energy EA are linearly proportional to VPN for entire range of forward bias VPN as indicated in (3.9b), since \( \cosh(UTI^*) \) is much greater than \( \exp(UPN/2) \) in this case. Again, Curves show the dependence in Figure 3.7(a), 3.7(b), 3.10(a) and 3.10(b). Density of interface states at each ET is a constant in silicon energy gap shown as in Figure 3.7(a) and Figure 3.10(a), while Figure 3.7(b) and Figure 3.10(b) show that density of interface states is a function of interface trap energy level.
When compared with the amplitude of IB-peak from an interface trap with a constant density of interface states at each ETI, the IB-peak increases on the order of cosh(ETI/ETIN) for an interface trap at which density of interface states is a function of ETI. The difference is more pronounced for shallow interface traps, such as the interface trap level ETI=±0.4eV, and±0.5eV, as shown in Figure 3.7.

For a constant distribution of density of interface traps in silicon energy gap, recombination peak current IB-peak is exponentially proportional to forward bias VPN/2 as shown in Figure 3.8(a). IB-peak–VPN curve with ETI=0 is essentially parallel to those curves with constant density of interface states in silicon gap, such as the number of interface trap level NETI=111 and 999. While, for a U-shape energy distribution of interface traps, the slope of IB-peak-VPN curve is a little bit higher than that with ETI=0 due to the contribution from the density of states at the interface traps around mid-gap. The reason for this is that RSS-peak in (3.9a) and (3.9b) is dominated by those interface traps around the silicon midgap or UTI*≈0 so

\[
\cosh(U_{\text{MI}}) = \cosh[(E_T - E_i)k_B T + \log_e (c_{ps}/c_{ns})^{1/2}] \approx 1
\]

While for those interface traps with shallower energy level (i.e., ETI≠0), they

\[
\cosh(U_{\text{MI}}) = \cosh[(E_T - E_i)k_B T + \log_e (c_{ps}/c_{ns})^{1/2}] >> 1,
\]

which makes RSS-peak<<1. Thus, these interface trap levels would not significantly contribute to the amplitude of recombination current. For the same reason, the thermal activation energy EA has the same forward bias dependence as recombination peak current IB-peak for a constant density of interface traps or a U-shaped density of interface traps in silicon energy gap.
Experiment data cannot uniquely determine the interface trap energy level, which is measured from the intrinsic Fermi level $E_I$ or near silicon mid-gap as defined by $E_{TI} = E_T - E_I$, because the measurement of the amplitude of peak current $I_{B-peak}$ and thermal activation energy $E_A$ only give $\cosh(UTI^*)$ or the magnitude of $ETI^* = ETI + kBT\ln(cns/cps)$, but not the sign and not the ratio of electron to hole capture rate at the trap. The density of interface states would give one more uncertainty factor, normalized interface trap energy $ETIN$, if it is a function of interface trap energy level (i.e., $N_{IT} = f(ETI)$). The indetermination has been known in thermal activation measurements of the DC current due to electron and hole recombination and generation at bulk and interface traps in two-terminal and multi-terminal semiconductor devices since 1957 [31].

Temperature $T$ can significantly affect recombination peak current $I_{B-peak}$ as shown in Figure 3.9(a), 3.9(b), 3.12(a) and 3.13(a). The percentage deviation for five temperatures $T=293, 303, 313, 323$ and $333K$, using the curve with $T=296.57K$ as reference, are respectively given in Figure 3.12(d) and Figure 3.13(d) for a discrete interface trap level $ETI=0$ and a U-shaped distribution of density of interface traps. The dependence is mainly determined by intrinsic carrier concentration $n_i$, which is a function $T^{3/2}$. While, Figure 3.11 shows that temperature has negligible effect on thermal activation energy $E_A$.

3.4.2. Temperature Dependence of the $I_{B-V_{GB}}$ lineshape

The lineshape of the $I_{B-V_{GB}}$ curve can be characterized by its half-width at half-maximum (HWHM). The formulae in the accumulation and inversion sides of peak gate voltage $V_{GB-peak}$ are given in (2.16)
\[ \Delta V_{\text{GB}+} = \Delta V_S + 2\sqrt{V_{\text{AA}}} \left[ \sqrt{|V_{\text{S-peak}} - \Delta V_S|} - \sqrt{|V_{\text{S-peak}}|} \right] \quad \text{(flatband -- side)} \quad (2.16a) \]

\[ \Delta V_{\text{GB}^-} = \Delta V_S + 2\sqrt{V_{\text{AA}}} \left[ \sqrt{|V_{\text{S-peak}} + \Delta V_S|} - \sqrt{|V_{\text{S-peak}}|} \right] \quad \text{(intinsic -- side)} \quad (2.16b) \]

Where, \( V_{\text{S-peak}} \) is the surface potential at peak current \( I_{\text{B-peak}} \), \( \Delta V_S \) is the variation of surface potential within the \( \Delta V_{\text{GB}} \) range. For the case of an \( n^+ \) poly-silicon gate in an \( n\)-MOS transistor with negligible trapped oxide charge, the flat band voltage is given by

\[ V_{\text{FB}} = -E_G/2q - V_F \quad (3.10) \]

\( V_F \) is majority carrier Fermi potential. In the above equation, \( dV_F/dT \) arises from the temperature dependence of the intrinsic carrier concentration \( n_i \), which is given by

\[ \frac{dV_F}{dT} = \frac{d}{dT} \left( \frac{kT}{q} \log_e \left( \frac{p_{\text{AA}}}{\sqrt{N_C N_V} \exp \left( \frac{-E_G}{2kT} \right)} \right) \right) \]

\[ = \frac{k}{q} \log_e \left( \frac{p_{\text{AA}}}{\sqrt{N_C N_V} \exp \left( \frac{-E_G}{2kT} \right)} \right) \]

\[ + \frac{kT}{q} \sqrt{N_C N_V} \frac{d}{dT} (N_C N_V)^{-1/2} + \frac{1}{2q} \frac{dE_G}{dT} - \frac{E_G}{2qT} \quad (3.11) \]

For an \( n\)-MOS transistor with substrate concentration \( p_{\text{AA}} = 10^{17} \text{cm}^{-3} \) and oxide thickness \( X_{\text{OX}} = 3.5 \text{nm}, V_{\text{AA}} = 8.518 \times 10^{-3} \text{V} \). Thus, the temperature dependence of \( \Delta V_{\text{GB}} \) in (3.9a) and (3.9b) are dominated by the temperature dependence of \( \Delta V_S \) and other terms can be ignored

\[ \frac{d\Delta V_{\text{GB}}}{dT} \approx \frac{d\Delta V_S}{dT} \approx \frac{dV_{\text{FB}}}{dT} = \frac{d}{dT} \left( \frac{E_G}{2q} + V_F \right) \]

\[ = \frac{k}{q} \log_e \left( \frac{p_{\text{AA}}}{\sqrt{N_C N_V} \exp \left( \frac{-E_G}{2kT} \right)} \right) \]

\[ + \frac{kT}{q} \sqrt{N_C N_V} \frac{d}{dT} (N_C N_V)^{-1/2} + \frac{1}{2q} \frac{dE_G}{dT} - \frac{E_G}{2qT} \quad (3.12) \]
Figure 3.13  Temperature T dependence of the IB-VGB linewidth for interface trap energy level at mid-gap ETI=0.0eV: (a) IB vs. VGB in absolute scale; (b) normalized IB vs. VGB in linear scale. (c) normalized IB vs. VGB in linear scale; (d) normalized percentage deviation using the curve with T=296.57K as reference. Temperature T varies from 293K to 333K.
Figure 3.13 Continued
Figure 3.14  Temperature T dependence of the IB-VGB linewidth for a U-shaped distribution of interface trap energy level in silicon gap: (a) IB vs. VGB in absolute scale; (b) normalized IB vs. VGB in linear scale; (c) normalized IB vs. VGB in linear scale; (d) normalized percentage deviation using the curve with T=296.57K as reference. Temperature T varies from 293K to 333K.
Figure 3.14 Continued

The gate voltage variations \( \frac{dV_{GB}}{dT} \) are -1.0479 mV and -1.0687 mV at around 296.57K and 333.0K, respectively. These results show that the temperature variation has only a small effect on the IB-VGB linewidth. A 10K change of the temperature will give
only 10mV change in HWHM of IB-VGB curve. Figure 3.12 shows the temperature effect on R-DCIV lineshape for interface trap level at silicon midgap, while Figure 3.13 gives the temperature effect for a U-shape distribution of interface trap density in silicon energy gap. For ETI=0.0eV, gate voltage varies from -0.1eV to +0.1eV for peak current IB-peak down to 10% of the peak as shown in Fig 3.12(d). Using the curve with temperature T=296.57K as reference, the percentage deviation is less than 10% for the curves with temperature varying from 293K to 303K. As given in Fig 3.13(d), the percentage deviation for temperature varying the same range is less than 10% for a U-shaped energy distribution of interface traps. These results show that the temperature variation has only a small effect on the IB-VGB linewidth except large temperature variation. A 10K change of the temperature will give around 10mV change in HWHM of IB-VGB curve. Thus, the extraction of impurity dopant concentration profile from IB-VGB lineshape is expected to be rather insensitive to the transistor temperature that varies during the experimental measurements.

2.4.3. Temperature Dependence of peak gate voltage $V_{GB\text{-peak}}$

The dependence forward bias VPN of the peak gate voltage VGB-peak is another important characteristics which has been used to determine the flat-band voltage VFB and average surface dopant impurity concentration $P_{AA\text{-ave}}=[P_{AA}(x=0, 0<y<L)]_\text{AVE}$ [26]. The accuracy of the extracted $P_{AA\text{-ave}}$ may be limited by the temperature dependence of VGB-peak. Therefore, we shall investigate the temperature effect on VGB-peak. Since VGB-peak always falls in the flat-band to intrinsic gate voltage range where electron and hole concentrations are near equal at the interface, i.e., $PS=NS$, it can be evaluated from the surface potential $VS=VS(VGB)$ given by
$V_{G_{B-peak}} = V_{FB} + V_{S-peak} + (V_{AA})^{1/2}(V_{S-peak})^{1/2}$ \hspace{1cm} (3.13)

$V_{S-peak}$ is the surface potential at peak recombination current $I_B$. $V_{AA} = \varepsilon_S q P_{AA}/2C_{OX}^2$ where $P_{AA}$ is dopant impurity concentration and $C_{OX}$ is the oxide capacitance per unit area. For an MOS transistor, the $V_{S-peak}$ equation is given by

$V_{S-peak} = -kT/q \log_e (c_{ns}/c_{ps})^{1/2} + (V_p + V_N)/2 \hspace{1cm} (3.14)$

Substituting (3.14) and (3.12) into (3.13), we obtain the temperature dependence of $V_{GB-peak}$ equation

$V_{GB-peak} = -\frac{E_G}{2q} - V_F - (kT/q) \log_e (c_{ns}/c_{ps})^{1/2} + (V_p + V_N)/2$

$\hspace{1cm} + (V_{AA})^{1/2}(-(kT/q) \log_e (c_{ns}/c_{ps})^{1/2} + (V_p + V_N)/2)^{1/2} \hspace{1cm} (3.15)$

At high injection levels, the electron and hole concentrations are nearly equal at Si/SiO$_2$ interface, i.e., $V_p = -V_N$, and the maximum surface recombination rate is near the flat-band. As indicated in (3.15), peak gate voltage is mainly determined by four parameters (1) substrate dopant impurity concentration $P_{AA}$, (2) gate oxide thickness $X_{OX}$, (3) emitter junction forward bias $V_{PN}$, and (4) the ratio of electron and hole capture rate. For an nMOS transistor at a given forward bias $V_{PN}$, a higher dopant impurity concentration $P_{AA}$ or a thicker gate oxide thickness $X_{OX}$ will shift the peak gate voltage $V_{GB-peak}$ towards a more positive $V_{GB}$ as shown in Figure 3.14(a) and (b).

Since electron and hole capture rate ratio is a function of interface trap energy level $E_{TI}$, i.e., $c_{ns}/c_{ps} = f(E_{TI})$, peak gate voltage $V_{GB-peak}$ is $c_{ns}/c_{ps} = f(E_{TI})$. $V_{GB}$ peak value can be used to character the energy distribution of interface traps in silicon energy gap. At a given VPN, a higher $V_{GB}$ peak value signifies a higher interface trap energy level since a higher ratio of $c_{ns}/c_{ps}$ corresponds to a higher $E_{TI}$ as shown in Figure 3.14(c).
Figure 3.15 (a) effect on peak gate voltage $V_{GB\text{-}peak}$ from nine gate oxide thickness, $X_{ox}$. (b) effect on peak gate voltage $V_{GB\text{-}peak}$ from seven dopant impurity concentration Interface trap energy level $E_{TI}=0.0\text{eV}$. (c) peak gate voltage $V_{GB\text{-}peak}$ dependence of discrete Interface trap energy level, $E_{TI}=0, \pm 0.1, \pm 0.2, \pm 0.3, \pm 0.4, \pm 0.5\text{eV}$. (d) Peak gate voltage $V_{GB\text{-}peak}$ dependence of five temperatures, $T=293, 303, 313, 323, 333\text{K}$, for three Interface trap energy level, $E_{TI}=0, \pm 0.5\text{eV}$. 

Figure 3.15 (a) effect on peak gate voltage $V_{GB\text{-}peak}$ from nine gate oxide thickness, $X_{ox}$.

(b) effect on peak gate voltage $V_{GB\text{-}peak}$ from seven dopant impurity concentration Interface trap energy level $E_{TI}=0.0\text{eV}$. (c) peak gate voltage $V_{GB\text{-}peak}$ dependence of discrete Interface trap energy level, $E_{TI}=0, \pm 0.1, \pm 0.2, \pm 0.3, \pm 0.4, \pm 0.5\text{eV}$. (d) Peak gate voltage $V_{GB\text{-}peak}$ dependence of five temperatures, $T=293, 303, 313, 323, 333\text{K}$, for three Interface trap energy level, $E_{TI}=0, \pm 0.5\text{eV}$. 

Figure 3.15 (a) effect on peak gate voltage $V_{GB\text{-}peak}$ from nine gate oxide thickness, $X_{ox}$. (b) effect on peak gate voltage $V_{GB\text{-}peak}$ from seven dopant impurity concentration Interface trap energy level $E_{TI}=0.0\text{eV}$. (c) peak gate voltage $V_{GB\text{-}peak}$ dependence of discrete Interface trap energy level, $E_{TI}=0, \pm 0.1, \pm 0.2, \pm 0.3, \pm 0.4, \pm 0.5\text{eV}$. (d) Peak gate voltage $V_{GB\text{-}peak}$ dependence of five temperatures, $T=293, 303, 313, 323, 333\text{K}$, for three Interface trap energy level, $E_{TI}=0, \pm 0.5\text{eV}$. 
Figure 3.15 Continued

The temperature dependence of VGB-peak comes from the temperature dependence of energy gap $E_G$ and Fermi potential $V_F$ as shown in (3.15). This gives
Substituting (3.13) into (3.16), we then obtain

\[
\frac{dV_{\text{GB-peak}}}{dT} = -\frac{1}{2q} \frac{dE_G}{dT} \frac{dV_F}{dT} - \frac{k}{q} \log_e \left( \frac{c_{ns}}{c_{ps}} \right)^{1/2} \\
+ \left( V_{AA} \right)^{1/2} \frac{-0.5 \left( \frac{k}{q} \right) \log_e \left( \frac{c_{ns}}{c_{ps}} \right)^{1/2}}{\left( -\left( kT / q \right) \log_e \left( \frac{c_{ns}}{c_{ps}} \right)^{1/2} + \left( V_p + V_n \right) / 2 \right)^{1/2}}
\]

(3.16)

For an interface trap energy level at mid-gap, electron and hole capture rates are assumed equal, i.e., \( c_{ns}/c_{ps} \). Thus, the last two term can be dropped in (3.17) since \( \log_e (c_{ns}/c_{ps}) = 0 \). Then, we have the peak gate voltage variation \( dV_{\text{GB-peak}}/dT = 0.0107 \text{mV/K} \) at forward bias \( V_{PN} = 200 \text{mV} \) in an n-MOS transistor with \( PAA=1017 \text{cm}^{-3}, \ XOX=3.7 \text{nm} \) and \( T=296.57 \text{K} \). While for an interface trap energy level near conduction or valence bands in a transistor with the same parameters, \( dV_{\text{GB-peak}}/dT \) are respectively \(-0.9663 \text{mV/K} \) and \( 0.8185 \text{mV/K} \) for \( ETI=0.5 \text{eV} \) and \( ETI=-0.5 \text{eV} \). This shows that peak gate voltage \( V_{\text{GB-peak}} \) has very small temperature dependence: a 10K change of temperature will give a less than 0.01V shift of \( V_{\text{GB-peak}} \) for a discrete interface trap level in the silicon gap. Figure 3.14(d) shows the temperature dependence of \( V_{\text{GB-peak}} \). \( V_{\text{GB-peak}} \) value for interface trap energy level at mid-gap is essentially a constant for low injection level for temperature varying from 293K to 333K, and it shifts towards positive VGB at high injection level for interface trap at mid-gap \( ETI=0.0 \text{eV} \). Since IB-VGB lineshape is dominated by those interface trap level close to
mid-gap, the temperature fluctuations during R-DCIV measurement give negligible errors in peak gate voltage VGB-peak for both a continuous density distribution of interface traps and a discrete interface trap energy level at mid-gap.

3.4.4. Reciprocal slope

The key point for R-DCIV is that when surface electron and hole concentrations are nearly equal or $U_s^*$ is equal to 0, there is a peak of recombination rate. The reciprocal slope or normalize voltage swing, $n$, is another important characteristics that could provide further characterization of the interface traps. Using the definition for $n$ given by

$$I_{B-peak} = I_0 \frac{\exp(U_{PN}) - 1}{\exp(U_{PN}/2) + \cosh(U_{T1}^*)} = I_0 \exp(U_{PN}/n) - 1$$

(3.18)

Here, $I_0 = qn_i(c_{ns}c_{ps})^{1/2}N_{IT}WL/2$. It is evident that the interface trap with effective energy $U_{T1}^* = 0$ would give a constant $n = 2$ which is totally independent of forward bias $U_{PN}$. This is the classic exponential to the $qV_{PN}$ over $2kT$ dependence $\exp(qV_{PN}/2kT)$. The $n$ value is computed by taking logarithm and differentiating forward bias $U_{PN}$ in both side of (3.18) given by

$$\frac{\exp(U_{PN})}{\exp(U_{PN}/n) - 1} - \frac{\exp(U_{PN}/2)}{2[\exp(U_{PN}/2) + \cosh(U_{T1}^*)]} = \frac{\exp(U_{PN}/n)}{n[\exp(U_{PN}/n) - 1]}$$

(3.19)

As peak current $I_{B-peak}$, the reciprocal slope is completely independent of the surface potential $U_s$ and other material properties, such as surface impurity concentrations, oxide thickness, interface trap concentration and carrier capture rate. For a discrete interface trap, the reciprocal slope $n$ strongly depends on the energy position of interface trap as
Figure 3.16  (a) Reciprocal slop discrete interface trap energy level, ETI=0, ±0.1, ±0.2, ±0.3, ±0.4, ±0.5eV. (b) Temperature. T=293-333K.
showed in Figure 3.15. The n value approach the ideal Shockley value of n=1 at low forward bias for the non-midgap traps, increasing towards n=2 at high V_{PN} or surface electron and hole concentrations are near equal in a small voltage range about 300mV for deep interface traps, such as E_{TI}=±0.1 and ±0.2eV. Compared with deep traps, the n value of shallow traps, such as E_{TI}=±0.4 and ±0.5eV, deviates from n=1 line towards n=2 only after high forward bias (V_{PN}>700mV).

The cns/cps ratio can significantly effect on n value. For those interface traps with U-shaped cns/cps ratio, n value approaches the idea value n=1 more than those traps with constant cns/cps ratio in silicon energy gap. Compared with cns/cps ratio, temperature has minor effect on n value since the temperature dependence is from the thermal energy. For a constant or U-shaped energy distribution of interface traps, the reciprocal slope is similar the n value from interface trap with ETI=±0.1eV since R-DCIV lineshape is mainly dominated by those interface traps around the midgap. The insensitivity of reciprocal slope on material properties of MOS transistors allows an accurate determination of the effective energy level of interface traps.

3.5 Summary

The effect of energy distribution of interface traps on R-DCIV lineshape is analyzed using the Shockley-Read-Hall band-trap thermal recombination kinetics. Comparison are given on R-DCIV lineshape among three density distributions of interface traps (1) a U-shaped DOS, (2) a constant DOS, and (3) a discrete interface trap energy level at mid-gap. The results show that the broadened lineshape in experiments not only can be accounted for by the spatial variation of surface dopant concentration but also by the energy distribution of interface traps in silicon gap. Slater’s perturbation theory indicates that the most probable density distribution of interface traps is U-shaped
in Si-gap. Thus, the extraction spatial profiles of the dopant impurity concentration, the interface trap concentration, and oxide thickness should use a U-shaped density of interface traps, instead of using a discrete interface trap level at mid-gap $E_{IT}=0$ or a constant energy distribution of interface traps in silicon gap.

Peak current $I_{B\text{-peak}}$ has large temperature dependence, while thermal activation energy $E_A$, $I_{B\text{-}V_{GB}}$ lineshape, reciprocal slope $n$, and peak gate voltage $V_{GB\text{-peak}}$ all have negligible temperature dependence, for both a continuous energy distribution of interface traps and a discrete interface trap energy level at mid-gap.
CHAPTER 4
IMPURITY DEIONIZATION

4.1 Introduction

Dopant impurity concentration, at the SiO2/Si interface and its vicinity in the source, channel and drain ranges under gate insulator, dominantly controlled the electrical characteristics of the MOS transistors. For future generations of smaller dimensions (<90nm), higher impurity concentration is necessary to reduce the channel in order to maintain the desirable and high performance characteristics of the transistor [46-49]. In this case, we shall consider dopant impurity deionization effect when using R-DCIV methodology to investigate transistor characteristics. The related discussion is still on silicon because it is the material almost universally preferred for most of semiconductor devices.

There are three conditions under which impurity are not completely ionized. One of these is that electrons are trapped at dopant donor levels and holes are trapped at the acceptors levels at low temperatures, kT<<EC-ED, or kT<<EV-EA. This is easy to understand that there is not enough thermal energy to release the trapped electron from the donor level or the trapped holes from the acceptor level at sufficient low temperature. The second is that impurity deionization occurs at high impurity or carrier concentration. If a semiconductor is doped with a shallow-level impurity, the impurity is typically expected to be fully ionized at room temperature. For a material with dopant impurity concentration NDD=1018cm-3 and room temperature T=25C, there is an appreciable fraction of the donor impurity is not ionized if the donor impurity level is 2kT below the
conduction band edge, \( EC = ED + 2kT \) since the Fermi level is about 3\( kT \) below the conduction band edge. At the interface \( \text{SiO}_2/\text{Si} \) of a MOS transistor, positive gate voltage can attract electrons to donor traps and negative gate voltage can attract holes to acceptor traps, even for low dopant impurity concentration. Thus, some dopant impurity atoms near the interface of \( \text{SiO}_2/\text{Si} \) are occupied by electrons at positive gate voltage and some acceptor impurity atoms are occupied by holes at negative gate voltage. This is the third deionization condition. Therefore, the ionized impurity density is a function of the temperature, the dopant concentration or Fermi level and surface potential or gate voltage in the MOS capacitance structure.

The impurity deionization effect at \( \text{SiO}_2/\text{Si} \) interface can occur in two ranges along the channel in a MOS transistor, the non-compensated range and compensated ranges, such as n+/p junction range for short channel transistor, as shown in Fig. 4.1 and 4.2, respectively. The three band diagrams in Figure 4.1 are for N type silicon. The first figure is for flat-band case. The second band diagram is for accumulation case. In this case, the positive gate voltage attracts electrons to the \( \text{SiO}_2/\text{Si} \) interface. Thus, some electrons are trapped at the donor impurities near the \( \text{SiO}_2/\text{Si} \) interface. In another word, the some dopant impurities are not completely ionized at positive gate voltage, which is deionization. The band diagram in Fig. 4.1(c) shows that the negative gate voltage will push electrons away from the interface in inversion range. Thus, the donor impurities at the \( \text{SiO}_2/\text{Si} \) interface are still ionized at the inversion range.

Fig. 4.2 shows the energy band diagram for compensated ranges. For a short channel MOS transistor, these ranges are very important since the length of the space charge range is comparable to channel length. In accumulation case, positive gate
Figure 4.1. Impurity deionization effect at the SiO₂/Si interface in non-compensated range. (a) Flat-band case, (b) surface at accumulation range, and (c) surface at inversion range.

Figure 4.2. Impurity deionization effect at the SiO₂/Si interface in compensated range. (a) Flat-band case, (b) surface at accumulation range, and (c) surface at inversion range.
voltage attracts electrons to interface and push holes away from interface. Thus, some
donor impurities atoms near the SiO₂/Si interface are occupied by the electrons and are
deionized while the acceptor impurities are still ionized as shown in Fig. 4.2(b). In
inversion range, gate voltage will push electrons away from interface and attract holes to
interface. Thus, donor impurities are still ionized and acceptor impurities get holes at
interface and are deionized which is illustrated in energy diagram Fig. 4.2(c).

Accounting to energy band diagram in Fig. 4.1 and 4.2, the dopant impurity
deionization effect is entirely negligible except in the strong accumulation region for non-
compensated ranges. While, we shall still consider deionization effect in both
accumulation and inversion ranges, for a moderate doped MOS transistor operating at
room temperature though the inversion will always give better results since impurity
deionization will be less significant in inversion range assuming no measurement related
problems.

Compared with the increase in accuracy gained by switching from Boltzmann
statistics to Fermi statistics, there is a very small gain in accuracy from the switch from
full ionization to deionization models. However, once the temperature is very low and/or
the dopant concentration is very high, deionization effects are not negligible. Also, if the
dopant impurity produces a deep trap level, deionization would become a significant
factor regardless of the doping concentration and/or temperature.

In the chapter, we will investigate the deionization effect dependence on the two
most important device parameters of the MOS transistor: the dopant impurity
concentration PAA and the oxide thickness XOX. As analyses in chapter 2, we will still
use percentage deviation and %RMS deviation of Fermi ionization model to judge
impurity deionization effect by comparing the exact Fermi deionization theory. For this thesis, a metal gate transistor with an interface trap at midgap level is assumed and impurity deionization at non-compensated range will be analyzed.

It will be shown that dopant impurity deionization gives negligible effect on DCIV lineshape for both dopant impurity concentration and oxide thickness dependences, which we match 90% of DCIV curve from peak current IB-peak to 10% of the peak. The fundamental reason is because electron and hole concentrations are near equal at around the peak current, both carrier concentrations are low (<10^{18} \text{cm}^{-3}) at the interface of SiO2/Si even under high injection level, and surface potential at recombination peak current lies in the flat-band to the intrinsic gate voltage range. Thus, impurity deionization effect does not carry much weight under this condition.

4.2 Dopant Impurity Concentration Dependence

Generally, it is reasonable to assume that all the surface impurities are completely ionized in doped silicon devices at room temperature because shallow level impurities are used and transistor operates between flat-band voltage and the intrinsic gate voltage. However, once transistor operates in strong accumulation or strong inversion ranges, the impurity deionization effect can not be neglected since gate voltage can attract significant electrons or holes to the impurity atoms near the SiO2/Si interface.

From the analyses of theory in chapter 2, it is evident that the impurity deionization effect will change the charge density equation, which is given by

\[ \rho = q(-N + P - N_A + P_D - n_+) \]  (2.4.1)

The ionized donor concentration \(N_A\) and acceptor concentration \(P_D\) are respectively given by (2.4.2a) and (2.4.2b)
At the SiO₂/Si interface, the donor level and acceptor level could lie around Fermi level for respectively n type and p type materials due to energy band bending which is from gate voltage attracts electron or hole to the interface. Thus, the probability of impurity deionization is very high. Therefore, the surface potential will be changed. As a result, impurity deionization effect could distort the DCIV lineshape from the recombination current at the SiO₂/Si interface under the gate contact.

The impurity Deionization effect on the error analyses of using Fermi-Ionization (FI) approximation is compared with the exact Fermi-Deionization (FD) results. The result using Boltzmann-Ionization (BI) approximation is also included the analyses. Fig. 4.2 shows a family of normalized theoretical recombination DCIV curves using BI approximation solution in dash line, FI approximation solution in solid line with dots and the FD exact theory in solid line. These figures give the recombination DCIV current for impurity concentration from 10¹⁷ to 10¹⁹ per cubic centimeters. In Fig. 4.3(a), the 90% peak current from 100% IB-peak down to 10% the IB-peak, is covered by a gate voltage range from -0.1V to +0.1V for 10¹⁷ impurity concentration and -0.2V to +0.2V for 10¹⁹ impurity concentration. We can see that the error or % deviation of the Fermi-ionization approximation solution is much less than 1% for 10¹⁷ impurity concentration and less than 10% for 10¹⁹ impurity concentration as shown in Fig. 4.3(c). When it comes to 5*10¹⁷ impurity concentration, which is in practical range, the percentage deviation is still less than 1%.

\[
N_A = \frac{P_{AA}}{1 + g_A \exp([E_A - E_f]/kT)} \quad (2.4.2a)
\]

\[
N_D = \frac{N_{DD}}{1 + g_A \exp([E_f - E_D]/kT)} \quad (2.4.2b)
\]
Figure 4.3 Deionization effect of dopant impurity concentration on the DCIV on the normalized IB vs. VGB lineshape. (a) IB vs. VGB in linear scale, (b) IB vs. VGB in semilog scale (c) percentage deviation and (d) %RMS deviation.

T=296.57K.
Fig. 4.3(d) gives the %RMS deviation by matching the theoretical curve to the experimental data. We can see that the Fermi-ionization approximation gives less than 4% RMS deviation at $10^{19}$ impurity concentration. If impurity concentration is less than
When matching 90% of the theoretical curve to the experimental data, the %RMS deviation is less than 1% and 50% DCIV curve from peak current $I_{B\text{-peak}}$ down to 50% of the peak, the %RMS deviation is less than 2 as shown in Fig. 4.3(d).

The value of percentage deviation and %RMS deviation indicates that the surface impurity deionization is negligible when dopant impurity concentration is in practical range, such as at around $10^{18}$ cm$^{-3}$. From these figures, we can see that the values of percentage deviation and %RMS deviation of FI are nearly equal to those of BI approximation solution. The basis reason is that we use FI theory to match the DCIV curves around the peak current $I_{B\text{-peak}}$, at which surface potential falls between flat-band and instinct gate voltage. Thus, gate voltage only attracts a very small amount of electrons or holes to the impurity atoms near the SiO$_2$/Si interface. Thus, impurity deionization does not carrier more weight than BI approximation solutions.

### 4.2 Oxide Thickness Dependence

The dimensions of Metal-Oxide-Silicon (MOS) field-effect transistors have continued to decrease for achieving higher packing density, faster circuit speed and low power dissipation [1, 67-68]. Aggressive scaling, propelled by the rapid advancement of VLSI technology, has reduced the oxide thickness at 1.2nm in 2002 [2]. At this scale of oxide thickness, the surface impurity deionization effect may be negligible since the increasing electrical field, which is due to the decreasing of oxide thickness for the same gate voltage, would attract more electrons or holes to impurity atoms near the SiO$_2$/Si interface.

Figures 4.4 give one family of normalized $I_B$ vs. $V_{GB}$ to show the lineshape dependence on the one of the most basic MOS transistor design parameters, the oxide thickness. It varies from 10A to 200A, which covers all practical range. For thin oxide
MOS transistors, gate voltage covers from -0.1V to +0.1V for peak current down to 10 percent of the peak. While, gate voltage should change from -0.3V to +0.3V for peak current down to 10 percent of peak for thick oxide MOS transistors. Fig. 4.4(c) shows the %deviation using the Fermi approximation and full ionization of impurity by comparing with the exact Fermi distribution and impurity deionization. We see that the deviations are less than 2% and 4% respectively for thin oxide and thick oxide MOS transistors when matching peak current down to 10% of the peak. The %RMS deviation for $10^{18}$ impurity concentration is given in Fig. 4.4(d). The error is less than 2% for thick oxide devices, while %RMS is less than 1% for thin oxide transistors, such as $X_{OX}$<50A. If we use only 50% of the measured DCIV curve (FWHM) from peak current down to 50% of the peak, %RMS error is less than 0.4% for all the oxide thickness smaller than 200A.

From the comparison between Fermi ionization approximation solution and the exact FD theory, we can conclude that the errors are very small for oxide thickness covering all practical range. This indicates that the impurity deionization doses not distort the DCIV curve a lot at around the peak current. Also, the confident level of BI approximation is nearly equal to the error of FI approximation.

The recombination current reaches its maximum when the gate voltage is varied to make the local surface concentration of electron and hole nearly equal. From (2.11b) equation, $U_{S-peak}=-\ln(c_{ns}/c_{ps})+U_F-U_{PN}/2$, the $U_{S-peak}$ shows that recombination peak current lies in the flat-band to the intrinsic gate voltage range ($0<U_S<U_F$ for p-Si). Thus, there are no many electrons or holes are attracted to impurity atoms near the SiO$_2$/Si interface.
Figure 4.4. Deionization effect of oxide thickness on the DCIV on the normalized IB vs. VGB lineshape. (a) IB vs. VGB in linear scale, (b) IB vs. VGB in semi-log scale. (c) percentage deviation and (d) %RMS deviation. T=296.57K.
Fig. 4.4. Continued

Therefore, it is reasonable to expect that the percentage deviation and %RMS deviation of FI approximation are essentially identical to the confident level of BI solutions for the
injected minority carrier concentration, interface trap energy level and temperature
dependences. Also, we can expect that there is a negligible difference between BI and FI
approximation solutions when matching 90% DCIV curve form peak current $I_{B,\text{peak}}$ down
to 10% of the peak, for both metal gate and silicon gate MOS transistors. In another
words, the percentage deviation and %RMS deviation of FI approximation confirms that
the simple and time-saving BI approximation solutions can used to extract the dopant
impurity concentration, interface trap concentration, oxide thickness profiles in MOS
transistors in all practical range, including dopant impurity concentration, oxide
thickness, injected minority concentration, interface trap energy level and temperature.

4.4 Summary

Impurity deionization effect of dopant concentration and oxide thickness on DCIV
lineshape has been obtained and presented. From the percentage deviation and %RMS
deviation of Fermi ionization approximation solution, it shows that there is a negligible
impurity deionization near the SiO2/Si interface in MOS transistors when matching 90%
of experimental data from peak current down to 10% of the peak. We can expect that the
errors of FI approximation are nearly identical to the confident level of BI for device
parameters in practical range, such as dopant impurity concentration, oxide thickness,
injected minority concentration, interface trap energy level and temperature, for both
metal gate and silicon gate MOS transistors.

The analyses of impurity deionization confirms that the time-saving and simple
Boltzamann ionization is a good approximation to extract the spatial profiles of device
and material parameter from experiment data, such as the dopant impurity concentration,
interface trap concentration, oxide thickness, since it has a good physical basis at around
the recombination peak current.
CHAPTER 5
SUMMARY AND CONCLUSIONS

The success of today’s semiconductor industry can be partially attributed to the passivation of intrinsic defects at the interface between the silicon channel and the thermal gate oxide to give extremely low interface trap density in a MOS transistor. Continued scaling down of the MOS transistor increases the importance of the impurity distribution along the channel on device’s electrical performance and manufacturing yield. The increasing importance of understanding the precise impurity concentration profile have made the experimental determination of impurity profile one of the major challenges in the development of the next generations of VLSI technology [4, 26], in order to provide the feedbacks for optimization the design and fabrication. The direct-current current voltage (DCIV) methodology has the sensitivity to extract the interface trap and impurity concentration profiles along the surface channel by measuring the gate bias VGB and the forward junction bias VPN modulated electron-hole recombination currents at the SiO2/Si interface. This unique sensitivity of DCIV makes it a powerful tool for monitoring the transistor reliability and for diagnosis of transistor design.

In the previous chapters, fundamental theories which relate DCIV characteristics to device and material parameters are presented. It is shown that the recombination peak current, gate voltage at the peak current and DCIV lineshape can be used to extract device parameters. In order for routine monitoring of surface impurity concentration profile, interface trap concentration profile and oxide thickness profiles during transistor fabrication, it is necessary to obtain the confident level of the fast Boltzmann fully
ionization solutions. The accuracy of the time-saving and simple BI approximation is obtained by comparing with the exact Fermi deionization theory showing excellent accuracy. The fundamental physical basis for high accuracy of the BI approximation to extract device parameters data is that the electron and hole concentrations are near equal at around recombination peak current and surface potential at around peak current lies in flat-band to intrinsic gate voltage. This means that both carrier concentrations near IB-peak can not be very high even under high injection condition from the forward junction bias.

The dependence of the confident level or accuracy of the BI approximation on the dopant impurities concentration PAA, oxide thickness XOX, the injected minority carriers VPN, energy position of interface trap level ETI and temperature T on the lineshape of the DCIV IB-VGB curves are computed by matching the exact Fermi Deionization theory. Results are obtained for both metal gate and silicon gate MOS transistors. When matching 90% of DCIV curves from the peak current IB-peak down to %10 of IB-peak, the percentage deviation and %RMS deviation, for metal gate and silicon gate MOS transistors, are respectively less than 8%, 4% and 10%, 5% when PAA varying from 1016 to 1019cm-3 with XOX=35A and VPN=200mV; 2%, 2% and 4%, 2% when XOX varying from 10A to 300A with VPN=200mV and PAA=1018cm-3; 6%, 3% and 10%, 4% for VPN varying from 100 to 800mV with XOX=35A and PAA=1018cm-3; 8%, 2% and 15%, 5% for ETI varying from 0 to 300mV with VPN=200mV, XOX=35A, PAA=1018cm-3 and T=296.57. The values are 2%, 1% and 5%, 2% respectively for metal and silicon gate transistors when T varying from 293K to 333K with VPN=200mV, XOX=35A and PAA=1018cm-3.
For a practical MOS transistor with $\text{VPN}=200\text{mV}$, $\text{XOX}=35\text{A}$, $\text{PAA}=1018\text{cm}^{-3}$, $\text{ETI}=0$ and $\text{T}=296.57\text{K}$, the percentage deviation and %RMS deviation are respectively less than 2% and 1% for metal gate devices, and 4% and 2% for silicon gate transistors when matching 90% of DCIV curves from peak current down to 10% of the peak using Boltzmann ionized approximations. These results indicate that the time-saving and simple BI approximation solutions of R-DCIV methodology are good enough to extract the spatial profiles of the dopant impurity concentration, interface trap concentration spatial and oxide thickness along the channel surface in modern MOS transistors.

Three density distributions of interface traps on DCIV lineshape: (1) a U-shaped DOS, (2) a constant DOS, and (3) a discrete interface trap energy level at mid-gap were analyzed using the Shockley-Read-Hall band-trap thermal recombination kinetics. One important result was that the broadened lineshape in experiments can not only be accounted for the spatial variation of surface dopant concentration but also by the energy distribution of interface traps in silicon gap. Thus, the parameter profile extraction of impurity concentration and interface trap concentration, and oxide thickness should use a U-shaped density of interface traps, instead of using a discrete interface trap level at mid-gap $\text{ETI}=0$ or a constant energy distribution of interface traps in silicon gap since the most probable density distribution of interface traps is U-shaped in Si-gap, which is from random variations of bond length and bond angle of Si-Si and Si-O structures based on Slater’s perturbation theory.

The ratio of electron and hole captures has a minor effect on the R-DCIV lineshape for both a single interface trap at mid-gap and a U-shaped distribution of interface trap energy. R-DCIV lineshape is dominated by those interface traps at around midgap while
other interface traps broaden the lineshape at either accumulation or inversion sides. The analyses of temperature dependence of the peak current, R-DCIV lineshape and peak gate voltage show that peak current IB-peak has large temperature dependence, while thermal activation energy EA, IB-VGB lineshape, reciprocal slope n, and peak gate voltage VGB-peak have negligible temperature dependences, for both a continuous energy distribution of interface traps and a discrete interface trap energy level at mid-gap.

The comparisons of BI, BD, FI and FD models shows that BI and FI approximations are respectively found to be nearly as good as BD and FD solutions. The analyses of impurity deionization effect indicate that deionization will be less significant in inversion range than in accumulation range assuming no measurement related problems.

The results of percentage deviation and %RMS deviation of FI approximation shows that there is a negligible impurity deionization near the SiO₂/Si interface in MOS transistors when matching 90% of experimental data from peak current down to 10% of the peak. It is reasonable to expect that the errors of FI approximation are nearly identical to the confident level of BI for all device parameters in practical range, such as dopant impurity concentration, oxide thickness, injected minority concentration, interface trap energy level and temperature, for both metal gate and silicon gate MOS transistors.

The analyses of impurity deionization confirms that the time-saving and simple BI is a good approximation of real phenomenon to extract the spatial profiles of device parameters from experiment data, such as the dopant impurity concentration, interface trap concentration and oxide thickness, since it has a good physical basis at around the recombination peak current.
Therefore, the results of the confident level of BI approximation, impurity deionization effect and distribution of interface trap energy investigated in this dissertation is expected to be useful for determining the spatial profiles of device parameters as well as for diagnosis of transistor design in the current and next generations of semiconductor technologies.
APPENDIX
ACCURACY OF ITERATIVE ANALYTICAL SOLUTIONS

The Appendix is to test the accuracy of iterative analytical solutions of surface potential $U_S$ and the related electron-hole recombination current $I_B$ at SiO$_2$/Si interface. The degeneracy is important in the inversion and accumulation regions of a MOS transistor, and there is no analytical solution to the Fermi integral. Thus, a full-range analytical approximation to the Fermi-Integral must be used, such as those shown in Blackmore’s paper on the subject of F-D integrals [34]. In addition the equation for $U_S$ is a transcendental equation, so iterative solution must be employed, such as the rational Chebyshev approximations [35, 36] used in this thesis. In this appendix, we check the $U_S$ and $I_B$ accuracy obtained from Boltzmann statistics and fully ionized impurity approximations.

There are two ways to check the accuracy of these two values of BI approximation solutions. One is to check them in accumulation and inversion ranges. At these two ranges, either surface majority carrier concentration or surface minority carrier concentration dominates in the electric field formula. Thus, we can simplify the formula, to give an analytical surface potential $U_S$ formula. Another way is to calculate the surface potential $U_S$ and gate voltage $V_{GB}$ from a given recombination current $I_B$.

Accumulation Region

The non-degenerate, fully-ionized solution is simplest when we assume that the minority carrier terms are negligible and the majority surface concentration is much larger than the bulk concentration. This assumption is somewhat indicative of strong
accumulation, which would invalidate the Boltzmann assumption, but it allows us to find an analytical solution. Electric field equations (2.4.11) at substrate is converted to the simplest forms

\[
E_{sx}^2 = \frac{2kT}{\varepsilon_{sx}} \left\{ N_v \left[ \exp(-U_{sx} - U_v + U_{fx}) - \exp(-U_v + U_{fx}) \right] + N_c \left[ \exp(U_{sx} + U_c - U_{fx} + U_{pn}) - \exp(U_c - U_{fx} + U_{pn}) \right] + P_{AA} U_{sx} \right\} \quad \text{for BI (2.4.11)}
\]
\[
\approx \frac{2kTN_v}{\varepsilon_{sx}} \exp(-U_{sx} - U_v + U_{fx})
\]
\[
= \frac{2kTP_{AA}}{\varepsilon_{sx}} \exp(-U_{sx}) \quad \text{Accumulation (A.1.1)}
\]

For an n+ doped poly-silicon nMOS transistor, the electric field formula at poly-silicon gate side has the similar form as that of in substrate side. The difference is that the minority carrier in substrate is electron, while minority carrier is hole in silicon gate. Thus, the \( V_{PN} \) in the formula of electric field at gate side should be in a place different from that of in the formula of electric field at substrate side. The surface potential at poly-silicon gate side is positive in accumulation range for an n+ doped nMOS transistor. Thus, the simplified electric field equation is given by

\[
E_{sg}^2 = \frac{2kT}{\varepsilon_{sg}} \left\{ N_v \left[ \exp(-U_{sg} - U_v + U_{fg} + U_{pn}) - \exp(-U_v + U_{fg}) \right] + N_c \left[ \exp(U_{sg} + U_c - U_{fg}) - \exp(U_c - U_{fg}) \right] + P_{GG} U_{sg} \right\} \quad \text{for BI (A.1.2)}
\]
\[
\approx \frac{2kTN_c}{\varepsilon_{sg}} \exp(U_{sg} + U_c - U_{fg})
\]
\[
= \frac{2kTP_{GG}}{\varepsilon_{sg}} \exp(U_{sg}) \quad \text{Accumulation (A.1.3)}
\]
Inversion Region

Derivation of the inversion of BI approximation solution is quite similar to that of accumulation side. The surface minority carrier terms are expected to dominate the majority carrier terms. Thus, the majority carrier terms are neglected and the sign of electric field is positive for p-type inversion. Starting with equation (2.4.11), and neglecting the majority carrier terms, gives

\[ E_{sx}^2 \approx \frac{2kTn_i^2}{\varepsilon_{sx}} \exp(U_{sx} + U_C - U_FX + U_{PN}) \]

\[ = \frac{2kTn_i^2}{\varepsilon_{sx} P_{AA}} \exp(U_{PN} + U_{sx}) \]

Inversion (A.1.4)

Similarly, the surface potential at silicon side \( U_{SG} \) is negative at inversion range, and the electric field \( E_{SG} \) is similar to \( E_{SX} \) at accumulation side. What we need to do is just to change the notations. The electric field is given by

\[ E_{sg}^2 \approx \frac{2kTn_i^2}{\varepsilon_{sg}} \exp(-U_{sg} - U_v + U_{FG} + U_{PN}) \]

\[ = \frac{2kTn_i^2}{\varepsilon_{sg} P_{GG}} \exp(-U_{SG} + U_{PN}) \]

Inversion (A.1.5)

We assume that the oxide charge \( Q_{OTT} \), and interface trap charge at gate \( Q_{ITG} \) and at substrate \( Q_{ITX} \) are zero, the dielectric constants in poly-silicon gate \( \varepsilon_{SG} \) and at substrate \( \varepsilon_{SX} \) are the same. Thus, the second voltage equation [5] is given by

\[ \varepsilon_{SG} E_{SG} = - (\varepsilon_{sx} E_{sx} + Q_{ITG} + Q_{ITX} + Q_{OTT}) \]

\[ \Rightarrow E_{SG} = - E_{SX} \]  

(A.1.6)

For the case of an n+ poly-silicon gate in an nMOS transistor, the surface potential at poly-silicon gate side \( U_{SG} \) is in inversion range when the surface potential at substrate side \( U_{SX} \) is in accumulation range. From the equations (A.1.1), (A.1.5) and (A.1.6), we
have the surface potential at silicon gate side when substrate is in accumulation range
given by

\[ U_{SG} = U_{SX} + \ln \left( \frac{n_i^2}{P_{GG}P_{AA}} \right) + U_{PN} \] 

Accumulation at substrate \hspace{1cm} (A.1.7)

Note that, in accumulation range, the sign of electric field \( E_{SX} \) is negative, the gate
equation (2.4.7) can be transformed into

\[ V_{GB} = V_{FB} + V_{SX} + V_{SG} + \text{sign}(V_{S})e_{SX}E_{SX} / C_{OX} \] 

\[ = V_{FB} + 2V_{SX} + \frac{kT}{q} \ln \left( \frac{n_i^2}{P_{GG}P_{AA}} \right) - \text{sqrt}(2kT\varepsilon_{SX}P_{AA} \exp(-U_{SX}) / C_{OX}^2) \] 

(A.1.8)

Dropping the surface potential term \( 2V_{SX} \), we have the \( U_{SX} \) at accumulation range given
by

\[ U_{SX} \approx -2 \ln(V_{FB} + \frac{kT}{q} \ln \left( \frac{n_i^2}{P_{GG}P_{AA}} \right) + V_{PN} - V_{GB}) + \ln \left( \frac{2kT\varepsilon_{SX}P_{AA}}{C_{OX}^2} \right) \] 

(A.1.9)

Similarly, the surface at poly-silicon side is in accumulation range when surface at
substrate side is in inversion range. The surface potential at poly-silicon side in
inversion range has the same form as in accumulation range given by

\[ U_{SG} = U_{SX} + \ln \left( \frac{n_i^2}{P_{GG}P_{AA}} \right) + U_{PN} \] 

Inversion at substrate \hspace{1cm} (A.1.10)

In this case, the sign of electric field \( E_{S} \) is positive, the gate equation (2.4.7) can be
transformed into

\[ V_{GB} = V_{FB} + V_{SX} + V_{SG} + \text{sign}(V_{S})e_{SX}E_{SX} / C_{OX} \] 

\[ = V_{FB} + 2V_{SX} + \frac{kT}{q} \ln \left( \frac{n_i^2}{P_{GG}P_{AA}} \right) + V_{PN} + \text{sqrt}(\frac{2kT\varepsilon_{SX}n_i^2}{P_{AA}C_{OX}^2} \exp(U_{PN} + U_{SX})) \] 

(A.1.11)
Therefore, we have the surface potential at substrate side when surface is at inversion range given by

\[ U_{SX} \approx 2 \ln(V_{GB} - V_{FB}) - \frac{kT}{q} \ln\left(\frac{n_i^2}{P_{GG} P_{AA}}\right) - V_{PN} - \ln\left(\frac{2kT \varepsilon_{SX} n_i^2}{P_{AA} C_{OX}}\right) \exp(U_{PN}) \]  

(A.1.12)

For a metal gate nMOS transistor, the electric field \( E_{SG} \) and surface potential \( U_{SG} \) at gate side are zero. Following the same procedures, we have the surface potential \( U_{SX} \) at accumulation and inversion ranges given by

\[ U_{SX} \approx -2 \ln(V_{FB} - V_{GB}) + \ln(2kT \varepsilon_{SX} P_{AA} / C_{OX}^2) \]  

Accumulation  

(A.1.13)

\[ U_{SX} \approx 2 \ln(V_{GB} - V_{FB}) - \ln\left(\frac{2kT \varepsilon_{SX} n_i^2}{P_{AA} C_{OX}^2}\right) \exp(U_{PN}) \]  

Inversion  

(A.1.14)

Since only one surface potential term \( V_{SX} \) is dropped for metal gate case, while \( 2V_{SX} \) is dropped for silicon gate case. Consequently, the \( V_{SX} \) computation for metal gate case is more accurate than that of silicon gate case. For the same reason, both results are close to but not equal to that of iterative computations. The unit Shockley-Read-Hall steady-state electron-hole recombination rate \( R_{S1} \), effective surface potential \( U_s^* \) and effect interface trap energy \( U_{TI}^* \) are given by (2.7b), (2.8b) and (2.9).

\[ R_{S1} = \frac{2}{(c_{ps} c_{n})^\frac{1}{2} n_i} \frac{[\exp(U_{PN}) - 1]}{\exp(U_{PN} / 2) \cosh(U_s^*) + \cosh(U_{TI}^*)} \]  

(2.7b)

\[ U_s^* = U_s + \log_e \left(\frac{c_{ns}}{c_{ps}}\right)^\frac{1}{2} - U_F + U_{PN} / 2 \]  

for p-Si  

(2.8b)

\[ U_{TI}^* = \frac{E_{TI}}{k_B T} = \frac{[(E_T - E_i) / k_B T + \frac{1}{2} \ln(c_{ns} / c_{ps})]} {2} \]  

(2.9)

The recombination current \( I_B \) is given by integrating \( R_{S1} \), through the channel length from the source to drain junction-space-charge regions, and the channel width from 0 to W. The analytic solutions can allow us to evaluate the accuracy that of from iterative computations. The result from iterative computation and analytic solution is
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Table A.2: Silicon Gate nMOS Transistors

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<td>3.3906972917D-23</td>
</tr>
<tr>
<td>10</td>
<td>0.90944930</td>
<td>0.92586751</td>
<td>5.3120797958D-23</td>
<td>2.7913769844D-23</td>
</tr>
</tbody>
</table>
given by table A.1 and table A.2 for metal gate and silicon gate case, respectively. In these two tables, the subscript ‘iter’ means the related values are from iterative computations, while subscript ‘anal’ means the values are analytical solutions.

The related parameters for an nMOS transistor are that dopant impurity concentration $P_{AA} = 1.0 \times 17 \text{cm}^{-3}$, oxide thickness $X_{OX} = 35 \text{A}$, forward bias $V_{PN} = 200 \text{mV}$, flat-band voltage $V_{FB} = 0.01 \text{V}$, interface trap energy level $E_{TI} = 0.0 \text{V}$ and temperature $T = 296.10 \text{K}$. From these two tables, the analytical solutions of surface potential $U_S$ and the related recombination current $I_B$ are close to those from the iterative computations since the surface potential term $V_S$ was dropped in the gate voltage equation. These results only check the trend of $U_S$ and $I_B$ in accumulation and inversion regions, but cannot tell us the accuracy of iterative computations.

Now, I will give the second way to check accuracy of iterative computations. In this method, the recombination current $I_B$ is as a known value, which is from iterative computations. Since every parameter is as a known value in the formula of unit Shockley-Read-Hall steady-state electron-hole recombination rate $R_{SSI}$, except parameter surface potential $U_S$. Thus, once we have an $I_B$ value, we can calculate the related surface potential $U_S$. From gate voltage equation, given in (2.4.7), we can calculate gate voltage $V_{GB}$ for metal gate case and $V_{GB} - V_{SG}$ for silicon gate devices once $U_S$ value is available. Gate voltage varies from $-1.0 \text{V}$ to $+1.0 \text{V}$ for iterative computations in the following two tables.

The result from iterative computation and analytic solution are given by table A.3 and table A.4 for metal gate and silicon gate case, respectively. The related parameters are: Temperature $T = 296.10 \text{K}$, oxide thickness $X_{OX} = 35.000 \text{A}$, dopant impurity concentration
\( P_{AA}=1.0 \times 17 \text{cm}^{-3} \), forward bias \( V_{PN}=200.00 \text{mV} \), temperature \( T=296.10 \text{K} \), interface trap energy level \( E_{TI}=0.0 \text{V} \) and flat-band voltage \( V_{FB}=0.01 \text{V} \). It is very clear that the errors between analytic and iterative solutions are very small, less than 0.05\% for surface potential \( U_{SX} \) and 0.006\% for gate voltage \( V_{GB} \) or \( V_{GB-V_{SG}} \). Actually, the iterative solutions can be very close to true values only if the iterative accuracy is set to a small enough. One shortcoming for this, it needs to take more computation time. However, we do not need care about it for running a small program in modern computers and a ‘true’ value is not necessary for our analysis. Thus, iterative computation is a good to way to compute transcendental equations.

**Table A.3: Metal Gate nMOS Transistors**

<table>
<thead>
<tr>
<th>( I_B(A) )</th>
<th>( V_{SX-iter}(V) )</th>
<th>( V_{SX-anal}(V) )</th>
<th>( V_{GB-iter}(V) )</th>
<th>( V_{GB-anal}(V) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.5757737591D-21</td>
<td>-0.17116026</td>
<td>-0.1711603150</td>
<td>-1.000</td>
<td>-1.000000180</td>
</tr>
<tr>
<td>7.5443371213D-21</td>
<td>-0.15840173</td>
<td>-0.1584017828</td>
<td>-0.800</td>
<td>-0.8000001529</td>
</tr>
<tr>
<td>1.4453229184D-20</td>
<td>-0.14181327</td>
<td>-0.1418133234</td>
<td>-0.600</td>
<td>-0.6000001259</td>
</tr>
<tr>
<td>3.6150491271D-20</td>
<td>-0.11842092</td>
<td>-0.1184209781</td>
<td>-0.400</td>
<td>-0.4000001006</td>
</tr>
<tr>
<td>1.5958819985D-19</td>
<td>-0.08053210</td>
<td>-0.0805321537</td>
<td>-0.200</td>
<td>-0.2000000779</td>
</tr>
<tr>
<td>3.0304050347D-18</td>
<td>-0.00541678</td>
<td>-0.005416834835</td>
<td>0.000</td>
<td>-0.62253D-7</td>
</tr>
<tr>
<td>6.1813348838D-16</td>
<td>0.13027819</td>
<td>0.1302781295</td>
<td>0.200</td>
<td>0.1999999422</td>
</tr>
<tr>
<td>3.0349853227D-13</td>
<td>0.29439343</td>
<td>0.2943933724</td>
<td>0.400</td>
<td>0.3999999428</td>
</tr>
<tr>
<td>1.7729689476D-15</td>
<td>0.46742467</td>
<td>0.4674246148</td>
<td>0.600</td>
<td>0.5999999434</td>
</tr>
<tr>
<td>2.0436699472D-18</td>
<td>0.64005960</td>
<td>0.6400595438</td>
<td>0.800</td>
<td>0.7999999420</td>
</tr>
<tr>
<td>7.0738732109D-20</td>
<td>0.72588281</td>
<td>0.7258827508</td>
<td>1.000</td>
<td>0.9999999192</td>
</tr>
</tbody>
</table>
Table A.4: Metal Gate nMOS Transistors

<table>
<thead>
<tr>
<th>$I_B$ (A)</th>
<th>$V_{SX}$-iter (V)</th>
<th>$V_{SX}$-anal (V)</th>
<th>($V_{GB}$-$V_{SG}$)-iter</th>
<th>($V_{GB}$-$V_{SG}$)-anal</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.854869D-21</td>
<td>-0.169650</td>
<td>-0.1696496086</td>
<td>-0.973816</td>
<td>-0.973816641</td>
</tr>
<tr>
<td>8.012867D-21</td>
<td>-0.156864</td>
<td>-0.1568644100</td>
<td>-0.778878</td>
<td>-0.778877830</td>
</tr>
<tr>
<td>1.535316D-20</td>
<td>-0.140272</td>
<td>-0.1402720706</td>
<td>-0.584221</td>
<td>-0.584220779</td>
</tr>
<tr>
<td>3.831240D-20</td>
<td>-0.116939</td>
<td>-0.1169389323</td>
<td>-0.389773</td>
<td>-0.389773156</td>
</tr>
<tr>
<td>1.673160D-19</td>
<td>-0.079326</td>
<td>-0.07932556737</td>
<td>-0.195271</td>
<td>-0.195271071</td>
</tr>
<tr>
<td>3.041451D-18</td>
<td>-0.005324</td>
<td>-0.005323997026</td>
<td>0.174e-3</td>
<td>0.174154946e-3</td>
</tr>
<tr>
<td>5.757235D-16</td>
<td>0.128465</td>
<td>0.1284644751</td>
<td>0.197671</td>
<td>0.1976711156</td>
</tr>
<tr>
<td>2.803055D-13</td>
<td>0.291192</td>
<td>0.2911914878</td>
<td>0.396227</td>
<td>0.3962271008</td>
</tr>
<tr>
<td>2.096752D-15</td>
<td>0.463144</td>
<td>0.4631442428</td>
<td>0.595123</td>
<td>0.5951234007</td>
</tr>
<tr>
<td>2.445692D-18</td>
<td>0.635477</td>
<td>0.6354773616</td>
<td>0.794020</td>
<td>0.7940199912</td>
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<tr>
<td>7.779777D-20</td>
<td>0.723456</td>
<td>0.7234556842</td>
<td>0.989398</td>
<td>0.9893974529</td>
</tr>
</tbody>
</table>
REFERENCES


BIOGRAPHICAL SKETCH

Zuhui Chen was born in Fujian, China, on October 7, 1973. He received the Bachelor of Science degree in physics in 1998 from Fujian Normal University and the Master of Science degree in physics in 2001 from Xiamen University, China. Since the fall of 2002, he has been studying in Electrical and Computer Engineering at the University of Florida. He is currently working toward his Ph.D. under the guidance of Professor Chih-Tang Sah. His Ph.D. dissertation research concerns investigation of theoretical limitations of recombination DCIV methodology for characterization of MOS transistors.