A study of dislocations in lattice-mismatched semiconductors

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2011

Yu, Y. (2011). A study of dislocations in lattice-mismatched semiconductors. Master's thesis, Nanyang Technological University, Singapore.

<https://hdl.handle.net/10356/46845>

<https://doi.org/10.32657/10356/46845>

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A STUDY OF DISLOCATIONS IN LATTICE-MISMATCHED SEMICONDUCTORS

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School of Electrical & Electronic Engineering

A thesis submitted to the Nanyang Technological University
In partial fulfillment of the requirement for the degree of
Master of Engineering

2011

Statement of Originality

I hereby certify that the work embodied in this thesis is the result of original research and has not been submitted for a higher degree to any other University or Institution.

19/01/2010

Date

余穎

Yu Ying

Acknowledgment

I would like to express my sincere gratitude to my supervisor Professor Yoon Soon Fatt for his guidance, support and encouragement. With his attention and patience, I have overcome a number of difficulties in my research and am fully aware of that I have learnt not only knowledge from the project itself, but also the way to become a professional researcher.

At the same time, I also appreciate all help from Dr. Hendrix Tanoto so that I can broaden my view and sharp my creativity by grasping his shared experience. Like Dr. Liu Chong Yang, Dr. Loke Wan Khai and Dr. Lew Kim Luong also impart, enlighten and assist me on mastery of all tools.

The dedicated contribution helps me also from my group-mates, all clean room technicians and the lab-mates working together in the experiments during the past years.

Last, but not least I want to thank my wife Xiao Lihua and my parents and for their love and support throughout my studies.

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Summary

Recently heteroepitaxy of III-V semiconductors with Si microelectronics on a single substrate has attracted great interest due to the ability of integrating optoelectronics on a silicon-based substrate. However, the fundamental differences in material, namely the 4% lattice mismatch and > 64% thermal expansion coefficient mismatch between GaAs and Si, epitaxial GaAs/Si integration are significantly maneuvered by the threading dislocations and the anti-phase defects (APDs). In the experiment that researcher applies to compositionally step-graded SiGe buffer layer up to ~100% Ge, which is lattice-matched to GaAs, the dislocation density successfully decreases to less than 10^6 cm^{-3} in fully relaxation of Ge/SiGe/Si virtual substrates.

The residual threading dislocation, which exists in the SiGe substrate, can propagate into the epitaxially grown III-V layer and thus influence the performance of grown materials. In this thesis, a series of quantitative calculations have been carried out based on the W. T. Read's model. The results show the effects of dislocation on the material's electrical properties, unveiling relationships among mobility, dislocation density and free carrier concentration. In addition, etch hillock density is checked in order to reveal the dislocation density. This newly deployed method offers a better solution than the conventional TEM inspection. At last, the calculation results are verified by the comparison with the experimental data.

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List of Symbols

Symbol	Description
a_0	Effective Bohr radius of the donor
a_f	Lattice constants of the epitaxial layer and the substrate
a_s	Lattice constants of the substrate
b	Absolute value of the Burger's vector
c	Space between two dangling bonds
e	Electron charge
E_0	Energy of nearest neighbor e-e interaction
E_e	Electron-electron interaction energy
E_{ep}	Interaction energy of electrons at positively space-charged region
E_F	Fermi energy
E_p	Energy stored in the surrounding positively space-charged region
E_{pe}	Interaction energy of electrons
E_T	Dislocation energy level
f	Fraction filling factor
f	Amount of lattice mismatch, or misfit
$\hbar$	Reduced Planck constant
h_c	Critical thickness
h_{pz}	Piezoelectric constant
K_o	Modified Bessel function
k_B	Boltzmann constant
L	Space between two occupied sites
m^*	Effective electron mass in GaAs
n	Free carrier concentration
n'	Effective screening concentration
N_A	Bulk acceptor concentration
N_D	Bulk donor concentration

N_{dis}	Dislocation density
N_I	Ionized impurity concentration
N_n	Neutral impurities concentration
R	Radius of the cylinder
T	Absolute temperature
ν	Poisson's ratio
Ze	Ionic charge
ϵ	Permittivity ($\epsilon_r \epsilon_0$)
ϵ_r	Relative permittivity
ϵ_0	Permittivity in vacuum
θ	Angle between the dislocation line and Burgers vector
λ	Screening parameter
λ_D	Debye length
μ	Mobility
μ_{dis}	Dislocation mobility
μ_{dp}	Deformation potential mobility
μ_H	Hall mobility
μ_{ii}	Ionized impurities mobility
μ_{ni}	Neutral impurities mobility
μ_{pe}	Piezoelectric potential mobility
μ_{po}	Polar optical phonons mobility
ρ_p	Charge density in compensated material
τ	Scattering time
τ_{dis}	Dislocation scattering time

List of Abbreviations

Abbreviations	Description
APD	Anti-phase defects
EPD	Etch pit density
KOH	Potassium Hydroxide
MBE	Molecular-beam epitaxy
MEE	Migration enhanced epitaxy
MOCVD	Metal-organic chemical-vapor deposition
SLS	Strained layer superlattice
TDD	Threading dislocation density
TEM	Transmission electron microscope

Chapter 1 INTRODUCTION AND MOTIVATION

1.1 Introduction

In the photonics industry, III-V compound semiconductor material is the most important material for the manufacturing of light emitting devices such as semiconductor lasers, light emitting diodes and optical detectors. Their direct bandgap, whose energies of the various III-V materials cover the entire spectrum from ultra-violet to near-infrared, permit very efficient photon coupling, making them become the ideal material in fiber optical applications typically operated in the 850 nm, 1300 nm or 1550 nm optical fiber transparency windows for free space optical transmission and visible display. High speed (GHz range) electronic devices, such as RF modules for cellular telephones, have a tendency to utilize III-V heterostructures due to the large electron mobility and relatively short lifetimes, a consequence of the direct bandgap, which permits extremely high speed switching speed.

Recently heteroepitaxy of III-V semiconductors combined with group IV material and alloy of those on a single substrate has attracted great interest. It is known that group IV elemental semiconductors, including silicon (Si), germanium (Ge) and alloy $\text{Si}_x\text{Ge}_{1-x}$, crystallize in the cubic “diamond-like” structure. The III-V compound semiconductors (i.e. GaAs) are formed in the cubic “zincblende” structure which is similar to the “diamond-like” structure.

Although Ge is the first type of material used to fabricate solid-state semiconductor transistors, today it is rarely used in an active device. The properties of Ge are strongly temperature dependent because of its small bandgap. Moreover, it lacks of high-quality electrically insulating native oxide. However, recently the commercial interest of Ge greatly arises because it has been found that Ge is a suitable substrate material for GaAs to be grown on in the applications of solar cells because of their similar structure, very close lattice constants and close thermal expansion coefficients. In GaAs/Ge heteroepitaxy, the presence of dislocations is not a serious issue as the material's dislocation density is as low as 10^5 cm^{-2} . However, the anti-phase domains (APDs) are adversely generated as crystalline defects in the GaAs epitaxial layer due to the imperfection of symmetry of the III-V zincblende crystal structure compared with the group IV diamond-like crystal, i.e. Ge. Currently, both metal-organic chemical-vapor deposition (MOCVD) and molecular-beam epitaxy (MBE) are used to grow GaAs on Ge. By suppressing APD formation and applying reproducible simultaneous control of both APD's and Ge out-diffusion, high quality GaAs/Ge heterojunction can be achieved.

Compared with Ge, Si completely dominates the modern conventional microelectronic industry for its very low material cost and the ease of fabricating the high quality silicon dioxide. However, because of its indirect bandgap, the light coupling ability of Si is relatively poor. Together with its relatively large electron effective mass, these drawbacks make Si one kind of poor material in optoelectronic

and high speed electronic application. In order to exploit technologies from two different platforms, high-speed or photonic technology from III-V and VLSI technology from Si, new ways must be explored to circumvent all the problems mentioned above. However, if III-V layers were deposited directly on the Si substrates, high material quality will be difficult to be obtained because of the high defect density resulting from the fundamental material differences, i.e. the 4% lattice mismatch and >64% thermal expansion mismatch [1]. To reduce the dislocation density in the GaAs film, several techniques have been developed, including misoriented substrates, strained layer superlattice (SLS) buffers and various annealing steps [2]. Although all the above methods can reduce the number of the defects to as low as the 10^6 cm^{-2} level [3-5], it is much higher than the $10^3 - 10^5 \text{ cm}^{-2}$ level required by the high quality devices [3], [5].

So far, inserting a graded $\text{Si}_x\text{Ge}_{1-x}$ buffer between the heteroepitaxy of GaAs and Si substrate is one of the best solutions. By slowly increasing the Ge content of the SiGe buffer during the epitaxy from the top of Si substrate, usually in the order of micrometers (e.g., a typical grading rate would be 10% Ge / μm), a $\sim 10 \mu\text{m}$ thick graded buffers from Si to $\sim 96\%$ Ge is obtained [6]. This strain relaxed buffer provides a “virtual substrate” as the $\text{Si}_x\text{Ge}_{1-x}$ buffer layer lattice-matched to GaAs. Samavedam and Fitzgerald [7] have demonstrated Ge (100) with 6° offcut towards (111) plane, the phenomena leading to more than an order of magnitude reduction in dislocation pileups compared with non-vicinal Si, which reduces the dislocation density to $10^5 \sim$

10^6 cm^{-2} . Growth of epitaxial by MBE/MEE (migration enhanced epitaxy) helps to reduce the density of APDs (anti-phase domains) and further improve the quality of grown material.

As mentioned above, high density of dislocations, which significantly degrades the quality of material, must be suppressed to below certain level, therefore, a clear understanding of the mechanism of dislocations is essential. In the past 50 years, several dislocations models were established to explain the effect of dislocation density on material's electrical and optical properties. From 1954, W. T. Read has published a series of papers regarding the dislocations as a sort of space-charged pipe lines in Ge [8-10]. This model assumes that the electrical properties of dislocations in *n*-type material are dominated by the dislocation's strong acceptor tendency. This acceptor behavior stems from the dangling bonds was first postulated by Shockley [11]. Such behavior occurs at the presence of the extra atomic half-plane associated with a dislocation with an edge component.

1.2 Motivation

Dislocation is one of the dominant factors which seriously affect the electrical and optical properties of the material. For deposition of GaAs directly on Si substrate, the dislocation density can be as high as 10^9 cm^{-2} , which will greatly degrade the electrical properties of the GaAs/Si heterostructure. Although the problem has been

partially solved in the experiment of GaAs on GeSi/Si buffer layer, theoretical explanation of this phenomenon is not available. Such a model using dislocation density to quantitatively describe the quality of the material in GaAs/GeSi heterostructure is still under development. However, there are several mature models suggesting a similar mechanism on other materials. As mentioned previously, Read reported a model which successfully quantified the electrical effects of dislocations on Ge substrate [8]. In his model, dislocations are treated as negatively-charged lines, which behaved as Coulombic scattering centers for the conduction electrons. Recently, Gurusinghe et al successfully adopted Read's model for wurtzite GaN [12-14]. Read's model is also adopted in this work because of the similarities of the crystal structure and the types of dislocations between Ge and GaAs.

The density is an important parameter to characterize the dislocations since it defines material quality. However, the measurement is very tedious and time consuming because it requires transmission electron microscope (TEM) pictures need to be taken or etch pit density needs to be measured after chemical etching.

1.3 Challenges and Objective

Basic fundamental lattice structure differences among Ge, GaN and GaAs should be taken into consideration for the reason that Read's model is originally built on Ge system, which is a diamond structure [8] and successfully adopted in GaN system as

reported in a later work [12-14]. It is better to take the fundamental structure differences among Ge, GaN and GaAs into account when this theory is applied into GaAs/GeSi/Si system. In GaAs bulk material, Read's model is used for grain boundaries calculation in early 80's as well [15]. In this research, GeSi/Si virtual substrate is incorporated into a new system, which provides us many research opportunities through the study of different material properties.

The purpose of this research is to investigate and study the electrical properties of dislocations in GaAs film, an epitaxial layer grown on GeSi/Si substrate, and the factors affecting the electron mobility. When Read's model is applied into our GaAs/GeSi/Si systems, a series of equations involving dislocation density, free carrier concentration and mobility can be obtained. Through the input of necessary data, the dislocation density can be calculated instead of performing the actually measurement. Experiment can be conducted to verify these calculated results. In the experiment, the Hall mobility of the GaAs/GeSi/Si samples is measured and dislocation density is revealed when the samples are etched by mixture of Chromium Oxide (CrO_3) and Hydrofluoric (HF) solution (HF-CrO_3). The calculated results will be tested for their consistency with the experiment results. Through this exercise, the relationships among the mobility, dislocation density and free carrier concentration can be established. The research does not only improve the understanding of dislocations in III-V/IV heterostructures, but also provides another effective method to estimate the defect density in the grown materials.

1.4 Contributions

An effective method has been developed to successfully characterize the dislocations in the GaAs/GeSi/Si system based on the Read's model on Ge. In this research, the difference of two types of lattice structures of materials (GaAs and Si) is taken into account. Meanwhile, a missing entropy term in Read's model is also considered. Detailed calculations were made to establish relationships among dislocation density, free carrier concentration and Hall mobility. The experimental data justify the calculated results and no fitting parameter is used in this calculation. The results show that dislocation density of GaAs material can be estimated from Hall mobility and free carrier concentration measurement.

1.5 Thesis Overview

Chapter 1 introduces the background and the motivation of this work. In Chapter 2, a review on Read's model is illustrated in detail. In addition, relationships among dislocation density, mobility and free carrier concentration are described. The experimental setup and the method to calculate results are presented in Chapter 3 and Chapter 4, respectively. The last chapter gives a summary to the whole thesis and draws a possible direction for future research.

Chapter 2 THEORETICAL REVIEW AND DERIVATION

The technological benefit of III-V/Si deposition was introduced in Chapter 1. In this chapter, the research theoretical background including the research methodologies is discussed in detail.

2.1 Lattice Mismatch

Since the scope of the research covers lattice mismatched materials, it is necessary to give a brief introduction about the lattice mismatch in the beginning. GaAs and Si are two absolutely different materials each with a unique lattice constant. The lattice mismatch between GaAs and Si (~ 4%) is responsible for the inability to achieve high material quality and produce high performance devices through epitaxial integration. The process of lattice mismatched heteroepitaxy involves the epitaxial growth of a layer with a lattice constant which is different from the underlying substrate. The amount of lattice mismatch, or misfit (f), is defined in Equation (2.1).

$$f = \frac{a_f - a_s}{a_s} \dots\dots\dots (2.1)$$

where a_f and a_s are the lattice constants of the epitaxial layer and the substrate, respectively [16]. Figure 2.1 shows a schematic representation of epitaxial growth of an epitaxial layer material with either same or different relaxed lattice parameter comparing with the lattice parameter of substrate material. This results in a

tetragonally distorted lattice in which the in-plane lattice constant of the layer material conforms to the atomic spacing of the substrate material.

Figure 2.1 The growth of an epitaxial layer of lattice constant, a , on a substrate of lattice constant, a_0 where a) $a = a_0$, b) $a > a_0$ and c) $a < a_0$. If lattice mismatch exists, either tensile or compressive strain can be incorporated into the epitaxial layer [17].

The epitaxial layers will continue to grow in this “tetragonally distorted” or pseudomorphic form until the layer thickness reaches the critical thickness, h_c . The

critical thickness is defined as the maximum thickness of an epilayer grown on the substrate. Beyond the critical thickness, it becomes energetically favorable to relieve the strain by other methods, such as the generation of one or more dislocations.

A number of models have been developed to calculate the value of the critical thickness. A typical one is typically described by the Matthews Blakeslee criteria [16]. This model uses an equivalent approach of balancing the forces for a propagating and threading dislocation. By balancing the force of the threading dislocation in an uncapped epilayer with the restoring tension force from the extra interfacial dislocation, the critical thickness (h_c) could be expressed by:

$$h_c \equiv \frac{b}{2\pi f} \frac{1 - \nu \cos^2 \theta}{(1 + \nu) \cos \lambda} \left[\ln \left(\frac{h_c}{b} \right) + 1 \right] \dots\dots\dots (2.2)$$

where ν represents the Poison's ratio and b is the absolute value of the Burger's vector which represents the magnitude and direction of the lattice distortion of dislocation in a crystal lattice. θ is the angle between the dislocation line and its Burgers vector, and λ is the angle between the Burger's vector and the direction in the interface perpendicular to the dislocation line.

Figure 2.2 plots the critical thickness versus Ge fractions in $\text{Si}_{1-x}\text{Ge}_x$ pseudomorphically grown on a Si (100) substrate calculated by employing the Matthews and Blakeslee's theory. As indicated in this figure, the critical thickness

varies with the change of Ge composition. It changes from 1 nm on Ge/Si material system to ~220 nm on the Si/Si material system.

Figure 2.2 Plot of critical thickness versus germanium fraction of pseudomorphic $\text{Si}_{1-x}\text{Ge}_x$ layers grown on bulk (100) silicon. The data is calculated using the Matthews and Blakeslee's model. A metastable curve for MBE growth at 550 °C is also included [19].

Because of the large lattice mismatch between Si and GaAs (4%), the critical thickness for these two materials is quite small which can explain the extremely high dislocation created in the direct deposition. The Ge buffer layer is introduced to reduce the dislocation density. The grading rate is 10% Ge per μm , which yields $\sim 10 \mu\text{m}$ thick graded buffers from Si to $\sim 96\%$ Ge [6]. Meanwhile, a model is required to explain the relationship between dislocations and the material electrical properties. The Read's model is introduced and discussed in detail below.

2.2 Read's Model

W. T. Read proposed a model to analyze the behavior of dislocations in Ge system in 1954 [8]. The original model described the acceptor-like nature of dislocations as negatively charged lines surrounded by positively charged cylindrical region to achieve charge balance.

Read's model is built on Ge system, whose crystal structure is diamond-like. The 60° dislocation is the most common in this structure. When dislocation is introduced, it appears as an extra plane in the system, which somehow distorts the crystal structure and creates some dangling bonds with one free electron for each atom. The detail is graphically illustrated in Figure 2.3.

Figure 2.3 (a) Perfect diamond structure; (b) an extra plane creating the 60° dislocation.

This extra plane brings some energy states into the bandgap associated with dislocation, which are acceptor-type because that the unpaired dangling bond each tends to capture an electron and forms a more stable state. Therefore, the dislocations can be treated as a row of closely spaced acceptor centers. Since they are filled by electrons, the dislocation lines are negatively charged.

In this thesis, all dangling bonds are called sites and those who still have the ability to capture electrons are empty sites while the rest are filled sites. In general, not all the sites are filled. To account for that, the filling factor, f , which describes the fraction of the sites that are occupied, is introduced. Illustrated in Figure 2.4, L is defined as the spacing between occupied sites. c is the spacing between two dangling bonds, which is defined as $c = b \sin 60^\circ / \sin \theta = 0.866b \operatorname{cosec} \theta$. Here b is the lattice constant of GaAs and θ is the angle between dislocation and Burgers vector. In this manner, the fraction of charged site is $f = c / L$. For edge ($\theta=90^\circ$) orientation, the spacing c is minimum.

Figure 2.4 Definition of fraction filling factor.

The corresponding density of electrons which occupies these sites is $(f/c)N_{dis}$ where N_{dis} is the dislocation density. Since the dislocation is negatively-charged, the bulk charge balance equation is defined as: $N_D = n + N_A + f \cdot (N_{dis} / c)$. N_D and N_A are the bulk donor and acceptor concentrations, respectively. The negatively charged line

repels the conduction electrons and a positive cylindrical space-charged region is formed surrounding the dislocation. The radius of the cylinder is defined as R , a radius containing an amount of fixed positive charge equal to the negative charge on the dislocation. This defines the charge balance within the cylinder. The relationship between R and L is shown as:

$$\pi R^2 \cdot (N_D - N_A) = 1/L = f/c \dots\dots\dots (2.3)$$

This space-charged region is assumed to have a sharp boundary. It is a good approximation at low temperature when the potential ψ rises by kT/q in a distance that is small compared with the radius R of the space-charged cylinder. Thus an electron that strikes the cylinder head-on penetrates only a negligible distance (compared to R).

The model is graphically illustrated below in Figure 2.5.

Figure 2.5 Graphically illustration of Read’s model.

A unit value of the fraction filling factor f is defined as f_0 when the radius of the space-charged cylinder is equal to lattice constant a . Then the relationship between f and f_0 can be written as $R = a \cdot (f/f_0)^{1/2}$. The calculation of the radius R will be given and discussed in Chapter 4.

2.3 Total Electrostatic Energy

In order to calculate the f value, the system's electrostatic energy must be taken into account. When the empty sites along the dislocations are filled by the conduction-band electrons, the electrostatic energy of the system increases. The potential energy of these states rises and thus the total electrostatic energy increases until nothing is gained energy-wise. The transfer of electrons from the conduction band to the dislocations will cease when the total electrostatic energy becomes constant. This electrostatic energy determines the distribution of electrons in the dislocation lines which affect the fraction filling factor.

In order to derive an analytical expression for the total electrostatic energy (E_s), three contributions are considered. They are electron-electron interaction energy (E_e), energy stored in the surrounding positively space-charged region (E_p) and interaction energy of electrons at the dislocation lines (E_{pe}) and the positively space-charged regions (E_{ep}), respectively [13]. All the three interactions will be discussed in detail. The total electrostatic energy per site is calculated by adding all the three contributions $E_s = E_e + E_p + E_{ep} + E_{pe}$ as discussed above.

At first, the electron-electron interaction energy per electron per length, E_e , at the dislocation line is calculated by:

$$E_e = E_0 f [\ln(f/2c) + 0.577] \dots\dots\dots (2.4)$$

where E_0 is the energy of nearest neighbor electron-electron interaction at the dislocation line. E_0 is expressed as $E_0 = q^2 / 4\pi \cdot \epsilon \cdot c$. 0.577 is the value of Euler's constant, where ϵ is permittivity defined as $\epsilon_r \epsilon_0$. ϵ_r is relative permittivity. ϵ_0 is permittivity in vacuum.

The second contribution is the energy stored in the surrounding positively space-charged region (E_p). In order to derive an expression for the interaction energy of the positive charge in the space-charged region, the Poisson's equation is solved around the dislocation for $r \leq R$ by:

$$\frac{1}{r} \frac{d}{dr} \left(r \frac{dV}{dr} \right) = -\frac{e\rho_p}{\epsilon} = -\frac{e(N_D - N_A)}{\epsilon} \dots\dots\dots (2.5)$$

which leads to:

$$V(r \leq R) = (e\rho_p / 4\epsilon)(R_0^2 - r^2) \dots\dots\dots (2.6)$$

Here ρ_p is the charge density in compensated material which contains both donors and acceptors. R_0 is a constant of integration and is determined by the continuity of the potential at $r = R$. Since $r \geq R$, the potential is the same as when all charges are concentrated along the axis of the cylinder. It is convenient to use the integral form of Gauss's law. In this case, the potential is given by:

$$V(r \geq R) = (eR^2 \rho_p / 2\epsilon) \ln(1/r) \dots\dots\dots (2.7)$$

By equating these potentials in Equations (2.6) and (2.7) at $r = R$ and applying the relation $\rho_p R^2 = f / \pi c$, the potential term becomes:

$$V(r \leq R) = \frac{ef}{4\pi\epsilon} \left[1 - 2 \ln(R) - \frac{r^2}{R^2} \right] \dots\dots\dots (2.8)$$

The total interaction energy for a site due to positively space, E_p , can be written as:

$$E_p = (1/2)l \int_0^R e\rho_p V(r \leq R) \cdot 2\pi r dr \dots\dots\dots (2.9)$$

Substituting the potential term from Equation (2.8) and integrating, we get:

$$E_p = E_0 f [1/4 - \ln(R)] \dots\dots\dots (2.10)$$

The third contribution is the interaction of electrons at the dislocation lines and the positively space-charged regions. The interaction energy of the positively space-chargers and electrons at the dislocation lines (E_{pe}) equals to the integral of $(1/2)e\rho_p V_e(r, z)$ with respects to both r and z . However, the interaction energy at the dislocation line with the positively space-charged (E_{ep}) is provided by the conservation of energy. The interaction energy of electrons and the positively space-charged is $E_{ep} = -(1/2)eV(r=0)$. This energy equals to the interaction energy of the positive charges and electrons. Hence, from Equation (2.8) E_{pe} is given as:

$$E_{ep} = E_{pe} = -\frac{1}{2}E_0 f [1 - 2\ln(R)] \dots\dots\dots (2.11)$$

As mentioned previously, the total electrostatic energy per site (E_s) is calculated by $E_s = E_e + E_p + E_{ep} + E_{pe}$. Substituting the equations for E_e , E_p , E_{pe} and E_{ep} into the above expression leads to:

$$E_s(f) = fE_0 \left[\frac{3}{2} \ln\left(\frac{f}{f_0}\right) - 0.866 \right] \dots\dots\dots (2.12)$$

A mathematical description is brought out for the above phenomenon by considering the formation energy per electron at a site. As is mentioned above, a degenerate energy level E_T is associated with the sites localized along the dislocation line. If a dislocation has q number of electrons out of p number of possible sites, then the

numbers of ways of arranging q electrons among p sites are $p!/(p-q)!q! = {}^pC_q$. The free energy per site can be written as [8]:

$$f \cdot G(f) = f \cdot [E_T - E_F + E_s(f) - \frac{k_B T}{f p} \ln({}^pC_q)] \dots\dots\dots (2.13)$$

where T is absolute temperature and k_B the Boltzmann constant. In the model we assumed that a site can have only one electron. Now at statistical and thermal equilibrium this free energy should be minimized with respect to f , which in turn depends on all parameters that contribute to the line charge. Subsequently, we take the derivative of Equation (2.13) with respect to f . Here, f , the fraction charge occupation in the dislocation, is given by the Fermi distribution-like function:

$$f = \frac{1}{[1 + \exp(\frac{E(f) - E_F}{k_B \cdot T})]} \dots\dots\dots (2.14)$$

where $E(f)$ is given as:

$$E(f) = E_T + \frac{d}{df} [f \cdot E_s(f)] \dots\dots\dots (2.15)$$

The E_T in the above equation represents the localized energy state of the dislocation within the bandgap. However unlike Ge system, GaAs system has two types of termination of the extra plane. The dislocations may be formed either by terminating the extra atomic half-plane on a row of group III elements (α dislocations) or on a row of group V elements (β dislocations) [20]. Since, in general, a grain boundary may have both α and β dislocations present and the exact position of the neutrality levels are unknown, a neutrality level near the mid-gap ($E_T = 0.71$ eV) will be selected. Such selection is appropriate because the neutrality levels for α and β have been predicted to be above and below the mid-gap region, respectively [19].

2.4 Mobility Due to Dislocations

In the previous sections, the dislocations are described as negatively charged lines surrounded by cylindrical positively space-charged regions. The negativity of the line is described by the fraction filling factor, f , in Read's model. In the positively space-charged region, any electron – positive charge recombination is prohibited, whose behaviors are similar to depletion region. Because of charge balancing of the negatively charged dislocation lines and the positively space-charged regions, all electrons which move near a negatively charged dislocation line are scattered, which eventually turn the dislocation lines into scattering centers. The corresponding relaxation time of this scattering line has been analytically solved by Pödör [22], by considering a continuously charged negative line screened by ionized impurities and free electrons.

The potential profiles from the dislocation lines have a pronounced effect on electron scattering. When the currents flow normal to the dislocations, the electron mobility is affected by the scattering effect due to dislocation lines. Because the impact due to the momentum component of electrons paralleling to the dislocation line is very small, the three-dimensional scattering is considered as two-dimensional scattering, i.e. electron motion is considered to be normal to the dislocations only.

Several assumptions are made in order to simplify the model. Firstly, it is assumed

that all the dislocations are straight lines, parallel one to another, so no crossover of dislocations are founded in this system. Secondly, the distance between two dislocations is long enough so that the electric field of one dislocation has a negligible effect on another dislocation's. The cylindrical boundaries of the positively space-charged region are assumed to be sharp and perfectly cylindrical. When the electrons collide with the cylinders, the scatterings are elastic and the electrons only penetrate a depth negligible in the positively space-charged region. In this case, there is no electron which penetrates the whole cylinder region.

The screened potential energy at a distance, r , from a charged dislocation line was given by Boch-Bruevich and Glasko [23] as:

$$V(r) = \frac{e}{2\pi\epsilon c} K_o(r/\lambda) \dots\dots\dots (2.16)$$

Here K_o is the modified Bessel function and λ is the screening parameter which will be discussed in detail later. The above equation describes the screened potential energy from a charged dislocation line. The result is inconclusive because it fails to consider how negatively the dislocation lines are being charged. In order to consider the negative charges carried by the dislocation lines, Read's model is adopted, meaning the fraction filling factor, f , added in the equation as an additional parameter, which modified the equation as:

$$V(r) = \frac{ef}{2\pi\epsilon c} K_o(r/\lambda) \dots\dots\dots (2.17)$$

Here f is the probability for the electrons to occupy vacancies along dislocation lines. c is the space between two dangling bonds. ϵ is the static dielectric constant. As mentioned previously, λ is the screening parameter, given by $\lambda = (\epsilon k_B T / e^2 n')^{1/2}$. Here n' is the effective screening concentration, involving possibly both free and bound carriers:

$$n' = n + (n + N_A) \left(1 - \frac{n + N_A}{N_D}\right) \dots\dots\dots (2.18)$$

where N_D and N_A are bulk donor and acceptor concentrations, respectively. The Fourier transform of the scattering potential given in Equation (2.18) can be rephrased as [24]:

$$V(\vec{q}) = \frac{f e^2 \lambda^2}{\epsilon c (1 + q^2 \lambda^2)} \dots\dots\dots (2.19)$$

where $q^2 = \left| \vec{k}_\perp' - \vec{k}_\perp \right|^2$. $k_\perp$, the wave vector normal to the dislocation line, is deduced from $E = (\hbar^2 / 2m^*) k_\perp^2$.

The relaxation time for electrons moving perpendicular to a group of parallel dislocations is:

$$\tau_{dis}(k) = \frac{\hbar^3 \epsilon^2 c^2}{f^2 N_{dis} m^* e^4} \frac{(1 + 4 \lambda^2 k_\perp^2)^{3/2}}{\lambda^4} \dots\dots\dots (2.20)$$

The mobility component due to a time relaxation, e.g., from dislocation scattering, can be calculated by energy averaging [25]:

$$\mu_{dis} = \frac{e \langle \tau_{dis} \rangle}{m^*} = \frac{4(k_B T)^{-5/2}}{3\pi^{1/2}} \frac{e}{m^*} \int_0^\infty \tau_{dis} E^{3/2} \exp\left(-\frac{E}{k_B T}\right) dE \dots\dots\dots (2.21)$$

In general, according to Equation (2.20), the dislocation mobility is inversely

proportional to the $f^2 N_{dis}$. Since f depends on N_{dis} through the charge balance, its effect on the mobility goes explicit. In the Chapter 4, the effect will be illustrated graphically.

2.5 Total Mobility

Besides charged dislocation lines, there are various scattering mechanisms in a semiconductor, which can be divided into three categories, they are, consisting of defect scattering, carrier-carrier scattering and lattice scattering. The total average mobility is calculated by considering the main scattering mechanisms in order to get a more precise result [32], [27].

2.5.1 Matthiessen's Rule

When several scattering mechanisms are involved, the mobility is given by $\mu = e \langle \tau \rangle / m^*$, where [23]:

$$\langle \tau \rangle = \left\langle \frac{1}{\tau_1^{-1} + \tau_2^{-1} + \tau_3^{-1} + \dots + \tau_n^{-1}} \right\rangle \dots\dots\dots (2.22)$$

If all the relaxation times are independent of energy, as would be the case with degenerate electrons, then the total relaxation time is given as

$$\tau^{-1} = \tau_1^{-1} + \tau_2^{-1} + \tau_3^{-1} + \dots \tau_n^{-1}$$

Or the total mobility is shown below.

$$\mu^{-1} = \mu_1^{-1} + \mu_2^{-1} + \mu_3^{-1} + \dots \mu_n^{-1} \dots\dots\dots (2.23)$$

Equation (2.23) is known as Matthiessen's rule, a preliminary approach widely

applied in semiconductors with its advent.

Matthiessen's rule is used to calculate the whole mobility. Besides the scattering due to the dislocations, the Matthiessen's rule includes the scattering caused by ionized impurities, polar optical phonon and so on:

$$\mu^{-1} = \mu_{dis}^{-1} + \mu_{ii}^{-1} + \mu_{ni}^{-1} + \mu_{dp}^{-1} + \mu_{pe}^{-1} + \mu_{po}^{-1} \dots\dots\dots (2.24)$$

Several mobility components due to dislocations (μ_{dis}), ionized impurities (μ_{ii}), neutral impurities (μ_{ni}), deformation potential (μ_{dp}), piezoelectric potential (μ_{pe}) and polar optical phonons (μ_{po}) are used for total mobility (μ) calculation. The descriptions of them are explained in detail below.

2.5.2 Ionized Impurities

In the case of ionized impurities scattering, the carrier and the charged impurities interact directly as the Coulombic interaction. Ionized impurities scatter electrons through their screened coulomb potentials:

$$\Delta V = \frac{Ze^2}{4\pi\epsilon r} e^{-r/\lambda_D} \dots\dots\dots (2.25)$$

where Ze is the ionic charge and λ_D the Debye length. In the non-degenerate case, $\lambda_D^2 = \epsilon kT / e^2 n$ for free-electron screening alone. Then:

$$A(q) = \frac{Ze^2}{\epsilon V_c} \frac{1}{a^2 + \lambda_D^{-2}} \dots\dots\dots (2.26)$$

Considering the non-degenerate statistics, we have the expression of mobility for ionized impurities [28]:

$$\mu_{ii} = \frac{128\sqrt{2\pi^{1/2}\epsilon^2(kT)^{3/2}}}{N_I Z^2 e^3 m^{*1/2} [\ln(1+y) - y/(1+y)]} \dots\dots\dots (2.27)$$

where N_I is the ionized impurity concentration and:

$$y = 24\epsilon m^{*1/2} / \hbar^2 e^2 n \dots\dots\dots (2.28)$$

2.5.3 Neutral Impurities

When an electron passes close to a neutral atom, momentum can be transferred through a process in which the free electron exchanges with a bound electron on the atom. Erginsoy [29] has calculated that $\tau_{ni}(\xi) = m^* / 20N_n \hbar a_0$, independent of energy, so that:

$$\mu_{ni} = \frac{e}{20N_n \hbar a_0} = \frac{e^3 m^*}{80\pi N_n \hbar^3 \epsilon} \dots\dots\dots (2.29)$$

where a_0 is the effective Bohr radius of the donor and N_n is the concentration of the neutral impurities.

2.5.4 Acoustic Phonons: Deformation Potential

The acoustic-mode lattice vibrations induce changes in lattice spacing, which results in the bandgap changing from point to point. Since the crystal is deformed at these points, the potential is called the deformation potential. The corresponding relaxation time can be written as [25]:

$$\tau_{dp} = \frac{\pi \hbar^4 \rho s^2}{\sqrt{2} E^2 m^{*3/2} (kT)} \xi^{-1/2} \dots\dots\dots (2.30)$$

where ρ is the crystal density, s is the averaged velocity of sound, and E , the deformation potential is about 9.3 eV [30]. Here $\rho s^2 \equiv c_l$, the longitudinal elastic constant, is about 14.5×10^{10} N/cm² in GaAs.

2.5.5 Acoustic Phonons: Piezoelectric Potential

The atomic displacements produced by the acoustic-mode lattice vibrations introduce a second potential if the atoms are partially ionized. This effect, called the piezoelectric effect, occurs in those crystals without a center of symmetry, which is suitable for all compound semiconductors. A relaxation time can be defined for the piezoelectric-potential mechanism because energy changes during the collisions are small. The relaxation time is [25]:

$$\tau_{pe}(\xi) = \frac{2\sqrt{2}\pi\hbar^2\rho s^2}{(eh_{pz}/\epsilon)^2 m^{*1/2}(kT)} \xi^{-1/2} = \frac{2\sqrt{2}\pi\hbar^2\epsilon}{eP^2 m^{*1/2}(kT)} \xi^{-1/2} \dots\dots\dots (2.31)$$

where h_{pz} is the piezoelectric constant and $P \equiv (h_{pz}^2/\rho s^2 \epsilon)$ is the piezoelectric coupling coefficient. The mobility for the relation time is:

$$\mu_{pe} = \frac{16\sqrt{2}\pi^{1/2}\hbar^2\epsilon}{3eP^2 m^{*3/2}(kT)^{1/2}} \dots\dots\dots (2.32)$$

At 300 K, the piezoelectric-potential scattering rate is about five times smaller than the deformation-potential rate.

2.5.6 Optical Phonons: Polar

The dominant scattering mechanism at 300 K in GaAs is the scattering due to the

dipole moments formed by the interaction of the ionic charges on the atoms with the optical-mode lattice vibrations. This mechanism is called polar optical-mode scattering. Putley [31] writes mobility for the relation time as:

$$\mu_{po} = \frac{2^{9/2} \pi^{1/2} \hbar^2 (kT)^{1/2} (e^{T_{po}/T} - 1) \chi(T_{po}/T)}{3 e(kT_{po}) m^{*3/2} (\epsilon_{\infty}^{-1} - \epsilon^{-1})} \dots\dots\dots (2.33)$$

2.5.7 Total Mobility

As mentioned in section 2.5.1, by applying Matthiessen's rule, the total mobility is calculated by considering the mobility components in different scattering mechanisms.

As mentioned in section 2.5.1, the total mobility is written as:

$$\mu^{-1} = \mu_{dis}^{-1} + \mu_{ii}^{-1} + \mu_{ni}^{-1} + \mu_{dp}^{-1} + \mu_{pe}^{-1} + \mu_{po}^{-1} \dots\dots\dots (2.24)$$

Among these components, in most cases, lattice scattering and ionized-impurity scattering are the dominant mechanisms in GaAs, because μ_{ni} , μ_{dp} , μ_{pe} , and μ_{po} are almost independent on the free carrier concentration, which tends to have negligible effects on the change of the mobility when the free carrier concentration changes. The detailed calculated results are shown in Chapter 4.

Chapter 3 EXPERIMENTAL BACKGROUND AND RESULTS

3.1 Defect Revealing Methods

Threading dislocation density (TDD) characterization is an effective method to evaluate the quality of the material among those defect-engineering approaches. This implies the ability to examine the overall defect morphology on a wafer-scale when sufficient sensitivity and resolution to distinguish individual threading dislocations maintain.

Unfortunately, high resolution inspection typically implies the characterization at a diminished scale. Transmission electron microscope (TEM), for example, is a poor choice of defect revealing method for TDD measurements despite its high resolution and sensitivity adequate to directly image the diffraction in contrast with individual dislocations. The volume of sampled material in a typical TEM sample is so tiny that for TDD on the scale of 10^6 cm^{-2} , it is hard to observe a threading dislocation and the statistical defect relevance is very low.

TDD characterization by etch pit density (EPD) lies in the opposite end comparing to TEM, allowing the wafer-scale characterization. Molten Potassium Hydroxide (KOH), for example, is one of the most commonly used etchants for characterizing the low

TDD for bulk GaAs wafers. However, it has been observed that the size of KOH etch pits themselves can limit the resolution of closely spaced dislocations and such discrepancies between actual TDD and measured EPD increases with the actual TDD [32]. As revealed by Ishida *et al.*, KOH EPD values are essentially useless for the characterization of GaAs/Si with TDD at the order of 10^8 cm^{-2} [33]. Meanwhile, the high temperature (300 °C) required for the molten KOH also restricts the application of this technique.

Besides the methods mentioned above, another method to mix Chromium Oxide (CrO_3), Hydrofluoric (HF) with DI water (H_2O) to form the $\text{CrO}_3\text{--HF--H}_2\text{O}$ solution as an etchant has received much attention. Such method is suitable to reveal the defects on GaAs both with and without light illumination. The etch rate is controlled by the ratio of compositions among CrO_3 , HF and H_2O . Thus, a large variety of etchants with different etch rates can be used to reveal the defects. The ratio of compositions has to be carefully selected in order to achieve an optimal etch rate target.

In this study, HF and CrO_3 are mixed together as basic mixture. The etching solutions were then prepared by diluting the basic mixture with DI water. The notation $D_{1:x}S_{a/b}L$ for these etchants has been adopted [34].

$D_{1:x}$ – dilution of 1 volume part of basic mixture with x volume parts of water;

$S_{a/b}$ – basic mixture consisting of a and b volume parts of HF (48 wt%) and CrO_3

(33 wt%) aqueous solutions, respectively;

L or I – designates that a laser or another source of illumination has been used during etching.

A characteristic feature of this CrO_3 -HF- H_2O system is that neither precipitates are formed during the preparation of the basic $S_{a/b}$ mixtures nor ageing of concentrated or diluted etchants has ever been noticed. The samples were etched without stirring in a Teflon beaker at room temperature.

Surface structures changing with the compositions are obtained after etching and the result is indicated in the ternary diagram as shown below [35].

Figure 3.1 Regions of different surface morphology after etching: (I) etch rate zero, (II) defect revealing action; (III) rough surface; (IIIa) large etch hillocks. Dashed region indicates the recommended range of composition for defect revealing [35].

In the above diagram, lines of constant HF/CrO₃ ratio are drawn, which result from the preparation procedure of different S_{a/b} diluted mixtures. Three main regions can be morphologically distinguished in this diagram.

- (I) no etching was detected;
- (II) defects are seen after removal of 0.5 – 5 μm;
- (III) rough surfaces are produced during etching.

Within region III, the sub-region (IIIa) must be discriminated. In this region, besides micro-roughness, large hillocks are created (macro-roughness) as shown in Figure 3.2. These features are not due to the dislocation as they are randomly distributed among the whole surface.

Figure 3.2 Large hillocks are created because of gas bubbles.

This phenomenon is attributed to the formation of gas bubbles when the HF concentration is very high [36]. These bubbles reduce the etch rate or even block the

etching process, leading to the formation of large hillocks. Bubble formation in these solutions caused rough surfaces, which also hampered the accurate etch depth determination, and also introduced some stirring effects. The bubble formation during etching in these solutions is related to the amount of gases already dissolved in the solution before etching and only occurs in solutions with HF concentration larger than ~ 10 molar. A possible explanation for this phenomenon is that heat is produced in the strongly exothermic reaction of arsine in the etchant, resulting local gas supersaturation and bubble formation. For the status of the surfaces, the recommended region for defect revealing without applying any light illumination is indicated as a dashed field in Figure 3.1, region II. The etch rates at different solution compositions are shown in the figure below [35].

Figure 3.3 Etch rate of (100) Si-doped GaAs as a function of composition of basic mixtures (Sa/b) for different dilution ratios ($D_{1:x}$) [35].

Several concentrations of the etching solutions have been selected in the experiments. Comparing with those in the figure above, the actual etch rates in our experiments are just consistent with the reported etch rates in Figure 3.3.

By considering both the defects reveal abilities and the etch rates, the solution composition $D_{1:1}S_{1/2}$ without illumination is chosen as our etchants. It is in the dashed region shown in Figure 3.1 and the etch rate is moderate. In our study, $D_{1:1}S_{1/2}$ is ideal for shallow defect-revealing of thin epitaxial GaAs layers, while the actual etch rate calculated from experimental data is about $0.766 \mu\text{m}/\text{min}$.

3.2 Design of Experiments

As mentioned previously, from the model the dislocation density can be predicted by measuring Hall mobility and free carrier concentration. In order to verify the calculated results, all the three parameters above have to be measured. The Hall mobility and free carrier concentrations are relatively easier to be obtained. The dislocation density is tallied in the etching process as mentioned in Section 3.1.

In order to have in depth understanding of the correlation between dislocation density and mobility, several samples, each of which has different orders of dislocation densities, are prepared. These samples are GaAs substrate, GaAs homoepitaxy, GaAs/GeSi heterostructure, and some of them are with or without migration enhanced

epitaxy (MEE) process, respectively. MEE is a process that repeats 1 monolayer deposition of Ga atoms followed by deposition of As atoms to conserve a flat epitaxial surface. The process can greatly reduce the anti-phase domain (APD) which is a one type of commonly observed defect for epitaxy of GaAs so as to improve the quality of material.

The schematic diagram in Figure 3.4 shows a structure of the GaAs/GeSi sample. For GeSi/Si material, on the top surface after depositing the $\text{Si}_x\text{Ge}_{1-x}$ buffer layer, the defect density is relatively high. With 200 nm undoped GaAs buffer layer, the defect density will be greatly suppressed to 10^5 cm^{-2} . The thick 1 or 1.5 μm GaAs layer is designed to be n doped with a doping density of about $5 \times 10^{18} \text{ cm}^{-3}$. The actual carrier concentration is obtained through Hall measurement and it varies from sample to sample. The 1 or 1.5 μm thick GaAs layer also increases the accuracy of the Hall measurement results by reducing the background noise from the GaAs undoped layer and SiGe/Si substrate. The bulk residual concentration of the GaAs buffer layer is around $9.632 \times 10^{14} \text{ cm}^{-3}$. Comparing to the top GaAs layer, whose doping density is around $5 \times 10^{18} \text{ cm}^{-3}$, the undoped GaAs buffer layer acts well as semi-insulating layer.

GaAs layer (1 or 1.5 μm) (Si Doped, n-typed)
GaAs Buffer (200 nm) (Undoped)
GeSi/Si Substrate (n-type)

Figure 3.4 The structure of GaAs/GeSi/Si samples.

3.3 Appearances of Different Defects

Different defects such as growth striations, dislocations and microprecipitates can be distinguished even after the removal of 0.5 μm GaAs. However, well resolved etch patterns are produced after deeper etching. These etch features are mainly etch hillocks. The examination results of a large number of GaAs crystals after etching are summarized in the table below. In this table, schematic drawings of the most important types of dislocation-related etch features are shown.

Scheme of geometry of dislocations and the corresponding etch features	Notation	Comments
D-1	Grown-in dislocations with Cottrell atmosphere
D-2	Glide dislocations which are moved by stress exceeding the CRSS (critical resolved shear stress)
D-3	Low-angle grain boundary dislocations after glide-climb re-alignment
D-4	Dislocations within an area of non-uniform distribution of electrically active impurities
D-5	"pure" dislocations with $\langle 101 \rangle$ or $\langle 011 \rangle$ type directions of the dislocation lines
D-6	Threading dislocations in epitaxial layers
D-7	Misfit dislocations in epitaxial layers

Table 1 Most important etch features related to dislocations after etching [37].

The first type of hillocks, marked D-1, are formed during etching on the outcrops of grown-in dislocations in *n*-type GaAs crystals on all low index planes. They are randomly observed in our experiments and are highlight in circles in Figure 3.5.

Figure 3.5 Dislocation-related etch hillocks of D-1 type after etching

The second type of hillocks, marked D-2, are formed on glide dislocations which are induced by stresses during post-growth cooling. By studying the mechanisms of their formation, above two types of dislocations can be distinguished. Firstly, D-1 dislocations can be introduced to the free surface of the crystal and move forming characteristic slip lines. Secondly, some of the grown-in D-1 dislocations move when the critical-resolved shear stress for dislocations is exceeded. However, both D-1 and D-2 types of dislocations do not have as significant impact to the mobility as threading dislocation does.

D-3, D-4 and D-5 types of hillocks are mainly observed on semi-insulating (SI) GaAs. Since our material is highly *n*-doped, these three types of hillocks are very much

minimized. D-6 and D-7 types of hillocks are caused by threading dislocation and misfit dislocation, respectively. D-6 type of the dislocation has the most significant impact on the mobility. Their densities vary with the different structures, i.e. GaAs bulk material and GaAs/GeSi heterostructure. D-6 type of dislocations is greatly eliminated by applying the 6 degree offcut during growth, which helps to improve the material's quality. They are pointed out in circles as shown in Figure 3.6(a) and Figure 3.6(b).

Figure 3.6 a) Etch hillocks of D-6 type after etching on GaAs; b) Etch hillocks of D-6 type after etching on SiGe/Si substrate.

For GaAs substrate, few D-6 and D-7 types of dislocations, which are the threading dislocation and misfit dislocations, are observed after etching. However, in the GaAs/GeSi/Si system, D-6 and D-7 are the most commonly observed types of dislocations. The existence of misfit dislocations helps release the stress. Misfit dislocation tends to have minor effect on the material's electrical properties.

Threading dislocations have a greater effect, for they affect the properties of material such as mobility and PL intensity. The ways to etch can differentiate these two types of effects. The threading dislocations are revealed after a shallow etching, while the misfit dislocations can only be observed after deeper etching.

The measured Hall mobility, dislocation density and their free carrier concentration (doping) are listed in the Table below.

Sample	Hall Mobility (cm ² /Vs)	Dislocation Density (cm ⁻²)	Doping (cm ⁻³)
A: GaAs Substrate	~3400	<5000	~5x10 ¹⁸
B: GaAs Substrate	~3300	<8000	~5x10 ¹⁸
C: GaAs Substrate	~3100	<10000	~5x10 ¹⁸
D: GaAs Substrate (Mechanical Graded)	~1920	~2x10 ⁵	~5x10 ¹⁸
E: GaAs Homoepitaxy	~1020	~8x10 ⁵	~3.4x10 ¹⁸
F: GaAs on SiGe with MEE	~972	~2x10 ⁶	~8.9x10 ¹⁸
G: GaAs on SiGe with MEE	~540	~3x10 ⁶	~5.4x10 ¹⁸
H: GaAs on SiGe without MEE	~64	~2x10 ⁷	~5x10 ¹⁸

Table 2 Hall mobility and dislocation densities of all the samples prepared.

As the dislocations are not evenly distributed on the whole surface, especially for the GaAs substrate, several photos are taken at different areas of every sample in order to obtain an average value. The variation of the dislocation density is shown as the error bar in next chapter.

Chapter 4 RESULTS AND DISCUSSION

All the necessary parameters such as fraction filling factor, space-charged cylindrical radius and mobility etc, have been calculated using the equations listed in Chapter 2. In this chapter, these results will be tabulated and presented formally and systematically. Several samples mentioned in Chapter 3 have been prepared so that enough experimental data has been collected. In order to verify the model, these recorded data, associated with calculated results are plotted in the same graph to exploit the feasibility.

4.1 Fraction Filling Factor

As described in previous chapter, the fraction filling factor is also one of the most important parameters contributing to the finding. It can be, extensively, used to calculate the mobility component due to the dislocations and describe how much the dislocation lines are negatively charged. As defined in Equation (2.14) and (2.15), the fraction filling factor, f , is a function of E_s . Together with expression of E_s from Equation (2.12) and the charge balance equation $N_D = n + N_A + f \cdot (N_{dis} / c)$, the values of f are calculated through averaging all the electrons' distribution in the dislocations, as illustrated in Figure 4.1.

Since every calculated result on different GaAs platform is very similar to each other, only the f value of Si doped n -type GaAs substrate is chosen for illustration. The

doping level N_D set to be $5 \times 10^{18} \text{ cm}^{-3}$, close to the actual doping density of the GaAs substrates ($\sim 5 \times 10^{18} \text{ cm}^{-3}$ from the substrates' specifications) in usage. It is purposely chosen for further comparison as it is the designed doping density for all the samples ranging from $3.4 \times 10^{18} \text{ cm}^{-3}$ to $8.9 \times 10^{18} \text{ cm}^{-3}$.

The unintentional doping N_A is assumed to be zero. The none zero N_A will compensate the N_D , thus the free carrier concentration in the material will be reduced accordingly. In Hall measurement, only the free carrier concentration is measured and this free carrier concentration is resulted from the combination of N_D and N_A . As our consideration is based on the relationship between mobility and free carrier concentration (rather than N_D and N_A) under different dislocation density, the change of N_A does not have direct impact on the curve. However, if in plot mobility is against N_D , the original curve for mobility component in dislocation will be shifted down and the total mobility will be affected accordingly by the unintentional doping N_A . This effect enlightens the clue for further research. Meanwhile, because the material used in the experiment is heavily n -doped, in most cases, the concentration of unintentional doping N_A is insignificant, compared with that of the n -type dopant. Further study to evaluate the impact of different N_A and N_D ratio on mobility is meaningful. The fraction filling factors are calculated under the assumption that the value of dislocation density is $1 \times 10^6 \text{ cm}^{-2}$.

As shown in Figure 4.1, the probability of occupying the dislocation acceptor centers

(sites) increases while the free carrier concentration increases. However, at high free carrier density zone, i.e. $n > 10^{19} \text{ cm}^{-3}$, f value reaches its maximum and maintains at one, indicating that nearly all the dislocation sites are filled by electrons.

Figure 4.1 Fractional filling of electrons versus free carrier concentration.

As mentioned earlier, in all the calculations, the fraction filling factor curves do not significantly varies with dislocation density changes for the experiment samples, where the dislocation density is not high. When the material is highly n -doped, the free carrier concentration is very high too. Thus, although a small number of electrons are captured by the dislocations, they are insignificant when compared with the total population of electrons. However, small changes of the curves are still found when free carrier concentration is lower, i.e. at $n \sim 10^{15} \text{ cm}^{-3}$. Since the doping concentration of the GaAs samples are purposely set to be more than 10^{18} cm^{-3} , these small changes are out of the region we are interested in.

Take note that high dislocation density does have impact on the f curve when the dislocation density is high. It is testified that when the dislocation density is about 10^9 cm^{-2} , the electrical properties of the GaAs samples will be very poor, in other words, it has very low mobility. When the dislocation density increases to about 10^{10} cm^{-2} , the shapes of the curves are distorted. Such high density of dislocations is able to capture almost all the free electrons and affect the filling factor. To establish the correlation between mobility and dislocation density, the transition region of mobility from high to low is required to be focused. The region where the dislocation density rises to an extremely high extent is not necessary to be taken into consideration.

4.2 Free Carrier Concentration and Dislocation Density

Based on the acceptor's nature of dislocations, the relationship between free electron concentration and the doping concentration previously obtained is not applicable, although it is generally useful in evaluating defect free materials. It shows a mixed dependency on the dislocation density as well. As is mentioned in Chapter 2, the free electron concentration is given from the electrostatic energy by taking into account the charge balance equation.

The established relationship, $N_D = n + N_A + f \cdot (N_{dis} / c)$, between the free electron concentration and dislocation density under different doping densities, calculated when the fraction filling factor is considered, is presented in Figure 4.2. The doping

density values in each of four curves are $5 \times 10^{18} \text{ cm}^{-3}$, $1 \times 10^{18} \text{ cm}^{-3}$, $5 \times 10^{17} \text{ cm}^{-3}$ and $1 \times 10^{17} \text{ cm}^{-3}$ respectively. The acceptor density is assumed to be zero as it only compensates the N_D concentration and shifts the curve and does not change its shape.

Figure 4.2 Free Carrier Concentration as function of dislocation density for four different donor concentrations calculated from the charge balance equation.

As is shown in Figure 4.2, when the dislocation concentrations are relatively low, the values of the free carriers almost do not depend on the dislocations, assuming all the donors are ionized. However, increase of dislocation density drains more and more carriers from the conduction band until there is a sudden drop in the free carrier concentration. When the dislocation density increases further, most of free electrons will be trapped by the dislocations so the conductivity of the sample is very low. In

such case, the mobility of the material greatly depends on the dislocation density, especially when the dislocation density is high enough to capture most of the free electrons.

The above behavior can be understood from the charge balance equation $N_D = n + N_A + f \cdot (N_{dis} / c)$ mentioned in Chapter 2. When the dislocation density (N_{ds}) is low, the value of $f \cdot (N_{dis} / c)$ is much smaller than N_D . In order to achieve charge balance, nearly all the electrons provided by donors are free carriers (N_A is assumed to be negligible). So we have $N_D \approx n$. Meanwhile, the value of $f \cdot (N_{dis} / c)$ component increases due to the increase of dislocation density. When the dislocation density is so high that the value of $f \cdot (N_{dis} / c)$ becomes comparable to N_D , nearly all the free electrons that are generated by donors are captured by the acceptor centers of dislocation. Thus, the decrease of the free electrons density leads to a sudden drop of free carrier concentration in the curve, while N_A is not taken into consideration here. With the presence of N_A , the electrons provided by the donors are captured by the acceptors, leading to a downward shift of the curve without significantly changing the shape of the curve.

4.3 Space-charged Cylindrical Radius

As mentioned in Chapter 2, when the sites in a dislocation attract electrons, the dislocation becomes negatively charged. In order to neutralize this negatively charged

line, a cylindrical positively space-charged region is formed. As is assumed in Chapter 2, this positively space-charged region has sharp boundary and it can be treated as a cylinder with radius R .

Not only f , but also the radius of the positively charge region (R) varies with n . R , which is a function of n in the charge balance equation, decreases when the free carrier concentration increases. From Equation (2.3), it is determined by $R = [f / (\pi N_D c)]^{1/2}$. With the f values obtained previously, the radius R versus n can then be calculated. R decreases when the free carrier concentration increases. The results are shown in Figure 4.3.

Figure 4.3 Space-charged cylindrical radius R , as a function of free carrier concentration n , for an isolated dislocation in GaAs.

As shown above, the radius of the space-charged cylinder R decreases from 0.155 μm

at free carrier concentration $n=1 \times 10^{16} \text{ cm}^{-3}$ to $0.005 \text{ } \mu\text{m}$ at $n=1 \times 10^{19} \text{ cm}^{-3}$. As mentioned in Chapter 2, the positively space-charged regions have similar behavior like the depletion regions, since the electron-hole recombination is prohibited in these regions. When free carrier concentration increases, the density of the electrons increases too. To balance the charge, the decrease of the volume of the depletion region makes the radius R decrease as well.

As mentioned in the previous chapter, the dislocations are assumed to be parallel to one another with enough spacing between the lines. So the volume of these depletion regions can be calculated by multiplying the cross sectional area with the dislocation density. It is assumed that the electrons can only penetrate a negligible depth in the positively space-charged region. In such case, these cylindrical positively space-charged regions will become scattering centers and block the movement of electrons. Increasing volume of the space-charged region causes the chance of electrons being scattered to increase as well. In these positively space-charged regions, the electrons are easily scattered and their mobilities are greatly reduced. It helps to explain the phenomenon that the mobility decreases with the increase in dislocations.

4.4 Mobility Due to Dislocations

Using the equations provided in Chapter 2, after the fractional filling factor, f , is calculated, the mobility component due to dislocation can be obtained. The calculated result by applying Equation (2.21) is shown in the figure below.

Figure 4.4 Mobility component due to the scattering effect of dislocations only.

In Figure 4.4, the numerically calculated mobility component due to the scattering effect of the dislocations is shown as a function of the free electron concentration. In general, according to Equation (2.20), the relaxation time directly linked to dislocation density is inversely proportional to $f^2 N_{dis}$. Since value of f depends on N_{dis} through the charge balance equation, the effect on the mobility is unnoticeable unless the value of f was rightly extracted from Figure 4.1 and substituted into Equation (2.21). Explicitly, Figure 4.4 clearly shows that the mobility component due to dislocations increases when dislocations decrease and increases linearly for a given dislocation density when free carrier concentration increase.

As shown above, the value of the mobility component due to dislocations becomes larger than $10^4 \text{ cm}^2/\text{Vs}$ when the dislocation density is relatively lower, i.e. $\sim 10^4 \text{ cm}^{-2}$. However, the actual values of the mobility from Hall measurement for GaAs at room temperature are less than $3000 \text{ cm}^2/\text{Vs}$, i.e. $\sim 3000 \text{ cm}^2/\text{Vs}$ for GaAs substrate, $\sim 1000 \text{ cm}^2/\text{Vs}$ for GaAs on GaAs homoepitaxy or $\sim 1000 \text{ cm}^2/\text{Vs}$ for GaAs on Ge heterostructure respectively. This phenomenon can be explained by Matthiessen's rule. At room temperature, some other mobility components whose values are close to the Hall mobility also have a contribution. When the dislocation density is lower than 10^5 cm^{-2} , the value of the mobility component due to dislocation is much higher than the actual measured value and its reciprocal is much smaller than the reciprocal of the actual value. In this case the reciprocal of the mobility component due to dislocation will play little part in the value of the sum when all the reciprocals are added to calculate the total mobility.

4.5 Total Mobility

Other scattering mechanisms, i.e. ionized impurities, acoustic phonons (deformation and piezoelectric), and polar optical phonons are studied to calculate the total mobility term. All the components (μ_{dis} , μ_{ii} , μ_{dp} , μ_{pe} , μ_{po}) should be calculated out to obtain the value of the total mobility by Matthiessen's rule [25]. The total mobility under different dislocation conditions is shown in Figure 4.5.

Figure 4.5 The calculated average transverse room-temp mobility from Equation (2.24).

As shown in Figure 4.5, when the dislocation density is less than 10^5 cm^{-2} , the mobility tends to saturate at around $3000 \text{ cm}^2/\text{Vs}$ when the free carrier concentration increases to be larger than 10^{19} cm^{-3} . At lower carrier concentration, scattering effect due to dislocations is significant, so the total mobility tends to increase first. With further increase of free carrier concentration, the mobility component caused by scattering of impurities becomes dominant and helps stabilize the curve at around $3000 \text{ cm}^2/\text{Vs}$.

When the dislocation density is low (less than 10^5 cm^{-2}), the contribution of the scattering effect due to dislocations to the total mobility is insignificant and it behaves in the similar manner as the dislocation free materials. As is shown in Figure 4.4, the mobility component caused by dislocation is much higher than the actual mobility value, meaning that its effect on the total mobility under Matthiessen's rule is negligible. When the dislocation density is very high in material, according to previous calculated results, the mobility due to dislocations is much lower compared with the mobility components from all other scattering terms. By Matthiessen's rule, mobility due to dislocation becomes the dominant factor that determines the quality of the material.

4.6 Mobility Change due to Temperature Variation

It is well known that the temperature variation is a key factor to change materials' electrical properties, i.e. mobility, free carrier concentration, etc. Whenever the temperature varies, so does mobility. The mobility change due to temperature variation is also taken into consideration in this research. The total mobility is calculated under different temperatures and shown below.

Figure 4.6 shows the temperature dependence of the mobility at different dislocation densities. Here, values of $1 \times 10^5 \text{ cm}^{-2}$, $1 \times 10^6 \text{ cm}^{-2}$ and $1 \times 10^7 \text{ cm}^{-2}$, are selected for the dislocation density. For each dislocation density, the mobility contribution due to

scattering mechanism at dislocation lines and the overall mobility are calculated and plotted in the graph.

Figure 4.6 Changes of mobility as function of temperature.

At extremely low temperature, the overall mobility only depends on the mobility component due to dislocation. The reason is that all other mechanisms are greatly suppressed under extremely low temperature condition while dislocation mobility does not change so significantly. Thus it becomes a dominant factor. The mobility components due to scattering at dislocation lines remain almost unchanged for the

whole range of the temperature variation. They are much less temperature-dependent than scattering of ionized impurities, phonons and other factors.

When the temperature increases to approximate 300 K, the dislocation density becomes one of main factors affecting the mobility. When dislocation density is low, i.e. $\sim 10^5 \text{ cm}^{-2}$, the overall mobility is dominated by other scattering mechanisms such as lattice scattering and ionized-impurity scattering. The contribution to the overall mobility by dislocation is insignificant. If the dislocation density increases to 10^6 cm^{-2} , the contribution to the overall mobility term caused by dislocation lines becomes significant. When dislocation density increases further ($N_{dis} > 10^7 \text{ cm}^{-2}$), the dislocation scattering becomes a dominant mechanism compared to other scattering mechanisms. As shown in Figure 4.6, the overall mobility almost remains the same because the mobility component due to dislocations does not change when the temperature varies.

4.7 Overall Experimental Verifications

To verify the model and the calculated results, the experimental results were analyzed. Several GaAs samples in different structures are prepared as shown in Table 2. The Hall mobility, free carrier concentration and the most important, the dislocation density are measured on these samples. The experimental data found to agree well with the calculated results from Equation (2.24) as shown in Figure 4.7 below.

Figure 4.7 Verifications of the overall results at 300 K.

For comparison, all the samples are purposely fabricated with doping densities around $5 \times 10^{18} \text{ cm}^{-3}$. With a fixed doping density, the comparison on how the dislocation density affects the mobility becomes easier. Although all the samples are prepared with care, the actual doping densities vary from $3.4 \times 10^{18} \text{ cm}^{-3}$ to $8.9 \times 10^{18} \text{ cm}^{-3}$.

(detailed values refer to Table 2) In order to verify the process more precisely, besides the calculated results obtained when N_D is at $5 \times 10^{18} \text{ cm}^{-3}$, two auxiliary lines as boundaries are also plotted when N_D are set to be $3 \times 10^{18} \text{ cm}^{-3}$ and $8 \times 10^{18} \text{ cm}^{-3}$ respectively. The purpose of sketching these two lines is not only to draw boundaries, so that almost all the data are within this range, but also to examine the sensitivity and accuracy of the model.

In Figure 4.7, samples A to D are GaAs substrates. Samples A, B and C have very good quality and high mobility. For all the three samples, their dislocation densities are lower than 10^4 cm^{-2} . These values are provided by the substrate suppliers rather than from actual Hall measurement. In the region around their mobility values (in Figure 4.7), the dislocations do not have much impact on the overall mobility. The mobility, which is mainly affected by other factors, changes little at this region. No matter how the dislocation density varies, it does not affect the actual mobility.

Sample D is a mechanical grade substrate. Therefore its material quality is not as good as that of samples A to C. As shown in the Figure 4.7, its worse material quality leads to lower mobility, with a value around $2000 \text{ cm}^2/\text{Vs}$ only. This mobility value is from Hall measurement while the dislocation density is from the suppliers. The slightly higher dislocation density of sample D causes poorer mobility compared with samples A to C. Sample E to H are all prepared using the MBE chamber. Sample E has a GaAs

on GaAs homoepitaxy structure, and its mobility is around $1000 \text{ cm}^2/\text{Vs}$. Samples F and G were fabricated by the MEE process and have same GaAs/GeSi heterostructures. These three samples have moderate dislocation densities. This point is helpful to verify the model because their values are sitting at the transition range of the curve. The calculated values of mobility as a function of actual doping density for sample F and G show a good fit to the measured data. The measured data also fall between the two boundary conditions with the same trend. Sample D to Sample G are the most important four samples in this research as their mobility values fall into the transition region of the mobility curve. When the dislocation density increases, the mobility value decreases from $\sim 2000 \text{ cm}^2/\text{Vs}$ to $\sim 500 \text{ cm}^2/\text{Vs}$. The excellent match between the experimental data and calculated results suggests a clear relationship between the dislocation density and the mobility, which enables the prediction of dislocation density.

Sample H has a GaAs on SiGe heterostructure grown without the MEE process. Its defect density is much higher and is around 10^7 cm^{-2} . These dislocations greatly affect the electrical properties of the sample and cause a low mobility, which is less than $100 \text{ cm}^2/\text{Vs}$ by measurement. Obviously for Sample H the dislocation scattering becomes a dominant factor. Meanwhile, the further increase in the dislocation density does not have much effect on the quality of material. The tail of the curve becomes flat since the mobility value is close to zero.

As shown in Figure 4.7, the experimental data agree well with the calculated result. This indicates that the model proposed in this work is robust to predict the dislocation density from the measured Hall mobility and the free carrier concentration data. Although a precise value of the dislocation density is barely to be obtained, this model provides a reasonable way to estimate the sample quality without tedious experiments incurred.

4.8 Discussion

Read's model is somehow limited in the calculations as in this model other factors exist and affect the final result, so it is needed to be further exploited. The way to improve the model will be discussed in detail. Read's model has been used to describe the Hall Effect data at room temperature. In Read's model, for germanium at low temperature, the free energy is minimized without considering the entropy term. This assumption overestimates the effect of free energy, reduces the probability of the occupation occurred. From a theoretical point of view, an accurate result at elevated temperatures should be obtained as expected, when the entropy term is taken into account.

In Read's study [10], the drift mobility was calculated by using Matthiessen's rule and compared with the experimental Hall mobility data. The mobility from dislocation and ionized impurity scattering was combined with a constant background mobility

component, which value is $450 \text{ cm}^2/\text{Vs}$. This value is a fitting parameter used to fit his experimental result. However, no further information and explanation about this value was provided. Other scattering mechanisms and the unintentional acceptors are not taken into account in the calculation, which affects the accuracy of the model. In this research, although the Hall mobility was calculated using Matthiessen's rule and compared with experimental results in the Figure 4.6 as before, no fitting parameter was used in this calculation. Detailed calculations were constructed on the basis of the relationships among dislocation density, free carrier concentration and Hall mobility.

When calculating the total mobility, there are a few things one should take note of. Experimental Hall mobility and scattering time are related by $\mu_H = (\langle \tau^2 \rangle / \langle \tau \rangle^2) (e \langle \tau \rangle m) = r \mu_D$, where r is the Hall factor and μ_D is the drift mobility. Therefore, using the drift mobility to describe the experimental data may cause an error up to 70% in some materials [22]. In this research, the value of Hall factor r is always close to one, which greatly reduces its impact and improves the accuracy of this calculation.

Matthiessen's rule is a common method used to calculate the mobility. Although the concept of calculation based on Matthiessen's rule is commonly accepted, using this method can double the deviation of error of the mobility if Matthiessen's rule is not properly applied [22]. This rule could produce accurate mobility values if the relaxation times would be independent on energy. However, in reality all scattering

rates are functions of energy, E . So by applying Matthiessen's rule, the accuracy of this calculation is inevitably affected. In order to overcome this drawback, energy averaging is a good method worthy to improve the accuracy of the simulated results. In this research, the results given by Matthiessen's rule are good enough to predict the dislocation density, as they are verified in this chapter.

What is more, some conditions have been assumed to be ideal to carry out the calculation in Chapter 2. Firstly, only electrons moving normal to the negatively charged dislocation lines are taken into account. It greatly simplifies the calculation as it turns a 3-D problem to 2-D one. However, in reality, there is also a velocity component parallel to the dislocation line, which has a very little impact on the mobility component due to the dislocation. Meanwhile, the unintentional acceptors are out of scope because of the nature of high n -type doping. They do not affect the accuracy of the calculation in this work unless their values are close to the n doping density. As recommended, it is worthy to be included in future research.

Furthermore, for the derivation of the free energy of the dislocation lines, the spaced electrons along the lines are assumed to be distributed evenly, which is also an idealized approximation as compared with the real situation. It can happen only when the temperature is at absolute zero. Moreover, the interactions among the electrons in dislocations are neglected in this report in order to simplify the model. This assumption is reasonable and logically sounded as the spacing between two

dislocations is big enough so the interaction is negligible. This is justified when the dislocation density is relatively low. However, when the dislocation density increases, the impact from the interactions becomes more and more significant. Because the dislocation density of the greatest concerned is around 10^5 cm^{-2} , the assumption is provided to be valid in this range. The dislocations are treated as straight parallel lines in the material in the model as previously mentioned in Chapter 2. Here, no cross-over of lines are allowed in the materials, which reduces the complexity when the impact of the positively space-charged region is considerable.

Chapter 5 SUMMARY AND FUTURE WORK

5.1 Summary

In this thesis, the relationships among the dislocation density, mobility and free carrier concentration have been developed for the GaAs/GeSi/Si heterostructures based on the Read's model. An in-depth understanding of the mechanism of dislocations has been obtained which built up the theory. The calculated results were verified with the experimental data collected.

Read's model has been introduced in details in the beginning. He treated the dislocations as negatively charged lines surrounded by a positively space-charged region. From his model, the most important parameter namely the fraction filling factor f is calculated. Meanwhile, the radius of the cylindrical space-charged region is obtained as the function of free carrier concentrations.

The incorporation of Read's model and scattering mechanism gives the freedom to predict the dislocation density by measuring the Hall mobility of the samples. Not only mobility component due to the scattering at dislocation lines is calculated, but also other scattering mechanisms are introduced and Matthiessen's rule is applied in order to obtain the total mobility. Last but not the least, the mobility variation with

temperature change is calculated.

Hall mobility and free carrier concentration are obtained experimentally through Hall effects measurement. Several samples are etched using the diluted HF – CrO₃ solution, a more accurate new etch process, in order to reveal the dislocation density by counting the number of the etch hillocks. These samples include GaAs substrates, GaAs homoepitaxy and GaAs/GeSi heterostructures with and without MEE process.

The model shows an excellent consistency between the experimental data and the calculated results. The objective of this project is fulfilled and the dislocation density can be predicted using the correct Hall mobility and free carrier concentration.

5.2 Future Work

Although success has been achieved, in the establishment of the most important relationships among dislocation density, free carrier concentration and Hall mobility, there are still some assumptions in the model which limit its application range. In my model, the unintentional acceptor concentration is treated as zero. It is worthy to explore the model from the view of donor to acceptor ratio. Secondly, all the dislocations are treated as straight lines, one parallel to one another with enough spacing between two lines. Last but not least, the interactions among dislocations are

not considered. Further study on the above can be expected to increase the accuracy and extend the application range of the model.

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