Chapter 1: Introduction
1.1 Basic Device in Electronic Engineering

The metal oxide semiconductor field effect transistor (MOSFET) is the most fundamental unit in micro process. Fig 1.1 shows a simplified MOSFET, in which terminals as S for source, G for gate, D for drain and B for body (more usually sub for substrate instead of B) exist. B is often ignored in a simplified model. Such terminals are for different voltage to apply. Difference of the voltage cause a meaningful current change in this structure for use in electronic engineering. Concretely, when a sufficiently large voltage is applied to the gate, a channel for carriers in the pink area in Fig 1.1 is formed, which means that the voltage difference between the ends of this channel can flow the current in this channel.

What must be paid attention in this structure is that, semiconductor material is used in pink area in Fig 1.1. Therefore, for obtaining relatively large carrier concentration in these semiconductor area, doping of impurities in always used in semiconductor manufacturing. As activation rate decreases in high doping density, larger carrier concentration is difficult to obtain in high doping density.

As known, the electrical resistivity can be written as

\[ \rho = \frac{1}{q n \mu} \]  \hspace{1cm} (1.1)

\( q \) is the charge on the particle; \( n \) is the majority carrier density; \( \mu \) is the mobility of the carrier.

From (1.1), we know that the resistivity can be reduced by increasing the carrier
density, so a large carrier concentration is fatal in some electronic device.

Compared to MOSFET, heterojunction field effect transistors (HFETs) develop a channel by a junction between two materials with different band gaps. In such a device, the two kinds of materials form a heterojunction for carrier channel, rather than a doped semiconductor for carrier channel. The materials to form heterojunction are usually compound semiconductor materials rather than Group-IV simple semiconductor. As undoped material in used here, theoretically a higher mobility and concentration can be obtained than MOSFET.

As shown in Fig 1.2 and Fig 1.3, the difference of the band of the spacer and the substrate leads to a quantum well, an uncontinuous area of the band. The quantum well leads to an area where the Fermi level is higher than the edge of conduction band. This develops the two dimensional electron gas (2DEG).
1.2 Gallium Nitride

As mentioned above, materials to form heterojunction in HFET are usually compound semiconductor materials, in which III-V components are commonly used. GaAs, GaAlAs are firstly used, and then In-compounds are researched for their high frequency properties.

Gallium nitride (Molecular formula: GaN) is a kind of III-V component and has been being used in semiconductor industry since the 1990s, especially LED.

Gallium nitride has a Wurtzite crystal structure. Wurtzite crystal structure is an example of hexagonal crystal system, and often refered as the structure of zinc sulfide (ZnS). The structure of gallium nitride is shown in Fig 1.4. [1]
shown in Table 1.1. [2]

<table>
<thead>
<tr>
<th></th>
<th>Si</th>
<th>GaAs</th>
<th>4H-SiC</th>
<th>GaN</th>
</tr>
</thead>
<tbody>
<tr>
<td>Band Gap [eV]</td>
<td>1.1</td>
<td>1.4</td>
<td>3.3</td>
<td>3.4</td>
</tr>
<tr>
<td>Breakdown Voltage [MV/cm]</td>
<td>0.3</td>
<td>0.4</td>
<td>3.0</td>
<td>3.3</td>
</tr>
<tr>
<td>Saturated Electron Velocity [10^7 cm/s]</td>
<td>1.0</td>
<td>2.0</td>
<td>2.0</td>
<td>2.5</td>
</tr>
<tr>
<td>Electron Mobility [cm^2/Vs]</td>
<td>1500</td>
<td>8500</td>
<td>1000</td>
<td>1200</td>
</tr>
<tr>
<td>Hole Mobility [cm^2/Vs]</td>
<td>600</td>
<td>400</td>
<td>115</td>
<td>~10</td>
</tr>
<tr>
<td>Coefficient of Thermal Conductivity [W/cmK]</td>
<td>1.5</td>
<td>0.5</td>
<td>4.9</td>
<td>2.1</td>
</tr>
</tbody>
</table>

As shown in Table 1.1, the band gap of gallium nitride, which is nearly equal to that of silicon carbide, is 3 times as silicon. On-resistance of gallium nitride device is thought one third of silicon device, for the breakdown voltage of gallium nitride is 3 times higher than silicon.

Compared to silicon carbide, a great advantage of gallium nitride is, that GaN has relatively large discontinuity in bandgap with materials such as AlGaN, so it can be used to form good heterojunction structure.

### 1.3 2-Dimensional Hole Gas (2DHG)

The electrical characters of HFETs with two dimensional electron gas (2DEG) have been reported in several articles. It is reported that high density 2DEG can be obtained by using positive polarization charges at the AlGaN/GaN interface. Therefore, the 2DEG mobility is as high as 1000 cm^2/Vs, so it is treated as important candidate for next generation power device.

Similar with 2DEG, two dimensional hole gas (2DHG) has been predicted in several articles, but reports in which 2DHG is observed are few. According to the prediction, 2DHG should have properties as high mobility and high density.

According to A. Özgür et al, using positive polarization charges at the AlGaN/GaN interface leads to high density 2DEG with the densities over 10^{13} cm^{-2} can be obtained. [3,4] In this research, a sheet carrier density of AlGaN/GaN interface of about 1.8 × 10^{13} cm^{-2} at room temperature has been confirmed.

### 1.4 Background of Energy Saving Devices
According to the survey of R&D Association for Future Electron Devices (FED) in Japan, 57% of total energy consumption in Japan, 573 billion kWh is used for devices in motors. Therefore, they also gave prediction, that the number would be 396 kWh if energy saving device was widely used. (Fig 1.5)

Thus, to decrease the energy consumption in motors is treated fatal to the human society. In order to realize this, HFET is regarded as promising candidate for its high breakdown voltage as a property of compound semiconductor material, especially GaN can be used for drivers in transverse power device.

Fig 1.5 Flow chart of electronic motor system

Fig 1.5 shows a simple flow chart of electronic motor system. The right down area in shallow blue colour is what often called driver, which is controlling the whole system. In traditional motor system, all of the electronic device are made of silicon material. To overcome the lower breakdown voltage of silicon material, GaN is gradually used in such devices instead of silicon, which is shown in Table 1.2.
### Table 1.2 Materials used in motor system

<table>
<thead>
<tr>
<th></th>
<th>Power device</th>
<th>Driver</th>
<th>Logic</th>
</tr>
</thead>
<tbody>
<tr>
<td>Discrete</td>
<td>Si IGBT</td>
<td>Si DMOS</td>
<td>Si CMOS</td>
</tr>
<tr>
<td></td>
<td></td>
<td>+ Si CMOS</td>
<td></td>
</tr>
<tr>
<td>Hybrid IC</td>
<td>GaN HEMT</td>
<td>Si DMOS</td>
<td>Si CMOS</td>
</tr>
<tr>
<td></td>
<td></td>
<td>+ Si CMOS</td>
<td></td>
</tr>
<tr>
<td>Monolithic IC</td>
<td>GaN HEMT</td>
<td>GaN CMOS</td>
<td>Si CMOS</td>
</tr>
</tbody>
</table>

In discrete semiconductor system, all parts of the system is made of silicon, but in hybrid IC system, power device is changed by GaN HEMT. In monolithic IC system in the future, it is promised that driver part will be changed by GaN CMOS devices.

Possible structures to realize GaN CMOS have been reported. One of them is shown as Fig 1.6, a device using both n-ch and p-ch by same materials. [5]

![Fig 1.6 A possible structure for GaN CMOS device](image)

The advantages of this device is apparent: firstly, the low resistance of GaN- transverse device leads to low consumption of the whole system, even in multistage circuits. Then, assumption of the system into one chip decrease of wiring among chips. Finally, assumption to one chip leads to a high efficiency including the high efficiency in manufacturing process, which will contribute to the energy saving.

By combining p-ch and n-ch GaN device as shown in Fig 1.7, assumption to on chip is predicted to be realized in future.
1.5 Piezopolarization in Heterostructure

Piezoelectricity is a physical phenomenon discovered in 18th century, referred to electrical charge in response to the physically mechanical pressure. The reason of this phenomenon can be attributable to the electric dipole in molecular structure. Mechanical stress in particular materials will break the total balance of electric dipole in the material.

Based on the same idea, a method to cause changes in electric dipole in manufacturing of heterostructure has been discovered. This phenomenon, which is usually called piezopolarization, shows a possibility of deepen the concentration of carriers in undoped semiconductor heterostructure.

1.6 Monte Carlo Method

Monte Carlo method is a calculation method in which random numbers are used in order to solve physical and mathematical problems, especially in the field of optimization, numerical integration and generation of draws from a probability distribution. This method is discovered to solve problems of physical phenomenon with inner random variables.

In the field of carrier movement, Monte Carlo method is useful on account of the uncertainty of carrier movement. Under modern theory of micro particle, it is difficult to know an exact state of a micro particle, which we call uncertainty.

Uncertainty of particles shows impossibility of calculating movement of particle by traditional methods, but it also shows utility of Monte Carlo method. In Monte Carlo
methods, we can give random states to a certain particle, and then giving random states again and again. The energy conservation must be considered and by this we can obtain several data about the movement states of the partial, and then use these data to calculate the characteristics of whole device.

The details of Monte Carlos used in device simulation field will be described later, here a simple example will be shown for Monte Carlo simulation used for the calculation of mathematical constant $\pi$.

Consider a 1×1 square shown as Fig 1.8, a pie (1/4 of a unit circle) which radius is 1 is inside of this square. The area of the square should be 1×1=1, and the area of the pie should be $\pi\times 1^2 \times 1/4 = \pi/4$. The ration of the two areas should be $\pi/4$.

![Fig 1.8 A model for calculation of Pi](image)

Now we try to approximate the numerical value of $\pi$ by placing points randomly in this square. Therefore, we can judge whether the point is in or outside the circle by calculating the distance of the points and the origin point and comparing it with the radius 1.

For instance, if point (0.5, 0.5) is placed in this square, and the distance of (0.5, 0.5) and the origin $O$, $\sqrt{0.5^2 + 0.5^2} = \sqrt{2}/2 < 1$, so the point (0.5, 0.5) is inside the circle.

Also, if point (0.75, 0.75) is placed in this square, and the distance of (0.5, 0.5) and the origin $O$, $\sqrt{0.75^2 + 0.75^2} = 3\sqrt{2}/4 > 1$, so the point (0.75, 0.75) is outside the circle. The two points, which are coloured red and blue, are shown in Fig1.9.
Fig 1.9 Judgment of the points inside or outside

By the way described above, we can place numerous random points in this square and then calculate the ration of number of points inside and whole points. After placing enough points, an approximated value of Pi can be obtained. (Fig 1.10)

The ratio of the number of the points inside the circle, which are coloured red, and the number of whole points, should be the ratio of the two areas, which is $\pi/4$. By letting the number of red points be $N_r$, and the number of whole points be $N$, $\pi$ should be equal to $4N_r/N$. By increasing the number of whole points placed, an approximate value of Pi can be obtained.

In Fig 1.11, a simple chart of the result of calculation of Pi by Monte Carlo method by using MATLAB is showed. By increasing the numbers of the points, the result is closing to the proper value.
Fig 1.11 Result of calculation of Pi by Monte Carlo method
Reference


Chapter 2: Equipment and Techniques
2.1 Transmission Electron Microscope (TEM)

Transmission Electron Microscope is a kind of microscope, which is often used to observe the structure of ultra-thin semiconductor materials. It is important equipment in not only electronics but also in other fields like biology. [1]

In transmission electron microscopy technique, electrons from an electron gun will transmit through the specimen, and the image of the specimen will be formed from the information obtained through the interaction of the electrons and specimen.

Resolve detail in an object was limited approximately by the wavelength of the light used in imaging. In optical microscopy technique, it is hard to observe specimens under a few hundred nanometers for this reason. Let $\lambda$ be the wavelength of photons, and $NA$ be the numerical aperture of the system, so the maximum resolution is

$$d \approx \frac{\lambda}{2NA} \tag{2.1}$$

For the small de Broglie wavelength of electrons, the TEM has a resolve detail about tens of thousands times better then optical microscope. Considering the relativity, the de Broglie wavelength of electron is

$$\lambda_{e} \approx \frac{h}{\sqrt{2m_{0}E(1 + \frac{E}{2m_{0}c^{2}})}} \tag{2.2}$$

$h$ is Planck’s constant, $m_{0}$ is the rest mass of an electron and $E$ is the energy of the accelerated electron. Highly accelerated electrons lead to high resolution. The electron beam will transmit through the specimen and then contains the information of electron density, phase and periodicity. The information will be analyzed and used to form the image of the specimen. Let $\Psi$ be the wave function of the electron transmitted from the specimen, so the observed intensity of the image is

$$I(x) = \frac{k}{t_{1} - t_{0}} \int_{t_{0}}^{t_{1}} \Psi^{*} \psi' \, dt \tag{2.3}$$

2.2 Secondary Ion Mass Spectrometry (SIMS)

The secondary ion mass spectrometry (SIMS) is a technique used to analyze the composition of the material. The model of SIMS is shown schematically in Fig 2.1.

Primary ions (usually Cs+ or O2 ) are accelerated to high speed with a kinetic energy
of about 10kV by an ion gun. The primary ions will sputter the surface of the specimen and the secondary ions will eject from the specimen. Then analyzers of the machine will collect information such as the type and the mass of the secondary ions. Through the SIMS measurement, we can obtain the dependence of the concentration of the elements and depth.

![Diagram](image.png)

**Fig 2.1 Model of secondary ion mass spectrometry**

### 2.3 Hall Effect Measurement

#### 2.3.1 Hall Effect

The Hall Effect is a phenomenon in which a conductor or semiconductor that carries an electric current perpendicular to an applied magnetic field develops a voltage gradient transverse to both current and field. The voltage is known as the Hall voltage.

Consider the sample shown in Fig 2.2 has height, width, depth $a, b, d$, and the current flows through the plane $ad$, and the magnetic field is parallel to the plane $ad$.

Under this situation, the Lorentz force is

$$F_L = qvB$$

where $q$ is the electrical charge on the particle; $v$ is the velocity of the particle; $B$ is the strength of the magnetic field.

The current which flows through the plane can be written as

$$I = qvnad$$

where $n$ is the carrier density.

So we have

$$v = \frac{I}{qnad}$$

(2.6)
From (2.4) and (2.6), we have

\[ F_L = q \cdot \frac{I}{qnad} \cdot B = \frac{IB}{nad} \]  \hspace{1cm} (2.7)

On the other hand, the voltage developed will lead to an electrical field, and this field will cause a force on the carrier, as

\[ F_E = q \cdot \frac{V}{a} \]  \hspace{1cm} (2.8)

where \( V \) is the voltage.

The Lorentz force balances the Coulomb's force, because the current continues to flow along the sample, so

\[ \frac{IB}{nad} = q \cdot \frac{V}{a} \]  \hspace{1cm} (2.9)

Hence

\[ V = \frac{IB}{nqd} \]  \hspace{1cm} (2.10)

Then we can rewrite (2.10) by sheet carrier density \( n_s \) as
\[ V = \frac{IB}{n_s q} \]  

(2.11)

It shows that we can know sheet carrier density by measuring the Hall voltage.

Therefore, as the direction of flow of current is depend on both the direction of the velocity of the move of the carriers and the type of the electric charge of the carriers, we can judge whether the carriers are holes or electrons by the polarization of the Hall voltage.

2.3.2 Hall Effect Measurement

Van der Pauw method was used in this experiment in order to measure the properties of the samples. The van der Pauw method, which was first propounded by Leo J. van der Pauw in 1958, is a technique widely used in measure electrical properties of two-dimensional samples.

2.3.2.1 Conditions of the Samples

Firstly, the sample to be measured by the van der Pauw method should be two-dimensional; namely the samples should be of a flat shape of uniform thickness, and the sample should not have any isolated holes.

Although the van der Pauw method is designed for sample of arbitrary shape, it is found that the measurement error is smaller if using a homogeneous and isotropic sample. So it is better to make the sample homogeneous and isotropic.

In order to flow currency to the samples, we also need add contacts to the surface of samples. Four contacts are needs, and in order to minimize the measurement error, the contacts should be sufficiently small compared to the size of the sample, and be located at the edge of sample.

As discussed below, necessary conditions of sample for the measurement can be listed as:

a) The sample must have a flat shape of uniform thickness.

b) There are no isolated holes in the sample.

c) The sample must be homogeneous and isotropic.

d) Four contacts must be located at the edges of the sample.

e) The area of contact of any individual contact should be small compared to the size of sample.

2.3.2.2 Necessary Conditions for the Contacts: Non-Rectifying

Another necessary condition for the contact is that the contacts should be ohmic. Namely, the contacts should be non-rectifying, which means that the current–voltage
curve of the region is linear and symmetric.

When metal and semiconductor are in contact, a barrier will exist between the two kinds of materials. The barrier is called Schottky Barrier (Fig 2.3). The Schottky Barrier prevents the move of the carrier between metal and semiconductor, so the contact becomes rectifying. This kind of rectifying behavior can be found in almost all metal-semiconductor contacts.

In measurement using van der Pauw method, the Schottky Barrier between metal contacts and semiconductor sample is treated as a problem. Basically we want an ohmic contact, which obeys Ohm’s law. Some properties of the sample, such as resistance, cannot be measured correctly if the Schottky Barrier exists.

\[ \phi_{SB} = \phi_m - \chi \]  

(2.12)

\( \phi_{SB} \) is the SBH; \( \phi_m \) is the work function of metal; \( \chi \) is the electron affinity.

We can choose the proper metal, whose work function is nearly equal to the electron affinity of semiconductor which we use as sample, in order to lower the SBH.

Another method to lower the SBH is to create an alloy at the interface between metal and semiconductor, by heat treatment such as annealing, which is widely used.

b) To create Quantum tunnelling

According to the theory of quantum mechanism, a particle, which behaves itself as
wave due to the wave–particle duality, is possible to tunnel through a barrier, through which it cannot tunnel under classic mechanism theory. If we can make the possibility to tunnel though the SBH high sufficiently to make the carrier move freely to both directions, we can make the metal-semiconductor contact ohmic. According to the mathematical analysis using the wave function in the Schrödinger equation, if SBH is extremely thin, the carrier will have relatively high possibility to tunnel through it. We can make the barrier very narrow by doping it very heavily, so the impurity concentration in the semiconductor in very important. Although change the impurity concentration is not easy considering other properties of the sample (e.g. the impurity concentration will effect on the mobility and resistance), we can make the impurity concentration near the surface between the two materials by heat treatment. By this method we can also obtain non-rectifying contact. [2]

2.3.2.3 Measurement of Resistance

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{sample.png}
\caption{Sample for Hall Measurement}
\end{figure}

Let us consider a sample which satisfies the conditions mention in section 2.3.2.1, as shown in Fig 2.4. Four contacts are at the edges of a sample of sharp of square and named A, B, C, and D. If the current flows between contact A and B is defined as \( I_{AB} \) and the potential difference between D and C \( (V_D - V_C) \) is \( V_{CD} \).

Then we define \( R_{AB,CD} \) as:

\[ R_{AB,CD} = \frac{V_{CD}}{I_{AB}} \quad (2.13) \]

Likely, we can define \( R_{BC,DA} \) as:

\[ R_{BC,DA} = \frac{V_{DA}}{I_{BC}} \quad (2.14) \]

\( R_{AB,CD} \) and \( R_{BC,DA} \) can be shown that they follow:

\[ \exp \left( -\pi \frac{R_{AB,CD}}{R_s} \right) + \exp \left( -\pi \frac{R_{BC,DA}}{R_s} \right) = 1 \quad (2.15) \]
\( R_s \) is the sheet resistance, and it can be rewritten as:

\[
R_s = \frac{\pi}{\ln 2} \left( \frac{R_{AB,CD} + R_{BC,DA}}{2} \right) f\left( \frac{R_{AB,CD}}{R_{BC,DA}} \right)
\]

(2.16)

where

\[
\frac{R_{AB,CD} - R_{BC,DA}}{R_{AB,CD} + R_{BC,DA}} = f \text{arcosh} \left( \frac{\exp(\ln 2/f)}{2} \right)
\]

(2.17)

We can use Taylor expansion to estimate the function \( f \).

\[
f = 1 - \left( \frac{R_{AB,CD} - R_{BC,DA}}{R_{AB,CD} + R_{BC,DA}} \right)^2 \ln 2 \frac{2}{2} - \left( \frac{R_{AB,CD} - R_{BC,DA}}{R_{AB,CD} + R_{BC,DA}} \right)^4 \left\{ \frac{(\ln 2)^2}{4} - \frac{(\ln 2)^3}{12} \right\} + \ldots
\]

(2.18)

From the equation (2.18), apparently, if

\[
f = 1 \text{ when } R_{AB,CD} = R_{BC,DA}
\]

(2.19)

As the sample has a flat shape of uniform thickness and it is homogeneous and isotropic, we can say that \( R_{AB,CD} = R_{BC,DA} \) so the function \( f \) should be 1. So (2.16) can be rewritten as

\[
R_s = \frac{\pi R_{AB,CD}}{\ln 2}
\]

(2.20)

As in fact \( R_{AB,CD} \) differs slightly from \( R_{BC,DA} \) we always measure data for different directions and use the average of them to calculate the sheet resistance. The 8 data of the sample are

\[
R_{AB,CD}, R_{BA,CD}, R_{CD,AB}, R_{DC,AB}, R_{BC,AD}, R_{CD,AD}, R_{AD,BC}, R_{DA,BC}
\]

(2.21)

We use the average of these 8 data to calculate the sheet resistance. [3]

### 2.3.2.4 Measurement of Sheet Carrier Density and Mobility

Consider a sample shown in Fig 2.2, firstly we flow the current from contact A to contact C, while let the magnetic field be perpendicular to the surface of the sample, and measure the potential difference between contact B and contact D \( (V_D - V_B) \). Then we reverse magnetic polarity, and measure the potential difference between contact B and contact D again. One of the two results of the measurement of the potential difference should be positive, and the other should be negative. Let us define the positive one, \( V_{AC-p} \), because this potential difference is measured when the current flows from contact A to contact C. Likely, we can define the negative on \( V_{AC-n} \). Then we define that

\[
V_{AC} = V_{AC-p} - V_{AC-n}
\]

(2.22)

Likely, we can have \( V_{CA}, V_{BD} \) and \( V_{DB} \).

The overall Hall voltage is
\[ V_H = \frac{V_{AC} + V_{CA} + V_{BD} + V_{DB}}{8} \]  \hspace{1cm} (2.23)

We can use this voltage to calculate the sheet carrier density like
\[ n_s = \frac{IB}{qV} \]  \hspace{1cm} (2.24)

We can calculate the mobility by the data of carrier density.
The resistivity can be written as
\[ \rho = \frac{1}{q(n\mu_n + p\mu_p)} \]  \hspace{1cm} (2.25)

When \( q \) is the charge on the particle, \( n \) is the concentration of negative carrier, \( p \) is the concentration of positive carrier, and \( \mu_n, \mu_p \) are the mobility of negative and positive carrier.

If we ignore the minority carrier, (2.25) can be written as
\[ \rho = \frac{1}{qn_m\mu_m} \]  \hspace{1cm} (2.26)

\( n_m \) is the concentration of majority carrier and \( \mu_m \) is the mobility of majority carrier.

We can use sheet carrier density \( n_s \) and sheet resistance \( R_s \) to rewrite (2.26)
\[ R_s = \frac{1}{qn_s\mu_m} \]  \hspace{1cm} (2.27)

Hence
\[ \mu_m = \frac{1}{R_sqn_s} \]  \hspace{1cm} (2.28)

As sheet resistance \( R_s \) can be obtained by (2.27), we can calculate the mobility by using (2.28).

2.3.3 Equipment for Hall Effect

The equipment used for Hall Effect is shown in Fig 2.5 and Fig 2.6. Fig 2.5 is the equipment for Hall Effect at high temperature (Room Temperature~900K) and low temperature (80K~Room Temperature). Liquid Nitrogen is used in the Hall Effect measurement at low temperature to lower the temperature.
Fig 2.5 Equipment for Hall Measurement at Low Temperature
2.4 Rapid Thermal Annealing (RTA)

Rapid thermal annealing (RTA) is a piece of equipment used for heat treatment. Using the equipment shown in Fig 2.7 sample can be annealed in different atmosphere, to heal the crystal structure of the wafer. A great advantage of the RTA equipment is that temperature can fall and rise rapidly. The temperature change of 1000°C can be achieved in about 10-20 seconds. Due to the short processing time, the further diffusion of the dopants can be limited to a minimum.
As shown in Fig 2.8, the sample is under heat treatment in atmosphere in N$_2$/O$_2$ (8:2) gas, and N$_2$ gas is used to surge pressure. [4]

### 2.5 Probe Station

The probe station is a machine used to acquire the signals from a semiconductor device. The total view of probe station is shown in Fig 2.9. The microscope is used to observe the sample and the location of the sample and probes. The probes can be controlled to contact the electrodes in the sample and obtain signals from the sample.

The image of the part of plate under the microscope is shown in Fig 2.10.
Photolithography is a method using light-like material applied on the surface of a flat thin sample to produce particular pattern on the sample. The light-like material is called “resist”, and the light used in photolithography is usually ultraviolet (UV) light. The photolithography technique is used to produce metal contact to the surface of sample, which will be mentioned in Chapter 3.
The process is shown as Fig 2.11:
1) Applying the resist to the sample. In the application, we usually use a machine call spin coater. A spin coater can rotate to high speed, and the sample can be placed on it. As the resist must be applied to the surface of the sample uniformly, we can use the centrifugal force to ensure it. First we apply the resist to the sample placed on the spin coater, and then rotate it to a high speed, and finally the resist will become a uniformly flat thin layer. After this, we should use a photomask which the light shines through but blocks light in some areas and lets it pass in others. The photoresist is exposed to
the UV light after aligning the photomask on the sample.

2) The exposure leads to a chemical change in resist. As a result, the exposed region and unexposed region become different chemically so the one of them can be removed by a special solution call photographic developer. Which one can be removed is depend on resist, and there are two kinds of resist: positive and negative. With positive photoresist, exposed regions are soluble in the developer. On the other hand, with negative photoresist, unexposed regions are soluble in the developer. The Fig 2.10 shows the situation of positive resist.

3) The region of upper layer to the substrate which is not protected by resist can be removed by some chemical materials in the process of etching. The chemical materials used in etching can be liquid or plasma.

4) After etching, the rest resist should be removed. A liquid call resist stripper can be used for the removal of resist. Another way to remove resist is ashing. In ashing a kind of plasma containing oxygen is used. The reactive species combines with the photoresist to form ash which is removed with a vacuum pump.

2.7 Ellipsometry

Ellipsometry is an optical technique to obtain permittivity characteristics of pellicle materials. On account of that during its measurement, material samples will not be touched and broken, it is treated as a sensitive measurement to measure tiny size samples. This technique measures change of polarization on reflection or transmission and compares it to a model, which is set previously.
Shown as Fig 2.12, radiation is emitted from the light source and polarized as a linear light by the polarizer. Then, it may pass through an optional compensator and fall into the sample. After reflection on the sample, the light will pass through an analyzer, and finally into the detector. Light which is polarized parallel to the plane of incidence is named $p$-polarized. Another polarization direction perpendicular is called $s$-polarized.

Then we can compare the two polarized light $p$ and $s$. Amplitude component is defined as $\psi$ and the phase difference is defined as $\Delta$. Through these data we can calculate physical parameters such as thickness of the samples.
In multi-layer sample as Fig 2.13, advanced calculation must be done in order to obtain the proper data we need.

The equipment used in our research is shown as Fig 2.14, in which two black box, detector and light source can be seen.

### 2.8 Atomic Force Microscope

Atomic Force Microscope (AFM) is nano-meter level scanning probe microscopy, in which atomic force is used here to measure surface statues of a sample.

![A flow-chart of AFM](Fig2.15)

A simple flow-chart of AFM system is shown in Fig 2.15. A cantilever in the machine will touch or approach in no contact mode to a sample. The tip will bend according to
Hooke’s Law. The force measured during this bend may be Mechanical contact Forces, van der Waals Forces, chemical bonds, static electricity, Casimir Force, Solvent Force or so on. This bend will be measured through laser on photodiode, and measured data will be analyzed by the machine, and then graphs about surface statues will be obtained.

The equipment used in our research is shown as Fig 2.16, and the cantilever is shown as Fig 2.17.
One can see in Fig 2.17, that a tiny tip at the top. The cantilever is made of silicon, covered with allium, and needed to be changed after using for a period of time.

On account of in the situation that the tip contacts samples, samples will sometimes attract the tip into itself, a mode called DFM is always used in our measurement. In this mode, the tip will not contact the sample directly, but operate as frequency modulation. The atoms in samples, sometimes also moves as frequency modulation, so by adjusting the distance of tip and sample, frequency can be measured and the surface statues can be measured by the distance data obtained.
Reference

Chapter 3: Experiments on Material Properties
3.1 Samples and General View of Experiments

In this research, two kinds of samples were prepared, as shown in Fig. 3.1. Sample-A in Fig. 3.1 (a) is the sample where polarization doping technique is used. The layer structure of the sample was grown on 3-inch c-plane sapphire substrate by metal organic chemical vapor deposition (MOCVD). Firstly, a layer of undoped GaN was grown, then undoped AlGaN, and undoped GaN. Finally, a Mg-doped GaN layer was grown to support Ohmic contact formation to 2DHG, which is necessary for electrical property evaluations. A detail layer structure was confirmed by X-ray diffraction (XRD) measurements and cross-sectional transmission electron microscope (TEM) observations as reported later. In Sample-A, 2DEG exists at the lower AlGaN(000)/GaN(0001) heterointerface, as reported in several previous studies[1,2,3]. Additionally, 2DHG generation at the upper GaN (000)/AlGaN(0001) heterointerface is expected due to negative polarization effect at the heterointerface. We have also prepared Sample-B illustrated in Fig. 3.1(b), to compare electrical property of sample-A with that in Mg doped conventional p-type GaN. Sample-B was grown on c-plane sapphire substrate, and consists two layers of 1.5μm-thick undoped GaN and 500-nm Mg-doped GaN. Van der Pauw square configurations for Hall Effect measurement were fabricated as follows. The both wafers were diced in 5 mm square. Ni/Au (20 nm/ 20 nm) electrodes were deposited on the tops of the both samples. Subsequently, the samples were annealed in air ambient to reduce contact resistance between the electrodes and 2DHG. Finally, Ti/Au (20 nm/ 100 nm) was deposited on the electrodes. Several experiments were conducted in order to clarify layer structures, crystal quality and electrical properties of the both samples, including XRD, TEM, atomic force microscope (AFM), secondary ion mass spectroscopy (SIMS), capacitance-voltage (C-V), and temperature dependence Hall Effect measurements.
Fig 3.1 Structure of the samples used in the Hall Effect measurement

3.2 XRD Measurements

Fig 3.2 Measured (0004) $2\theta-\omega$ curve of sample-A (solid line) and a simulation result (dashed line).
Firstly, XRD measurements were performed here in order to characterize a layer structure and crystal quality of Sample-A. Figure 3.2 shows a measured $2\theta-\omega$ curve, where GaN(0004) and AlGaN(0004) peaks, and also several satellite peaks is observed. We have simulated diffraction curves with assuming GaN/AlGaN/GaN double heterostructure and the best fitting to the measured curve was obtained when a GaN cap layer thickness is 38 nm, an AlGaN barrier thickness is 48 nm, and an Al composition is 23%, as shown in Fig.2. We have also measured a rocking curve of the GaN(0004) diffraction and a full-width at half-maximum value of 290 arcsec was obtained.

![Fig 3.3 TEM image of the GaN/AlGaN/GaN layer structure](image)

In Fig 3.3, we confirmed the existence of three layers, and the depth of each layer was measured through the enlarged view of the upper surface shown at Fig 3.4. The measured depth of the layers approaches to the designed. Though the interface of Mg doped GaN and undoped GaN is not clear, the total depth of the layers of Mg doped GaN and undoped GaN can be confirmed in this image. What is important, that abrupt heterointerface is seen in these figures.
Fig 3.4 Enlarged view of the upper surface of the GaN/AlGaN/GaN layer structure

3.3 AFM

Figure 3.5 shows AFM images of Sample-A surface. Atomically flat morphology with step and terrace structures are observed without any cracks. Measured RMS roughness was 0.2 nm. Some pits located at the step edges were also observed, as shown in Fig. 3.5.
3.4 CV Characteristics

Electrical properties of the both samples were evaluated. We have measured C-V characteristics at 100 kHz by putting Hg probes on the sample surfaces. Figure 3.6 shows a carrier distribution profile calculated from a measured C-V curve. The peak of the carrier concentration is located at 40 nm depth which is correspond to the position of the upper GaN/AlGaN heterointerface confirmed by TEM observation, and then the concentration decreases in the inner part of the sample.

![AFM images of Sample-A surface at the scan size of 3 μm × 3 μm (left) and 1 μm × 1 μm (right).](image)

![Carrier concentration profile of Sample-A from CV measurement.](image)
3.5 SIMS

Fig 3.7 SIMS depth profiles of Sample-A

Mg impurity distribution in Sample-A was clarified through SIMS measurements. Figure 5 shows distributions of Al and Mg atoms, and relative intensities of CsN and CsGa signals in Sample-A, from the surface to 100-nm-depth. We observed that Mg exists in the whole GaN region, even though the 20-nm-thick GaN layer on the AlGaN layer was grown with no doping. The Mg concentration of the undoped GaN region was about
4×10^{18} \text{ cm}^{-3} \text{ which is an order of magnitude lower than that in Mg-doped GaN. This existence of Mg in undoped GaN, should be due to the thermal back diffusion of Mg atoms during MOCVD growth[4].}

3.6 Hall Effect Measurement

3.6.1 Steps of Experiment

The steps of experiment are shown in Fig 3.8. Firstly organic solvent cleaning using acetone is performed, and then the sample is blowed the samples by gas gun. After this, the sample is place in Hydrogen fluoride solution (40\%) for 1 minute. Then nickel 20nm and Au 20nm is added as electrode to the sample. After heat treatment in RTA for 10 minutes at 550°C in air atmosphere (N\textsubscript{2}:O\textsubscript{2}=8:2), Titanium 20nm and gold 100nm is added to the sample.

In the step of metal deposition, at beginning the method of lithograph which is was mentioned in Chapter 2 has been tested, but we found that the ashing, which is used to remove the photoresist from the sample, is not so good, especially in lowering the Schottky Barrier Height.

Fig 3.8 Experiment step of adding contacts
Inside of the lithograph, we use a metal mask to deposit the metal to the surface of sample. The metal mask is a plate made of metal and there are small holes which is 0.3mm in diameter and equal to the diameter of metal electrode of the experimental producers in the plate. The steps of adding electrodes to the sample is shown schematically in the Fig 3.69,

![Diagram of adding electrodes to the sample]

**Figure 3.9 Steps of adding electrodes to the sample**

### 3.6.2 Results of Hall Effect Measurement

Hall measurement by van der Pauw method is used in this research to obtain the relationship between sheet carrier density, sheet resistance, mobility and temperature. The structure we used in this measurement is shown in Fig 3.1 (b), and we also demonstrate the same Hall measurement on another sample shown in Fig 3.1 (a) as control. The graphs of the measurement results are shown schematically in Fig 3.7, Fig 3.8, and Fig 3.9.
Fig 3.10 Sheet carrier density dependence on temperature

Fig 3.11 Sheet resistance dependence on temperature
Fig 3.12 Mobility dependence on temperature

We did a calculation on the effect of top Mg layer in Sample-A, shown as Fig 3.13.

Fig 3.13 Modified sheet carrier density

In Fig 3.13, The dashed line shows the sheet carrier density of Sample-A after
departing the carriers from the top layer Mg-doped GaN, by using the result of sheet carrier density of Sample-B, while assuming the carrier distribution of the 30-nm Mg doped layer of Sample-A was the same as 500-nm Mg doped layer of Sample-B. As shown in the graphs, the existence of the AlGaN layer leads to a great change in electrical properties, and somehow it is certain that this kind of change owns to the 2DHG.

3.7 Analysis of Measured Results

Here a detailed analysis on mobility of Sample-A is done here and it will be introduced in this section. Unless mentioned otherwise, it is referred to [5].

3.7.1 Acoustic phonon scattering

Piezoelectric scattering is treated as a kind of acoustic phonon scattering in 2DHG system. To distinguish it from ‘common’ acoustic phonon scattering, ‘deformation potential scattering’ is used here, which comes from that deformation potential which will mentioned in Chapter 4.

3.7.1.1 Acoustic Phonon Scattering

The momentum relaxation rate is given by [6]

\[
\frac{1}{\tau_{DP}} = \frac{3E_D^2 k_B T m^* b}{16 \rho \mu_l^2 \hbar^3} J_{DP}(k) \tag{3.1}
\]

here, \( \rho \) is the density of crystal, \( \mu_l \) is longitudinal acoustic phonon velocity, \( E_D \) is deformation potential constant, \( m^* \) is electron effective mass, \( k \) is electron wavevector and \( k_B \) is Boltzman constant. And

\[
J_{DP}(k) = \int_0^{2k} \frac{1}{2\pi k^3 (q + q_s)^2 \sqrt{1 - (q/2k)^2}} q^4 dq \tag{3.2}
\]

\[
b = \left( \frac{33e^2 m^* N_S}{8\varepsilon_S h^2} \right)^{1/3} \tag{3.3}
\]

\[
q_s = \frac{e^2 m^*}{2\pi \hbar^2 \varepsilon_S} F_{11}(q) f(0) \tag{3.4}
\]

3.7.1.2 Piezoelectric Scattering

The scattering rate is given by [6]

\[
\frac{1}{\tau_{PE}} = \frac{e^2 K^2 k_B T m^*}{\pi \varepsilon_S h^3 k} J_{PE}(k) \tag{3.5}
\]
and $K$ is electromechanical coupling coefficient

$$K^2 = \frac{\varepsilon_{LA}^2}{\varepsilon_S c_{LA}} + \frac{\varepsilon_{TA}^2}{\varepsilon_S c_{TA}}$$

and

$$J_{PE}(k) = \int_0^{2k} \frac{F_{11}(q)}{4k^2(q + q_s)^2\sqrt{1 - (q/2k)^2}} q^3 dq$$

### 3.7.3 Polar-optical Phonon Scattering

According to Gelmont et al., the mobility of polar-optical phonon scattering should be [7]

$$\mu_{2p0} = \frac{\kappa^* k_0 h^2}{2\pi \varepsilon_0 \omega_0 m^2 n_G(k_0)} \left( 1 + \frac{1 - \exp(-y)}{y} \right)$$

$y$ here should be

$$y = \frac{\pi h^2 N_S}{m_n k_B T}$$

here

$$G(k_0) = \frac{b(8b^2 + 9k_0 b + 3k_0^2)}{8(k_0 + b)^3}$$

and parameter $b$ should be

$$b = \left( \frac{33\pi m_n e^2 N_S}{2\kappa_0 h^2} \right)$$

### 3.7.4 Dislocation Scattering

Scattering rate of dislocation scattering should be

$$\frac{1}{\tau_{\text{dis}}} = N_{\text{dis}} \left( \frac{m^*}{2\pi h^3 l_F^3} \right) \int_0^{2k_F} \frac{|A(q)|^2}{\sqrt{1 - \left( \frac{q}{2k_F} \right)^2}} dq$$

$$A(q) = \frac{e}{2\varepsilon_S q(q + q_{TF})}$$

here $\varepsilon_S$ is dielectric constant. $\rho_L$ is line charge density, which can be given an approximation by $ef/c_0$. Here, $c_0$ is lattice constant and $f$ is fraction of filled state, and here we assumed $f = 1$, which means that all the donor states in the dislocation are filled. $q_{TF} = 2/a^*_b$, and $a^*_b$ is effective Bohr radius in the material.

### 3.8 Mobility Analysis

A fitting of mobility analysis is shown as Fig 3.14. The calculation here is based on
the fitting of effective mass being 0.24 $m^*$. 

![Fig 3.14 Fitting of Mobility](image)

In this figure, several lines here show us possible mobility when only one scattering exists. In this calculation, it is deformation potential scattering that limit the mobility of 2DHG, which will be base for our discussion by Monte Carlo method.

### 3.9 Effect of SPM on AlGaN/GaN Samples

SPM is abbreviation for Sulfuric acid-Hydrogen Peroxide Mixture. This word here stands for a cleaning way in semiconductor production. Firstly, the sample will be put in a mixed liquid of sulfuric acid and hydrogen peroxide, and heated to 180°C for 5 minutes. Then the sample will be put in 20% HF for 2 minutes. We repute this process for numerous times, and take investigation of the relationship of surface statues and SPM by AFM.

A figure of sample surface without any treatment is showed as Fig 3.15. Several dislocation can be seen in this image. In this 1000 nm $\times$ 1000 nm image, dislocations are measured no more than 30 nm.
Fig 3.15 AFM image of no SPM treatment (1000 nm × 1000 nm)

Image of the sample after 5 times SPM treatment is shown as Fig 3.16. In this image, we can confirm more dislocations on the surface. As it is an image of 1000 nm × 1000 nm, we give another image of (10000 nm × 10000 nm) shown as Fig 3.17. In this image, no dislocation can be confirmed, being thought that the dislocations are too tiny.

Fig 3.16 AFM image of 5 times SPM treatment (1000 nm × 1000 nm)
Fig 3.17 AFM image of 5 times SPM treatment (10000 nm × 10000 nm)

Fig 3.18 AFM image of 15 times SPM treatment (1000 nm × 1000 nm)
Image of the sample after 15 times SPM treatment is shown as Fig 3.18. Dislocations are clearer in this image, and we can also confirm the number of dislocations becomes more, but dislocations cannot confirmed on image of 10000 nm × 10000 nm as Fig 3.19.

Fig 3.19 AFM image of 15 times SPM treatment (10000 nm × 10000 nm)

However, after 20 times of SPM treatment, dislocations can be slightly confirmed at
the surface as shown in Fig 3.20, and a detailed image of 1000 nm × 1000 nm as Fig 3.21 shows more clearly the larger dislocation image.

**Fig 3.21** AFM image of 20 times SPM treatment (1000 nm × 1000 nm)

This trend was confirmed in following experiment, as shown in Fig 3.22~3.25.

**Fig 3.22** AFM image of 30 times SPM treatment (10000 nm × 10000 nm)
Fig 3.23 AFM image of 40 times SPM treatment (10000 nm × 10000 nm)

Fig 3.24 AFM image of 55 times SPM treatment (10000 nm × 10000 nm)
Fig 3.25 AFM image of 60 times SPM treatment (10000 nm × 10000 nm)

Other images of size 1000 nm × 1000 nm are also confirmed, shown as Fig 3.26~3.30.

Fig 3.26 AFM image of 30 times SPM treatment (1000 nm × 1000 nm)
Fig 3.27 AFM image of 40 times SPM treatment (1000 nm × 1000 nm)

Fig 3.28 AFM image of 50 times SPM treatment (1000 nm × 1000 nm)
Detailed sizes of dislocations are measured through AFM images, from 30 nm from firstly, to a largest of 200-nm level for 60 times of SPM treatment. Complicated data are involved in this experiment, which leaves difficulty in expressing it objectively, but it is apparent from the figures which we gave, that dislocations at AlGaN/GaN heterostructure
sample surface are increasing in size and numbers. This phenomena, is thought to be needed to considered in any experiments concerning with SPM treatment of AlGaN surface.

From the experiments conducted above, the harm of SPM treatment to AlGaN/GaN heterostructure samples can be confirmed; that is, dislocations at sample surface are becoming larger and more, due to SPM treatment. For this reason, least time of SPM treatment is required in surface treatment of AlGaN/GaN heterostructure samples, considering effect of dislocations to the surface.

A possible explanation of the increasing dislocations is shown as Fig 3.31, which shows that AlGaN solutes by reactions with SPM solution after treatment. Another possible explanation is given by Fig 3.32, which shows that inner side of dislocation on surface of AlGaN is oxidized by SPM solutions. Anyhow, SPM is harm to surface of AlGaN, and may influence the quality of samples.

![Fig 3.31 Image of SPM inverse ion AlGaN](image1)

![Fig 3.32 Image of oxidation on AlGaN surface](image2)

A revision of experiments in this section is shown in Fig 3.33. This figure is made by counting dislocations in 1000 nm×1000 nm image.
Fig 3.33 Revision of SPM effect on AlGaN surface
Reference


Chapter 4: Monte Carlo Simulation for 2DHG
4.1 Basic Theory of Quantum on Scattering

As mentioned in Section 1.6, Monte Carlo method is a useful method for probability physics, simulations of random carriers in semiconductor included. In this section, the theoretical basic of this method used will be introduced simply. The method introduced here, is referred to Semiconductor Device Simulation by Dr. Tomizawa. [1]

Transition probability can be shown under first order perturbation theory as

\[ i\hbar \frac{\partial \psi(r, t)}{\partial t} = (H_0 + H')\psi(r, t) \]  

(4.1)

Unperturbed Hamiltonian \( H_0 \) is assumed to be arisen from Schrödinger Equation as

\[ H_0\psi_k = E_k\psi_k \]  

(4.2)

, when \( \psi_k \) is characteristic vector and \( E_k \) is energy eigenvalue.

A possible solution of Equation (4.2) should be

\[ \psi_k(r, t) = \sum c_k \psi_k^0(r) e^{-iE_k t/\hbar} \]  

(4.4)

If substituting (4.4) for (4.1),

\[ i\hbar \sum_k \frac{\partial c_k(t)}{\partial t} \psi_k(r) e^{-iE_k t/\hbar} = \sum_k H' c_k(t) \psi_k(r) e^{-iE_k t/\hbar} \]  

(4.5)

, can be obtained.

Multiplied by \( \psi_k^\ast e^{iE_k t/\hbar} \) and then integrated of the both sides of (4.5) with respect of \( r \), we can obtain a new integration equation about \( c_k(t) \) as

\[ i\hbar \frac{\partial c_k(t)}{\partial t} = \sum_k \langle k' | H' | k \rangle e^{i(E_{k'} - E_k) t/\hbar} \]  

(4.6)

Let us consider a single carrier in a single energy eigenvalue, we have

\[ i\hbar \frac{\partial c_k(t)}{\partial t} = \langle k' | H' | k \rangle e^{i(E_{k'} - E_k) t/\hbar} \]  

(4.7)

As \( H' \) is considered to be harmonic as

\[ H'(t) = H' e^{\mp i\omega t} \]  

(4.8)

Substituting (4.4) for (4.1),

\[ i\hbar \frac{\partial c_k(t)}{\partial t} = \langle k' | H' | k \rangle e^{i(E_{k'} - E_k - \hbar \omega) t/\hbar} \]  

(4.9)

, and then we integrate it from 0 to \( t \).
\[ c_{k'}(t) = \frac{1}{i\hbar} \langle k'|H'|k \rangle e^{i(E_{k'} - E_k + \hbar \omega)t/\hbar} - \frac{1}{i\hbar} \langle E_{k'} - E_k \mp \hbar \omega \rangle \]  \hspace{1cm} (4.10)

Let us assume that
\[ \xi = \frac{1}{2\hbar} (E_{k'} - E_k \mp \hbar \omega) \]  \hspace{1cm} (4.11)
so we can rewrite (4.10) as
\[ c_{k'}(t) = \frac{1}{i\hbar} \langle k'|H'|k \rangle e^{i\xi t} \frac{\sin(\xi t)}{\xi t} - \frac{1}{i\hbar} \langle E_{k'} - E_k \mp \hbar \omega \rangle \]  \hspace{1cm} (4.12)

Transition probability from state \( k \) to \( k' \) per unit time should be
\[ S(k, k') = \lim_{t \to \infty} \frac{|c_{k'}(t)|}{t} \]  \hspace{1cm} (4.13)
So,
\[ S(k, k') = \lim_{t \to \infty} \frac{|\langle k'|H'|k \rangle|^2}{\hbar^2} \left( \frac{\sin(\xi t)}{\xi t} \right)^2 t \]  \hspace{1cm} (4.14)

Finally through calculation of the equation, we can have
\[ S(k, k') = \frac{2\pi}{\hbar} |\langle k'|H'|k \rangle|^2 \delta(E_{k'} - E_k \mp \hbar \omega) \]  \hspace{1cm} (4.15)

Equation (4.15) also shows energy conservation. The minus-plus sign indicates that carrier whether obtain or emit a quantum with energy \( \hbar \omega \). Therefore what is more important in some calculations, it is when \( \hbar \omega = 0 \) that, elastic scattering without energy change happens.

Scattering rate, which is one of the most important parameters in Monte Carlo simulation, should be
\[ W(k') = \frac{\Omega}{(2\pi)^3} \int S(k, k') d\mathbf{k}' \]  \hspace{1cm} (4.16)
Or
\[ W(k') = \frac{2\pi}{\hbar} \frac{\Omega}{(2\pi)^3} \int |\langle k'|H'|k \rangle|^2 \delta(E_{k'} - E_k \mp \hbar \omega) d\mathbf{k}' \]  \hspace{1cm} (4.17)

### 4.2 Scattering Rate for Acoustic Phonon Scattering

Lattice vibration of basic vibration in crystal can be written as
\[ \mathbf{u}(r, t) = \sum_q \left( \frac{\hbar}{2\rho \omega_q \Omega} \right)^{1/2} e_q (a_q + a_q^\dagger) e^{iq \cdot r} \]  \hspace{1cm} (4.18)
\( a_q, a_{-q}^\dagger \) are used here as creation and annihilation operators, and Hamiltonian of perturbation can be written as
\[
H' = \Xi_d \mathbf{\nabla} \cdot \mathbf{u}(r, t)
\] (4.19)
\( \Xi_d \) is what we call deformation potential, and finally we can have
\[
H' = \sum_q i q \Xi_d \left( \frac{\hbar}{2 \rho \omega_q \Omega} \right)^{1/2} (a_q + a_{-q}^\dagger) e^{iqr}
\] (4.20)

Under a parabolic band structure,
\[
\langle \mathbf{k}', n_q - 1 | H' | \mathbf{k}, n_q \rangle = i q \Xi_d \left( \frac{\hbar}{2 \rho \omega_q \Omega} \right)^{1/2} \sqrt{n_q} \delta(\mathbf{k}' - \mathbf{k} - \mathbf{q})
\] (4.21)

\[
\langle \mathbf{k}', n_q + 1 | H' | \mathbf{k}, n_q \rangle = i q \Xi_d \left( \frac{\hbar}{2 \rho \omega_q \Omega} \right)^{1/2} \sqrt{n_q + 1} \delta(\mathbf{k}' - \mathbf{k} + \mathbf{q})
\] (4.22)

Then we substitute (4.21), (4.22) for (4.15),
\[
S(\mathbf{k}, \mathbf{k}') = \frac{\pi \Xi_d^2 q^2}{\rho \omega_q \Omega} \left( n_q + \frac{1}{2} \mp \frac{1}{2} \right) \times \delta(\mathbf{k}' - \mathbf{k} \mp \mathbf{q}) \delta(E_{kr} - E_k \mp \hbar \omega)
\] (4.23)

Considering conservation of energy and momentums, we have
\[
E_{kr} = E_k \pm \hbar \omega_q
\] (4.24)
\[
\mathbf{k}' = \mathbf{k} \pm \mathbf{q}
\] (4.25)

, and when energy band is parabolic and isotropic, we have
\[
\frac{\hbar^2 k'^2}{2m^*} = \frac{\hbar^2 k^2}{2m^*} \pm \hbar \omega_q
\] (4.26)

Combining (4.25) and (4.26), we have
\[
\delta(\mathbf{k}' - \mathbf{k} \mp \mathbf{q}) \delta(E_{kr} - E_k \mp \hbar \omega) = \delta \left( \frac{\hbar^2 q^2}{2m^*} \pm \frac{\hbar^2 k q \cos \theta'}{m^*} \mp \hbar \omega_q \right)
\] (4.27)

\( \theta' \) here is for the angle between \( \mathbf{k} \) and \( \mathbf{q} \).

With assuming the scattering is elastic, we have
\[
S(\mathbf{k}, \mathbf{k}') \approx \frac{\pi \Xi_d^2 k_B T_L}{\hbar c_L \Omega} \frac{k}{qE_k} \delta \left( \frac{q}{2k} \pm \cos \theta' \right)
\] (4.28)

, so
\[
W(\mathbf{k}') = \frac{\Omega}{(2\pi)^3} \int S(\mathbf{k}, \mathbf{k}') d\mathbf{k}' = \frac{\Xi_d^2 k_B T_L}{8\pi^2 \hbar c_L E_k} \frac{k}{q} \int \frac{1}{q} \delta \left( \frac{q}{2k} \pm \cos \theta' \right) d\mathbf{q}
\] (4.29)
\[
\int \frac{1}{q} \delta \left( \frac{q}{2k} \pm \cos \theta' \right) dq = \int_{0}^{\infty} \int_{-1}^{+1} \int_{0}^{2\pi} \delta \left( \frac{q}{2k} \pm \cos \theta' \right) d\phi d(\cos \theta') dq
\]
(4.30)

\[
= 2\pi \int_{q_{\min}}^{q_{\max}} q dq = \pi (q_{\max}^2 - q_{\min}^2) = 4\pi k^2
\]

Scattering rate can be written as

\[
W(k') = \frac{2\pi \frac{\sigma_d^2 k_B T_L}{h c}}{N(E_k)}
\]
(4.31)

Here, \( N(E_k) \) stands for state density of carriers, which should be

\[
N(E_k) = \frac{(2m^*)^{3/2} \sqrt{E_k}}{4\pi^2 \hbar^3}
\]
(4.32)

### 4.3 One-particle Monte Carlo Method

One-particle Monte Carlo Method is introduced in this section. One-particle Monte Carlo Method is used to simulate carrier movement problems through considering one single particle. In this method, a model where one particle changes its movement by numerous scatterings is used, in order to solve several problems about carrier transport. This method can be used directly, without assuming shape of distribution function.

Fig 4.1 shows a simple flow-chart of one-particle Monte Carlo Method. A particle moves freely, drifting under some electrical field, then scatters under one particular scattering mechanism. Finally, after scattering of times indicated, we calculate for several physical quantities by the data obtained in this simulation process.

#### 4.3.1 Total Scattering Rate

Here we give a definition to total scattering rate by free time.

Consider a particle which drifts in time of \( \tau \), then the possibility of scattering is set to be

\[
P(\tau) = W_T(E_k) \exp \left( - \int_{0}^{\tau} W_T(E_k) dt \right)
\]
(4.33)
Here

\[ W_T(E_k) = \sum_{j=1}^{N} W_j(E_k) \]  

(4.34)

For convenience of calculation, we assume that

\[ \Gamma = \sum_{j=0}^{N} W_j(E_k) \]  

(4.35)

here a virtual \( W_0(E_k) \) is used.

So we can rewrite (4.33) to

\[ P(\tau) = \Gamma \exp \left( - \int_0^{\tau} \Gamma dt \right) = \Gamma e^{-\Gamma \tau} \]  

(4.36)
and free time is decided as
\[ \tau = -\frac{\ln(r_1)}{\Gamma} \] (4.37)
here \( r_1 \) is a random number between 1 and 0.

### 4.3.2 Drift Process
In drift process, change of movement statues in free time \( \tau \) is,
\[ \Delta k = -\int_{t}^{t+\tau} \nabla H dt' \] (4.38)
here \( H \) is total energy of the particle. So\[ H = E_k - e\varphi(r) \] (4.39)
here \( E_k \) is kinetic energy and \( e\varphi(r) \) is potential energy. When a uniform electric field \( \mathbf{F} \) is applied,
\[ \Delta k = -\frac{eF}{\hbar} \tau \] (4.40)

### 4.3.3 Scattering Process
Firstly one of several scattering mechanisms must be chosen. We give a definition to
\[ \Lambda_n(E_k) = \frac{\sum_{j=1}^{n} W_j(E_k)}{\Gamma} \] (4.41)
Then we use a random number \( r_2(0 < r_2 < 1) \) to judge as whether it satisfy\[ \Lambda_{n-1}(E_k) < r_2 \leq \Lambda_n(E_k) \] (4.42)
If (4.42) is satisfied, \( n^{th} \) scattering mechanism will be chosen. Then movement statues \( \mathbf{k}' \) after scattering must be chosen. Length of vector \( \mathbf{k}' \) can be determined by conservation of energy. For an isotropic scattering, we use two random numbers \( r_3, r_4 \) to determine angle after scattering.
\[ \varphi' = 2\pi r_3 \]
\[ \cos\theta' = 1 - 2r_4 \] (4.43)
Then these angles are used to determine the components of \( \mathbf{k}' \).
\[ k'_x = k'\sin\theta'\cos\varphi' \]
\[ k'_y = k'\sin\theta'\sin\varphi' \]
\[ k'_z = k'\cos\theta' \] (4.44)

### 4.3.4 Drift Velocity
Drift velocity of one carrier at point \( \mathbf{k} \) should be
\[ \mathbf{v} = \frac{1}{\hbar} \nabla_k E_k \] (4.45)
So the average velocity during free time $\tau$ should be

$$\langle v \rangle \tau = \frac{1}{\hbar} \frac{\Delta E_k}{\Delta k}$$

(4.46)

$\Delta E_k$ and $\Delta k$ are change of energy and momentum during free time $\tau$.

So,

$$\langle v \rangle \tau = -\frac{\Delta E_k}{eF\tau}$$

(4.47)

For the total time $T$.

$$\langle v \rangle_T = \frac{1}{T} \sum_{j=1}^{N} \langle v \rangle_{\tau T} = -\frac{1}{eFT} \sum_{j=1}^{N} \Delta E_k = -\frac{1}{eFT} \sum_{j=1}^{N} (E_f - E_i)$$

(4.48)

$E_i$ and $E_f$ stand for the start and end of each free time.

Mobility here, should be

$$\mu = \langle v \rangle_T / F$$

(4.49)

### 4.4 Premise of Monte Carlo Method Calculation

Here let us review mobility simulation conducted in Chapter 3. In that section, a calculation conducted by fitting shows us that deformation potential scattering limits mobility of 2DHG at GaN/AlGaN heterostructure most. Deformation potential scattering approach the value of total mobility at almost any temperature in our measurement.

On account of this and for the convenience of calculation, we firstly conduct a Monte Carlo simulation on deformation potential as Fig 4.1. The constants in this simulation are referred to [2], and initial conditions are: electrical filed strength is set to be $5 \times 10^7$ V/m, which should be no effect on results if time of calculation is long enough; initial energy is set to be 0.1 eV, which also should not concern the results, when time of calculation is long enough, for carriers absorb enough energy in the electrical field. Direction of momentum is set to be $+x$, for the convenience of calculation, and also will not influence on the results.

As a short revision of the process in this chapter above, a simple image of our calculation is shown in Fig 4.2.
1) Giving initial energy

\[ W(k) = \frac{2n \Xi_k^2 k_B T_L}{\hbar c_L} N(E_k) \]

\[ \tau = -\frac{\log r_1}{W(k)} \]

2) Calculation for scattering rate and free time

3) Giving a uniform electric field

\[ d k_x = \frac{eF}{\hbar} \cdot \tau \]

4) Calculation for increment of momentum in drift process

\[ E' = E + E_{phonon} \]

\[ E' = E - E_{phonon} \]

5) Deciding energy after scattering

\[ k = \sqrt{2E'm^*/\hbar^2} \]

\[ x' = 2\pi r_2 \]

\[ k_x' = \cos \varphi, k_y' = \sin \varphi \]

\[ k_x'^2 + k_y'^2 = 2E'm^*/\hbar^2 \]

6) Deciding momentum

Fig 4.2 Image of Drift Process Simulation
4.5 Results of Monte Carlo Method Calculation

Results of our calculation is shown as Fig 4.3.

![Fig 4.3 Result of Monte Carlo Method](image)

Red dotted line in this figure, shows simulation results of Monte Carlos method. Green solid line, shows fitting results of mobility. The two lines show same trend, but not close enough. Possible reason for this difference, may be the uncertainty of physical constants in initial conditions.

Firstly, compared to effective mass of electrons in 2DEG, effective mass of holes in 2DHG do not have a generally acknowledged value. In our calculation we use $m^* = 0.24m_0$, for this is the result in mobility fitting, but as referred as [3], different reports of effective mass are there.

Secondly, convergence may not be enough. As introduced in Chapter 1, convergence is needed in order to obtain the final result. However, right result may be not obtained in each calculation model, because random values are used in this method, and it will lead to uncertainty of the results. In order to solve this problem, times of simulation, which here should be scattering must be more enough, but it will be limited by the hardware conditions. We tried best in laboratory computer, but still found that convergence might be not good enough, which lead to an error in calculation.

However, in this simulation, we can confirm the decreasing trend of mobility with
increasing temperature and same order with mobility fitting, considering the errors.

**4.6 Influence of Initial Conditions**

As mentioned above, electric field in initial conditions should not effect on results of mobility, due to independent of physical identity of mobility in materials. Here we tried to use different electrical field to complete the calculation, in order to confirm the effect of electrical field at room temperature, whose result is shown in Fig 4.4.

![Fig 4.4 Mobility Dependence on Electrical Field](image)

In lower electrical field, mobility simulation results show higher value, but it is thought that result here did not convergence. On higher electrical field, results show certain values, which are approximately $10\sim20\ \text{cm}^2\text{/Vs}$. The values are close to experiment results.

In our simulation, effective mass obtained from fitting of results of Hall Effect measurements. We tried another simulation by using 10 times of this effective mass, in order to confirm the effect of effective mass in this simulation. Results of simulation by using $m=2.4m_0$ are shown in Fig 4.5. Lower mobility in this graph can be confirmed, and it convergence in a relatively lower electrical field.

We also tried to change the initial momentum of carrier (direction, magnitude), and then no apparent change in results can be confirmed. Motilities are still $10\sim20\ \text{cm}^2\text{/Vs}$, and final energy is about $10000\sim20000\ \text{eV}$. 

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4.7 Further Research about Mobility of 2DHG

To obtain a relatively high mobility, is thought to be important in further application of 2DHG. As the mobility is limited by deformation potential, a proper method to decrease it is required.

According to well-known Fang-Howard model, effective quantum well width should be

\[ w \propto \frac{m^*}{P_{2DHG}^3} \]  

(4.50)

where \( P_{2DHG}^3 \) is the 2DHG density.

Deformation potential scattering is thought to be proportional to effective quantum well [5], so it should be important to decrease 2DHG density, only considering mobility. As stronger polarization will lead to high 2DHG density, less aluminum in AlGaN is needed to realize this.
Reference


Chapter 5: Surface Passivation in GaN Structure
5.1 Passivation in GaN Related Structures

To obtain good electrical characteristics, passivation is thought an important part in device. Insert of passivation can sometimes greatly improve device characteristics.

In GaN related materials, passivation have been an important theme for long time. Many materials for passivation are reported in both surface and interface, and electrical properties were reported. [1-3]

In this research, passivation with SiO$_2$ on $n$-GaN by TEOS and EB will be introduced.

5.2 Ohmic Contact on $n$-GaN

This experiment is started with obtaining Ohmic contact on $n$-GaN materials, for it is necessary to have an Ohmic contact on samples, to ensure signals in this sample can be obtained.

As mentioned in Chapter 3, SPM treatment give bad influence to surface of GaN materials, only HF was used in the pre-process. Ti (15 nm)/Al (60 nm)/Mo (35 nm)/TiN (50 nm) multi-layer was sputtered in $n$-GaN samples, and CTLM patterns are made in this samples. This pattern is made to measure sheet resistance [4], but calculation of resistance is neglected here. The samples were heat-treated in RTA for 1 minute at different temperature.

![TCLM Pattern](image)

*Fig 5.1 TCLM Pattern*

$IV$-characteristic is measured by using probes, and two probes are set to inner and outer
contact of this pattern. To illustrate, data of $a_1=90 \, \mu m$, $d=30 \, \mu m$ is shown in Fig 5.2.

Fig 5.2 IV characteristic result of TCLM pattern

At 700 °C nitrogen ambient, an IV characteristic close to Ohmic is obtained. In further experiment, this temperature will be used for heat treatment.

5.3 Structure of Sample

A sample shown as Fig 5.3 is used for this experiment. 100 nm silicon dioxide is made by EB and another sample by TEOS, then Ti/Al/Mo/TiN contact was add on a side where silicon dioxide had been removed. Another Al contact was added to the top of silicon dioxide.

Fig 5.3 Structure of sample

5.4 Experiment Steps
Process of this experiment is as: after cleaning in 20% HF for 2 minutes, firstly a 100-nm SiO$_2$ is added to $n$-GaN, by TEOS, and another same sample was made by EB. Liftoff procedure was conducted here, in order to conduct wet etching for SiO$_2$ in next step. After these, sample with resist was added with Ti/Al/Mo/TiN contact for Ohmic electrode. Then the sample was treated under acetone and ethanol to remove resist and metals attached to it. Here, the sample was conducted heat treatment first time at 700 °C for 1 minute.
nitrogen ambient, in order to obtain Ohmic contact. Then aluminum was added to this sample on its surface, another pattern was used for wet etching of aluminum, in order to limit aluminum only appear on top of silicon dioxide in this structure. Finally, the sample is treated in forming gas for 30 minutes at 420°C, for forming of aluminum contact.

Fig 5.5 CV characteristics of TEOS sample

Fig 5.6 CV characteristics of EB sample
5.5 C-V Characteristic

C-V characteristics of the two samples have been obtained by probe, shown as Fig 5.5 and Fig 5.6.

Comparing the two graphs, we can find obviously, that EB sample has a better quality, for a stable characteristic in high frequency, and no hysteresis showed here. Hysteresis in CV characteristics is usually treated as an evidence of the existence of traps, which leads to another evidence of existence of dislocations. At least in our experiments, silicon dioxide made by TEOS, can be treated better for passivation in GaN-related materials.
Reference


Chapter 6: Conclusion & Towards Future
Detailed conclusion of each chapter is written in that chapter, in this chapter we give a mainly revision and try to connect present researches with future researches.

6.1 Control and Limit of Mobility and Carrier Density

In this thesis, we conducted a series of experiments, with a sample of 2DHG utilizing polarization at AlGaN/GaN heterostructure. Density of holes in this sample is as large as $1 \times 10^{13} \text{cm}^{-2}$, which is the top of world as we know. Maximum 2DHG mobility of 16 cm$^2$/Vs at room temperature was obtained. We gave analyze to this result, and showed deformation potential scattering in transport mechanism, limits the mobility most.

As mentioned in Chapter 3, deformation potential scattering can be lessened by lessening carrier density. It is thought that wider effective quantum well will lower deformation potential scattering.

In a published article of our group, we showed a relationship of sheet carrier density and depth of undoped AlGaN layer. [1] It is thought that polarization changes due to sheet carrier density.

![Fig 6.1 Relationship of sheet carrier density and depth of undoped AlGaN layer](image)
Considering deformation potential should weaken in lower density, we gave a simple method to obtain higher mobility by adjusting depth of undoped AlGaN layer. Absolutely, in practice, we should consider more elements and conditions to decide to use which sample, but we gave a method for more alternative.

6.2 Passivation of GaN Device

Silicon dioxide was chosen in this thesis for experiment of passivation, for its high resistance and convenience of producing. TEOS and EB were tried in this thesis, because the two methods has their own advantage. TEOS is used widely and treated best method for manufacture of silicon dioxide in industry, and EB is comparably used in laboratory for particular structures. In our experiment, EB is treated as a better method to add silicon dioxide to GaN samples. In order to obtain an improved quality of GaN material devices, it is treated indispensable to have a good passivation. Although this part is just a tiny part of this thesis, it needs more researches in future.

6.3 Toward Realize of Monolithic IC

Exist of 2DHG at GaN related material heterojunctions, especially at undoped GaN compounds interface, shows a high possibility of realizing monolithic IC, which was mentioned in Chapter 1. For this goal, further research on GaN related devices utilizing 2DHG need to be conducted.
Reference

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