NEUTRON TRANSMUTATION AND HYDROGENATION STUDY OF Hg$_{1-x}$Cd$_x$Te

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Anomalous Hall behavior of HgCdTe refers to a "double cross-over" feature of the Hall coefficient in p-type material, or a peak in the Hall mobility or Hall coefficient in n-type material. A magnetoconductivity tensor approach was utilized to identify presence of two electrons contributing to the conduction as well as transport properties of each electron in the material. The two electron model for the mobility shows that the anomalous Hall behavior results from the competition of two electrons, one in the energy gap graded region near the CdZnTe/HgCdTe interface with large band gap and the other in the bulk of the LPE film with narrow band gap.

Hg$_{0.78}$Cd$_{0.22}$Te samples grown by LPE on CdZnTe(111B)-oriented substrates were exposed to various doses of thermal neutrons (~1.7 x 10$^{16}$ – 1.25 x 10$^{17}$/cm$^2$) and subsequently annealed at ~220°C for ~24h in Hg saturated vapor to recover damage and reduce the presence of Hg vacancies. Extensive Magnetotransport measurements were performed on these samples. SIMS profile for impurities produced by neutron irradiation was also obtained. The purpose for this study is to investigate the influence of neutron irradiation on this material as a basis for further study on HgCdTe$^{74}$Se. The result shows that total mobility is observed to decrease with increased neutron dose and can be fitted by including a mobility inverse proportional to neutron dose. Electron introduction rate of thermal neutron is much smaller than that of fission neutrons. Total recovering of the material is suggested to have longer time annealing. Using Kane’s model, we also fitted carrier concentration change at low temperature by introducing a donor level with activation energy changing with temperature.
Results on Se diffusion in liquid phase epitaxy (LPE) grown HgCdTe epilayers is reported. The LPE Hg\(_{0.78}\)Cd\(_{0.22}\)Te samples were implanted with Se of \(2.0 \times 10^{14}/\text{cm}^2\) at 100keV and annealed at 350-450°C in mercury saturated vapor. Secondary ions mass spectrometry (SIMS) profiles were obtained for each sample. From a Gaussian fit we find that the Se diffusion coefficient \(D_{\text{Se}}\) is about one to two orders of magnitude smaller than that of arsenic. The as-implanted Se distribution is taken into account in case of small diffusion length in Gaussian fitting. Assuming a Te vacancy based mechanism, the Arrhenius relationship yields an activation energy 1.84eV.

Dislocations introduced in HgCdTe materials result in two energy levels, where one is a donor and one is an acceptor. Hydrogenation treatment can effectively neutralize these dislocation defect levels. Both experimental results and theoretical calculation show that the mobility due to dislocation scattering remains constant in the low temperature range (<77K), and increases with temperature between 77K and 150K. Dislocation scattering has little effect on electrical transport properties of HgCdTe with an EPD lower than \(10^7/\text{cm}^2\). Dislocations may have little effect on carrier concentration for semiconductor material with zinc blende structure due to self compensation.
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CHAPTER 1

INTRODUCTION

1.1. Overview

This thesis reports preliminary results of neutron transmutation doping and hydrogenation of molecular beam epitaxy (MBE) grown mercury cadmium telluride (HgCdTe) on silicon (Si). The results of this work are divided into six chapters. Chapters 1 provides a comprehensive overview of this thesis. Chapter 2 introduces characterization and experimental methods including transport and glow discharge plasma apparatus. Chapter 3, 4 and 5 discuss the results of the neutron transmutation doping study. Chapter 3 covers the theoretical aspects of the magnetoconductivity tensor analysis, which is then utilized to extract individual carrier information in mixed conduction based on magnetic field dependent transport measurements. Mixed conduction of two electrons from a graded layer of liquid phase epitaxy (LPE) grown HgCdTe is proposed to explain the anomalous Hall behavior observed in this material. The effects of neutron irradiation on the anomalous Hall behavior are also examined. This analysis is also used in Chapter 4 to analyze the transport results presented in the chapter.

Chapter 4 covers the results of the neutron transmutation study of HgCdTe material as a basis for neutron transmutation p-type doping. Samples were exposed to various amounts of thermal neutron flux, and the effects of thermal neutron irradiation damage on the transport properties and recovery annealing are investigated. Kane’s $k \cdot p$ theory is used to calculate the Fermi level of n-type material, and a model incorporating a pinning behavior of the donor level is used to describe the anomalous behavior of Hall electron concentration at low temperature.
Chapter 5 examines selenium (Se) diffusion in HgCdTe. The purpose of this study was to investigate the thermal stability and diffusion mechanisms of Se in HgCdTe. Samples implanted with Se were annealed at various temperatures, and the diffusion coefficient of Se was obtained by Gaussian fitting the SIMS depth profile of Se concentration was found to satisfy an Arrhenius relationship. A method for fitting the diffusion coefficient for small diffusion length is also described.

Chapter 6 covers the preliminary results of a hydrogenation study on MBE grown HgCdTe/Si material with threading dislocations. Two samples were treated by the glow discharge plasma method in two successive runs. Hall measurements were obtained after each hydrogenation. The effects of hydrogenation on the sample transport properties are presented and discussed. Both experimental results and theoretical calculations show that electron mobility resulting from dislocation scattering is a constant in the low temperature regime, and increases with temperature at higher temperatures. A model of two energy levels introduced by threading dislocations are used to describe the experimental results.

1.2. Background of Hg$_{1-x}$Cd$_x$Te Material and Devices

1.2.1. Historical Aspects

It has been almost five decades since the first report of the semiconductor ternary compound HgCdTe (MCT) in 1959 [1]. With the development of new material growth and device fabrication technologies, HgCdTe has become the dominant material system for infrared (IR) sensors. Three properties make it unique among all infrared materials — high quantum efficiency, tailorable energy band gap by varying composition, and favorable recombination mechanisms. The main applications of this material are for space and military purposes, such as space telescopes development, target detection and identification, and threat warning.

Early MCT materials were grown by bulk methods. Although not suitable for fabricating large focal plane arrays (FPAs) due to defects, bulk materials are still used for photoconductor and small photovoltaic detectors. Bulk materials are usually grown by three methods:
solid state recrystallization [2, 3], the Bridgman [4], and the traveling heater method [5]. The desire for large FPAs and higher quality devices with enhanced capabilities led to the development of various epitaxial growth methods in the last two decades: these are liquid phase epitaxy (LPE) [6, 7], metal-organic vapor phase epitaxy (MOCVD) [8], and molecular beam epitaxy (MBE) [9, 10]. Due to its well-developed growing and processing techniques, LPE materials are being grown routinely for large FPAs. Double-layer heterojunction devices are also made with LPE material. But the LPE method has limitations in controlling the composition and doping profile for multi-layer structures, whereas MBE technology provides better control of these properties and has the capability of growing complex structures. These advantages have made MBE the most attractive method for developing the latest generation of IR detectors. Vast resources are being invested for acquiring premium MBE material and related technologies such as doping and alternative substrates.

Production of the first generation photoconductor devices began in the late 1970s. Signal processing in the element, or SPRITE detectors [11] used time-delay and signal integration techniques, leading to improvement in detection systems compared to early photoconductors. The second generation devices began with FPAs of photodiodes in the 1980s. The advantages of photodiode detectors are high impedance, low power dissipation and high-frequency operation.

Current interest, as well as future trends, concentrates on a third generation of infrared sensors. Third generation usually refers to large arrays with enhanced capabilities, e.g., multi-spectral detectors, high performance uncooled systems, and low cost uncooled imagers [12]. Two-color 20µm unit-cell HgCdTe/CdZnTe triple layer heterojunction 1280×720 FPAs [13] and hybrid FPAs as large as 2048×2048 elements [14] have been reported. Two main types of hybrid MCT FPAs are the front-illuminated loophole configuration [15] and the back-illuminated bump-interconnected configuration [16]. The front-illuminated configuration has the advantage of more stable thermomechanical properties but is not suitable for band gap
engineering. In the back-illuminated configuration, both the detector and read-out integrate circuit processing are optimized. Figure 1.1 shows typical architectures of the two types.

![Figure 1.1. MCT hybrid FPA architecture of (a) front-illuminated loophole, and (b) back-illuminated bump-interconnection.](image)

Despite the fact that MBE-grown HgCdTe epilayers have become the most attractive candidate for third generation detectors, there are many difficulties to overcome. These include p-type doping and alternative substrates, which are the motivation of this research and will be detailed in section 1.3.

1.2.2. Band Structure and Transport Properties

The unique features of HgCdTe band structure and its transport properties deserve a brief account for a better understanding of this work. The binary compounds HgTe and CdTe are mutually soluble in arbitrary proportion, forming the single phase disordered zinc blende ternary alloy Hg$_{1-x}$Cd$_x$Te with the cadmium mole fraction $x$ covering the entire range from 0 to 1. The lattice constant of HgTe is 6.462Å which increases almost linearly with $x$ to that of CdTe, 6.482Å [17]. The temperature variation of the lattice parameter is also very small. These properties are very important for growing high quality heterostructures
in band gap engineering. Band structure models for HgCdTe were originally extended from that of gray tin proposed by Grove and Paul [18]. It is widely accepted [19, 20] that, as shown in figure 1.2, HgTe is a semimetal with zero band gap and CdTe is a wide band gap semiconductor. At \( x \sim 0.15 \), the material system changes from a semimetal structure to a semiconductor. At wave vector \( k = 0 \), the conduction band possesses a \( \Gamma_6 \) symmetry. The valence bands have \( \Gamma_8 \) symmetry and separate into a heavy hole band and light hole band which are degenerate at \( k = 0 \). The spin-orbit split-off band exhibits \( \Gamma_7 \) symmetry. The band gap \( E_g \) is determined by energy difference \( \Gamma_6 - \Gamma_8 \) at \( k = 0 \).

\[
\begin{align*}
E_0 &= E_{\Gamma_6} - E_{\Gamma_8} = -0.3 \text{eV} \\
\Delta &= E_{\Gamma_8} - E_{\Gamma_7} = 1 \text{eV} \\
E_0 &= E_{\Gamma_6} - E_{\Gamma_8} = 1.61 \text{eV} \\
\Delta &= E_{\Gamma_8} - E_{\Gamma_7} = 0.81 \text{eV}
\end{align*}
\]

Figure 1.2. Band structure of Hg\(_{1-x}\)Cd\(_x\)Te for various \( x \) at \( T=0K \) and \( k=0 \).

The increase of the direct energy gap, \( E_g \), with composition \( x \) for \( x > 0.15 \) enables the material to detect IR radiation in the 1-20\( \mu \)m region. This is one of the unusual properties that makes this material system most interesting for infrared sensors. In contrast to most other semiconductor materials, the band gap of HgCdTe increases rapidly with temperature for small \( x \). The temperature dependence of \( E_g \) given by Seiler et al [21] and widely used, is

\[
E_g = -0.302 + 1.93x - 0.81x^2 + 0.832x^3 + [5.35(1-2x)(10^{-4})(-1822+T^3)/(255.2+T^2)].
\]  \( (1) \)
The conduction band, light hole valence band and split-off band also show nonparabolicity. These properties are successfully described by Kane’s model derived for InSb [22]. According to Kane’s model based on three bands, the conduction band can be described as

$$\gamma(E) = E(1 + \frac{E}{E_g}) = \frac{\hbar^2 k^2}{2m_e}. \quad (2)$$

where the electron effective mass $m_e$ depends on wave vector and is given by $m_e \approx (3E_g/2E_P)m_0$ [20], where $E_P$ is the momentum matrix element expressed in terms of energy. An empirical expression for $E_P$ is

$$E_P = (18 + 3x)(eV).$$

This expression gives a very small electron mass, e.g., $\sim 8 \times 10^{-3}m_0$ for $x = 0.22$, where $m_0$ denotes free electron mass, in good agreement with results from magneto-optical and magneto-transport experiments [23, 24]. The small electron effective mass results in a very large electron mobility. Since $\mu_e = \tau_e/m_e$, electron mobilities as high as $3 \times 10^5 (cm^2/Vs)$ have been reported for LPE grown Hg$_{0.78}$Cd$_{0.22}$Te [25]. The heavy hole effective mass, $m_{hh}$, is believed to range from 0.28$m_0$ to 0.7$m_0$ [26, 18, 24] and experiments show no dependence of $m_{hh}$ on composition. The heavy hole mobility $\mu_{hh}$ is typically in the range of 100-1400 $cm^2/Vs$ at 77K for $x=0.2$, and decreases with net hole concentration [27, 28, 29]. As a consequence of the small electron-to-heavy-hole effective mass ratio, for n-type HgCdTe, the Fermi energy $E_F$ lies very close to the conduction band at low temperature. The LPE n-type samples used in this study have a moderate electron concentration ($\sim 10^{14}/cm^3$) with $x = 0.22$. According to calculation, the Fermi level lies near the conduction band for temperatures lower than 30K.

Undoped HgCdTe materials usually contains residual donors even after receiving a standard annealing. Those donors have near-zero activation energy and thus are ionized at temperatures lower than 4K. This makes it difficult to measure the intrinsic carrier densities in the low temperature range.
1.3. Motivations

Although tremendous progress has been made in material growth and processing technologies, some properties of this material are not yet well understood, and challenges still remain in acquiring both higher quality materials and cutting-edge device technologies.

Transport measurements are usually employed to obtain semiconductor material parameters such as carrier type, resistivity, carrier and dopant concentration, and carrier mobility. But mixed conduction makes the transport data difficult to interpret. Anomalous Hall behavior is a transport phenomenon where the temperature dependence of Hall mobility or Hall coefficient deviate from the classical behavior as a consequence of mixed conduction. One common anomalous Hall behavior observed in p-type HgCdTe materials is due to the large $\mu_e$ to $\mu_h$ ratio, and is identified by a "double crossover" feature, where the Hall coefficient changes sign twice in the low temperature range [30]. In contrast, anomalous Hall behavior in n-type material is identified as a peak in the temperature dependence of the mobility or Hall coefficient. Although it is accepted that mixed conduction accounts for the anomalous Hall behavior, there is no agreement on the origin of the multiple carriers. Understanding the physics behind this phenomenon not only is important for correctly interpreting the transport data and describing the transport properties, but it also helps determine the electrical and optical properties of the material. As one part of the transmutation doping study, the effect of neutron irradiation on this anomalous behavior was investigated. The conductivity tensor analysis was used in this case for delineating the effect of each carrier on the transport properties, allowing for a more concise model of the anomalous behavior.

Most of the difficulties in HgCdTe originate from the volatile nature of mercury, which makes both growing and processing extremely difficult. The high Hg diffusivity creates a graded junction in high temperature processes, which severely degrades device performance. Particularly in the HgTe/HgCdTe superlattice, annealing at even a moderate temperature ($225^\circ C$) can totally destroy the structure [31]. In addition, annealing is usually performed in a sealed ampoule with mercury vapor to avoid the formation of excess Hg vacancies. Mercury
vapor pressure can reach \( \sim 4\text{atm} \) at 450\(^\circ\)C and \( \sim 8\text{atm} \) at 500\(^\circ\)C. Given that Hg is toxic, the high Hg vapor pressure is extremely dangerous and should be avoided if possible. But current p-type doping techniques requires high temperature activation. Arsenic (As) has grown in popularity as a p-dopant because of its low diffusivity. However, arsenic is amphoteric within the HgCdTe lattice, occupying both the metal and nonmetal sites, resulting in both donor and acceptor characteristics [32, 33], respectively, and thus requires complex deposition and annealing schemes to activate the p-type dopants. For example, studies have shown that arsenic(As)-doped in LPE grown HgCdTe under Hg-rich condition can be 100% activated as a p-type dopant [32], but in the MBE process it remains problematic [34, 35, 36]. Post growth annealing at high temperature, typically 500\(^\circ\)C, is required to activate the As atoms at the Te sites. But this high temperature annealing will result in the serious problems mentioned above. To assure that As will only reside on the nonmetal sites, two techniques, elemental transmutation doping (TD) and neutron activated elemental transmutation doping (NTD), were recently proposed [37]. In the case of TD, the radioactive isotope \(^{75}\text{Se}\) is incorporated into HgCdTe, \textit{in situ} or \textit{ex situ}, and allowed to decay naturally to \(^{75}\text{As}\). In the case of NTD, a HgCdTe\(^{74}\text{Se}\) alloy (with \(^{74}\text{Se}\) at dopant level) is irradiated by a thermal neutron flux. After neutron capture, The \(^{74}\text{Se}\) atoms are transmuted into \(^{75}\text{Se}\) and subsequently decay to \(^{75}\text{As}\). Because \(^{75}\text{Se}\) is group VI element, it only occupies the Te site and the resulting \(^{75}\text{As}\) will remain at this position. This work will concentrate on the thermal neutron irradiation of HgCdTe as a basis for future research of transmutation doping.

The mobility of Se in a HgCdTe lattice is another concern, if neutron transmutation doping is employed. In addition, this feature is also of interest in the development of new substrate buffer layers containing Se. In this work, the first Se diffusion behavior in HgCdTe is reported. Methods of chalcogen self-diffusion can be utilized to analyze the diffusion mechanisms of Se since Se is group VI element.

Another difficulty in HgCdTe comes from MBE growth of HgCdTe/Si. Lattice matched CdZn\(_{0.04}\)Te is widely used as a substrate for both LPE and MBE growth of HgCdTe due
to a better surface morphology and smaller dislocation densities in the resulting HgCdTe epilayer than for CdTe substrate [38, 39]. Dislocation densities as low as $5 \times 10^4 \text{cm}^{-2}$ are reported in MBE grown HgCdTe/CdZnTe [40]. But as size of MCT hybrid FPAs increases, thermal expansion mismatch between the Si chip and CdZnTe substrate becomes a serious concern, and the thermal reliability of the array is compromised. Thus, Si is a natural choice as an alternative substrate. Additional reasons for using Si as a substrate are its availability in large size, good mechanical properties, and much lower cost than CdZnTe substrate. But MCT grown directly on Si suffers from high dislocation density due to the 19% lattice constant mismatch between MCT and Si. Dislocations can thread into the surface and junctions, and degrade device performance. For example, the $R_0A$ product, a measure of the detection properties, is found to decrease dramatically with dislocation density, particularly at temperature lower than 78K [41]. At 77K for electric fields near $3000 V/cm$, dark current is proportional to dislocation density for densities between the low-$10^5$—low-$10^7 \text{cm}^{-2}$ range [42]. The effect of dislocations on mobility comes from the dangling bonds along the dislocations which tend to pair with electrons and behave as acceptors and trap centers. Defect centers with dangling bonds paired with electrons become negatively charged and will contribute to scattering.

Hydrogenation provides a promising method to reduce the defect scattering. Hydrogenation is the process of introducing hydrogen (deuterium) atoms into semiconductor materials. The single electron of hydrogen (deuterium) atoms can pair with the dangling bonds of dislocations, hence reducing the defect effect. Our preliminary results of hydrogenation passivation are presented in this thesis.
CHAPTER 2

EXPERIMENTAL ASPECTS

2.1. Hall Measurement

The Hall effect is a powerful tool to characterize the electrical transport properties of conductors or semiconductor materials. Edwin Hall discovered this effect in 1879 [43] and presented it in his doctoral thesis. Carriers moving at a right or oblique angle to a magnetic field will be deflected due to the Lorentz force, resulting in a potential difference across a conducting material. From measurements of this Hall voltage and the material resistivity, conduction carrier information, such as mobility, concentration and magneto-conductivity, can be obtained. There are two sample configurations in Hall measurements—Standard Hall configuration and Van der Pauw configuration. The advantages and disadvantages of each will now be discussed.

2.1.1. Standard Hall Configuration

Figure 2.1 shows a standard Hall configuration. A current $i$ runs through a long rectangular strip of length $l$. The thickness $t$ and width $w$ are much smaller than the length so that current flows parallel to the edge of the strip.

As electrons are deflected from the direction of current flow by a magnetic field $B$ which is perpendicular to the current direction, a Hall field, $\varepsilon_H$, is built up in the transverse direction to balance the Lorentz force, or

$$e\varepsilon_H = eBv_x,$$

(1)

where $v_x = -\varepsilon_x \mu_e$ is electron drift velocity. $\varepsilon_x$ is electrical field in the $x$ direction and $\mu_e$ is electron mobility. The Hall voltage is given by

$$V_H = \varepsilon_H w = -B\mu_e\varepsilon_x w,$$

(2)
Figure 2.1. Standard Hall configuration.

and the Hall coefficient, $R_H$, is defined by

$$\epsilon_H = R_H J_x B \quad \text{or} \quad V_H = R_H i B / t. \quad (3)$$

From equation 2 and 3, we have

$$R_H = -\mu_e \varepsilon_x w t / i = -\mu_e \varepsilon_x / J_x, \quad (4)$$

where $J_x$ is current density in the $x$ direction and $n$ is electron density. If the conductivity is given by $\sigma = n e \mu_e$, then

$$J_x = -n e v_x = n e \mu_e \varepsilon_x = \sigma \varepsilon_x \quad (5)$$

Finally, the Hall coefficient for a single carrier n-type sample is given by

$$R_H = -\frac{1}{ne}. \quad (6)$$
Similarly for p-type semiconductors,

\[ R_H = \frac{1}{pe}. \]  

(7)

The sign of Hall voltage indicates whether the sample is n-type or p-type. If the electrical current and magnetic field are configured as in figure 2.1, \( V_H \) (or \( R_H \)) will be positive for p-type (holes) and negative for n-type (electrons). Conductivity by electrons or holes \( \sigma = ne\mu_e \) or \( \sigma = pe\mu_p \) is related to \( R_H \) by

\[ |R_H|\sigma = \mu. \]  

(8)

By measuring the Hall voltage and conductivity, one can calculate the Hall coefficient, carrier concentration and mobility from equation 6 and 8. In actual measurements, contact asymmetry must be considered. This can be reduced by averaging the values for \( V_H \) obtained by reversing the current and/or magnetic field. Current-voltage (\( I-V \)) measurements should also be performed to assure that the sample being measured is operating in the ohmic regime.

2.1.2. Van der Pauw Configuration

Van der Pauw Hall measurement [44] provides a method to characterize lamella samples with irregular geometry if they meet the following requirements:

(i) the contacts on the sample are sufficiently small,

(ii) the contacts are on the periphery of the sample, and

(iii) the lamella is of uniform thickness \( t \) and free of voids.

Theoretically, the Van der Pauw method will apply for arbitrary geometry and arbitrary contact location as long as the above conditions are met. A cloverleaf as shown in Figure 2.2 is the preferred geometry for the Van der Pauw method due to its small effective contact size. However, a cloverleaf is hard to fabricate and the typical geometry is a square or a rectangle with contacts on the corners.
If current $i_{12}$ is applied to contacts 1 and 2 and the potential drop $V_3 - V_4$ is measured across contacts 3 and 4, $R_{12,34}$ is defined as

$$R_{12,34} = \frac{V_3 - V_4}{i_{12}}.$$  

Similarly we define

$$R_{14,23} = \frac{V_2 - V_3}{i_{14}}.$$  

Van der Pauw proved that resistivity of the lamella, $\rho$, fits the Van der Pauw equation 9,

$$exp\left(-\frac{\pi t}{\rho} R_{12,34}\right) + exp\left(-\frac{\pi t}{\rho} R_{14,23}\right) = 1.$$  \hspace{1cm} (9)

After determining $R_{12,34}$ and $R_{14,23}$ experimentally, the Van der Pauw equation can be numerically solved for $\rho$.

The Hall coefficient can also be measured for arbitrary lamella provided it meets the same criteria. If a magnetic field $B$ is induced perpendicular to the lamella surface, $R_{13,24}$ will change by an amount $\Delta R_{13,24}$. Van der Pauw also showed in [44] that the Hall coefficient $R_H$ is given by

$$R_H = \frac{t}{B} \Delta R_{13,24}.$$  \hspace{1cm} (10)
The Hall carrier concentration and Hall mobility can then be calculated using equation 6–8. Just as in the standard configuration, an $I - V$ curve is used to determine the ohmic regime and $R_H$ is obtained by measuring $\Delta R_{24,13}$ for reversed field and current and averaging the results. Van der Pauw method can not be used for tensor analysis because of lack of symmetry.

2.1.3. Experiment Set-up for Hall Measurements

The samples measured were mounted on a copper sample holder within a Janis ST-300 cryostat as illustrated in figure 2.3. Good ohmic contacts are very important to ensure reliable experimental results. Contacts on n-type HgCdTe samples were made by direct indium soldering. The $I - V$ characteristics were obtained at various temperatures to verify ohmic contacts and determine the proper current to use. The cryostat chamber is evacuated to $2 \times 10^{-6} \text{torr}$ by a diffusion pump to minimize heat transfer. Temperatures as low as 77.2K can be achieved for liquid nitrogen and 4.4K for liquid helium. The sample temperature can be controlled to an accuracy of less than ±0.2K.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig23.png}
\caption{Schematic of Janis ST-300 cryostat.}
\end{figure}
Figure 2.4 is diagram of the Hall experimental set-up. Uniform magnetic fields as high as 19KG are obtained by an electromagnet. The voltage in Hall measurements is averaged over all contact combinations and polarities of current bias and magnetic field. A computer-controlled switching device is used to apply current and measure voltage using different contact combination. Data acquisition and control of the voltmeter, current source, switching device, and temperature controller are through an IEEE488 interface. The analog signal of the magnet control panel is interfaced to the computer by a Keithley STA300 A/D converter and KPCI-3101 card. The whole system is integrated by Labview software.

![Figure 2.4. Schematic of Hall experimental set-up.](image)

2.2. Glow Discharge Plasma

A plasma is a partially ionized gas. The term "glow discharge" refers to the state in which the plasma is luminous. A glow discharge can be produced by applying an electrical potential difference between two electrodes in a gas. Figure 2.5 shows the schematic of the DC plasma apparatus. Two parallel plates of 5 × 5cm were mounted in a vacuum chamber and attached to a DC supply. The typical pressure for the plasma process is 2 torr. A high voltage source is connected to the circuit to start the plasma. The spacing of the two parallel
plates is $3cm$. The typical operating voltage of the plasma apparatus is around $400V$. Gas flow through the vacuum tube is metered using the inlet line. A pressure gauge was installed at the inlet side and a thermocouple was placed directly on the metallic sample mount. After ionization by the high starting voltage, ions and electrons are accelerated by the electric field and strike the electrode. Usually only a very small portion of the gas atoms are ionized. The charged species in the plasma is on the order of $10^{10}cm^{-3}$ (only 0.01% of total particles). In a high density plasma reactor, the ion concentration can reach $10^{12}cm^{-3}$.

![Figure 2.5. DC parallel plate plasma reactor.](image)

Glow discharge has been widely used in microelectronic processing such as plasma sputtering deposition and plasma etching. In this work, hydrogenation was used to neutralize the dangling bonds of the dislocation line in the samples studied. Samples to be treated are placed on the cathode. Hydrogen or deuterium gas is fed into the chamber through the gas inlet. Due to its small size, accelerated hydrogen and deuterium ions can penetrate the sample surface to a depth of more than $10\mu m$. The $H^+(D^+)$ injection dosage can be calculated by measuring the current and recording the sputter time. The depth distribution of $H^+(D^+)$ is calibrated by a SIMS depth profile. Figure 2.6 shows a picture of the the apparatus.

If the material on the electrode is insulating, charge accumulates on the surface, the field is reduced during the exposure and the plasma will finally be extinguished. To solve this
problem, a radio frequency (RF) modulation is superimposed on the DC current. In the hydrogenation study of HgCdTe/Si, even though the Si substrate is insulating, the HgCdTe epilayer is conducting so that both DC and RF glow discharge can be used. In DC glow discharge, a conducting clip holds the sample on the electrode and serves as electrical contact to the HgCdTe epilayer without requiring a path through the Si substrate.
CHAPTER 3

INVESTIGATION OF ANOMALOUS HALL BEHAVIOR OF HGCDTE USING MAGNETOCONDUCTIVITY TENSOR ANALYSIS

3.1. Introduction

Classical Hall behavior is usually observed in short wavelength material or n-type bulk HgCdTe. It can be identified by high constant mobility at low temperature, and decreasing mobility as $T^{-\alpha}$ ($1.5 < \alpha < 2$) at higher temperature. In contrast to the classic case, anomalous Hall behavior of HgCdTe refers to a “double cross-over” feature of the Hall coefficient in p-type material, or a peak in the Hall mobility or Hall coefficient in n-type material at temperatures around 100K where devices usually operate. Thus, it is very important to understand the physics behind this behavior and investigate its effect on device performance.

Unlike the classic case, anomalous Hall mobility can not be modeled by taking into account only common scattering mechanisms. Many models have been proposed to explain this behavior. Anomalous Hall behavior in p-type material has been modeled by an n-type inversion layer on the surface [45, 30, 46, 47, 48], where the mixed conduction of holes and electrons results in anomalous peak. Chen’s study [49] of n-type LPE HgCdTe also shows that the anomalous feature remains after surface treatment including anodization and etching by lactic acid or Br-MeOH solution. Chen proposed a model of p-type microscopic inclusions in an n-type matrix. Hyliands’ study [50] of MOVPE p-type HgCdTe on a CdTe substrate revealed that the anomalous feature appears to be related to the interface with the substrate, and can be eliminated after removal of the CdTe substrate and growth interface. Hence, Hyliands suggested that the anomalous behavior in this material is due to contamination at substrate-layer interface.
Regardless of the different models describing the anomalous Hall behavior, it is accepted that this feature results from mixed conduction of multiple carriers. In the present work, the anomalous behavior has been studied in various n-type samples grown by the LPE or MBE methods and it is proposed that the behavior results from the mixed conduction involving two electrons [51]. One of them originates from the bulk of the thin film and the other from the graded layer at the HgCdTe/CdZnTe interface.

3.2. Theoretical Considerations

3.2.1. Transport Theory for Multicarrier System

In deriving equation 6 for the Hall coefficient, it was assumed that one carrier dominates in transport properties. In this case, the Hall coefficient, and Hall mobility are independent of magnetic field. The conductivity \( \sigma \) is defined as the proportionality constant in equation 5, where \( \sigma = ne\mu_e \). However, in many circumstances, more than one carrier contribute to conduction. The experimental Hall mobility, Hall concentration, and Hall coefficient are usually measured and calculated by a one-carrier model in standard practice, which reflect the averaged effect of mixed conduction, resulting in misleading results. For example, in p-type HgCdTe material, the large electron to hole mobility ratio may result in a negative Hall coefficient at intermediate and high temperatures, making the sample look n-type. The measured Hall carrier concentration reflects neither the actual electron concentration, nor the hole concentration. Even for n-type material with multiple conduction electrons, one must be very careful how to interpret the experimental results since the Hall mobility, and Hall concentration are now magnetic field dependent.

Magnetoconductivity tensor analysis has been used in the past to describe magnetic field transport properties [52] of narrow gap semiconductors. In this study it is used to extract individual carrier information and model the anomalous Hall behavior of n-type LPE HgCdTe material.
In general conductivity and resistivity can be defined in terms of a tensor relationship between the current density and electrical field,

\[ \mathbf{J} = \hat{\sigma} \mathbf{E} \]  

(1)

where \( \mathbf{J} \) and \( \mathbf{E} \) are defined as follows:

\[ \mathbf{J} = \begin{pmatrix} J_x \\ J_y \end{pmatrix} ; \quad \mathbf{E} = \begin{pmatrix} \varepsilon_x \\ \varepsilon_y \end{pmatrix} . \]  

(2)

\( \hat{\sigma} \) is described by a \( 2 \times 2 \) matrix in the two dimensional case. For cubic symmetry, this tensor reduces to [53]

\[ \hat{\sigma} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} \\ -\sigma_{xy} & \sigma_{xx} \end{pmatrix} . \]  

(3)

The tensor components can be derived by solving the equation of motion for electrons. Considering the one electron case first, the equation of motion can be written in the form

\[
\begin{align*}
\dot{v}_x &= -(e/m_e) \varepsilon_x - \omega v_y, \\
\dot{v}_y &= -(e/m_e) \varepsilon_y + \omega v_x,
\end{align*}
\]  

(4)

where \( \omega = eB/m_e \). Smith gives a detailed solution to equation 4 in reference [13], in which complex variable \( Z = v_x + iv_y \) is used to simplify the form. After averaging \( Z \) over all collision times \( \tau \), one gets

\[ \bar{Z} = \bar{v}_x + i\bar{v}_y = -\frac{e}{m_e} (\varepsilon_x + i\varepsilon_y) \frac{\tau}{1 - i\omega \tau}. \]  

(5)

Using \( J = -en\bar{v} \), expressions for the current density component can be obtained from the real and imaginary parts:

\[ J_x = \frac{ne^2}{m_e} \left( \frac{\tau \varepsilon_x}{1 + \omega^2 \tau^2} - \frac{\omega \tau^2 \varepsilon_y}{1 + \omega^2 \tau^2} \right) \]  

(6)

and

\[ J_y = \frac{ne^2}{m_e} \left( \frac{\tau \varepsilon_y}{1 + \omega^2 \tau^2} + \frac{\omega \tau^2 \varepsilon_x}{1 + \omega^2 \tau^2} \right) . \]  

(7)
The conductivity tensor components can be determined by comparing equation 1, 3, 6, and 7, and are found to be

\[ \sigma_{xx} = \frac{\tau}{1 + \omega^2 \tau^2}; \quad \sigma_{xy} = -\frac{\omega \tau^2}{1 + \omega^2 \tau^2} \]  

(8)

In multi-carrier systems, the conduction tensor components are obtained by summing over individual carriers. Hence we have

\[ \sigma_{xx} = \frac{\rho_{xx}}{\rho_{xx}^2 + R_H^2 B^2} \approx \sum_{i=1}^{M} \frac{n_i |e| B_i}{B_i^2 + B^2}, \]  

(9)

and

\[ \sigma_{xy} = \frac{R_H B}{\rho_{xx}^2 + R_H^2 B^2} \approx \sum_{i=1}^{M} \frac{n_i e B}{B_i^2 + B^2}, \]  

(10)

where \( \rho_{xx} \) and \( R_H \) are the transverse magnetoresistance and Hall coefficient using the one carrier model, respectively. The resistivity \( \rho_{xx} \) is also the inverse of the conductivity \( \sigma \) defined in equation 5 and can be determined experimentally. The label \( M \) is the number of carrier types, and \( n_i \) and \( B_i \) are the concentrations and critical magnetic fields (the value of \( B \) at the peak position) for the \( i \)th carrier. The mobility for each carrier, \( \mu_i \), can be calculated using the relationship \( B_i = 1/\mu_i \), where we have used \( \mu = e\tau/m_e \) in the above expression. The sign of \( \sigma_{xy} \) is indicative of the type of carrier dominating the transport properties, being negative for electrons and positive for holes.

By judicious choice of \( M \), the magnetic field dependent experimental data can be modeled using standard multivariable fitting programs, allowing \( n_i \) and \( \mu_i \) to be extracted from the fitting variables. The conductivity tensor component \( \sigma_{xy} \) is chosen in this study to fit the experimental data because it provides information about carrier type.

The Hall coefficient is a function of magnetic field in multiple carrier systems. In a two electron system, if the concentration and mobility of the two electrons are given by \( n_1, n_2, \mu_1, \) and \( \mu_2 \), respectively, and taking \( J_y = 0 \), we can obtain the following expression from
equations 6 and 7,
\[
\varepsilon_y = -\frac{(n_1 b + n_2)}{(n_1 b + n_2)^2 + \mu_1^2 B^2(n_1 + n_2)^2} e J_x B,
\]
where \( b = \mu_1 / \mu_2 \). Comparing equation 11 and 3, the Hall coefficient of two electron system is
\[
R_H = -\frac{(n_1 b + n_2)}{(n_1 b + n_2)^2 + \mu_1^2 B^2(n_1 + n_2)^2} e.
\]
Equation 12 shows that the Hall coefficient is magnetic field-dependent for a two electron system. However if \( \mu_1^2 B^2 \) is much smaller than 1, the Hall coefficient becomes
\[
R_H = -\frac{n_1 \mu_1^2 + n_2 \mu_2^2}{e(n_1 \mu_1 + n_2 \mu_2)^2}.
\]

### 3.3. Experiments and Two Electron Model for Mobility

Results of magnetotransport measurements of three samples are presented in this section. Sample information is listed in Table 3.1. Sample 1 and sample 2 are LPE grown Hg\(_{0.78}\)Cd\(_{0.22}\)Te on CdZnTe substrate from the same lot. Sample 2 is irradiated by thermal neutrons with a dose of \( 1.7 \times 10^{16} / \text{cm}^2 \). Sample 3 is MBE grown Hg\(_{0.78}\)Cd\(_{0.22}\)Te on Si substrate with a buffer layer. All three samples were annealed and etched by 0.3% Br-MeOH solution for 1.5 minutes to remove possible contamination from the surface layer. The standard Hall configuration is used in making the measurements. The temperature dependence and magnetic field dependence at various temperatures of the transport properties were measured.

<table>
<thead>
<tr>
<th>Sample #</th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Growth Method</td>
<td>LPE ( \text{Hg}<em>{0.78}\text{Cd}</em>{0.22}\text{Te} )</td>
<td>LPE ( \text{Hg}<em>{0.78}\text{Cd}</em>{0.22}\text{Te} )</td>
<td>MBE ( \text{Hg}<em>{0.78}\text{Cd}</em>{0.22}\text{Te} )</td>
</tr>
<tr>
<td>Treatment</td>
<td>annealed, etched</td>
<td>neutron irradiated, annealed, etched</td>
<td>annealed, etched</td>
</tr>
</tbody>
</table>

**Table 3.1.** Sample growth methods and post-growth treatment received.
Figure 3.1 shows a plot of Hall mobilities vs. temperature for samples 1 through 3. Sample 1 and sample 2 exhibit an anomalous Hall behavior, evidenced by the peak in the mobility at ~100K. Sample 3 exhibits a temperature dependence for the classical mobility. It is also seen that the mobility of sample 2 is different from that of sample 1. As will be discussed in chapter 4, this change in the anomalous peak is caused by ionized impurity scattering due to neutron irradiation, which results in mobility reduction at the low and intermediate temperature range.

![Figure 3.1. Anomalous hall mobility versus classic case.](image)

Figure 3.2 shows plots of conductivity tensor component $\sigma_{xy}$ vs $ln(B)$ at $T = 77K$ for sample 2. Using the conductivity tensor analysis discussed in Section 3.2.1, the carrier concentration and mobility of individual electrons can be extracted. In Figure 3.2 (a) only one electron is used to describe the data, resulting in a poor fit. Figure 3.2 (b) illustrates the results of a fit using $M = 2$, describing two electrons (high mobility (HE) and low mobility (LE)) of differing concentration $n$ and mobility $\mu$. This shows an excellent fit to
the experimental results. Thus, it is seen that two electrons of differing mobility, rather than one, are necessary to describe the magnetic field dependence for this sample at 77K.

A series of magnetic field dependent measurements were also taken on each sample. The results are shown in Figure 3.3 (a) and 3.3 (b) for sample 2. The data were modeled using the tensor analysis at each temperature to determine the temperature dependence of concentration and mobility for each electron. It is seen that, at low temperature ($T < 110K$), $\sigma_{xy}$ vs $B$ can be modeled well using two electrons. However, at higher temperature ($T > 110K$), the higher mobility electron dominates and only one electron is necessary to describe the results.

Using the results obtained from the magnetoconductivity tensor analysis, the Hall coefficient of two electrons can be calculated from equation 13 for small magnetic field,

$$R_H = \frac{-n_{HE}\mu_{HE}^2 - n_{LE}\mu_{LE}^2}{(n_{HE}\mu_{HE} + n_{LE}\mu_{LE})^2},$$

An effective mobility can be calculated by equation 8. In equation 14, $n_{HE}, n_{LE}, \mu_{HE}, \mu_{LE}$ are the concentrations and mobilities extracted from the magnetoconductivity tensor analysis at each temperature. As shown in Figure 3.3 (b), the features of the effective mobility $\mu_{EFF}$, determined from equation 8 and 14, matches the mobility $\mu_{EXP}$ obtained directly from the temperature dependent transport data and modeled using only one carrier. Both $\mu_{EFF}$ and $\mu_{EXP}$ exhibit an anomalous peak at 110K, where the high mobility electron begins to dominate. Separately, however, neither temperature dependence of the individual electron contributions $\mu_{HE}$ or $\mu_{LE}$ exhibit the anomalous behavior. This indicates that the anomalous Hall feature observed results from the competition of two electrons of differing concentration and mobility.

Although sample 3 exhibits classical mobility, the conductivity tensor analysis shows there are also two electrons contributing to conduction, as shown in figure 3.4. The ratio of $\mu_{HE}/\mu_{LE}$ is $\sim 4.8$ for sample 3 but only 2.8 for sample 2. The large mobility ratio of sample 3 makes the higher mobility electron dominate so that it shows classical behavior.
Figure 3.2. Magnetic field dependence of conductivity at $T = 77\text{K}$ for the neutron irradiated sample 2. (a) One electron fit. (b) Two electron fit. Curves LE and HE are the conductivity for electrons with lower mobility and higher mobility, respectively.
Figure 3.3. Two electron model for anomalous Hall behavior of irradiated sample 2. Concentration (a) and mobility (b) are obtained by conductivity tensor analysis for each electron at various temperatures. High mobility electrons dominate for $T > 110K$. 
Figure 3.4. Two electron fitting of MBE grown sample 3 at 77K. The large mobility ratio of two electron results in classical behavior.

The data have also been analyzed [51] using different scattering mechanisms in an attempt to clarify the physical mechanisms responsible for the temperature dependence of the mobility. The main scattering processes considered were ionized impurity, polar optical phonon, and alloy scattering. In calculating the alloy scattering component for this narrow gap material, it was necessary to include the temperature dependence of the effective mass. A model taking into account the presence of electrons in two different conduction channels of differing thickness was used to describe the experimental results. As seen in Figure 3.5, the effective mobility corresponds well to the experimental mobility over the temperature range studied. The conduction channel thicknesses for the fit were 10µm at an average x-value (composition of Cd) of 0.65 for the lower mobility carrier and 40µm at an average x-value of 0.22 for the high mobility carrier. Since it is known that there exists a graded energy gap region starting at the CdZnTe/HgCdTe interface and continuing into the HgCdTe, one can concluded that the lower mobility carrier results from electrons in the graded region.
Thus, the two conduction channels in the LPE film, of differing mass and mobility, give rise to the anomalous increase in the effective one-carrier mobility shown in Figure 3.1.

![Figure 3.5. Two electron scattering for neutron irradiated sample 2.](image)

3.4. Conclusion

A magnetoconductivity tensor approach was utilized to identify the presence of two electrons contributing to the conduction as well as transport properties of each electron in the material. The two electron model for the mobility shows that the anomalous Hall behavior results from the competition of two electrons, one in the energy gap graded region near the CdZnTe/HgCdTe interface with large band gap and the other in the bulk of the LPE film with narrow band gap.
4.1. Introduction of Neutron Transmutation Doping

Damage resulting from high energy electrons, ion implantation, and fission neutrons to HgCdTe have been investigated in detail, but there is limited information about thermal neutron irradiation effects on this material. Since infrared sensors may need to function in hazardous environments including that of thermal neutron irradiation, the resulting damage to devices will affect their functionality and its life time, and should be investigated. Recovery from this damage via thermal annealing is also of interest. Finally, the feasibility of neutron transmutation doping as an alternate means to dope HgCdTe has been recently proposed [37] and should be investigated.

Arsenic is widely used as a p-dopant for HgCdTe grown by various methods due to its low diffusion coefficient. Current arsenic doping techniques concentrate on direct doping, either in situ or ex situ. While this technique has proven successful in liquid phase epitaxy material [54], in molecular beam epitaxy, however, it remains a challenge to growers due to the amphoteric behavior of arsenic, especially when incorporated under Te-rich growth conditions [55, 56]. To avoid the difficulties in direct As doping, two novel indirect doping technique, namely elemental transmutation doping (TD) and neutron activated elemental transmutation doping (NTD), have been proposed by Golding et al [37]. In the case of NTD, a HgCdTe$^{74}$Se alloy is irradiated by a neutron flux. After neutron capture, the $^{74}$Se atoms are transmuted into $^{75}$Se and subsequently decay to $^{75}$As. The two reactions are written as

$$\begin{align*}
^{74}_{34}\text{Se} + n &\rightarrow ^{75}_{34}\text{Se} \\
^{75}_{34}\text{Se} \rightarrow ^{EC}^{75}_{34}\text{Se} &\rightarrow ^{75}_{33}\text{As}. 
\end{align*}$$

(1)
However, the elements Hg, Cd, and Te within the lattice are also irradiated. Their transmutation products and their influence on thermal neutron irradiated HgCdTe material must also be investigated. As a result, this research is concentrated on the influence of thermal neutron irradiation on LPE $Hg_{0.78}Cd_{0.22}Te$ samples. Typical reactions are thermal neutron capture ($n, \gamma$) with some followed by electron capture (EC) or $\beta$ decay:

\[
\frac{A}{Z}X + n \rightarrow \frac{A+1}{Z}X, \tag{2}
\]

\[
\frac{A+1}{Z}X \xrightarrow{EC} \frac{A+1}{Z-1}Y \tag{3}
\]

or

\[
\frac{A+1}{Z}X \xrightarrow{\beta^-} \frac{A+1}{Z+1}Y. \tag{4}
\]

All reactions are accompanied by $\gamma$ emission. Some isotopes, such as $^{113}Cd$, $^{123}Te$, $^{199}Hg$, etc., produce the stable isotopes $^{114}Cd$, $^{124}Te$, $^{200}Hg$, respectively, and do not exhibit EC or $\beta$ decay. However, if these atoms possess a high recoil energy, numerous vacancies and interstitials will result, producing electrically active states in the bandgap. By using the relative neutron capture cross-sections for all isotopes of Hg, Cd, Te, and the natural abundance of each isotope, the numbers of atoms produced for every $^{197}Au$ atom produced in $Hg_{0.78}Cd_{0.22}Te$ alloy are shown in Table 4.1, where the isotope ratios ($\frac{\# \text{final product}}{\#^{197}Au}$) greater than 0.1 are listed. It is seen that the most important new elements produced by neutron irradiation are $^{197}Au$ and $^{203}Tl$. Gold has been reported to be a p-type dopant [57, 58] and thallium to be an n-dopant [59] at metal sites in HgCdTe and will contribute to electrical conduction. Early work has shown that n-type bulk HgCdTe was converted to p-type upon thermal neutron irradiation followed by 1h annealing in mercury-saturated vapor at 200$^\circ$C [60].

Another concern is thermal neutron damage. The fission neutron has an electron introduction rate of $3 - 8/cm$ and mobility damage has been observed [61]. Thus, baseline studies
of the influence of thermal neutron irradiation on HgCdTe material should be performed before proceeding to NTD of the HgCdTe\textsuperscript{74}Se alloy.

The recoil energy of the transmuted atoms on the lattice accounts for most of the irradiation damage. If the recoil energy is greater than the enthalpy sufficient to displace the lattice atoms, point defects such as vacancies, interstitial atoms or even anti-sites may result. For example, the enthalpy to produce a vacancy is 2.2eV at a mercury site and 4.7eV at a cadmium site for Hg\textsubscript{0.8}Cd\textsubscript{0.2}Te material [62]. As seen in Table 4.1, most transmuted atoms are \textsuperscript{113}Cd and \textsuperscript{199}Hg. The recoil energy from the decay reaction 4.1 or 4 is usually less than 1eV and can be neglected. The recoil energy of neutron capture, \( E_r \), can be calculated from the nuclear reaction energy and the conservation of momentum to be

\[
E_r = \frac{E_\gamma^2}{2Mc^2},
\]

where \( M \), \( E_\gamma \), and \( c \) are the nuclear mass, emitted \( \gamma \)-ray energy and speed of light, respectively.

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Product of ((n, \gamma))</th>
<th>Product of decay</th>
<th>Decay half life</th>
<th># final product #\textsuperscript{197}Au</th>
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<tbody>
<tr>
<td>\textsuperscript{111}Cd</td>
<td>\textsuperscript{112}Cd (stable)</td>
<td></td>
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<td>0.2</td>
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<tr>
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<td>\textsuperscript{114}Cd (stable)</td>
<td></td>
<td></td>
<td>146</td>
</tr>
<tr>
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<td>\textsuperscript{124}Te (stable)</td>
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</tr>
<tr>
<td>\textsuperscript{196}Hg</td>
<td>\textsuperscript{197}Hg</td>
<td>\textsuperscript{197}Au (EC)</td>
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<td>\textsuperscript{203}Tl(\beta^-)</td>
<td>46d</td>
<td>0.3</td>
</tr>
</tbody>
</table>

Table 4.1. Main products of thermal neutron irradiation.
Figure 4.1. $\gamma$ energy distribution of neutron capture by $^{113}$Cd (from NNDC).

$I_\gamma$ is the $\gamma$ intensity for a specific transition, and $I_{\text{max}}$ is the $\gamma$ intensity for the strongest transition.

Neutron capture reaction energy is emitted in the form of $\gamma$ radiation which follows a characteristic distribution. Figure 4.1 shows the $\gamma$ energy distribution for neutron capture by $^{113}$Cd. This figure is plotted from the data provided by the National Nuclear Data Center (NNDC).

As calculated from the gamma radiation energy distribution, upon neutron capture more than 40% of transmuted $^{113}$Cd and approximated $\sim$ 60% transmuted $^{199}$Hg have recoil energies high enough (>2.2eV for $^{199}$Hg and >4.7eV for $^{113}$Cd) to be displaced from the lattice point. If Se is incorporated, around 60%-70% will be displaced from lattice site. Some highly energetic recoiled atoms may result in multiple displacements and the total number of displaced atoms can get even larger. As a result, a total concentration of point
defects can reach $10^{17}/cm^3$. Hence the recovery from irradiation damage by annealing is also investigated in this work.

4.2. Experiment

Indium-doped LPE $Hg_{0.78}Cd_{0.22}Te$ samples on CdZnTe (111B)-oriented substrates were provided by DRS Infrared Technologies. SIMS analysis was done in Evan Analytical Group. From SIMS analysis, the indium level was measured to be $2 \times 10^{14} cm^{-3}$. The epilayer thickness for all samples was $55 - 59 \mu m$. Samples from the same lot were irradiated in the NIST Center for Neutron Research. Table 4.2 lists the sample specification and corresponding treatment. Sample 1 was not irradiated and served as a control sample. The initial attempt at neutron irradiation used a thermal neutron flux $1.2 \times 10^{17}/cm^2h$ for 3 minutes. However, as a result of gamma heating at this flux, the temperature of the sample exceeded $100^\circ C$, which melted the sample mounting adhesive. To avoid overheating, sample 2 to 5 were irradiated by neutrons with a thermal flux $1.3 \times 10^{15}/cm^2h$, an epithermal flux $3 \times 10^{11}/cm^2h$, and a fast (fission spectrum) flux $1.8 \times 10^9/cm^2h$, reducing the gamma heating to acceptable levels. The epithermal and fast flux are so small when compared to thermal neutrons that they are neglected in the analysis. After irradiation, all samples except sample 3A were annealed at $220^\circ C$ for 24h in mercury vapor to recover from the irradiation damage[63].

Temperature dependent transport measurements were performed on all six samples to determine Hall mobility and carrier concentration. Each sample was etched in 0.3% Br-MeOH solution for 1-2 minutes. A VDP configuration, as shown in 2.2 (b), was used to make sample contacts. Error analysis on Hall mobility and Hall concentration was carefully performed. SIMS depth profiles were obtained to determine the impurity concentration produced by neutron transmutation.

4.3. Results and Discussion

Magnetotransport measurements show that the unirradiated sample 1 is n-type with an electron concentration of $2 \times 10^{14}/cm^3$ at 77K. All other samples remain n-type after neutron irradiation. The influence of thermal neutron irradiation on the transport properties were
Table 4.2. Sample specification and corresponding post-growth treatment.

<table>
<thead>
<tr>
<th>Sample #</th>
<th>1</th>
<th>2</th>
<th>3A</th>
<th>3B</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>DRS ID (14-01-916- )</td>
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<td>01</td>
<td>03</td>
<td>03</td>
<td>04</td>
<td>05</td>
</tr>
<tr>
<td>Cutoff at 77K (µm)</td>
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<td>10.92</td>
<td>10.91</td>
<td>10.91</td>
<td>10.89</td>
<td>10.91</td>
</tr>
<tr>
<td>Film thickness (µm)</td>
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<td>55</td>
<td>57</td>
<td>57</td>
<td>59</td>
<td>57</td>
</tr>
<tr>
<td>Dislocation density (cm⁻²)</td>
<td>$1.1 \times 10^5$</td>
<td>$1.3 \times 10^5$</td>
<td>$1.3 \times 10^5$</td>
<td>$1.3 \times 10^5$</td>
<td>$1.1 \times 10^5$</td>
<td>$1.2 \times 10^5$</td>
</tr>
<tr>
<td>Neutron flux ($10^{15} cm^{-2} h^{-1}$)</td>
<td>1.3</td>
<td>1.3</td>
<td>1.3</td>
<td>1.3</td>
<td>1.3</td>
<td></td>
</tr>
<tr>
<td>Irradiation time (h)</td>
<td>13</td>
<td>24</td>
<td>24</td>
<td>48</td>
<td>96</td>
<td></td>
</tr>
<tr>
<td>Neutron Dose (Φ) ($10^{16} cm^{-2}$)</td>
<td>No irradiation</td>
<td>1.7</td>
<td>3.1</td>
<td>3.1</td>
<td>6.2</td>
<td>12.5</td>
</tr>
<tr>
<td>Annealing (24h/220°C)</td>
<td>Yes</td>
<td>Yes</td>
<td>No</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
</tbody>
</table>

also investigated. As seen in Figure 4.2, in the entire temperature range of 4-300K, the mobility decreases as the thermal neutron dose is increased. Figure 4.3 shows mobility as a function of neutron dose for those samples at 77K.

According to theoretical studies on scattering mechanisms [64, 27], the mobility of ionized and neutral impurities is inversely proportional to the number of scattering centers, hence also inversely proportional to irradiation dose. This is seen in Figure 4.3 where mobility versus dose is shown for five samples. If $\mu_0$ is the mobility for an unirradiated sample and $\mu'$ is mobility corresponding to irradiation-induced defect scattering, the total mobility $\mu_t$ after irradiation can be written as

$$\frac{1}{\mu_t} = \frac{1}{\mu_0} + \frac{1}{\mu'}.$$  (6)
**Figure 4.2.** Temperature dependence of mobility for five annealed samples shows mobility decreases with increasing neutron dose.

**Figure 4.3.** Mobility vs neutron dose for five samples at 77K. The dashed curve is fitted by including a mobility which is inversely proportional to neutron dose.
Fitting $\mu_t$ in Figure 4.3 results in a relationship between dose and mobility, given by

$$
\mu' = \frac{1.72 \times 10^{21} V^{-1} s^{-1}}{\Phi},
$$

(7)

where $\Phi$ is neutron dose received.

Plot of mobility versus dose for the five samples at other temperatures also show the same behavior as seen in Figure 4.4 for 12K and Figure 4.5 for 100K.

![Graph](image)

**Figure 4.4.** Mobility vs neutron dose for five samples at 12K.

Figure 4.6 and 4.7 plot mobility and electron concentration for samples 3A (unannealed) and 3B (annealed) that were irradiated for 24 hours, compared with unirradiated sample 1. After annealing, the carrier concentration is restored to almost the same level of the unirradiated sample while the mobility does not completely recover. As discussed previously, thermal neutron irradiation can produce a large quantity of vacancies on both Te and metal sites. Some self-interstitial atoms can act as dopants, e.g., Hg interstitials were reported to be donors in this material [65]. From SIMS profiles, the $^{197}$Au reaches concentration of $7 \times 10^{14}$, $1 \times 10^{15}$, and $1.7 \times 10^{15}/cm^3$ for sample 3B, 4 and 5, respectively. In addition, the $^{203}$Tl level
Figure 4.5. Mobility vs neutron dose for five samples at 100K.

Figure 4.6. Temperature dependence of mobility of three samples shows irradiation damage can only be partially recovered by standard annealing ($24h/220^\circ C$).
Figure 4.7. Hall electron concentration of samples 1-3, showing that the carrier concentration can be almost completely recovered after a 24h anneal at 220°C in Hg vapor.

is \( \sim 2 - 7 \times 10^{14}/cm^3 \). Any gold and thallium atoms that remain on the lattice sites will also act as acceptors or donors. Thus, all irradiated samples may be compensated at a moderate to high level depending on the effectiveness of the recovery anneal. Defects produced by irradiation result in a decrease in mobility and increase in net electron concentration. Those defects can be either ionized or neutral.

Figure 4.8 shows the increase of electron concentration with increasing neutron dose at 77K, yielding an electron introduction rate of \( \Delta n_H/\Delta \Phi = 2.3 \times 10^{-3}/cm \). Compared to the rate of \( 3 - 8/cm \) for fission neutrons, this is quite small. This result is very important for the feasibility of neutron transmutation doping. Better recovery of the transport properties may require longer annealing time than standard method (24h at 220°C).

4.4. Analysis of Donor Energy Level

Another interesting result observed is the change of Hall electron concentration at temperatures below 92K. The activation energy of monovalent donors can be estimated using a
Figure 4.8. Electron Hall concentration vs neutron dose at 77K. Dashed line shows linearly fitting of the experimental data with electron introduction rate $2.3 \times 10^{-3}/cm$.

hydrogen atom model, where

$$
\epsilon_d = 2\pi^2 m^*_e q^4 / \hbar^2 \epsilon_0
$$

(8)

where $m^*_e$ is the electron effective mass, $q$ the electron charge, $\epsilon_0$ the low frequency dielectric constant. Since electrons in HgCdTe have a very small effective mass, the typical donor activation energy calculated from expression 8 is less than 0.5meV. Donors with such near-zero energy are ionized below 4K and the electron concentration is constant at low temperatures. However, this is not the case for the irradiated samples, as shown in Figure 4.9. At low temperature, the electron concentration of all irradiated samples increases with temperature and then decreases before going into the intrinsic region. This feature becomes more pronounced as the neutron dose increases.

Careful error analysis shows that fluctuation of carrier concentration due to error in the same set of measurements is $< 1.5\%$ as indicated by the error bar in Figure 4.9. thus, a change of carrier concentration with temperature appears to be due to the activation of
Figure 4.9. Hall electron concentration of four samples with a fitting curve using the shallow donor model with constant activation energy. Values of $N_d$ from fit are $\sim 0.9 \times 10^{14}, 3 \times 10^{14}$ and $7 \times 10^{14}/cm^3$, for sample 3B, 4, and 5, respectively. The activation energy determined by fitting is shown in the figure. Error bars for samples 3B, 4, and 5 indicate that the change of electron concentration cannot be attributed to error.

defect complexes resulting from neutron irradiation. In this work, this unusual temperature dependence of the Hall concentration will be described by a donor level which is pinned to the valence band.

According to the condition of electrical neutrality, the electron concentration can be written as

$$n = n_d + (N_{a0} - N_{d0})$$  \hspace{1cm} (9)

where $N_{a0}$ and $N_{d0}$ are the concentrations of acceptor and shallow donor levels, respectively. $n_d$ is the ionized donor concentration and is given by [66]

$$n_d = \frac{N_d}{1 + 2\exp[(\epsilon_d - E_F)/kT]}.$$  \hspace{1cm} (10)
where $E_F$ is the Fermi level, and $N_d$ is the donor concentration of non-zero activation energy $\epsilon_d$, the energy difference between the conduction band edge $E_c$ and donor energy level $E_d$. If the zero of energy is set at the conduction band edge, then $\epsilon_d = -E_d$. Since the hole concentration is very small in n-type material at low temperature, it is neglected in equation 9. In this study, the temperature dependence of the Hall electron concentration will be used to extract the donor level using equation 9 and 10. Assuming the Hall factor $r_H$ to be unity, the Fermi level can be determined by numerically solving the following equation derived from Kane’s model, for the concentration,

$$n = \frac{3}{4\pi^2} \left( \frac{3}{2} \right)^{1/2} \left( \frac{k}{P} \right)^3 T^3 \int_0^\infty \frac{X^{1/2}(X + \phi)^{1/2}(2X + \phi)dX}{1 + exp(X - \eta)}$$

where $\phi$, $\eta$, and $X$ are the reduced energy gap, reduced Fermi level, and variable of integration given by

$$\phi = E_g/kT,$$

$$\eta = E_F/kT,$$

$$X = \frac{-E_g + (E_g^2 + 8P^2K^2/3)^{1/2}}{2kT}.$$  

where $K$ is wave vector. A fitted expression for the resulting Fermi energy as a function of temperature is

$$E_F = 0.00256 - 5.6644 \times 10^{-6}T^{1.8} (eV)$$

4.4.1. Constant Activation Energy Donor Model

The activation behavior illustrated in figure 4.9 at $\sim 20 - 60K$ suggests that a shallow donor is present. A shallow donor is usually described as hydrogenic, where the donor is pinned to the conduction band edge, i.e., $\epsilon_d$ is constant. The solid curves in Figure 4.9 show the fitting results using equations 9 and 10 for a constant shallow activation energy. Although the activation process seen in the temperature regime of 20-60K can be explained
by a hydrogenic donor of different binding energy for different neutron dose, the higher
temperature results can not be described.

4.4.2. Deep Donor Model

Deep donor levels at $\sim 0.2E_g - 0.3E_g$ have been observed by various methods [67, 68,
69, 70]. Van Vechten used entropy to study temperature variation of the defect ionization
level in semiconductors [71, 72]. In this approach, $E_g$ can be defined as the standard chemical
potential $\Delta E_{cv}$ for creation of electron-hole pairs

$$0 \longrightarrow e^+ + e^-, \Delta E_{cv}$$

$\Delta E_{cv}$ is equal to the increase of Gibbs free energy for creation of one electron-hole pair at
constant temperature and pressure:

$$\Delta E_{cv} \equiv \frac{\partial G}{\partial n_p} \bigg|_{T,P}$$

(14)

where $G$, $P$, $n_p$ denote the Gibbs free energy, pressure and number of electron-hole pairs,
respectively. Then $\Delta E_{cv}$ can be decomposed into enthalpy $\Delta H_{cv}$ and entropy $\Delta S_{cv}$:

$$\Delta E_{cv}(T) = \Delta H_{cv}(T) - T\Delta S_{cv}(T)$$

(15)

The ionization energy of donor impurities can also be defined as the change of the stan-
dard chemical potential to create an ionized donor and an electron pair in the reaction

$$D^x \longrightarrow D^+ + e^-, \epsilon_d$$

(16)

where $x$ denotes a neutral defect before ionization. The ionization energy $\epsilon_d$ may be decom-
posed into the enthalpy of ionization $\Delta H_I$ and entropy of ionization $\Delta S_I$, where

$$\epsilon_d = \Delta H_I(T) - T\Delta S_I(T).$$

(17)

As a result, $\Delta S_{cv}(T)$, $\Delta S_I(T)$ can be derived from equation 15 and 17

$$\Delta S_{cv} = -\frac{\partial \Delta E_{cv}}{\partial T},$$

(18)

$$\Delta S_I = -\frac{\partial \epsilon_d}{\partial T}.$$
For shallow Coulombic donors, bound electrons are highly delocalized. The change of entropy is very small when they become free electrons upon ionization, i.e., \( \Delta S_f(T) \sim 0 \). According to equation 19, \( \epsilon_d \) is a constant and this level is then pinned to the conduction band. This is the case that was considered in the constant shallow donor model.

If the donors are deeper vacancies, isoelectronic impurities, or interstitials, two new carriers of opposite charge are created upon ionization. The electron becomes a free carrier while the positive hole is bound in the vicinity of the neutral core. Van Vechten’s analysis\[71, 72\] shows that, no matter what degree of localization the bound hole has, the entropy change upon ionization cannot be neglected and hence \( \epsilon_d \) will be temperature dependent. In the extreme case, i.e., when the bound hole is highly delocalized, entropy change will be very similar to reaction 13, i.e., \( \Delta S_f(T) \sim \Delta S_{ce}(T) \). In this case, the donor level will be pinned to the valence band instead of the conduction band. If the band gap change is very small as a function of temperature, this deep donor level will still remain at a constant position relative to the conduction band. However, when dealing with narrow band gap material such as Hg\(_{0.78}\)Cd\(_{0.22}\)Te, the results can be quite different, since its band gap increases substantially with temperature. As a result, the deep donor energy level of vacancies, isoelectronic defects or interstitials will also change substantially with temperature.

An empirical functional form may be chosen for \( \epsilon_d \) that is similar to \( E_F \), i.e.,

\[
\epsilon_d = a + bT^c (eV)
\]

is obtained. One advantage of this expression is that it has a minimal number of fitting parameters while providing a satisfactory fit. The solid curves in figure 4.10 were obtained by fitting the electron concentration. Fitting parameters were \( a = 0.00372 \), \( b = 1.8527 \times 10^{-7} \), and \( c = 2.6 \) for sample 5. The donor energy level \( E_d(T) = -\epsilon_d(T) \) of sample 5 is plotted as the dashed curve in figure 4.11. As can be seen, at 4K, \( E_d \) is below \( E_F \) so that this donor is not activated. As the temperature increases, the gap \( E_{df} \) between \( E_d \) and \( E_F \) becomes smaller and a small portion of the donors are activated. At \( \sim 60K \), the Hall electron concentration reaches the highest level where \( E_{df} \) becomes the smallest. But even at this point, there still
Figure 4.10. Hall electron concentration of four samples with fitting curves for sample 3B, 4 and 5 that included a deeper donor level which changes with temperature.

is only a small portion of donors that activated. As temperature continues to increase, $E_d$ begins to increase, which results in the decrease of the Hall electron concentration. Figure 4.11 also shows that both $E_F$ and $E_d$ move toward the center of gap as the temperature increases and $E_d$ does not stay at a fixed position relative to the conduction band, e.g., it changes from $\epsilon_d \sim 4meV$ at $4.4K$ to $28meV$ at $92K$. Since this change ($\Delta \epsilon_d$ is $\sim 24meV$) parallels the increase in the band gap ($\Delta E_g \sim 26meV$) for the same temperature range, this result supports Van Vechten’s analysis that this donor level is pinned to the valence band. Similar results are found for samples 3B and 4.

4.5. Conclusion

The effects of thermal neutron irradiation on LPE grown Hg$_{0.78}$Cd$_{0.22}$Te epilayers have been studied. The result shows that all irradiated samples remain n-type. The electron introduction rate is much smaller than those for fission neutron. The mobility decreases
Figure 4.11. In the deep donor level model, donor energy level $E_d$ plotted with $E_F$ shows that the change of electron concentration is due to the change of gap between $E_d$ and $E_F$.

with increasing neutron dose and can be fitted by including a mobility term that is inversely proportional to neutron dose. This is caused by the creation of additional ionized or neutral impurity scattering centers. By fitting the temperature dependence of Hall electron concentration at low temperature, a deep donor level is found to be pinned to the valence band as predicted by Van Vechten.
CHAPTER 5

DIFFUSION STUDIES OF SE IN HG$_{0.78}$CD$_{0.22}$TE GROWN BY LIQUID PHASE EPITAXY

5.1. Introduction

Atomic diffusion of dopants, including those from groups I [73], III [74], IV [75], and V [76, 40], have been extensively studied in HgCdTe. However, the diffusion behavior of the group VI element selenium(Se) in this material has not been reported, even though the diffusion characteristics of Se in HgCdTe have become interesting for the following reasons. Buffer layers grown using II-VI materials containing selenium, such as ZnTe/CdSeTe [77] and CdSeTe/CdTe [78], are promising candidates. Also, in order to achieve efficient p-type doping in HgCdTe, the transmutation of Se to As becomes a viable candidate[37, 51]. Thus, the diffusion characteristics of Se in HgCdTeSe are important if stable p-n diodes are to be synthesized by this technique. The objective of this study is to investigate the diffusion behavior of Se in HgCdTe material and provide a basis for further investigation of Si substrate buffer technology and the transmutation doping.

Atomic diffusion in a crystalline solid is the migration process of atoms by thermally hopping from one site to another. The diffusing species can occupy either lattice site of a binary compound or interstitial sites depending on the diffusion mechanism. Study of atomic diffusion can also provide an understanding of the structure of defects, which have significant effects on the electrical and optical properties of the material. The diffusion mechanisms can be divided into two categories — defect-independent processes and defect-dependent processes. Defect-independent processes include direct exchange of places between two atoms, and ring mechanisms, which occur when a group of neighboring atoms exchange
their sites in a cyclic manner. Although defect-independent processes are occasionally suggested as the mechanism for several diffusion phenomena in solids, they are usually neglected in a crystal due to the high activation energy required for these processes.

Defect-dependent processes dominate in the atomic diffusion of atoms in semiconductor materials, including interstitial, vacancy and dislocation mechanisms. More than one mechanism may contribute simultaneously to the diffusion profile of a given species. However, under specific conditions, usually one mechanism dominates. Dislocation-based diffusion is much faster than other mechanisms as a consequence of the short diffusion path for this mechanism. In materials with high etch pit density (EPD), this short circuit diffusion can create a tail component of the distribution of diffusion atoms which will severely compromise junction properties [79, 76]. In this study, the HgCdTe samples used have very low EPD ($\sim 10^5/cm^2$); hence short circuit diffusion will not occur. According to previous studies, interstitial and vacancy mechanisms are most likely to govern the behavior of chalcogen diffusion in II-VI materials. Figure 5.1 illustrates the vacancy mechanism and interstitial mechanism. In the latter case, impurities diffuse through interstitial spaces and return by either replacing a host atom or being captured by a vacancy.

A number of other possible mechanisms for diffusion have been proposed. Interstitialcy is a mechanism by which a self-interstitial host atom displaces a substitutional impurity, driving it to an interstitial site where it diffuses some distance before it returns to the lattice. Indirect interstitial mechanisms in self-diffusion are analogous to interstitialcy. The only difference is that the replaced atom is the same type of element instead of a substitutional atom. It is accepted that the Chalcogen self-diffusion in II-VI material under chalcogen rich conditions or low metal vapor pressure is governed by this method [80, 81].

Since Se is group VI element, it is valid to treat migration of Se atoms in HgCdTe as self-diffusion. Chalcogen self-diffusion in II-VI material has been studied in various materials such as CdTe, CdSe [82, 80, 83], ZnTe [84], CdS [81] and HgCdTe [75, 85]. The diffusion
Figure 5.1. Illustration of vacancy mechanism (a) and interstitial mechanisms (b).

mechanism is dependent on various conditions such as diffusion species, temperature, ambient partial vapor pressure and dopants. The diffusion coefficient $D$ for a specific mechanism is proportional to the corresponding defect concentration. Thus, analysis of the defect formation reaction and defect electrical properties, together with the experimental data, are usually employed to determine the diffusion mechanism. For example, the study of metal pressure dependence of electron concentration, chalcogen vacancy concentration, and chalcogen diffusion coefficient have revealed that vacancies on chalcogen sites govern the chalcogen self-diffusion behavior under metal-rich conditions. Taking Te self-diffusion in CdTe as an
example, Te vacancy formation in Cd rich gas is written as

\[ Cd(g) \leftrightarrow Cd^x_{Cd} \times V^\text{Te}_{Te} + 2e \] (1)

where the subscript denotes the position of the atom. \( V^\text{Te}_{Te} \) means that the Te vacancy is doubly ionized and \( e \) denotes the free electron. The mass action relation for this reaction is

\[ K_R = [V^\text{Te}_{Te}][e]^2/P_{Cd}. \] (2)

\( K_R \) is the reaction constant and only dependent on temperature. \([V^\text{Te}_{Te}]\) and \([e]\) denote \( V^\text{Te}_{Te} \) and \( e \) concentrations, respectively, and \( P_{Cd} \) is the Cd vapor pressure. The electroneutrality condition (ENC) for this process can be approximated as

\[ 2[V^\text{Te}_{Te}] = [e]. \] (3)

From the mass action relation, the \( P_{Cd}^{1/3} \) -dependence of the free electron and Te vacancy concentrations can be found:

\[ 2[V^\text{Te}_{Te}] = [e] = (2K_R)^{1/3}P_{Cd}^{1/3}. \] (4)

The same analysis for doubly activated Cd interstitial atoms gives the same relation for \([Cd^i]\) and the corresponding \([e]\). Many experiments [86, 87, 88, 89] have shown that \([e]\) is proportional to \( P_{Cd}^{1/3} \) in undoped CdTe. In a chalcogen self-diffusion study [75, 82], it was also observed that the diffusion coefficient increases with \( P_{M}^{1/3} \) (metal pressure) when the metal pressure approaches saturation. Since the metal interstitial mechanism involves formation of antisites, which requires higher energy, the \( P_{M}^{1/3} \) dependence of the diffusion coefficient leads to the mechanism based on doubly ionized vacancies on group VI sites.

5.2. Fick’s Law and Diffusion Coefficient for Small Diffusion Length

According to Fick’s first law, the mass flux \( J(z, t) \) at position \( z \) and time \( t \) is proportional to concentration gradient \( C(z, t) \),

\[ J(z, t) = -D \frac{\partial C(z, t)}{\partial z}, \] (5)

where \( D \) is the diffusion coefficient and usually conforms to the Arrhenius relationship,
\[ D = D_0 e^{x(E/kT)}, \]  

(6)

where \( D_0 \) is a constant, and \( E \) is the activation energy. The continuity equation of diffusion is expressed as

\[ \frac{\partial C(z,t)}{\partial t} = -\frac{\partial J}{\partial z}. \]  

(7)

Since there is no convenient way to measure \( J \), a second expression of Fick’s law, or Fick’s second law, can be derived through Fick’s first law and the continuity equation,

\[ \frac{\partial C(z,t)}{\partial t} = \frac{\partial}{\partial z} (D \frac{\partial C}{\partial z}). \]  

(8)

If the diffusion coefficient \( D \) is independent of position, equation 8 reduces to

\[ \frac{\partial C(z,t)}{\partial t} = D \frac{\partial^2 C(z,t)}{\partial z^2}. \]  

(9)

Generally, the diffusion process is very complex and equation 9 can only be solved numerically. However, under special boundary conditions, an analytical solution to equation 9 can be derived.

In drive-in diffusion, a fixed amount of impurities are introduced into a material. Under ideal conditions all impurities are incorporated into a very thin layer so that the initial impurity concentration can be approximated as a delta function,

\[ c(z,0) = Q_T \delta(z - z'). \]  

(10)

The solution to Fick’s second law under this boundary condition is a Gaussian:

\[ c(z,t) = \frac{Q_T}{\sqrt{\pi Dt}} e^{-(z - z')^2/4Dt}. \]  

(11)

In the case of a small diffusion coefficient, the diffusion length may be very small even after a long anneal time. In this case, the boundary condition can not be approximated by a delta function and the initial distribution of the impurity must be taken into consideration[90]. The
introduction of a certain amount of impurity into a material is usually done via implantation, and the initial profile of the impurity can be approximated by a Gaussian centered at $z' = R_p$:

$$c(z',0) = c_0 \exp \left( -\frac{(z' - R_p)^2}{2\Delta R_p^2} \right), \quad (12)$$

where $\Delta R_p$ is the standard deviation of the projected range. Then the impurity profile at time $t$ can be calculated by a convolution integral over depth $z'$ using the initial impurity distribution given in equation 12,

$$c(z,t) = \int_0^\infty \frac{dQ_T(z')}{\sqrt{\pi Dt}} e^{-\frac{(z-z')^2}{4Dt}} dz' = \int_0^\infty \frac{c(z',0)}{\sqrt{\pi Dt}} e^{\frac{(z-z')^2}{4Dt}} dz' = \frac{c_0}{\sqrt{\piDt}} \int_0^\infty e^{-\frac{(z-R_p)^2}{2\Delta R_p^2}} e^{-\frac{(z-z')^2}{4Dt}} dz'. \quad (13)$$

The final expression can be written as

$$c(z,t) = Ae^{-\frac{(z-R_p)^2}{(4Dt+2\Delta R_p^2)}} = Ae^{-\frac{(z-R_p)^2}{D'}} \quad (14)$$

where $A$ is an integration constant. The parameters $\Delta R_p$ and $D'$ can be obtained by fitting the as-implanted sample and the annealed sample, respectively, and the diffusion coefficient $D$ can be determined from

$$D = \frac{(D' - 2\Delta R_p^2)}{4t}. \quad (15)$$

5.3. Experiment and Discussion

In this study, five LPE Hg$_{0.78}$Cd$_{0.22}$Te samples, grown on CdZnTe substrates, were implanted with a Se dose of $2 \times 10^{14}/cm^2$ at 100keV under identical conditions. The thickness of the samples were $\sim 55\mu m$ and the etch pit density (EPD) was $\sim 1 \times 10^5/cm^2$. Following implantation, four samples were cut in two and the two halves were placed face to face to avoid loss of Se atoms from the epilayers. This face-to-face arrangement also assured the boundary condition of a constant initial concentration of Se atoms. The samples were annealed in mercury saturated vapor at various temperatures (see Table 5.1). After annealing,
the samples were easily separated and retained a smooth surface. SIMS profiles were obtained, for which the concentration routine precision and accuracy of depth calibration were \( \sim 10\% \) and \( \pm 3 - 5\% \), respectively.

<table>
<thead>
<tr>
<th>Sample #</th>
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<th>3</th>
<th>4</th>
<th>5</th>
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</thead>
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<td>Annealing Temperature(^\circ)C</td>
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<td>425</td>
<td>450</td>
</tr>
<tr>
<td>Annealing Time (hrs)</td>
<td>–</td>
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<td>72</td>
<td>24</td>
<td>24</td>
</tr>
</tbody>
</table>

**Table 5.1.** Tabulation of sample anneal times and temperatures.

**Figure 5.2.** SIMS Se profile of sample 2, annealed for 144\(hrs\) at 350\(\circ\)C, compared to as-implanted sample 1. Gaussian fitting yields \( D_{Se} = (4.5 \pm 0.007) \times 10^{-17} cm^2/s \).

Figure 5.2 to Figure 5.5 show SIMS profile of Se for each sample. Theoretical calculations show that the projected range \( R_p \) is about 50\(nm\). In addition, the Gaussian peak positions of all annealed samples do not change. Thus, the high concentration located at a depth of less than 20\(nm\) detected by SIMS is believed to be an artifact. All Se profiles exhibit
**Figure 5.3.** SIMS Se profile of sample 3, annealed for 72\textit{hrs} at 373\textdegree\textit{C}. Gaussian fitting yields $D_{Se} = (1.7 \pm 0.008) \times 10^{-16} \text{cm}^2/\text{s}$.

**Figure 5.4.** SIMS Se profile of sample 4, annealed for 24\textit{hrs} at 425\textdegree\textit{C}. Gaussian fitting yields $D_{Se} = (3.0 \pm 0.001) \times 10^{-15} \text{cm}^2/\text{s}$. 
Figure 5.5. SIMS Se profile of sample 5, annealed for 24 hrs at 450°C. Gaussian fitting yields $D_{Se} = (1.0 \pm 0.0001) \times 10^{-14} cm^2/s$.

As seen in Figure 5.2, the diffusion length of sample 2 is still small ($\sim 0.1 \mu m$) after a 144 hr anneal, thus the as-implanted distribution of Se must be taken into account in fitting for the diffusion coefficient. For the 350°C annealed sample, the fitting yields $\Delta R_p = (5.09 \pm 0.006) \times 10^{-6} cm$, $D' = (1.45 \pm 0.006) \times 10^{-10} cm^2/s$, and $D_{Se} = (4.5 \pm 0.007) \times 10^{-17} cm^2/s$. The uncertainties listed here are one standard deviation. Using the same method, the diffusion coefficient at 375°C is $(1.7 \pm 0.008) \times 10^{-17} cm^2/s$. For 425°C and 450°C, the diffusion length is large enough that the as-implanted distribution can be neglected. Fitting directly with equation 11 gives $D_{Se} = (3.0 \pm 0.001) \times 10^{-15} cm^2/s$ and $(1.0 \pm 0.0001) \times 10^{-14} cm^2/s$ for 425°C and 450°C, respectively. Comparing with arsenic diffusion, the diffusion of Se in Hg$_{0.78}$Cd$_{0.22}$Te is found to be much smaller, e.g., $D_{Se} \sim 1 \times 10^{-14} cm^2/s$ and $D_{As} \sim 2.6 \times 10^{-13} cm^2/s$ at 450°C. This suggests that Se redistribution is very small in HgCdTe at the temperatures studied.

Also seen from figure 5.2 to 5.5 is that the tail component of the depth profile becomes less pronounced as the annealing temperature is increased and almost vanishes at 450°C when
diffusion length becomes large (\( \sim 0.5\mu m \)). In the study of As and Sb diffusion in HgCdTe [76], the tail component was also observed. In material with large EPD (\( \sim 10^7/cm^2 \)), it does not vanish for large diffusion length. It is believed that the tail in high EPD material is due to occupancy of impurity atoms on metal sites and the diffusion is metal-vacancy-based atomic diffusion. This diffusion is enhanced by the dissociation of defects from the damaged surface and hence dependent on implant damage, vacancy distribution and EPD of the material. Thus the diffusion coefficient is large and not a constant. Since the LPE HgCdTe samples have low EPD (\( 10^5/cm^2 \)) and the tail vanishes for large diffusion length, it is suggested that the tail observed for small diffusion length is associated with the tail of the as-implanted distribution. As the anneal temperature increases, this component then merges with the Gaussian component of the diffusion.

Point defects play a dominant role in diffusion behavior of II-VI compounds. Previous chalcogen self-diffusion studies provide some valuable information for understanding Se diffusion behavior discussed in section 5.1. In their study of Te self-diffusion in HgCdTe, Gorshkov et al [75] found that \( D_{Te} \) at 450°C increased slowly with \( P_{Hg}^{1/3} \) when Hg vapor pressure \( P_H \) approaches saturation. In a Te self-diffusion study in CdTe [82], it was also observed that \( D_{Te} \) has a \( P_{Te}^{1/3} \) dependence. Other experiments [91] showed the free electron concentration has the same relation to the metal vapor. Based on his analysis using electroneutrality conditions (ENCs) and Brouwer approximations [92, 82], Shaw concluded that variation of chalcogen diffusion coefficient \( D_x \) with metal vapor pressure \( P_m^{1/3} \) points to nonmetal vacancy based mechanism. Since Se is also a chalcogen element, it is assumed that Se diffusion in HgCdTe is Te-vacancy based. In another study, implanted As diffusion in HgCdTe [76] shows the Gaussian component of the As profile is also due to Te vacancy based atomic diffusion. Since implantation creates a Hg-rich ambient and results in a large portion of As atoms occupying Te sites, As atoms start from Te sites. The constant diffusion
coefficient is a consequence of the stable Te vacancy concentration in bulk HgCdTe. Comparing to As, Se should be more likely to be incorporated into Te sites; hence the assumption is reasonable.

Since a Te-vacancy-based mechanism leads to a $P_{Hg}^{1/3}$ dependence, the Arrhenius equation 6 under Hg saturated vapor can be rewritten as

$$D = D_0 e^{-E/kT} P_{Hg}^{1/3}. \quad (16)$$

All the samples investigated were annealed in mercury saturated vapor, which changes significantly with temperature. Plotting $\ln(D_{Se}/P_{Hg}^{1/3})$ vs $1/kT$ in Figure 5.6 shows a good linearity, and $D_0$ and $E$ are found to be $0.12 \pm 0.11 cm^2/s$ and $1.84 \pm 0.05 eV$, respectively.

\begin{figure}[h]
\centering
\includegraphics[width=0.6\textwidth]{figure56.png}
\caption{Fitting $\ln(D_{Se}/P_{Hg}^{1/3})$ linearly, activation energy is shown to be 1.84eV.}
\end{figure}

Further study will concentrate on Se diffusion behavior as a function of Hg and Te partial vapor pressure, which will further clarify the diffusion mechanism.
5.4. Conclusion

In this diffusion study, the Se diffusion coefficient is seen to be constant and around one order of magnitude smaller than that of As in Hg$_{0.78}$Cd$_{0.22}$Te material. The tail component vanishes for large diffusion length and is associated with the tail of the as-implanted profile. The diffusion coefficient for small diffusion length can be obtained by integrating the initial concentration over depth. Assuming a Te vacancy based mechanism, the Arrhenius relation yields an activation energy 1.84eV.
6.1. Introduction

Silicon has become a promising substrate in MBE growth of HgCdTe material for long wavelength infrared focal plane array (IR FPA) imagers and complex structured devices. The advantage of the silicon substrate is obvious. First, large silicon wafers with excellent crystalline quality are available at low cost. Second, the silicon substrate can thermally match the ROIC in hybrid IRFPA and improve the thermal reliability of infrared devices. In addition, silicon has much higher mechanical strength than the CdZnTe substrate currently used for these imagers. However, there is a 19% lattice mismatch between HgCdTe and silicon, resulting in a high density of lattice dislocations. The edge dislocation has been shown to introduce deep energy levels in semiconductor materials[93, 94]. These levels result from the dangling bonds of the dislocations. These dangling bonds create space charge and behave as both scattering and recombination centers, severely compromising the electrical and optical properties of devices.

In as early as 1952, Gallagher [93] observed the increase of resistivity and decrease of minority carrier lifetime in plastically deformed germanium. He suggested that this phenomenon is due to acceptor-like defects. Pearson and Read’s work confirmed that the acceptor-like defects are associated with the edge component of the dislocation created in plastic deformation [94]. The dislocation can also scatter conduction electrons, thereby reduce the mobility.

In epitaxially grown semiconductor films, where dislocations advance from the substrate to the free surface of the film, threading dislocations occur. Threading dislocations are the
most deleterious because they span the film thickness and act as scattering centers for the conduction electrons.

In addition to the effort to reduce the dislocation density by employing composite buffer layer technologies, there is an increasing interest in passivating dislocations by hydrogenation [95, 96]. Hydrogen atoms introduced into the material can pair with the dangling bonds, and hence electrically neutralize the dislocation. Hydrogenation of GaAs has shown considerable progress in neutralization of defects, and can significantly improve the electrical and optical properties of the material [97, 98]. Increases in the minority carrier life time are also achieved in hydrogenated polycrystalline silicon solar cells [99, 100]. Various methods to incorporate hydrogen have been developed, including chemical diffusion [100], low-energy hydrogen ion implantation [101, 102, 103], remote plasma hydrogenation [104, 105, 99], and direct plasma hydrogenation [106, 99]. Ion implantation allows controllable high concentrations of H⁺ into targets. But the deleterious effect of damage and expensive equipment make it unfavorable. In direct plasma hydrogenation, samples are exposed directly to hydrogen plasma produced by a direct current (DC), radio frequency (RF), or electron cyclotron resonance (ERC) apparatus. This method is simple, fast, and provides excellent control of the hydrogen dose, and thus it has become the most common method of hydrogenation. In the remote plasma hydrogenation method, a low temperature plasma diffuses into the surface of the samples without any enhancement. As a result the damage to the surface is minimized. But the remote plasma method requires more complicated apparatus and usually needs to be combined with other methods (typically chemical diffusion) to achieve good results. Both plasma hydrogenation methods are illustrated in figures 6.1 and 6.2, respectively.

In this work, a preliminary hydrogenation study on MBE HgCdTe epilayer grown on silicon wafer is reported. Hydrogen atoms are introduced through a DC glow discharge plasma, and Hall measurements and SIMS analysis were used to characterize the hydrogenation efficacy in reducing defects. In addition, the method used to calculate the dislocation scattering
is discussed. A model of two energy levels due to different types of dislocation lines is used to describe the experimental results presented here.

6.2. Dislocation Energy Level and Scattering

It is worthwhile to discuss the dislocation formation process and properties in semiconductor materials, for analyzing the effects on the materials electrical and optical properties, as well as the effect of hydrogenation. In this chapter, explanations of the experimental
data of HgCdTe hydrogenation will be discussed in terms of dislocation energy levels instead of detailed hydrogenation kinetics, though the latter is of similar importance and will be investigated in future work.

Edge dislocations can be described as the insertion of an extra half-plane of atoms into a perfect crystal, or the slip of one plane with respect to another. The slip direction, or Burgers vector, is perpendicular to the dislocation line. In a diamond or zinc blende lattice, the most common slip plane is \{111\} and the dislocation runs along the \langle 110 \rangle direction. As shown in figure 6.3 for the diamond structure, a row of atoms above the slip plane (111) have no neighbors in the plane below, forming a row of dangling bonds in [01\overline{1}] direction.

![Figure 6.3](image)

**Figure 6.3.** A dislocation on a (111) plane in diamond structure, running at 60° to slip (Burgers) vector with both edge component and screw component.

However, the zinc blende structure is visualized as two face-centered cubic structures (fcc) displaced from each other by one-quarter of a body diagonal. The tetrahedral bonds of the lattice are not symmetric in the opposite direction. Hence, as shown in figure 6.4,
the insertion of a half plane from the opposite directions will result in a dislocation line of unpaired bonds of metal atoms and nonmetal atoms, respectively.

Figure 6.4. Dislocation on a (111) plane in zinc blende structure, running at 60° to slip (Burgers) vector with both edge component and screw component.

Unlike dislocations in the diamond structure, whereas only one energy level is created, the dangling bonds of the two types of dislocations in zinc blende structure will form two energy levels due to differing electron affinity. The terms $\epsilon_m$, $\epsilon_n$ denote the energy levels of metal dislocation and nonmetal dislocation, respectively. The position of these two levels in the band gap, as well as the Fermi energy $E_F$, governs the effect of the dislocation on electrical properties of the material. It is possible that one level is donor-like while another is acceptor-like, and both levels can be activated in the temperature range studied. If this is the case, donors and acceptors introduced by the dislocations will compensate each other when the dislocation densities of the two types are similar. This will result in a decrease
of carrier mobility due to scattering of ionized dislocation levels, while at the same time the carrier concentration is relatively constant. This result is different from the case of germanium, in which the dislocation only introduces an acceptor level, resulting in a change in both mobility and carrier concentration.

Read [107] derived a method to calculate the occupancy rate, \( f \), of acceptor-like dislocation levels in plastically deformed Ge. As a dislocation is introduced, the electrons begin to occupy the acceptor level, the dislocation line becomes negatively charged and the electrostatic energy of the negatively charged line, \( \epsilon_s \), increases. The occupancy rate \( f_{dsl} \) is determined by the equilibrium between the increase of electrostatic energy \( \epsilon_s \) and the decrease of free energy \( F(f_{dsl}) \) for moving a free electron to an acceptor level \( \epsilon_{dist} \).

In n-type narrow gap HgCdTe material, the Fermi level is very close to the conduction band at low temperature, so the acceptor-like dislocation level will be fully filled, i.e., \( f_{dsl} \) is equal to 1. On the contrary, if a donor-like dislocation is very shallow, as in HgCdTe, the corresponding occupancy rate will be 0.

When dislocation levels are activated, space charged lines act as Coulomb scattering centers. The potential \( V(r) \) satisfies Poisson’s equation in cylindrical coordinates,

\[
\frac{d^2V}{dr^2} + \frac{1}{r} \frac{dV}{dr} = \frac{(n - n_0)e}{\varepsilon \varepsilon_0}
\]

where \( n = n_0 \exp(-|e|V/kT) \) and \( n_0 \) are the carrier densities near and far away from the scattering center, respectively, and \( e \) is positive for holes and negative for electrons. Under the small screening effect approximation, \( n \) is given by

\[
n(r) = n_0[1 - |e|V(r)/k_BT];
\]

Then Poisson’s equation becomes

\[
\frac{d^2V}{dr^2} + \frac{1}{r} \frac{dV}{dr} = \frac{V}{\lambda_D^2}
\]

where the Debye length \( \lambda_D = \sqrt{\varepsilon \varepsilon_0 / e^2 n^*} \), and \( n^* \) is defined as [27]

\[
n^* = \frac{dn}{d\eta}
\]

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and $\eta$ is the reduced Fermi energy.

Bonch-Bruevich and Kogan [108] have solved the Poisson equation analytically for cylindrical symmetry. The screened potential of an acceptor-like charged line, at distance $r$ from the center of the dislocation, is expressed as,

$$V(r) = \frac{1}{4\pi \varepsilon \varepsilon_0} \frac{2e\bar{f}}{c} K_0\left(\frac{r}{\lambda_D}\right),$$

(5)

where $K_0$ is a zero-order Bessel function of the second kind; $c$ is the spacing between dangling bonds. Pödör calculated the differential cross section $\sigma(\theta)$ using Born’s approximation for small perturbation [109], from which the reciprocal of the momentum relaxation time is obtained:

$$\frac{1}{\tau_{dsl}} = N_{dsl}v_\perp \int_0^{2\pi} (1 - \cos \theta)\sigma(\theta) d\theta$$

$$= \frac{N_{dsl}e^4 f_{dsl}^2 \lambda}{8\varepsilon^2 \varepsilon_0^2 c^2 m^2} (v_\perp^2 + \hbar^2/4m^2\lambda^2)^{-3/2}$$

(6)

where $v_\perp$ is the velocity in the direction perpendicular to the dislocation line, and $m$ is carrier effective mass. For a donor-like dislocation, the momentum relaxation time can be obtained by replacing $f_{dsl}$ with $(1 - f_{dsl})$ in expression 6.

An analytical expression for the averaged relaxation time and mobility are available if the conduction band is nondegenerate and parabolic[109]. The mobility due to acceptor-like dislocation in n-type material can be expressed as

$$\mu_{dsl} = \frac{30\sqrt{2\pi \varepsilon^2 \varepsilon_0^2 c^2 (k_B T)^{3/2}}}{e^3 f_{dsl} \lambda D n_e^{1/2} N_{dsl}}.$$  

(7)

For n-type narrow band gap HgCdTe, the conduction band is nonparabolic according to Kane’s model. As a result, the mobility due to dislocation can only be calculated numerically, as

$$\mu_{dsl} = \frac{e \langle \tau_{dsl} \rangle}{m} = \frac{e}{m} \frac{\int_{-\infty}^{\infty} \tau_{dsl} v_x (-\partial f_0/\partial E) d^3k}{\int_{-\infty}^{\infty} f_0 d^3k}$$

(8)

Before calculating $\mu_{dsl}$, the Fermi energy and $n^*$ have to be determined from equations 11 and 4.
6.3. Experiments and Results

HgCdTe epilayers were grown by MBE on CdTe/Si substrate. Hall measurements show all samples are n-type with a carrier concentration of $\sim 1.5 \times 10^{15}/cm^3$. The samples were etched for 5min in 0.1% BrMeOH solution to remove the surface oxide and contamination before measurements were performed. The samples were then exposed to hydrogen plasma excited by a DC glow discharge. SIMS analysis was performed to obtain the depth profile of hydrogen concentration. Temperature-dependent Hall mobility and carrier concentration were determined by Hall measurement using a Van der Pauw configuration. No post hydrogenation annealing was performed on the samples.

A series of samples were treated in a deuterium glow discharge under various conditions. Figure 6.5 shows SIMS depth profiles of deuterium. The peaks of deuterium profiles match the location of the HgCdTe/CdTe interface, indicating that deuterium atoms are trapped at the HgCdTe/CdTe interface where impurities and dislocations exist. The untreated sample shows low deuterium concentration.

![SIMS depth profiles of deuterium for HgCdTe on CdTe/Si composite substrates treated in deuterium glow discharges.](image)

**Figure 6.5.** SIMS depth profiles of deuterium for HgCdTe on CdTe/Si composite substrates treated in deuterium glow discharges.

Two subsequent samples, RSC 3-1523A and RSC 3-1523B, were treated by DC hydrogen glow discharge in two successive runs to investigate the effect of dislocation on carrier mobility.
and concentration. Table 6.1 shows treatment details of the two samples. A microscopic image taken after etching (CrO$_3$(5M)+HCL+H$_2$O, 60:25:90 by volume, 15seconds [110]), shown in figure 6.6, shows that RSC 3-1523A has very large EPD in contrast to a LPE HgCdTe sample with EPD of $1 \times 10^6/cm^2$.

<table>
<thead>
<tr>
<th>Sample</th>
<th>run</th>
<th>This run</th>
<th>Cumulative</th>
</tr>
</thead>
<tbody>
<tr>
<td>3-1523A</td>
<td>1</td>
<td>0.0114</td>
<td>0.0114</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>0.0060</td>
<td>0.0174</td>
</tr>
<tr>
<td>3-1523B</td>
<td>1</td>
<td>0.0012</td>
<td>0.0026</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>0.0018</td>
<td>0.0044</td>
</tr>
</tbody>
</table>

Table 6.1. Tabulation of hydrogenation treatment.

Figure 6.6. Microscopic image of RSC 3-1523A after etching illustrating high EPD.

Hall measurements were performed before and after each hydrogenation treatment. Figures 6.7 and 6.8 show that hydrogenation dramatically increases electron mobility in both samples after each treatment. Matthiessen’s rule was used to determine the experimental dislocation mobility of sample RSC 3-1523A before and after hydrogenation, assuming only dislocation defects are present:

$$\frac{1}{\mu_{\text{untreated}}} = \frac{1}{\mu_{\text{dsl}}} + \frac{1}{\mu_{\text{treated}}}.$$  (9)
Figure 6.7. Mobility of sample RSC 3-1523A with high EPD before and after each hydrogenation.

Figure 6.8. Mobility of sample RSC 3-1523B with low EPD before and after each hydrogenation.

A theoretical calculation of dislocation mobility is also shown in figure 6.9 for sample RSC 3-1523A after the second treatment. In this theoretical calculation, it is assumed that the dislocations are perpendicular to the epilayer surface, all donor-like levels are empty and all
Figure 6.9. Dislocation mobility of sample RSC 3-1523A before and after the second hydrogenation treatment. Theoretical calculation of dislocation mobility shows a similar temperature dependence

acceptor-like level are filled, and the EPD was taken to be $2.5 \times 10^8/cm^2$. Both experimental and calculated dislocation mobilities show a constant value at low temperatures and increase with higher temperature. The theoretical calculation is based on Kane’s model, which is a good approximation at low temperatures. As temperature increases, this model tends to have larger error, which accounts for the deviation of the calculation from the experimental results at high temperatures.

Since the momentum relaxation time is inversely proportional to dislocation density, the dislocation scattering effect on carrier electrical transport properties will become negligible if the EPD is $< 10^7/cm^2$. This is also evidenced by our experimental results from sample 3-973, for which the EPD is $\sim 5 \times 10^6/cm^2$. As shown in figure 6.10, the mobility change of sample 3-973 after hydrogenation treatment is very small.

As discussed in the previous section, dislocations introduced in materials with a zinc blende structure will result in two energy levels and both levels can be activated and compensate each other, resulting in a small change in Hall concentration upon hydrogenation.
Since both donors and acceptors of dislocations are ionized and act as scattering centers, after hydrogenation, they are neutralized, resulting a dramatic change of mobility in contrast to carrier concentration. This phenomenon was observed in our experiments. As shown in figures 6.11 and 6.12, the electron concentrations of both 3-1523A and 3-1523B almost remain the same after being treated by hydrogen glow discharge.

6.4. Conclusion

Dislocations introduced in HgCdTe materials will result in two energy levels, where one is a donor and one is an acceptor. Hydrogenation treatment can effectively neutralize these dislocation defect levels. Both experimental results and theoretical calculation show that the mobility due to dislocation scattering remains constant at the low temperature range (< 77K), and increases with temperature between 77K and 150K. Dislocation scattering has little effect on electrical transport properties of HgCdTe with an EPD lower than 10⁷/cm². Dislocations may have little effect on carrier concentration for semiconductor material with zinc blende structure due to self compensation.
**Figure 6.11.** Electron concentration of RSC 3-1523A before and after hydrogenation.

**Figure 6.12.** Electron concentration of RSC 3-1523B before and after hydrogenation.
BIBLIOGRAPHY


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