Scattering Mechanisms and Transport Properties of Semiconductors at Low Temperatures

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Abstract

The purpose of this project is to verify scattering mechanisms in semiconductors by measuring transport properties and producing data that reflects existing research. The Hall effect is utilized to measure the resistivity, mobility and charge carrier concentration of the semiconductors: indium tin oxide (ITO), p-type silicon, and n-type silicon. By verifying and improving the measurement procedure, newer semiconductors can be produced and studied for desirable characteristics which are applicable throughout modern technology. Using liquid nitrogen to acquire the temperature dependent properties of the ITO and silicon samples, scattering mechanisms and trends related to the dopant concentration were measured. The temperature dependent electrical characteristics of three silicon samples doped with antimony, arsenic, and boron, produced carrier densities and mobilities that were consistent with existing research. At low temperatures, the samples' mobilities were impacted by impurity scattering and at higher temperatures the mobilities were impacted by phonon scattering, as seen in both the data and previous research. The carrier concentration of ITO was measured over a broad range of temperatures to be $1.0*10^{21}$ cm⁻³, which is large for a semiconductor causing the material to behave like a weak metal. By producing measurements consistent with theory, similar methodology can be applied to wide band-gap semiconductors which have been less researched in the past, specifically TiO₂ which is currently being produced by the Tate lab at Oregon State University.

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Chapter 1 – Introduction

We use electricity and complex pieces of technology on a daily basis. Most of today's devices are dependent on integrated circuits that are built on semiconducting layers that dictate how and where signals are transmitted. In the last century, humans have been constantly improving semiconductor technology to fit our needs. This has been accomplished a great deal through the use of silicon, which is the most abundant semiconducting material on our world. By purifying silicon found in the ground and altering it to have properties that fit our specific needs, we have been able to reduce the size of computer chips leading to the invention and alteration of devices throughout our society. We have learned so much by working with silicon for all these years that semiconductors have become their own branch in material sciences. Transport properties are related to how electricity is conducted within the material and help us understand electrical conduction mechanisms. Semiconductor transport properties are dependent on available energy, meaning their conduction changes through the addition of thermal energy (heat) or through the addition of atoms that alter the electron energy structure of a semiconducting material [1]. This relationship between applied energy and a semiconductor's ability to conduct electricity helps us understand and study their conduction mechanisms. Many semiconductors conduct electricity better at higher temperatures than lower temperatures due to their transport properties, the opposite trend of metals. Observing these trends closely has allowed us to fine tune existing semiconductors and to create new semiconductors based on our developed knowledge of their transport properties.

1.1 Motivation and Objective

The purpose of this research project is to measure, observe and verify the temperature dependent behavior of semiconductor transport properties: carrier concentration (carrier density), mobility, and resistivity. This research focuses on n-type silicon, p-type silicon, intrinsic silicon and indium tin oxide, which all have vast amounts of comparable data available from previous research. Producing results consistent with existing data helps correct systematic errors and solidifies our standard operating procedures which can then be applied to lesser-known semiconductors. The wide band gap semiconductor TiO2 is currently being produced and investigated by the Tate research group and shows possibilities of being widely used in condensed matter physics and industry. As the measurement processes for semiconductor transport properties are confirmed, the lab group can gather consistent and repeatable data on TiO2.

In this thesis, the background of semiconductor transport properties will be provided. In order to understand the measurements and results of this research, one must gain familiarity on the subjects involved, such as what each transport property is and the role each one plays. Along with the transport properties themselves, the reader must gain some background on how materials achieve conduction and the mechanisms which impede conduction. Then the specifics of how this research was conducted and how measurements were collected will be explained,

finally followed by the analysis and comparison of this data with previous research conducted on similar occurrences.

Chapter 2 – Theory



Figure 2.0 The general band structures for metals, semiconductors and insulators are shown. [1].

Mechanisms involving the movement of charges within materials can be studied through the temperature dependence of the transport properties: carrier concentration, resistivity, and mobility. Charge carrier concentration is the amount of charge carriers that are available for conduction, i.e. located in the conduction band. Resistivity is the opposition strength a material has against the flow of charge, which is also the inverse of conductivity. Finally, mobility is how quickly charge carriers can move when acted upon by an electric field[2].

In Fig 2.0 above, the Fermi level, E_f , is the highest state an electron can occupy at absolute zero temperature. In the metal band diagram, the valence band and conduction band overlap with the Fermi level lying within the conduction band. The charge carrier concentration is large for metals and equivalent at all temperatures because no thermal energy is required to promote electrons from the valence band into the conduction band. For semiconductors, the Fermi level lies between the valence and conduction bands, so in order for electrons to become mobile and conduct, energy must be added [3]. As will be discussed and viewed in the results of this research, this energy dependence can be altered by introducing dopants. In insulators, the band gap is so large due to the difference in the energy levels which electrons occupy; this makes insulators unable to achieve conduction.

2.1 Semiconductor Transport Properties

The three transport properties are present in equation 2.1 below which tells the story of how these charge carriers can move about various materials.

$$\sigma \equiv \frac{1}{\rho} = n e \mu , \qquad (2.1)$$

where σ is the conductivity, or the inverse of the resistivity ρ , which is equal to the product of the charge carrier density n, the electron charge magnitude e, and the mobility μ [4]. By applying

this equation to semiconductors, their use in everyday electronics becomes obvious through the ability to control the carrier concentration during the manufacturing process. In turn, this dictates the behaviors of the resistivity and mobility therefore controlling how electrical signals are transmitted.

2.1.1 Carrier Concentration

The carrier concentration is the density of mobile charges within a volume of material. In metals, the concentration of free electrons is higher, such as copper which contains 8.47×10^{22} per cubic centimeter [5]. The constant availability of these mobile charges due to the overlapping band gap is a key piece of determining metallic behavior. On the other hand, intrinsic, or pure, semiconductors have lower carrier concentrations than metals. At room temperature, intrinsic silicon has an equal amount of mobile electrons and holes, each with carrier concentrations of $1 * 10^{10}$ per cubic centimeter [6]. Holes are positively charged voids in a crystal lattice where an electron would be for a homogenous material. The reason metals usually have a higher carrier concentration than semiconductors, is because electrons in metals are readily available and mobile in the conduction band without the need for added energy. In intrinsic semiconductors, charge carrier concentration is dependent on energy added to promote electrons to the conduction band. In this research, we look at the thermal energy dependence of carrier concentrations within semiconductors, though other forms of energy can alter charge carrier concentration as well. This energy required to achieve conduction is known as the band gap, which is the difference in energy between the valence and conduction bands [3]. At absolute zero (0 K) the maximum energy an electron can have is known as the Fermi energy (E_t) , this is why semiconductor charge carrier concentration is smaller at lower temperatures, in turn lowering the conductivity. At zero Kelvin, intrinsic silicon has zero mobile electrons or holes, ten orders of magnitude less than its room temperature concentrations stated before! These two comparisons show just how much change can occur within the same piece of material over a fairly narrow region of temperature [7].

As can be seen in Fig 2.0, the semiconductor valence band contains holes left behind from the electrons which were excited over the band gap and into the conduction band. Carrier concentrations can be increased in semiconductors by adding elements, referred to as dopants and impurities, which have more electrons than required for ionic bonding, or fewer electrons that are required, leaving holes [1]. As the percentage of dopants increases so does the charge carrier density at any given temperature due to the extra electrons or holes attached to the added impurities.

2.1.2 Resistivity

Resistivity in metals can be understood as friction that moving charges have with the atomic structure of a material. When electrons in metals move through the crystal structure of the material, they have to pass between the atoms that are bound together. Metals have very low

resistivity due to their large constant carrier concentration and become less resistive at lower temperatures. This is caused by a smaller amount of thermal energy contributing to the vibration of a metal's crystalline lattice structure, making it easier for electrons to flow through. In semiconductors, the resistivity is impacted by the changing carrier concentration and the mobility. The mobility is dependent on the interaction of charge carriers with the lattice structure of material as seen in metals, and also by the attraction that charge carriers have with oppositely charged atoms within the material [8]. Semiconductors are known to have a drastic increase in resistivity at lower temperatures due to fewer mobile charge carriers and smaller mobilities.

2.1.3 Mobility

The mobility of a material is how easily a charge can flow through a material and can be seen as inversely related to resistivity and carrier concentration by rewriting equation 2.1,

$$\mu = \frac{1}{q\rho n'},\tag{2.1.3}$$

where μ is the mobility, q is the charge magnitude (+e for holes, -e for electrons), ρ is the resistivity, and *n* is the carrier density. The mobility is co-dependent on the resistivity and carrier density [2]. Note that since metals have a constant carrier concentration and charges remain constant, the relationship between mobility and resistivity causes mobility in metals to decrease as temperatures increase due to greater vibrations within the lattice. In semiconductors, this relationship is a bit more complex and relates to both the change in carrier concentration over varying temperatures as well as the lattice vibrations that occur in all solids. Scattering mechanisms cause the mobility to increase by obstructing the ease of charge carrier movement [9]. For most conducting and semiconducting materials, the mobility is temperature dependent and is affected by the different mechanisms, two of which, impurity and phonon scattering, will be discussed and observed in this research.

2.1.4 Intrinsic, n-type and p-type

There are three types of semiconductors, one of which is intrinsic such as pure silicon and gallium arsenide. This type features mobile charge carriers that are freed up from atoms within a homogenous material. When some thermal energy is put into pure silicon, electrons from the valence band of a silicon atom are able to reach the conduction band, leaving behind a positively charged "hole" in the valence band they originated from, as illustrated in Fig 2.0. When an electron leaves an atom it must find a new position within the lattice, which is in the form of a hole that an electron recently left. This constant movement of electrons and holes in intrinsic semiconductors leads to two separate conductivities, one of which is the classic negative electron movement, and the other is a less familiar movement of positively charged holes, known as positive conduction [10]. Since both positive and negative charge carriers originate from a neutral atom or molecule, such as silicon or gallium arsenide, intrinsic semiconductors have equal concentrations of holes and electrons.

The other two types of semiconductors are manufactured to allow specific charge carrier types at controlled concentrations. N-type semiconductors are created by doping an intrinsic semiconductor, usually silicon, with a group V element, known as a donor, so that an extra electron is readily available and closer to the conduction band. As energy enters this material, electrons are easily freed up from their atoms and become mobile within the material's lattice while leaving molecular bonds intact, *i.e.* no leftover holes. Similarly, for p-type semiconductors, an intrinsic semiconductor is doped with a group III element, known as an acceptor, which leaves one empty bond position, or "hole", for every acceptor atom introduced. As electrons from neighboring atoms fill a hole, they leave behind a hole which they occupied, creating an illusion that the holes are moving and there is a conduction of positive charges.

An important note for analyzing data related to donors and acceptors: N_D and N_A are known as donor and acceptor concentrations, which is not the same as the carrier concentration. N_D and N_A are impurity concentrations which mean that they are the fixed amount of dopant atoms present in a semiconductor, while charge carrier concentration is the dynamic amount of charge carriers that have been excited into the conduction band.

2.2 The Hall Effect



Fig. 2.2 The Hall Effect diagram illustrates an n-type material with an applied longitudinal voltage and current in the *x*-direction while a magnetic field is applied in the *z*-direction. The black dots represent mobile electrons that have been pushed in the negative *y*-direction by the cross product of their velocity and the induced magnetic field. The buildup of electrons creates an electric field force pointing in the opposite direction, bringing the total force in the *y*-direction to zero and establishes a negative Hall voltage, V_{H_i} across the width of the material [2].

The Hall effect is a phenomenon that allows transport properties to be studied in semiconductors by manipulating electrical forces, geometry, and magnetic fields. As can be seen in Fig 2.2, the Hall effect occurs when a longitudinal voltage is put over a material and current flows while a

perpendicular magnetic field is applied. The moving charges undergo the Lorentz force pushing the charges perpendicular to both the current flow and the magnetic field in the direction corresponding to both the cross product of the Lorentz force and the sign of the charges. As the flowing charge carriers are forced against the boundary of the material, the Lorentz force approaches zero. The accumulated charges produce an electric field equal to and against the Lorentz force pushing them which can be measured as a voltage. Depending on the type of charge carriers flowing, electrons or holes, the sign of this will reveal what the carrier type is and its concentration, from

$$V_H = \frac{BI}{qtn},\tag{2.2.1}$$

where V_H is the measured Hall voltage across the material, *B* is the applied magnetic field, *I* is the applied current, *q* is the charge magnitude, *t* is the thickness of the material over which the charges accumulate, and *n* is the carrier density. The Hall voltage can be measured as positive or negative depending on the type of charge carrier conducting, which corresponds to the sign of the charge contained in *q* from Eq. 2.2.1 [2][5].

The resistivity ρ can be calculated using Ohm's law with the longitudinal voltage V_H , current I, and the geometry of the material

$$\rho = \frac{wt}{L} * \frac{V_L}{I},\tag{2.2.2}$$

where w, t and L are the width, thickness, and length of the material, respectively. Since Eq. 2.2.1 produces the carrier concentration and carrier type and Eq. 2.2.2 produces the resistivity, there is now enough information to calculate the mobility using Eq. 1.2.3.

2.3 Scattering Mechanisms

As discussed in earlier sections, resistivity and mobility of semiconductors are dependent on both the vibration of the lattice due to thermal energy, as well as the attraction charge carriers have with oppositely charged atoms within the lattice. These occurrences are known as lattice scattering and impurity scattering and are caused by phonons and dopants, respectively.

2.3.1 Lattice Scattering and Phonons

All solids are composed of atoms that are positioned in a fixed structure, known as a lattice. Fig 2.3.1 below shows an image of the atomic structure of silicon.



Figure 2.3.1 Lattice structure of silicon

This image shows the complexity of the lattice structure of not only silicon, but all solid materials. As thermal energy is added to a solid material phonons increase. Though phonons are a quantum mechanical quasi-particle, they can be classically described as vibrations within the lattice structure of solids. As phonons increase at higher temperatures and a current is applied to a material, the charge carriers interact and essentially "bump into" phonons and atoms vibrating more frequently. These bumps cause charge carriers to slow down and is the root of why resistivity increases and mobility decreases at higher temperatures for all conducting materials, at lower temperatures, fewer phonons occur, which is why metals become less resistive since charge carriers are more mobile [9].

2.3.2 Impurity Scattering and Doping

In semiconductors, when the crystal is doped with impurity atoms carrying a different number of valence electrons, an extrinsic semiconductor is created, either n-type or p-type, because the material had to be doped with these atoms in order to achieve the specified properties. When current flows through a semiconductor, charge carriers must push through the lattice, but as temperatures decrease and the lattice vibrates slower, two things occur: The first is that fewer electrons possess enough thermal energy to become conductive, and the second is that more interaction can occur between charged ions within the lattice and the flowing charge carriers [11]. In an n-type semiconductor, as an electron flows by an atom such as arsenic with a missing electron, an electrical attraction takes place which slows the electron down causing resistivity to increase and mobility to decrease. This same process happens in p-type semiconductors, though with opposite charges. This phenomenon is known as impurity scattering and is caused by the dopants within the crystalline lattice.

2.4 Temperature Dependence in Transport Properties

Tying it all together, semiconductor transport properties can be temperature dependent for different reasons than conductors. It has been discussed how carrier concentration in semiconductors increases with temperature leading to greater conductivity. Though the higher carrier concentration the more conductive the material, as temperature continues to increase phonon scattering will occur and begin to dominate conduction by decreasing the mobility and producing higher resistivities at higher temperatures in all materials. At lower temperatures, there are fewer charge carriers in semiconductors which move slower and the entire material vibrates slower. The lack of speed and frequency give way to attractive forces between carriers and ionized impurities decreasing the mobility. This impurity scattering is unique to semiconductors and helps determine the behavior over different temperature ranges and different dopant/impurity concentrations.

These properties will be viewed experimentally in both traditional semiconductors as well as semiconductors with metallic characteristics.

Chapter 3 – Methods



Figure 3. The Lakeshore Hall System and schematic shown above [12].

Using the Lakeshore Hall system, the resistivity, carrier concentration and mobility can be measured for semiconductors at room temperatures, as well as low temperatures. The process begins by acquiring the thin film and preparing it for the system. The sample is then placed between two magnets, which can be seen in Fig. 3. A magnetic field is induced along with a voltage and current, allowing transport properties to be measured. This general process is repeated at different temperatures to gather information on the temperature dependence of semiconducting materials.

3.1 Van der Pauw Contact Method



Figure 3.1 (a) image of sample with attached contacts, (b) van der Pauw schematic of sample and ideal contact areas [12]

The Van der Pauw contact method allows for accurate measurements of currents and voltages over a material. This method lies in creating four contacts on the periphery of a uniformly thick sample, which can be used to apply current to as a voltage is measured in order to calculate resistance or resistivity [12]. It is important to make ohmic contacts so that all the current and voltage measurements are due to the material and not the buildup of charge within a contact, creating a Schottky barrier [13]. Figure 3.1 above shows an example of Van der Pauw contacts. Note that the contact widths, 'c' must be much smaller than the width of the sample 'L'. Creating contacts as similar to a point contact allows the voltage and current measurements to reflect properties of the sample rather than properties associated with the contact itself.



3.2 IV Curve Measurement

Figure 3.2a Ohmic IV curve

For every sample being measured, an IV curve measurement is administered to assure that the contacts are ohmic. An IV curve is completed for four pairs of contacts: 1-2, 2-3, 3-4, and 4-1. For each pair, current is applied at different amperage steps, and is then reversed. While this current is applied a voltage is measured over each current step to confirm contacts are secure and the current-voltage relationship is linear (ohmic), such as Fig. 3.2a. If one or more of the contacts are not securely set, the voltage measurements will be noticeably greater than the contacts that are set properly. The Lakeshore software notices high voltage readings as out of compliance, because the voltmeter in the system only measures accurately up to 6V, therefore the applied current must be chosen to achieve an appropriate voltage reading. Voltage readings that are too

high can be caused by inconsistencies within contacts which increase the total resistance and voltage measurements along the IV curve.



Figure 3.2b non-ohmic (Schottky) IV-curve

If a non-linear relationship such as in Fig. 3.2b occurs, but voltages were within compliance, the interface between the indium solder and the sample created a Schottky barrier. A Schottky barrier occurs when a metal and a semiconductor make contact but require different energies to allow conduction. This barrier is due to a potential difference and causes a buildup of charges at the low side of the barrier therefore altering the measured voltage due to the non-ohmic contact [2]. This is why diodes work, because the barrier created by the conducting metal wire and the semiconductor piece requires a bias voltage to allow conduction. If this occurs in an IV curve measurement, the material used for the contact must be changed because the semiconductor material cannot be altered in order to measure transport properties [13][14].

3.3 Hall System

Once ohmic contacts are completed and confirmed, the Hall card containing the sample is inserted into the Hall system sample arm by aligning the leads at the bottom of the Hall card with the sample facing north, which corresponds to the magnetic field produced by the system. The Gaussmeter is then positioned between the focus of the magnet and the sample holder encasement. The Gaussmeter must be positioned precisely between where the sample and the magnet pole in order to control the magnetic field at precise magnitudes giving accurate measurements. The operating conditions are then set on the Lakeshore software on the computer attached to the system [12]. The initial measurement of a sample is conducted at varying

magnetic fields between $\pm 8 \ kG$ at 1 kG increments. The thickness of the sample must be included to get accurate calculations for the carrier density, though this could be entered at a later time if the thickness is currently unknown. The variable field measurement setup is complete at this point and when the results are complete, a field can be chosen at which the mobility and carrier density converge. This field will then be used for the temperature dependent measurement, as there is not adequate time to do a full magnetic field sweep during this process.

3.3.1 Resistivity



Figure 3.3.1 Van der Pauw schematic showing applied current and measured voltage pairs. Resistivity is measured and calculated using contact configuration (a) while carrier concentration and mobility are calculated using the Hall voltage in configuration (b) [12].

The resistivity of the material is determined by the geometry of the material in the system, specifically the thickness of the material. Using the van der Pauw configuration of contacts, the voltage over and current through the contacts are measured and applied. By using the thickness of the sample and the current and voltage measurements to calculate a resistance, the process is repeated on different contact pairs to produce an average resistivity consistent throughout the sample [12]. An example of a contact pair used to calculate resistivity is shown in figure 3.3.1(a), depicting a longitudinal voltage measurement in the direction of the current. The longitudinal voltage and current along with the thickness is used to calculate the resistivity using an average of the equations:

$$\rho_{A} = \frac{\pi f_{A} t[m, cm]}{\ln(2)} \left\{ \frac{V_{12,43}^{+} - V_{12,43}^{-} + V_{23,14}^{+} - V_{23,14}^{-}}{I_{12}^{+} - I_{12}^{-} + I_{23}^{+} - I_{23}^{-}} \right\} \quad [\Omega \cdot m, \Omega \cdot cm]$$

$$\rho_{B} = \frac{\pi f_{B} t[m, cm]}{\ln(2)} \left\{ \frac{V_{34,21}^{+} - V_{34,21}^{-} + V_{41,23}^{+} - V_{41,23}^{-}}{I_{34}^{+} - I_{34}^{-} + I_{41}^{+} - I_{41}^{-}} \right\} \quad [\Omega \cdot m, \Omega \cdot cm]$$

Where f_A and f_b are factors that contain the length and width, but since the samples are square and contact distances are all equal from corner to corner, both f_A and f_b are equivalent to each other. These f-factors are critical in calculating the averages for the voltage and current between contact pairs, if the contact pairs are unevenly spaced, the system will alert the user that there are inconsistencies in the data collected. The collected data for the four contact pairs at each current step should fall within a ten percent tolerance of each other; otherwise contact adhesion and/or spacing must be investigated.

3.3.2 Carrier Density

The carrier density is calculated by the magnetic field magnitude, current measurement and Hall voltage measurement as previously explained in eq 1.2.2. The current and Hall voltage configurations measured by the system are different contact pairs which are perpendicular to each other, because the Hall voltage is the potential *across* the flow of charge. An example of this configuration can be seen in Fig. 3.3.1b. Using the input thickness of the material and the measured parameters, the Lakeshore software is able to calculate the number of charges per cubic centimeter by taking the average of these measurements for the four different sets and orientations of contacts. This measurement process also extracts the carrier type through the Hall voltage sign, as stated in eq 1.3 [2][12].

The Lakeshore system and software produce data that can be used to model the carrier density over a range of fields and temperatures in order to extract the semiconductor behavior.

3.2.3 Mobility

The mobility of the material is calculated by applying the calculated resistivity and carrier density to equation 1.2.3. The Lakeshore system uses the information gathered on resistivity and carrier density to do so.

3.3 Temperature Dependent Hall Measurements

To gather temperature dependent Hall data, a dewar is inserted between the magnets and filled with liquid nitrogen. This allows the sample to cool down to near zero temperature of 77 K. The transport properties are measured as the temperature rises from 77 K back to room temperature [12].

Both arsenic and antimony are group 5 elements meaning they have five valence electrons available to form bonds with silicon. When silicon is doped with either arsenic or antimony, four electrons are bonded with separate silicon atoms and leave one electron available for conduction. These extra electrons become free when thermal energy is added to the doped material, and this can be seen in the results, especially for antimony [15].

Chapter 4 – Results

4.1 Boron doped Silicon (P-type)

Boron doped silicon samples were the p-type silicon samples used. Since boron is a group III element, it brings one acceptor site per boron atom inserted in the silicon lattice. Each acceptor site is a hole in terms of conduction, and move in the opposite



Figure 4.1a Boron doped silicon resistivity versus temperature.



Figure 4.1b Boron doped silicon carrier concentration versus temperature.



Figure 4.1c Boron doped silicon mobility versus temperature.

4.2 N-type Silicon

The n-type silicon samples correlated closely with previous research done by Sheng S. Li for the National Bureau of Standards.



4.2.1 Antimony Doped Silicon

Figure 4.2.1a Antimony doped silicon resistivity versus temperature.



Figure 4.2.1b Antimony doped silicon carrier concentration versus temperature.



Figure 4.2.1c Antimony doped silicon mobility versus temperature.

4.2.2 Arsenic Doped Silicon



Figure 4.2.2a Arsenic doped silicon resistivity versus temperature.



Figure 4.2.2b Arsenic doped silicon carrier concentration versus temperature.



Figure 4.2.2c Arsenic doped silicon mobility versus temperature.

4.3 Indium Tin Oxide



4.3a ITO resistivity versus temperature



4.3b ITO carrier concentration versus temperature



4.3c ITO mobility versus temperature

Chapter 5 – Discussion

5.1 Silicon Results and Comparisons

When comparing data collected in the lab with previously collected data on similar materials, the transport property trends become clear and verify occurring scattering mechanisms.

5.1.1 N-type Silicon



Figure 5.1.1a The arsenic doped silicon and antimony doped silicon data correlate with previously collected data and with theoretical trends which represent resistivity as a function of impurity concentrations and temperature [16].

In figure 5.1.1a above, the resistivity vs. temperature plot compares theoretical plots with the recently collected resistivities of antimony and arsenic doped silicon. The theoretical model for resistivity was created by using equation 2.1.3 while the mobility figures were generated through a separate model accounting for various scattering mechanisms [16]. The antimony doped silicon is very closely aligned with donor concentrations between 1E18 and 2E18 antimony atoms per cubic centimeter. This correlation reinforces the understanding that in semiconductors with lower donor(dopant) concentrations, the resistivity increases at lower temperatures, the opposite of metals. Note that this is due to the smaller amount of electrons becoming excited into the

conduction band when less thermal energy is available within the material, which corresponds to the relation of equation 2.1.3.

As can be seen in figure 5.1.1a above, the arsenic data collected had an initial donor concentration much higher than previous predictions included. The resistivity trends for donor concentrations of about 1E19 atoms per cubic centimeter show that there is a reversal in the resistivity-temperature relationship. As the dopant concentration is increased, such as in the arsenic sample, electrons have a higher probability of being excited into the conduction band with a smaller thermal energy which in turn causes highly doped semiconductors to behave almost as a metal. As discussed previously for metals, resistivity increases at higher temperatures.



Figure 5.1.1b Room temperature electron mobility values for arsenic are overlaid onto existing theoretical and experimental values of mobility against room temperature carrier concentration [17]

In figure 5.1.1b, the room temperature mobility tends to decrease as carrier concentration increases. In arsenic doped silicon, this is due to lattice vibrations increasing electron-phonon interactions. As more impurity atoms are added to a semiconductor, the band gap decreases causing a higher probability of mobile electrons at room temperature, which leads to more electron-phonon interactions. As seen in the carrier density and resistivity plots from the results section, the arsenic doped silicon sample essentially has free and mobile electrons at any given temperature above 77 K, which only leaves phonon scattering as the impactful conduction mechanism.



Figure 5.1.1c N-type Si:As and Si:Sb mobility data overlaid onto theoretical contour lines for various donor concentrations at varying temperatures [16]

In the n-type mobility plot above, the antimony and arsenic doped silicon samples have differing trends. This leads one to believe that the trends change direction at about the same dopant concentration as the arsenic doped silicon sample used, which is about 10¹⁹ electrons per cm³. After some investigation into the Hall data, it was determined that the limits of the Lakeshore Hall system created this unexpected trend. Specifically, the Kiethley nanovolt meter had reached the lower boundary of measuring the Hall voltage across the sample that the Lakeshore system undergoes. The measured voltages were far too low to produce sensical and accurate carrier densities, which in turn produced inaccurate mobility data from the relationship in Eq. 2.2. In order to gather more reasonable mobility data for the arsenic doped silicon, the measurement process should be repeated with higher excitation currents that would keep the Hall voltage measurements within compliance and above the lower limits of the voltmeter.

5.1.2 P-type Silicon



Figure 5.1.2 Boron doped silicon resistivity data compared with existing experimental and theoretical results and trends [18]

The heavily boron doped silicon sample data shown in Fig. 5.1. continues the trends appearing in previous research done by Luis Linares at the University of Florida [18]. The temperature dependent resistivity trends show that for higher concentration of acceptor atoms semiconductor resistivity steadily decreases as temperature increases. This trend occurs because at lower temperatures, both the lattice and charge carriers have lower kinetic energy, which cause the mobility to be smaller. As seen from Eq. 2.1.3, the resistivity is inversely related to the mobility; therefore, as the resistivity decreases with temperature the mobility can be expected to increase, which does occur.



5.2 Temperature Dependent Mobility Trends

Figure 5.2a Antimony and arsenic silicon mobility data overlaid onto theoretical n-type mobility trends of various impurity concentrations [19].



Figure 5.2b Collected data for boron and antimony doped silicon mobilities overlaid onto theoretical and experimental trends for both p-type and n-type mobility [20].

The first figure, Fig 5.2a, shows clear mobility trends for n-type silicon which correlate to the recently collected antimony data. The antimony doped silicon data arches as the theory predicts, though in both figures 5.2a and 5.2b, the peak of the recently collected data is shifted to the left. Though this shift does not impact the understanding and verification of the occurring scattering mechanisms, it should be noted that the temperature probe may have an offset from the precise temperature of the sample. As can be seen in the antimony results section and using equation 2.1.3 to analyze this data, the interconnectedness of conductivity and scattering mechanisms can be pieced together. At lower temperatures, there are fewer electrons excited into the conduction band which contributes to a greater resistivity as there is an inverse relationship between resistivity and charge carrier concentration. In addition to the carrier density's resistivity contribution, the small mobility at lower temperatures increases the resistivity as well since they are also inversely related. The small mobility is caused by the attraction of mobile electrons to positively charged ionized antimony atoms throughout the lattice, causing the electrons to slow down under an electric field (voltage). This attraction occurs more frequently at lower temperatures because everything is moving slower creating more time for the interaction. This can be understood by Eq. 5.1.2 below which connects the thermal energy of atoms and charge carriers to the attraction of charge carriers with a charged nucleus as viewed quantum mechanically.

$$\frac{Ze^2}{4\pi\varepsilon_0 r_s} = \frac{3}{2} K_B T, \qquad (5.1.2)$$

As the temperature increases, the thermal energy of the lattice and charge carriers dominates and overcomes the atomic attraction [11]. At roughly 200 K, the mobility begins to decrease again due to the large amount of thermal energy now present in the lattice. The thermal energy induces lattice vibrations which induce quasi-particles called phonons that interact and interfere with electron mobility. This interference that phonons have with charge carriers is known as phonon scattering which produces the second half of the arch which can be seen in the antimony mobility data.

The recently collected data for boron doped silicon also shows that the mobility is minimal at lower temperatures but this time increases until it flattens out at room temperature where data collection stopped. This reinforces the expectation that impurity scattering dominates when more dopant atoms are present due to the greater amount of ionized atoms to attract mobile charge carriers. As seen with the antimony doped sample, the occurrence of impurity scattering at lower temperatures is due to both the molecular structure and positively-charged holes moving slower. The slow movement then increases the interaction time holes have with atoms which decreases the mobility of the holes due to the Coulomb attraction [11]. This is beautifully explained in Eq. 5.1.2 showing that the thermal energy between an electron moving through the material must equal, or at least compare to, the Coulomb potential of an atom with charge *Z*. The left hand side of this equation has been seen in quantum mechanics within Hamiltonians and perturbation theory, while the right hand side is the thermal-kinetic energy in a three-dimensional solid[15].

The mobility data for the arsenic doped silicon is not reliable as previously discussed in section 5.1.1 due to the limitations and wrong configurations of the Hall system. This data can be neglected for analysis, but is shown to reinforce that the data is nonsensical which led to tracking down the experimental error.

5.3 Indium Tin Oxide

ITO produced behavior that very closely related to previous research by Lin in the Journal of Condensed Matter physics. Lin pointed out that ITO produces metallic behavior and the resistivity of ITO should follow the Bloch-Gruneisen equation [21]:

$$\frac{\rho_{\mathrm{BG}} - \rho_0}{\lambda_{\mathrm{tr}} \omega_D / \omega_p^2} = f_{\mathrm{BG}}(T/\Theta_D) = (4\pi)^2 \left(\frac{2T}{\Theta_D}\right)^5 \int_0^{\Theta_D/2T} dx \frac{x^5}{\sinh^2(x)}$$
(5.3)

Comparing this model to resistivity measurements recently collected the curves in Fig 5.3 below were produced.



Figure 5.3. ITO temperature dependent resistivity data compared with the Bloch-Gruneisen[21]

Fig. 5.3 shows a strong correlation between the Bloch-Gruneisen model and ITO resistivity collected over various temperatures. The numerical correlation produced by the Pearson formula gave 0.9997 [22]. The Pearson correlation coefficient is a statistical method which normalizes the similarities and differences between datasets using the formula

$$r = \frac{\sum_{i}^{n} (x_{i} - \overline{x})(y_{i} - \overline{y})}{\sum_{i}^{n} (x_{i} - \overline{x})^{2} (y_{i} - \overline{y})^{2}}.$$
(5.3.2)

With the strong Pearson coefficient, both the data and model for ITO resistivity uphold each other. The numerical calculation and plot was produced using Mathematica.

As the resistivity was confirmed and the carrier density measurements seen in the results section appear to be relatively constant with an average at about 10^{21} cm⁻³, the expected mobility would decrease proportionately to the resistivity, given their inverse relationship [23]. It can be concluded that phonon scattering is the dominant mechanism which occurs in highly doped indium tin oxide when viewing the temperature dependent data from section 4.3.

Chapter 6 – Conclusion

The goal of verifying scattering mechanisms was achieved by observing the impurity and lattice scattering over a range of temperatures in silicon samples and indium tin oxide. This work was important and useful in determining the behavior of semiconductors at varying temperatures and impurity concentrations which can be applied to newly produced semiconductors such as TiO2. With silicon being the dominant semiconductor used throughout technology, it is important to know what the impact of donor and acceptor impurities are on conduction mechanisms, because conductivity allows information to be carried through electrical signals.

The room temperature carrier densities of boron doped silicon sample, antimony doped silicon sample, and arsenic doped silicon sample were measured to be $8*10^{18}$, $1.5*10^{18}$, and $3.4*10^{19}$ per cubic centimeter respectively. The antimony sample showed significant changes in carrier densities leading to the dominant impurity scattering at lower temperatures and phonon scattering at higher temperatures. The boron doped sample showed a relatively constant and large carrier concentration with lower mobility at lower temperatures because of impurity scattering.

The broad implications of this research are that transport properties in newly created semiconductor samples can be investigated with known and verified operating procedures within the Hall lab. As these newer semiconductors are researched, specifically the polymorphs: brookite, anatase and rutile of TiO2, more uses and manipulations of this material can be developed for custom uses. Most importantly, this research has verified scattering mechanisms which occur due to impurities and phonons within semiconductors and the changes which occur due to temperatures and impurity concentrations. Newer insights have been brought to light as the work with silicon samples has been done, which include making contacts ohmic. A different contact material, graphite adhesive, has been introduced to semiconductors that inhibit schottky barriers when soldered with indium. This should help in future research as the contact resistance has impacted measurements as additional contact resistivity throws off the already sensitive Hall voltage measurement. The intricacies of the Hall system have been investigated enough in this research so that future users can aim for certain voltage readings within the system to acquire dependable data, unlike that which occurred with the arsenic doped silicon sample. Though there are some TiO2 samples ready to measure, the hopes for completing a thorough investigation on intrinsic silicon are still present, as well as collecting sensical data on the arsenic doped silicon. As these last samples are confirmed and match the values expected of their dopant concentrations, the group can confidently move forward in collecting data for TiO2.

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