Kelvin probe microscopy on disordered semiconducting materials

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Preface

This thesis is written as graduation paper for my master degree on applied physics. This one year project is done in the research group molecular materials and nanostructures (MMN) at the technical university of Eindhoven. This research group focuses mainly on organic electronics, in both material research and organic PV-solar cells. Part of the group is chemistry related and their main activity is synthesizing and characterizing new materials. My work is done at the physics part of the group. The physics part of the group focuses on conduction mechanisms through small molecules, polymers and a variety of graphene like materials. Furthermore there is interest in a variety of new devices such as organic light emitting field effect transistors and light emitting electrochemical cells.

First of all I want to thank Christian Roelofs. Christian supervised my project, and guided me through this thesis. He taught me about the atomic force microscope, and how to work with an ultra high vacuum chamber. He explained me the measurement techniques used, and we have discussion about both my and his work. Last but not least, Christian supplied most samples with collaboration of the Holst centre Eindhoven, and Philips research.

Secondly my much gratitude and appreciation goes to dr. ir. Martijn Kemerink, who is the head of the physics subgroup of MMN. With dedication and patients he helped me with discussion about the physics I encountered.

Next I want to thank the group technician Marco for responding basically direct on anything what should be fixed. More specific he helped me with redesigning sample holders, and the two times adjustments had to be made and the vacuum had to be broken.

Finally the rest of my direct colleagues for all the knowledge shared which leads to my broad interest in the field. This useful knowledge transfer comes meanly by sharing findings on friday morning meetings. The more general every-day-live knowledge from cultures all over the world as well as dutch weekends was also highly pleasant to hear.

-Willem
Abstract

In disordered semiconducting materials the conduction is dominated by localized states that can be occupied by charge carriers. The energetic distribution of these states, i.e. the density of states (DOS), is crucial for modeling the charge transport in these types of materials and hence for better insight. Most conduction models assume an exponential or Gaussian DOS. Here, a Kelvin probe measurement technique in ultra high vacuum is used to directly measure this DOS for the active layer of a thin film field effect transistor (TFT). In a TFT, an appropriate gate bias induces an accumulation layer in the semiconducting layer, allowing charge to flow. The conventional mobility models, variable range hopping and mobility edge, are used to fit this charge transport. Second, assuming a constant DOS, a constant electric permeability and non-relevant surface states, the limited screening of the gate voltage as simultaneously probed by the Kelvin probe can quantitatively be related to the DOS. The results are corrected for the finite thickness of the active layer, so for the distribution of the accumulation layer in the normal direction. A third technique is used to examine the conduction namely the Seebeck coefficient \( S = -\Delta V/\Delta T \). With the conduction mechanism known the Seebeck coefficient can be directly calculated.

These techniques are used to examine conduction through oxidic as well as organic materials, for n-type, p-type and ambipolar semiconductors. In the report five different materials are examined, and mostly treated separately. The first material examined is Gallium Indium Zinc Oxide (GIZO). Mobility models are used to combine the DOS measurements mentioned above, temperature dependent mobility measurements and temperature dependent Seebeck coefficient measurements. For the DOS an exponential shape is found, with a slope of \( T_0 = 800K \). Using this as the tail of localized states, GIZO shows good fits for an extended mobility edge model. This is a mobility edge model which allows hopping conduction in the tail states and also accounts for the reported Hall effect in GIZO.

For Pentacene the DOS measurements show an exponential tail and fast increasing bulk states. The DOS shows good fits with use of a double exponential. It is shown that surface states are formed at the gate dielectric of the pentacene layer. Next the material PTAA is examined. PTAA shows typical mobility curves, with the mobility showing a rapid increase for low gate voltages, followed by a very slow increase at higher gate voltages. The DOS measurements show an exponential DOS. Using this DOS we show that the mobility is not decently described with either variable range hopping or mobility edge. With use of any arbitrary exponential DOS the fits are still poor. Hence, we conclude that the variable range hopping model in this state is unable to describe the conduction mechanism for the material PTAA.

Measurements are performed on the ambipolar polymer materials P17 and KH71. The materials are rather comparable in structure where KH71 has longer polymer chains and larger molecular mass than P17. Both materials show an asymmetry for electrons and holes for both the Kelvin probe as well as the mobility measurements. The bandgap of P17 shows up in Kelvin probe measurements, whereas the bandgap of KH71 is not observed. For use in ambipolar regime a recombination zone in a FET can be measured using scanning Kelvin probe microscopy. The stability of the position of this recombination zone is found to be critically dependent of the ratio between contact resistance and conductivity. This is confirmed using numerical simulations. However, many measurement phenomena remain unclear, which makes an actual DOS extraction from Kelvin probe measurements unreliable in this case.

Summarizing, the Kelvin probe technique is suitable to measure the DOS; for GIZO nice results are obtained. In the organic materials many unexplained things happen and the assumption of a position independent DOS and constant electrical permeability are doubtful.
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1. Introduction

Popularity of organic electronics is pushed by promises of low production costs, large area application, and the possibility for flexible devices. These promises are mostly a result of the solubility of many of the materials. Solution deposition is done at low temperatures in contrast to the deposition of conventional crystalline semiconductors. This low temperature process ability creates the possibility to deposit the material on plastics, for creating flexible electronics.

Most used device configurations are organic field effect transistors (OTFT), organic light emitting diodes (OLED) and organic photovoltaic cells. OTFTs are also useful in integrated circuitry. One of the applications for OTFTs is to drive OLEDs in an OLED display. OLED displays already hit the market. A key advantage of organic polymers is the tunability of the band gap. With the low cost, large areas, and tune ability great promises for the future are expected.

However the charge transport in organic materials is not well understood. The description of charge transport is depending on the disordered structure \(^1\)-\(^4\). Two models which are mostly used in literature to describe charge transport are variable range hopping, and mobility edge. Crucial in models for charge transport is knowledge of the density of states (DOS). \(^5\) In the absence of information about the DOS is normally assumed to be exponential or Gaussian. Several techniques are used to extract the DOS. \(^6\)-\(^11\)

We measure the DOS directly using scanning Kelvin probe microscopy (SKPM) from a functioning field effect transistor as introduced by Tal et al. \(^11\) Huge advantage of this technique above many others is the DOS is probed in an operational transistor. The DOS is measured while charge is accumulated and able to conduct. Therefore the DOS measured is the same DOS which is responsible for charge transport.

1.1. Project goal

The aim of this project is to use scanning Kelvin probe measurements to extract the density of states of several materials. This DOS is a basis for understanding transport measurements. The Kelvin probe measurements are now used for self assembled monolayers. First objective is to correct for finite thicknesses of thin films (<10nm).

Several different types of materials are investigated, n-type, p-type en ambipolar semiconductors. Gallium Indium Zink Oxide GIZO, is an amorphous oxide n-type semiconductor. For p-type both pentacene and PTAA are investigated. For the ambipolar semiconductors two polymers are investigated, P17 and KH71.

The buildup of this document starts with an explanation of the field effect transistor. These are the devices used for all measurements, and therefore of high importance. The second chapter deals with the specific conduction models used in this thesis. This chapter is kept short as this is mostly found in textbooks. Most of the measurement technique of the DOS measurements is explained using the results of GIZO to be able to use realistic values. The results are divided into four parts, as if they are all separate research subjects. All unipolar devices have a chapter dedicated to their results. The ambipolar devices are considered simultaneously.
2. Devices

In this study thin film field effect transistors (TFT) are used to examine the different organic materials. First the architecture of the materials as used in this rapport is discussed, followed with the operation of the TFT, and a brief discussion about contact resistance.

2.1. Field effect transistor

The field effect transistor consists of three electrodes, referred to as the source drain and gate, schematically shown in figure 1. The space between source and drain contacts is called the channel. The channel length (L) is the distance between source and drain contact. The channel width (W) is perpendicular to the channel length. It defines the length of area between source and drain contact. The channel width is typically in the order of centimeters where the channel length is in the order of micrometers. So the channel width is usually several orders of magnitude larger than the channel length. The channel is filled with an active semiconducting layer allowing conduction between source and drain. The gate electrode is separated from the channel by a dielectric layer, preventing any current to flow. With the gate the conductivity of the active layer between source and drain contacts can be controlled.

![Diagram of field effect transistor](image)

**Figure 1:** Schematic representation of an organic field effect transistor. The metallic source, drain and gate contacts are represented in blue, the active layer material in green and the electric isolating dielectric layer is represented in orange. The drain contact is typically grounded, $V_G$ is the gate voltage with respect to the drain contact, $V_{sd}$ is the voltage between source and drain contact.

2.2. Operation of Field effect transistors

Ideally there are no intrinsic free charge carriers in the semiconducting layer, therefore no current will flow between source and drain contact. The transistor works like a capacitor. By applying a bias on the gate electrode charges will build up at the gate. An equal number of charge carriers, opposite in sign, will be accumulated into the active layer. This charge will be near the gate dielectric in a so called accumulation layer. Charge carriers in the accumulation layer allow a current to flow between source and drain electrodes.
If a low gate voltage is applied $|V_G| < |V_{sd}|$ the charges in the accumulation layer vary along the length direction of the organic semiconductor. This operation mode is referred to as the saturation regime. If the gate voltage is high $|V_G| >> |V_{sd}|$, the variation of accumulated charges in the organic semiconductor are negligible, the transistor is in linear regime. To account for this variation in the channel the gate voltage has to be calculated with respect to the channel position. This variable potential $V(x)$ is given for constant mobility by:

$$V(x) = V_G - \frac{x}{L} \left( (V_G - V_{sd})^2 - V_G^2 \right) + V_G^2$$  \hspace{1cm} (1)

In which $x$ is the position in the channel length measured from the drain contact. With the assumption of a constant linear mobility and the channel length being much larger than the thickness of the gate dielectric, the current can be calculated for the linear regime $I_{SDLin}$ equation 2 and for the saturation regime $I_{SDSat}$ equation 3.

$$I_{SDLin} = \frac{W}{L} \mu C (V_G - V_T) V_{SD}$$ \hspace{1cm} \text{with} \hspace{0.5cm} V_D >> V_G$$  \hspace{1cm} (2)

$$I_{SDSat} = \frac{W}{L} \mu C (V_G - V_T)^2$$ \hspace{1cm} \text{with} \hspace{0.5cm} V_D \geq V_G$$  \hspace{1cm} (3)

With $C$ the area capacity and $\mu$ is the mobility. For determining the mobility the transistor is operated in the linear regime. By measuring the current, the mobility can be calculated:

$$\mu = \frac{L}{CWV_{SD}} \frac{I_{SD}}{(V_G - V_T)}$$  \hspace{1cm} (4)

In literature the current is generally calculated with use of the differentiation of the current to the gate voltage. The method has the advantage to be independent of threshold voltage.

$$\mu = \frac{L}{CWV_{SD}} \frac{\partial I_{SD}}{\partial V_G}$$  \hspace{1cm} (5)

### 2.3. Contact resistance

The contact resistance accounts for voltage drops at both contacts. For conventional metal semiconductor interfaces contact resistance can normally described as a Schottky barrier, such resistance is not ohmic. In order to get a good understanding about contact resistance the contact resistance can be modeled using advanced hopping injection models as Arkhipov\textsuperscript{12} model and Emtage/O’Dwyer model. In these models the resistance is gate voltage dependant for low gate voltages.

Without the modeling approach the contact resistance can be measured. This can be done by using the transmission line method (TLM, or transition length measurement) making one sample with TFT structures with increasing channel lengths. The value of the resistance of the total transistor is build up from two parts; the sheet resistance, and the contact resistance. The contact resistance is encountered twice, at the source and at the drain contact. After rearranging equation 3 and adding the contact resistance the next equation is obtained:

$$R = \frac{L}{\mu WC (V_G - V_T)} + 2R_C$$  \hspace{1cm} (6)
With $R_C$ the contact resistance. Plotting sever conductance measurements to different channel lengths, a plot appears with a linear slope. From the slope the mobility can be obtained, where from the y-intercept point the sum of both contact resistances is obtained.

### 3. Mobility models

Mobility models are crucial in understanding charge transport in materials. The modeling of charge transport in organic semiconductors in this report revolves around two models: Variable range hopping and mobility edge. Mobility edge is also referred to as multiple trapping and thermal release model. Both models assume disordered localized states to be of high importance. Variable range hopping is a theory which describes the charge carriers localized on different molecules. With use of phonon vibration these charge carriers can ‘hop’ to an energetically and spatially nearby molecule. Mobility edge model assumes a tail of localized states. The charge carriers occupying these states can be excited up to a state where they are spatially extended. These spatially extended state, which are in energy just above the ‘mobility edge’ allow for conducting current.

#### 3.1. Mott variable range hopping

In order to derive variable range hopping two assumptions have to be made. We assume a weak electronic coupling between the different electronic sites, so they can be treated as independent. Furthermore it is assumed that charge carriers tunnel from one molecular orbital to another. The hopping rates from state $i$ with energy $E_i$ to state $j$ with a higher energy $E_j$ is described by the Miller-Abraham\(^{13}\) expression:

$$v_{ij} = \begin{cases} v_0 \exp \left[-2\alpha r_{ij} - \frac{E_j - E_i}{k_B T} \right] & \text{if } E_j - E_i \geq 0 \\ v_0 \exp \left[-2\alpha r_{ij} \right] & \text{if } E_j - E_i \leq 0 \end{cases}$$  \hspace{1cm} (7)

Here $r_{ij}$ is the distance between state $i$ and state $j$, $K_B$ is the Boltzmann constant, $T$ is the temperature and $\alpha$ represents the inverse localization length of the decaying wave function. $v_0$ represents the attempt frequency, this frequency is related to molecular vibrations typically between (1-100) fs. For hops to lower energy this energy part drops out of this equation.

The conduction is closely related to the hopping rate, following Mott\(^{14}\) the conduction can be written as:

$$\sigma = \sigma_0 \exp \left[-2\alpha R^* - \frac{E^*}{k_B T} \right]$$  \hspace{1cm} (8)

$R^*$ represents the typical hopping distance, and $E^*$ the typical hopping energy. With the assumption that a typical hop takes place from the Fermi level, a relation between $R^*$ and $E^*$ can be obtained.

$$\frac{4\pi}{3} (R^*)^3 \int_{E_f}^{E_i+E^*} dE g(E) = B_c$$  \hspace{1cm} (9)

With $B_c$ is the number of bonds per site in the percolation cluster. We assume 3D hopping and use $B_c=2.8$ for the modeling. Next step is to find the most dominant hop by maximizing the conductivity (equation 8) with $R^*$ and $E^*$. Any DOS can be used and the mobility is very dependent to the shape of this DOS.

#### 3.1.1. Vissenberg and Matters mobility model
Disorder in organic material can lead to an exponential DOS.

\[ g(E) = \frac{N_0}{k_BT_0} \exp \left( \frac{E}{k_BT_0} \right) \]  (10)

In this equation \( E \) is the energy, \( N_0 \) represents the total number of states and \( T_0 \) determines the width of the exponential DOS. With the assumption the \( E_f \) is far in the DOS, and that \( E^* \ll k_BT_0 \), Vissenberg and Matters show the mobility of a field effect transistor can be calculated. 4

\[ \mu_{FE} = \frac{\sigma_0}{q} \left( \frac{T_0 / T}{2\alpha} \right)^{T_0/T} \left( \frac{C(V_G - V_T)}{2k_BT_0\epsilon_s} \right)^{T_0/T-1} \]  (11)

With \( V_G \) the gate voltage, \( V_T \) the threshold voltage, \( q \) is charge and \( C \) is the gate capacitance.

### 3.2. Mobility edge model

In conventional crystalline materials the conduction is described by bands of delocalized states. In amorphous oxide materials, conduction can be described by this type of transport. Added to this are localized trap states. Among these localized trap states no conduction is allowed in the pure mobility edge model. Charge transport takes place when a charge carrier gets thermally excited above a so called mobility edge. Above this mobility edge, the states are delocalized, and its transport is described as if it is a band like transport. Up to the point the charge carrier will fall back to a localized state. Therefore the conduction is linear with the amount of charges in above the mobility edge.

\[ \sigma_{ME} = e \mu_{free} \int_{E_{ME}}^{\infty} f_{FD}(E) g(E) dE \]  (12)

In this function \( f_{FD} \) is the Fermi Dirac distribution, where the integral start at the mobility edge energy \( E_{ME} \). \( g(E) \) represents the density of states, \( e \) the electron charge. \( \mu_{free} \) is the mobility of one free electron. In this single electron mobility are many unknowns, including the scattering time. Therefore the value of this variable is difficult to predict.

### 3.3. Extended mobility edge model

The mobility edge model explained above, has a tail of localized states. Mott showed the possibility that in these tail states hopping conduction exists. The fusion of these two models into one model is referred to as extended mobility edge (eME). The conduction in such material will follow a combination of both models shown above. Above a certain mobility edge energy \( E_C \), band like conduction takes place. In all localized tail states the Mott variable range hopping occurs.

\[ \sigma_{VRH} = \sigma_0 \exp \left[ -2\alpha R^* - (E^* - E_F) / (k_BT) \right] \text{ for } E < E_C \]

\[ \sigma_{ME} = e \mu_{free} \int_{E_C}^{\infty} f_{FD}(E) g(E) dE \text{ for } E \geq E_C \]  (13)

In the modeling used in this report, the localized tail states can have any shape. Most used are exponential tail states. The mobility edge DOS is assumed to be a constant DOS.
The two types of conduction can be seen as parallel paths. The total conduction through the investigated material can be described by the superposition of both separate conductions.

\[ \sigma_{eME} = \sigma_{ME} + \sigma_{VRH} \]  

(15)

Several parameters distinguish whether the variable range hopping or the band like conduction dominates the charge transport. For example if the number of charge carriers in the tail of localized states is much higher than the number of accumulated charges. Than this results in very few charges being able to jump above the mobility edge. This will favor hopping conduction. The shape of the DOS can also contribute to the distinction. Temperature can also distinguish between variable range hopping and band conduction. By increasing temperature, typical hops will get higher in energy, and the mobility edge will be reached more easily. If the typical hopping energy is above the mobility edge, the variable range hopping contribution will become negligible, the conduction will be totally dominated by band conduction.

### 3.4. Seebeck coefficient

The Seebeck coefficient \( S \) is alongside the Peltier coefficient \( \Pi \) part of the thermoelectric effect. The Seebeck coefficient describes the voltage response \( \Delta V \) form a temperature difference \( \Delta T \) along a material.

\[ S = \frac{\Delta V}{\Delta T} \]  

(16)

By applying a known temperature difference to a TFT, the voltage difference, and therefore the Seebeck coefficient, can be directly measured. All Seebeck measurements used in this document are performed by W.C. Germs.

The Seebeck effect is mainly caused by charge carrier diffusion. Charge carriers on a hot end of a material can diffuse differently than charge carriers on the cold end. The opposite effect is described by the Peltier coefficient. The Peltier coefficient is a measure for the heat flux carried per unit charge through a material. If the charge transport mechanism is known the Peltier coefficient can be calculated. By fitting with the model shown above all necessary parameters are known. The Seebeck coefficient can be calculated from the Peltier coefficient with use of the Onsager reciprocity relations.

\[ S = \frac{\Pi}{T} = \int \frac{(E - E_F)\sigma(E)dE}{eT\int \sigma(E)dE} \]  

(17)

The Peltier coefficient is written as the integral over the conduction with energy \( E \), normalized to the total conduction. It is straight forward to directly calculate the Seebeck coefficient from data of the conduction. For variable range hopping equation reduces to:

\[ S_{VRH} = \frac{(E^* - E_F)}{eT} \]  

(18)

Where \( E^* \) is the typical hopping energy. The hopping energy dominates conduction and therefore Seebeck coefficient.
For pure mobility edge all localized tail states can be ignored. The only states contributing to mobility, and therefore Seebeck coefficient, are the states above the mobility edge. The derivation from equation is done by setting limits to the integral. The function can be simplified by assuming all states above the mobility edge have the typical mobility edge energy ($E_C$). The correction factor $A$ is for additional energy transported by the states above the mobility edge.

$$S_{ME} = \frac{(E_C - E_F)}{eT} + A$$

$$A = \int_{E_C}^{\infty} \frac{E}{eT} \sigma_{ME}(E)dE \int_{E_C}^{\infty} \sigma_{ME}(E)dE$$  \hspace{2cm} (19)$$

The contribution of $A$ is mostly relatively small. In calculations in this thesis this $A$ is always taken into account. For the extended mobility edge both Seebeck coefficients must be combined. This is done weighted for the mobility contribution of both parts.

$$S_{\text{ext}} = \frac{S_{ME} \sigma_{ME} + S_{VRH} \sigma_{VRH}}{\sigma_{ME} + \sigma_{VRH}}$$  \hspace{2cm} (20)$$
4. Measurement technique

Several techniques can be used for measuring the DOS of organic material, such as ultraviolet photoemission spectroscopy, inverse photoemission spectroscopy and thermally stimulated luminescence. We use scanning Kelvin probe microscopy (SKPM) for measuring the DOS, SKPM is a technique used with an atomic force microscope (AFM) in non contact mode. Measurements were done on an Omicron variable temperature scanning probe microscope (VT-SPM).

The set up is conditioned in an ultra high vacuum (UHV) environment with a working pressure of less than $10^{-9}$ mbar. The UHV is to prevent stressing of the OTFTs by charge accumulation in the silicon oxide dielectric under influence of water vapor and present to reduce noise in measurements. In order to reach variable temperatures a flow cryostat with heating is present. The UHV system contains a heater to anneal the samples before going in the SPM.

The non contact AFM makes use of change in tip oscillations frequency to measure the topography of a sample. The oscillation is monitored using a laser pointed at the AFM-tip, its reflection is recorded by a photo sensitive diode (PSD). The signal of the PSD is used as a feedback signal to control the piëzo elements. These piëzo elements have a range of 10μm in both lateral directions and 2μm in the vertical direction. The course positioning of the piezo’s is done using a slip stick technique.

4.1. Scanning Kelvin probe microscopy

In addition to non-contact AFM, a conductive tip can be used for scanning Kelvin probe microscopy first demonstrated by Nonnenmacher et al.\textsuperscript{15} This technique measures the electrostatic potential between the tip and the substrate. For this measurement the electrostatic potential difference is nullified. This potential includes the bias applied to the tip, the work function difference and (unintentional) dopant. For the measurement an additional ac voltage ($V_{ac}\sin(\omega t)$) is applied to the tip. The force on this capacitor with capacitance ($C$), depending on the height of the tip ($z$) is then given as a function of the biases:

$$F = \frac{1}{2} \frac{dC}{dz} V^2 = \frac{1}{2} \frac{dC}{dz} \left[ V_{DC}^2 + V_{DC} V_{ac} \sin(\omega t) + \frac{1}{2} V_{ac}^2 \left[ 1 - \cos(2\omega t) \right] \right]$$

with $C$ the capacitance between tip and active layer, and $z$ the distance between the tip and the active layer. Using this function the second term in the straight brackets is measurable and can be nullified by adjusting $V_{DC}$ via the bias between tip and substrate.

The tip height is controlled with a proportional integral (PI-) controller. The resonance frequency of the tip is typically in the order of 10\textsuperscript{5} Hertz. The driving frequency for the SKPM measurement should be sufficiently high that the height controller can’t follow this frequency. Few hundred hertz is a good number for $V_{ac}$. To prevent aliasing the PI-controller should have at least 10 full cycles.

The accuracy of the measurements can be calculated by integrating over the surface which interacts with the conductive tip. Interactions of point charges have quadratic decay, therefore the area of relevant influence is in the order of 50 nm\textsuperscript{16}. This area is dependent on the tip shape, oscillation amplitude and the height of the tip above the surface. This area is also dependent on the surface roughness, and more strongly the gradient of the potential in the surface.
4.2. DOS measurements

The density of states of a material can be directly determined using SKPM, this is first demonstrated by Tal. et al. where a field effect transistor configuration is used. In our experimental setup a bias is applied on source and drain, the gate is grounded, but for a more general description with both source and drain contact grounded. These grounded source and drain contacts pin the Fermi level.

The electrostatic energy levels of the different parts are displayed in figure 2. In calculations not the HOMO and LUMO onset are used as a reference. The DOS is continued to fill up all number of states, estimated using the density of the material, the point where all states are filled is depicted as the reference point.

By applying a gate negative gate bias the electrostatic energy will shift up. The active layer will follow the gate in potential en will shift up. Up to the point the valence band crosses the Fermi level, charge carriers will distribute throughout the active layer. This distribution is governed by two potentials; the electrical potential and the chemical potential. The electrical potential is a result of the coulomb repulsion between the charge carriers. These two potentials results in a distribution of the charge carriers, therefore they are often combined in an electrochemical potential. The shift of the band at the sample surface is what is measured with the AFM tip $(q \Delta V_{skpm})$.

![Diagram](image)

Figure 2: Schematic view of the energy diagram for SKPM on an OTFT. HOMO and LUMO levels represent the onset of the valence and conduction band respectively. Black lines represent the energy scheme where source, drain and gate contact are grounded. The orange lines represent the energy scheme for applied gate bias. Both source and drain are grounded in order to keep the Fermi level of the semiconductor constant. Work functions of the different parts are indicated using $\varphi$. The electron affinity is shown as $ea$, and the ionization potential is indicated using $IP$.

4.3. DOS calculations

In this chapter it is shown how to calculate the DOS using the technique described. First there will be assumed that charge will spread equally throughout the active layer (a calculation without this assumption is made in the chapter band bending). We assume both a constant electric permittivity as a constant DOS throughout the layer. Not taking interaction of an active layer and the SiO₂ into account. The DOS could change while more charge carriers are injected. This effect favors this technique since
the DOS is exactly equivalently addressed in mobility measurements. The general expression for the number of holes is the integral over all states and the probability of occupation:

\[ p = \int_{-\infty}^{\infty} g(E) f(E, E_f^h) \, dE \]  \hspace{1cm} (22)

Where the DOS is represented by \( g \) and \( f \) is the familiar Fermi-Dirac function in which \( E_f^h \) is the energy relative to the Fermi level. The density of holes is directly dependent to the amount of screening.

\[ p = -V_{Gd} \frac{C}{d_{org} q g} = -(V_G - V_{skpm} - V_d) \frac{C}{d_{org} q g} \]  \hspace{1cm} (23)

In which the gate voltage \( (V_G) \) is the applied gate bias, Kelvin probe technique is used to measure \( (V_{skpm}) \), and the depletion voltage \( (V_d) \) is found by completely depleting the material of its charge carriers. The depletion voltage is typically a constant value in time and gate bias, it can depend on the position on the TFT and is affected by stress in the TFT. Taking the derivative of the charge carriers will rule out most of the unknown terms.

\[ \frac{dp}{qdV_{SKPM}} = \left[ \left( \frac{dV_{SKPM}}{dV_G} \right)^{-1} - 1 \right] \frac{C}{d_{org} q g} \]  \hspace{1cm} (24)

Equation (23) and (24) can be linked using the equality,

\[ E_f^h = q(V_G - V_d) - q V_{SKPM} \rightarrow dE_f^h = -q dV_{SKPM} \]  \hspace{1cm} (25)

Combining all will lead to a difficult function; in order to continue algebraically assumption should be made.

**4.3.1. Zero temperature assumption**

A way to continue calculations is using zero temperature dependence first derived by Tal et al.\(^{11}\) This is not very realistic unless the width of the DOS is much wider than the width of the Fermi-Dirac distribution i.e. \( T_0 \gg T \). Using equation and taking the derivative to \( E_f^h \) will give,

\[ \frac{dp}{dE_f^h} = \int_{-\infty}^{\infty} g(E) \frac{df(E, E_f^h)}{dE_f^h} \, dE = \int_{-\infty}^{\infty} g(E) \delta(E - E_f^h) \, dE = g(E_f^h) \]  \hspace{1cm} (26)

The Fermi-Dirac distribution will become a delta peak under the zero temperature assumption. Combining equation (22), (24) and (26) will lead to the zero temperature DOS;

\[ g(qV_{SKPM}) = \left[ \left( \frac{dV_{SKPM}}{dV_G} \right)^{-1} - 1 \right] \frac{C}{d_{org} q g} \]  \hspace{1cm} (27)

The value for \( qV_{SKPM} \) is relative to an energy which depends on several material and device characteristics; this is justified by the integration of equation (26). It is therefore more appropriate to set \( V_{SKPM} \) equal to zero for the case of no gate bias.

**4.3.2. Exponential DOS assumption**

The derivation of the zero temperature assumption is not that applicable. To make progress an assumption for the shape of the DOS should be assumed. This assumption is common in organic electronics.
\[ g(E) = \frac{N_{\text{exp}}}{k_B T_0} \exp \left( \frac{E}{k_B T_0} \right) \]  

(28)

This function crosses zero energy when all states are occupied, i.e. all states have negative energy. Using this assumption the integral of equation (22) can be solved.

\[ p = \int_{-\infty}^{\infty} N_0 \exp \left( \frac{E}{k_B T_0} \right) \frac{1}{1 + \left( \frac{E-E_f^b}{k_B T} \right)} \, dE \]

(29)

\[ N_0 \exp \left( \frac{E_f^b}{k_B T_0} \right) \Gamma \left( 1 - \frac{T}{T_0} \right) \Gamma \left( 1 + \frac{T}{T_0} \right) = N_0 \exp \left( \frac{E_f^b}{k_B T_0} \right) \frac{\pi T / T_0}{\sin \left( \pi T / T_0 \right)} \]

It is assumed that most carriers occupy the sites in the tail of the DOS \(-E_f^b \gg k_B T_0\) and with \(T < T_0\).

The derivative can be taken from equation (29):

\[ \frac{dp}{dE_f^b} = N_0 \frac{\exp \left( \frac{E_f^b}{k_B T_0} \right)}{k_B T_0} \frac{\pi T / T_0}{\sin \left( \pi T / T_0 \right)} = g(E_f^b) \frac{\pi T / T_0}{\sin \left( \pi T / T_0 \right)} \]

(30)

In order to determine the DOS of this expression the derivative of the holes should be found. An expression for the number of holes in a material is given using equation (27) and (30).

\[ g(q V_{skpm}) = \left[ \frac{dV_{SKPM}}{dV_G} \right]^{-1} \left( \frac{C}{d_{org} q^2} \right) \frac{\sin \left( \pi T / T_0 \right)}{\pi T / T_0} \]

(31)

This function equals the function for a zero temperature assumption only with a temperature dependent part. This function locally approximates the DOS as an exponential. This exponential is used to estimate the contribution of a finite temperature. This is a good approximation as long as \(T_0\) has small changes within the energy span of \(T\).

A disadvantage of this method is that it uses the derivative of a measured signal; low amount of noise would dominate the measurements. In order to generate trustworthy results the data points should be fitted and smoothened, giving rise to loss of accuracy and resolution. An alternative method is developed cancelling the derivative, equation (28) and equation (29) can be rewritten to give:

\[ g(E_f^b) = p \left( \frac{\sin \left( \pi T / T_0 \right)}{\pi k_B T} \right) \]

(32)

This function combined with the function for the number of holes leads to an expression for the DOS.

\[ g(q V_{skpm}) = (V_G - V_{skpm} - V_d) \frac{C}{d_{org} q^2} \frac{\sin \left( \pi T / T_0 \right)}{\pi k_B T} \]

(33)

4.3.3. Double exponential DOS

The double exponential is used later on to fit DOS of pentacene. The concept is to sum two exponents. The sum of these two exponents can be estimated as a single exponent. The number of variables to calculate the DOS does drastically increase from one static over the regime \((T_0)\), to two static and two depending on the energy. The advantage of this approach is it allows to directly calculate a DOS from the data points. This allows a fast iteration process in comparison with a guessed DOS. The DOS is first calculated using a single exponent approach; if this approach is unable to fit results the second exponent
can be added. The variables in the function of the double exponent are up front estimated by calculations with a single DOS.

The slope of both the sum of both exponential can be calculated using the sum of both derivatives. This can directly be translated into a global $T_0$. The exponential DOS is referred to as $g$, where the composite DOS $g_{12}$ consists of two exponential function $g_1$ and $g_2$. Both derivatives and values of the single exponential and the double exponential should be the same.

$$\frac{d g(E)}{dE} = \frac{d}{dE} \left( \frac{N_{exp}}{k_B T_0} \exp \left( \frac{E}{k_B T_0} \right) \right) = g(E) \quad (34)$$

$$\frac{d g_{12}(E)}{dE} = \frac{d}{dE} (g_1(E) + g_2(E)) = \frac{g_1(E)}{k_B T_{01}} + \frac{g_1(E)}{k_B T_{02}}$$

$$g(E) = \frac{g_1(E) + g_2(E)}{k_B T_{01}} + \frac{g_1(E)}{k_B T_{02}}$$

$$T_0 = \frac{g_1(E) + g_2(E)}{T_{01} g_1(E) + g_2(E)} \quad (35)$$

If $g_1/T_{01} >> g_2/T_{02}$, the global $T_0$ would equal $T_{01}$. This is also true for $T_{01}$ and $T_{02}$ interchanged. In the limits of either of one dominating the situation of a single exponential is back. Now a zero temperature assumption is used in order to calculate the number of particles from the DOS.

$$p = \int_{-\infty}^{\infty} dE \left[ \frac{N_{01}}{k_B T_{01}} \exp \left( \frac{E}{k_B T_{01}} \right) + \frac{N_{02}}{k_B T_{02}} \exp \left( \frac{E}{k_B T_{02}} \right) \right] U(E)$$

$$p = N_{01} \exp \left( \frac{E_f^h}{k_B T_{01}} \right) + N_{02} \exp \left( \frac{E_f^h}{k_B T_{02}} \right) = k_B T_{01} g_{01} + k_B T_{02} g_{02}$$

Unlike with the single exponential $g(E)$ is not recovered with one factor difference. To precede the DOS is forced extracted, the residue is in the division factor.

$$p(E) = k_B T_0 (E) g(E) \frac{T_{01} g_1(E) + T_{02} g_2(E)}{T_0 g_1(E) + T_0 g_2(E)} \quad (37)$$

The second term will vanish if either one or the other exponent is dominant. The term can be rewritten using $f = T_{01}/T_{02}$ and $F(E) = g_1(E)/g_2(E)$.

$$\frac{T_{01} g_1(E) + T_{02} g_2(E)}{T_0 g_1(E) + T_0 g_2(E)} = \frac{F^2(E) + (f + f^{-1}) F(E) + 1}{F^2(E) + 2F(E) + 1}$$

$$F = F^{-1}$$

Note that for both $F = F^2$ and $f = f^{-1}$ this factor is symmetric as it should. In case where this factor is largest, at $F = I$, to obtain a factor of 2, $f$ should be as large as 6. In the limit where both exponents share $T_0$, if $f \rightarrow I$, the expression reduces to unity. In the limit where either one or the other exponent dominates, $F \rightarrow 0$ or $F \rightarrow 0$, this factor also reduces to unity. Therefore this factor can be neglected for first estimations. Now considering a finite temperature and expression for $g(E)$, combining functions (30), (37) and (38)
\[ g \left( qV_{skpm} \right) = \left( V_G - V_{skpm} - V_d \right) \frac{C}{d_{org} q} \frac{\sin \left( \pi T / T_0 (E) \right)}{\pi k_B T} \frac{F^2 (E)^2 + 2F (E) + 1}{F^2 (E) + \left( f + f^{-1} \right) F (E) + 1} \]

With \( E = qV_{skpm} - E \Delta \) in which \( E \Delta \) is determined by definition of \( g(E) \). This value is related to the threshold voltage and the number of states chosen in the calculation with a single exponent. Note the use of a single exponent does not define a total number of states. As a small recap \( T_0 \) can be calculated using:

\[ T_0 = T_{0i} \frac{F_0 (E) + 1}{F (E) + f} \]

Where \( f = T_{0i}/T_{02} \) and \( F(E) = g_{1}(E)/g_{2}(E) \). It should be noted that the finite temperature adds an approximation. The two exponentials are summed and approximated as one exponential sharing the slope in each point. This is a crucial approximation in order to obtain equation (39).

### 4.3.4. Fitting measured DOS

In a realistic system the DOS can have any shape. A hybrid of a Gaussian and an exponential tail states is commonly used. The states measured, the tail states, are dominated by the exponential part. The states at higher energy’s are modeled using the Gaussian fit.

\[ g (E) = \frac{N_{\exp}}{k_B T_0} \exp \left( \frac{E}{k_B T_0} \right) + \frac{N_{Gauss}}{\sigma \sqrt{2\pi}} \exp \left( -\frac{E^2}{2\sigma^2} \right) \]

Any model of a DOS starts off with an exponential DOS fit. If this fit fails to predict descent results the a next step is to use a double exponential fit. In order to get to different DOS the easiest route is to use the double exponential, and after the procedure fit the Gaussian. Fitting with any arbitrary DOS is possible. But for any guess the Kelvin probe signal has to be calculated. This is a highly time consuming simulation.
4.4. Simulations

4.4.1. Band bending

Charge transport in OTFT’s is described by disordered localized states. The conduction is therefore enhanced with an increased number of free charges. The highest density of charges is near the dielectric of the TFT. This region is most vital for charge transport, and is referred to as the accumulation layer. A finite thickness of the active layer makes the measured potential different from the potential in the accumulation layer. This band bending can be explained by charge transfer shown by Lange et al.\textsuperscript{18} In order to correct for this band bending, Poisson’s equation is used;

\[
\frac{d^2V}{dx^2} = \frac{en(x)}{\varepsilon} \tag{42}
\]

In this function \(V\) is the local potential, \(e\) the elementary charge and \(\varepsilon\) the relative permittivity of the polymer. Charge neutrality of the device gives rise to the first boundary condition; the derivative of the electric field should be zero outside the device. The number of electrons \((n)\) should be calculated using the convolution of the Fermi-Dirac distribution with the DOS of the organic layer.

\[
n(x) = \int_{-\infty}^{\infty} \frac{1}{1 + \exp \left[ \left( E - E_f \right) / k_B T \right]} g(E + eV(x)) dE \tag{43}
\]

Where \(E\) is energy, \(k_B\) is Boltzmann’s constant, \(T\) is temperature, \(g(E)\) is the measured DOS and \(V(x)\) is the electrostatic potential.

The band bending model is written using Matlab. For both the Kelvin probe simulations as the mobility simulations a correction is made for band bending. To calculate the band bending the active layer thickness is cut in its thickness direction into 200 slices; above 30 slices no significant change in outcome is observed. All slices are considered independently. Starting from the slice at the gate dielectric the local potential is calculated. For the very first slide the potential is guessed. The density of occupied states is calculated using a finite temperature integral between the DOS and Fermi-Dirac statistics. This integral is put in a table with which the number of charges is fitted. From the local potential the number of charges is calculated. These number of charges leads to a change in potential for the next control volume using Poissont equation. The field at the vacuum surface of the material should have no gradient, to ensure charge neutrality of the device. The initial control volume is adapted to nullify this final gradient. Note that the assumption for a constant DOS and constant electric permeability throughout the layers has to be made.

4.4.2. Mobility simulations

All simulation performed use one of the above mentioned mobility models. A DOS is assumed or fitted to measurement the data. The modeling is performed using a 1D simulation with the transistor operating in the linear regime.

The thickness of the active layer is set to the actual measured thickness. For the unknown thicker layer the thickness is set to 50 nm where the accumulation layer does not exceed several nanometer. In this simulation the thickness of the active layer is set to 50nm, the active layer is divided into parts of 2.5Å. Simulation show larger layer thicknesses do not contribute to the result.

The fitting of the data is performed using minimalization of the absolute value of the difference between simulated and measured data. This approach is chosen above reducing the RMS value to involve the lower temperature, and therefore lower mobility sweeps. Furthermore the values below 3V gate bias are cut since simulation are in only performed in linear regime where \(|V_G| >> |V_{sd}|\).
4.4.3. SKPM DOS simulations

The simulation program for the correction of the data for band bending will be explained using amorphous Indium Gallium Zinc Oxide (GIZO) as example. This is convenient to run the program with realistic numbers. GIZO is known to have electron mobility up to the order of 10 cm²/Vs. The thickness of GIZO can be well controlled using sputtering techniques. The sample used in this measurement has a thickness of about 8nm. Both height and potential profile are measured using scanning lift mode AFM and SKPM simultaneously. An area of 1x1 μm² was scanned, a flat surface with no large defects was found. Peak to peak amplitude of the topography profile is within 1.5 nm. The potential profile did not exceed 20mV difference, which is about the thermal accuracy of the KPFM set up.

GIZO is an electron conductor, and therefore the theory shown in chapter ‘DOS measurements’ should be reproduced for electron conducting devices oppose to hole conducting devices. The energy scheme comprehensive to this is given in figure 3. Electrons accumulate when a positive voltage is applied to the gate dielectric with respect to the grounded source and drain contacts. The onset of the conduction band referred to as the LUMO. Under influence of the gate bias the LUMO of the active layer will shift below the Fermi level. All states below the Fermi level are occupied with electrons.

![Figure 3: Schematic view of the energy diagram for SKPM on an OTFT. HOMO and LUMO levels represent the onset of the valence and conduction band respectively. Black lines represent the energy scheme where source, drain and gate contact are grounded. The orange lines represents the energy scheme for applied gate bias. Both source and drain are grounded in order to keep the Fermi level of the semiconductor constant. Work functions of the different parts are indicated using φ. The electron affinity is shown as ea, and the ionization potential is indicated using IP.](image)

In order to calculate the band bending a DOS should be known and vice versa. Therefore the calculations are performed in an iteration process, where three iteration steps provide decent accuracy. The simulation is based on a one dimensional model. The semiconducting interface closest to the gate is set at \( x=0 \) and the semiconducting interface with the vacuum \( x=d_{org} \). Some device and material constants should be inserted as input; for the active layer, the thickness \( d_{org}=8\text{nm} \), the relative permeability \( (\varepsilon_r=11.517) \) and an initial guess for \( T_0 \). The DOS is shown in figure 4a, in the case of no energy shift all states are occupied, this electrostatic energy is set as zero. In normal situations this point is far above the Fermi level, showing a positive energy shift. The more charges accumulated the closer this energy is to its offset of zero. The device parameters are the thickness of the silicon oxide \( (d=200\text{nm}) \) and the relative permeability of the oxide \( (\varepsilon_r=3.8) \).

The program reads in the measurement data \( V_{skpm} \) vs. \( V_G \) performed with the SKPM setup (black data from figure 5a). The charges are considered equally spread throughout the active layer, with equation...
(33) and the assumed $T_0$ the DOS is calculated. Shown in figure 5b as black squares. In this calculated DOS the Fermi energy at a gate voltage of 0 V is set to the offset energy. Using the $T_0$ of an exponential fit the DOS as shown in figure 4a is obtained. With this DOS $V_{skpm}$ is simulated for both the situation with and without band bending. Results for one such measurement for one gate voltage is shown in figure 4b. Measurement data of $V_{skpm}$ is fitted to the simulation with band bending (black line). The fit is a shift in both the surface potential and the Gate voltage. The simulation data without band bending but equal DOS is shown as a red line. The measurement data points are corrected with the difference between the simulation with and without band bending resulting in the red triangles of figure 5a. This new dataset without band bending will give more accurate results for the DOS shown as the red squares of figure 5b.

This process is repeated for this new DOS, until no changes are observed. Note that the exponential DOS is the fit used. The simulations of the surface potential are used to give a correction for band bending. For this simulation the shape is not fitted, only the x-y position, so the surface potential and the gate voltage. This procedure is justified and contains information about the offset of the DOS, the absolute value of the Kelvin probe signal and the threshold voltage.

Figure 4: a) electron density of occupied states modelled according to a single exponential model, with the total number of charges being 1E26, before and after adding charge carriers in the material by applying a bias to the gate. Fermi energy in this model equals 0 volt (blue line). The vacuum energy level shift, and therefore the measured potential, equals the shift shown using the blue arrow. b) Simulation of the potential profile in an 8nm thick GIZO layer for the case with band bending and for the case where all charge is spread equally, the gate voltage is set on 8 volt. The triangles indicate the Kelvin probe potential. The black triangle should coincide with the measured Kelvin probe voltage shown in figure 5.
Figure 5: a) Measured Kelvin probe voltage vs. gate voltage data of GIZO (black triangles) corrected for both surface potential and threshold voltage to match the simulated data (solid black line). The solid red line shows the situation if no band bending and an equal distribution of charges in the active layer is assumed. The measured data corrected for the difference between the red and black line (red triangles) can be used to calculate the DOS. b) Calculated DOS using the dataset of figure a, for both the situation where no band bending is taken into account (black squares) and the situation where corrections are used to compensate band bending (red squares).

4.4.4. Thickness analysis

Simulations are performed to gain insight of the effect of band banding on the derived DOS for different thicknesses of the active layer (Figure 6). These simulations are made using the numbers for the GIZO TFT. The thickness of the layer is varied from 1nm up to 100nm. In figure 6a the potential in the material is shown as function of the distance from the gate dielectric is shown for a gate bias of both 8 V and in figure 6b for a gate bias of 24 V.

Figure 6: Potential profile vs. the relative thickness of the active layer a) for 8 volt gate bias, b) for 24 volt gate bias. The colours represent a different thickness of the active layer; 1nm (black), 2nm (red), 4nm (green), 8nm (blue), 20nm (cyan), 50nm (magenta), 100nm (dark yellow)

For thin layers the potential is almost constant throughout the channel, indicating that the charge is equally distributed and banding hardly plays a role. With increasing layer thickness the role of band bending increases. Furthermore, the potential decreases as a result of a less filled DOS because the charge can distribute over a larger area. From a thickness of about 20 nm the potential close to the dielectric doesn’t deaccrease anymore because the majority of the charge carriers is located in the first few nanometers and no notable difference in the accumulation layer is observed. Measurements are done on different thicknesses of the semiconductor by Lange et al. 18 They indeed report an increase of the measurable range of the DOS with decreasing layer thickness. The measurements of the DOS also worsen since the averaging is over a larger range. Furthermore the sensitivity decreases with increasing thickness of the layer. To illustrate this effect, the difference in Kelvin probe voltage is divided by the difference in Fermi level (figure 7).
Figure 7: simulation of the sensitivity defined as the difference in measured Kelvin probe voltage divided by the difference in Fermi level. This sensitivity is plotted with respect to the gate voltage.

For increasing thicker layer sensitivity of this measurement method is rapidly lost. For an infinitely thin layer the local potential will shift 1 volt with 1eV DOS level shift. The range over the DOS is decreased by increasing thickness. A layer, which is thinner than the typical accumulation layer thickness, will have a larger shift in the energy of the DOS.
5. Results GIZO

In this chapter the results of Gallium Indium Zink Oxide (GIZO) are presented. GIZO is in the class of amorphous oxide semiconductors (AOS). The application of AOS is in transparent electrodes, which finds application in both displays and photovoltaic cells. There is debate about the type of transport the materials show. The DOS is a key aspect, which is directly measured using Kelvin probe techniques. Temperature dependant measurements are performed for both the mobility as Seebeck coefficient. We show the extended mobility edge model to give good fits for the mobility. Using the same parameter set, decent predictions can be done for the Seebeck coefficient.

Capacitance voltage measurements are done by Jeon et al. to extract the DOS of GIZO. They extracted an exponential and a Gaussian or, a tail of two exponentials. 19,20 One percolation model by Kamiya et al. 21 is also popular in literature. 22,23,24 This model for AOS assumes a conventional square root DOS. In this DOS a Gaussian distribution of potential barriers limit the conduction.

5.1. Experimental details

The devices are delivered by Holst Centre. Devices were prepared using a highly doped Si substrate as the gate electrode and 200 nm of thermally grown SiO2 as gate dielectric. This bottom contact, blanket gate approach allows for excellent heat transfer through the substrate and the device. Source and drain electrodes are gold, deposited with standard lithography techniques. The channel length and width of the used devices were 5 µm and 10000 µm, respectively. A 10nm thick GIZO layer was then deposited via RF-sputtering from a GIZO target with a 2:2:1 Ga:In:Zn metal ratio. A partial pressure of oxygen in argon of 2% was maintained throughout the deposition in the sputter chamber. The resulting devices were annealed at 400C for 20min in air.

5.2. Results and discussion

First the structure of the GIZO TFT is examined for topography and defects, using both AFM and SKPM techniques.

![Figure 8: a) AFM image, b) SKPM image of 4nm thick layer of GIZO.](image)

The AFM image of figure 8 shows a flat surface with a variation less than 1.6 nm. The average thickness of the layer is 8 nm so a good coverage over the entire layer is expected. There is correlation in the image which implies island growth. The in space corresponding SKPM image shows very few
deviations. The deviations are in the order of magnitude of the thermal energy which implies that we approach about highest possible accuracy using this technique at room temperature.

5.2.1. Microscopic results

Kelvin probe measurements as a function of the gate voltage are performed on five different locations far from the contacts. Results are plotted in figure 9.

Figure 9: Measured surface potential, using Kelvin probe force microscopy, as function of the applied gate voltage on five different locations.

The density of states corresponding to these measurements is calculated as described in chapter 4. The results are shown in table 1.

Table 1: \( T_0 \) value results of exponential fits through the calculated DOS of the dataset shown in figure 9.

<table>
<thead>
<tr>
<th>( T_0 ) (K)</th>
<th>( T_0 ) corrected (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>593</td>
<td>743</td>
</tr>
<tr>
<td>682</td>
<td>836</td>
</tr>
<tr>
<td>1061</td>
<td>1231</td>
</tr>
<tr>
<td>601</td>
<td>758</td>
</tr>
<tr>
<td>692</td>
<td>836</td>
</tr>
</tbody>
</table>

The average \( T_0 \) of the DOS measurements is about 800K discarding the 1231K result. This value will be used for comparison with macroscopic results. The range of the measured DOS is about \( 2 \times 10^{19} \), which corresponds to about 0.08 eV above the Fermi level when no gate bias is applied.

By including band bending higher values of \( T_0 \) are obtained. The value for \( T_0 \) with respect to the assumed thickness of the layer is plotted in figure 10. The thickness at 0 nm is obtained making calculations without taking any band bending into account.
Figure 10: Deviation in $T_0$ with respect to varying assumptions for thickness. The data point at thickness of 0 nm is calculated without taking band bending into account

The sensitivity of $T_0$ to a variation in the thickness of the layer is about 20K/nm over the full range of the plot. The topography shown in figure 8 contains a deviation of about 1.5nm which results in an uncertainty of about 30K.

The Fermi level lies in a tail of exponential states. The exponential reaches over 80 meV above Fermi level, so has to be of high importance for the conduction.

The Kamiya model predicts a square root DOS, which is in contradiction with the exponential DOS that is measured. No further analysis is done here. W.C. Germs has shown that this model predicts the mobility and Seebeck measurements fairly well.
5.2.2. Transfer characteristics

Since the original sample broke down, samples were used from the same batch for measuring the transfer curves of GIZO. One measurement is performed using a sample from the same substrate. This sample has 40 μm channel length. Using Vissenberg-Matters model on a gate sweep an exponential DOS with a $T_{0_{VM}}$ of 430K is extracted.

In order to have temperature dependent measurements a dataset obtained by W.C. Germs is used. This dataset shows a Vissenberg-Matters $T_{0_{VM}}$ of 370K and a mobility of 6 cm$^2$/Vs this result is sufficiently close to the $T_{0_{VM}}$ 430K and mobility of 3 cm$^2$/Vs found using this theory on the original batch.

The dataset of Germs is fitted using variable range hopping theory. In the first fitting procedure the DOS is assumed to be an exponential, which leads to three fitting parameters; the exponential slope of the DOS ($T_0$), the decay length of an electron wave function in GIZO ($\alpha^{-1}$) and a density dependent mobility prefactor ($\sigma_0$). The low gate voltages make the relative occupation of the density of states low. Therefore the total number of states does not matter as long as it is sufficient. The exact number of the total density of states only shifts the threshold voltage slightly, in the order of 0.1 V for a factor of ten difference. The number of states is chosen to be $N_{tot} = 3 \times 10^28$ m$^{-3}$.

\[\text{Figure 11: Fit of dataset using an exponential DOS. Fit parameters are: } T_0 = 401K, \sigma_0 = 1.138 \times 10^6 \text{ S/m and } \alpha^{-1} = 1.77 \times 10^{-9} \text{ m.}\]

The modelled data is best fitted to the experimental data using the following fit parameters: The slope of the DOS found using transfer curves is marked with a small ‘t’ and has a value of $T_0t = 401K$. The conductivity of the charges is $\sigma_0 = 1.138 \times 10^6 \text{ S/m}$ and the inverse localization length $\alpha^{-1} = 1.77 \times 10^{-9} \text{ m}$. The result is plotted in figure 11. The result for the Seebeck coefficient is plotted in figure 12.
The DOS found fitting the transfer curves with variable range hopping is an exponential with $T_0=401K$ where the DOS found using a direct DOS measurements equals around $T_0=800K$. Results of the simulations for the Seebeck coefficient are about a factor of 4 higher than the measured data. The measured data is shown later in this chapter, in figure 20. To conclude, measurements do not coincide with one other if GIZO is simply modeled using variable range hopping.

5.2.3. Combining microscopic transfer characteristics

The Kelvin probe measurements show a DOS with a $T_0$ of about 800K where the transfer curve fitting gives a $T_0$ of 400K. In order to overcome this difference an approach is used where the DOS is modeled using both a Gaussian and exponential tail states. The tail states are modeled using an 800K exponential decay, shown in figure 14. The Fermi level of the variable range hopping model could be in the exponent where the transport level would be positioned in the Gaussian. The fitting parameters chosen are the total number of states ($N_{tot}$), the number of tale states ($N_{exp}$), the width of the Gaussian ($\sigma_{Gauss}$), the localization length ($\alpha^{-1}$) and a density dependent mobility prefactor ($\sigma_0$).

The fit turns out to be not uniquely defined; the transition region from exponent to Gaussian could shift in Fermi level offset by combination of all 5 variables. Therefore both the total number of charge carriers and the width of the density of states is fixed to reasonable parameters; $N_{tot} = 3e28$ and $\sigma_{Gauss} = 0.08$, this reduces the degrees of freedom to three, results are shown in figure 13.
Figure 13: Fit of dataset using an exponential DOS for the tail states and a Gaussian DOS for the bulk states. Fixed parameters for the DOS are $T_0=800$, $N_{tot}=3 \times 10^{28}$ and $\sigma_{Gauss}=0.08$ eV. Fit parameters are: $N_{exp}=3.64 \times 10^{25}$, $\sigma_0=2.56 \times 10^6$ S/m and $\alpha^{-1}=1.26 \times 10^{-9}$ m.

Figure 14: a) occupied states plotted against the Fermi level $e_n$ (eV). b) Average Fermi level with respect to the gate bias applied. Y-axis can be compared to the Fermi level plotted in figure a).

The average Fermi level over all occupied states of the active layer is calculated to show the position of the Fermi level in the occupied DOS. For a wide range of gate voltages the Fermi energy is positioned in exponential tail states. Calculations for the typical hopping energy show this value to be in the Gaussian part of the DOS.

The Kelvin probe measurements reach a DOS of $2 \times 10^{19} \text{[eV}^{-1} \text{cm}^{-3}]$, with use of equation (30) this can be converted to the number of occupied states. The number of occupied states obtained is temperature dependent, for all temperatures it is close to $n=1 \times 10^{18}$. This would already be in the Gaussian DOS fitted to the measurements. In order to check the validity of this DOS, it is directly used to fit the data obtained with the surface potential vs. gate voltage plots.
Figure 15: Measured surface potential vs. gate voltage data of GIZO (black squares) corrected for both the threshold voltage and surface potential to match the simulated data (solid black line). The simulation is performed using the obtained Gaussian DOS with exponential tail states.

The fit of surface potential made with the obtained DOS shown in figure 15. The data points do not coincide with the modelled data. The reason why the gate voltages higher DOS are reached using equal gate voltage is the thickness of the layer. The Kelvin probe measurements go up to higher values for the occupied states for comparable gate voltages. This effect is nicely illustrated in figure 6. Where we show, that because of a thin layer, the DOS will get occupied to higher energies.

The Seebeck coefficient of this model is plotted in figure 16. The simulated points are about a factor of 4 higher than the measurement points. The measured data is nearly temperature independent, it shows a slight increase in Seebeck coefficient for higher temperatures. The simulated data predicts a decrease for increasing temperature, this contradicts the measurements.
Figure 16: simulated Seebeck coefficient as a function of the applied gate voltage, plotted for several different temperatures. The DOS assumed is a Gaussian with an exponential tail with $T_0=800K$.

To conclude, this approach, where a Gaussian and an exponential DOS are combined in a VRH model, fails on predicting any of the measurements. Mainly because the DOS is known for fairly high energies with respect to the energies addressed at thicker layers.

### 5.2.4. Mobility edge model

Both variable range hopping approaches are unable to predict the experiments. Now a mobility edge model is fitted to the measurement results. Mobility edge is favored above variable range hopping because GIZO TFT’s show Hall mobility$^{24}$ Pure hopping conduction is not sufficient to understand the Hall Effect. The model considered in this part is the mobility edge model. The band is modeled by a constant DOS where all electrons have the same specific mobility ($\mu_{0,\text{ME}}$). The trap states, the tail of the DOS, are modeled using the exponential DOS found with using the SKPM method. In the tail states no conduction is allowed. The exponential decay length is obtained from the Kelvin probe measurements and has a value of $T_0=800K$. The other fit parameter is the trap states ($N_{\text{trap}}$).
Figure 17: example of a dataset using a mobility edge model with exponential tail state with a $T_0=800K$. The parameters chosen are $N_{trap}=9.943 \times 10^{25}$, $\mu_{0\ ME}=2.75 \text{cm}^2/\text{Vs}$.

The mobility edge is unable to fit the results shown in figure 17. In order to illustrate the trends of the mobility edge model reasonable values are inserted. This model is unable to predict the outcome of the transfer characteristics with use of reasonable values. Higher order terms dominate in this model. A reason for this behavior is the shallow slope, the high $T_0$ value, of the tail states in comparison to the width of the Fermi Dirac distribution function. The width of the Fermi Dirac function is determined by the temperature, the thermal energy ranges in the experiments range from about $10\text{meV}$ to $25\text{meV}$. The total shift in the Fermi level is in the order of $2\text{00}\text{meV}$ at gate voltage range of $20\text{V}$ in contrast to a gate voltage of zero volt. The exponential decay of the Fermi-Dirac distribution approaches this fixed mobility edge, and shows an exponential increase in mobility. Furthermore the accumulation layer does get smaller for increased voltage, strengthening the fast increase.

The Seebeck coefficients obtained, using this model, are close to one order of magnitude larger than the measurement data. It also depends on temperature, the 90K results are about a factor of three larger than the results for 310K. The measurements show the Seebeck coefficient to be nearly temperature independent.

This mobility edge model is not able to predict any of the measurements, and therefore insufficient to describe the conduction through GIZO TFT’s.

5.2.5. Extended mobility edge model

Mobility edge like conduction is unable to predict the mobility measurements. It is shown that there exists Hall mobility in GIZO TFT’s, therefore mobility edge is favored above variable range hopping. The extended mobility edge model combines both mobility edge and variable range hopping in the. The DOS consist of two parts. One part is a constant DOS located above the mobility edge; these charge carriers have band mobility ($\mu_{0\ ME}$). The tail states are modeled with the exponential DOS obtained from Kelvin probe measurements, with $T_0=800K$, and total amount of fail states ($N_{exp}$). In these tail states conduction takes place via hopping, with a mobility fitted using the prefactor ($\sigma_0$) and delocalization length ($\alpha^{-1}$). The fit obtained is shown in figure 18.
Figure 18: Fit of a mobility dataset using a mobility edge model. The tail states are modelled using an exponential DOS. In these tail states hopping mobility is allowed. Fixed parameters for the tail states is $T_0=800K$. The fitted constants are $N_{exp}=1.055 \times 10^{26}$, $\sigma_0=4.61 \times 10^4$ S/m, $\mu_{ME}=50.7$ cm$^2$/Vs and $\alpha^{-1}=4.84 \times 10^{-9}$m

The contribution of the conduction above the mobility edge compared to the total conduction is very low and is plotted in figure 19. The conduction of electrons in the mobility edge state is dependent on both the DOS and the band mobility. In figure 19, the part of the conduction of the electrons above the mobility edge is shown. This part is small and therefore irrelevant for the actual fit of the mobility, but necessary in order to explain the Hall measurements.

By neglecting the mobility edge part the fitting is done with 2 fit parameters only, the hopping mobility prefactor and the localization length.

Figure 19: Contribution of the conductivity of variable range hopping over the conductivity of mobility edge transport plotted as a function of the gate voltage.
The Seebeck coefficient of this simulation and the measurement data is plotted in figure 20. The simulated data is very close to the measurement data. The temperature dependence of both the simulation data as the measured data is very small.

The electron localization length is large for hopping in disordered materials ($\alpha^{-1} = 4.84 \text{nm}$). In order to show that this variable range hopping does not break down, the hopping energy and the hopping distance are calculated. The hopping distance should be larger than the electron localization length. The maximum Fermi level which determines the DOS with respect to the Fermi energy is plotted in figure 21. These maximal Fermi energies are directly translated hopping energy and hopping distance, shown in the graphs of figure 22. The typical hopping energy remains higher than the thermal energy. The typical hopping distance remains higher than the electron localization length.

**Figure 20:** simulated Seebeck coefficient as a function of the applied gate voltage, plotted for several different temperatures. The DOS assumed is a Gaussian with an exponential tail with $T_0=800\text{K}$.

**Figure 21:** maximal Fermi energy plotted against the gate voltage.
So this shows that hopping mobility is valid in the range of operation of these transistors. It is possible to mix in mobility edge without large consequences for the fits.

5.2.6. Conclusion

The DOS is calculated using both Kelvin probe technique and variable range hopping model on transfer characteristics. The extraction of the density of states via Kelvin probe microscopy route shows a DOS of about 800K. Variable range hopping model used on transfer characteristics shows a DOS of 400K. The model used is not sufficient to link both results.

A forced variable range hopping model with a DOS with $T_0 = 800K$, results in reasonable transfer characteristics fits. It should be noted that large electron delocalization lengths are found of 4.8nm. The Seebeck coefficient calculated using this fit is close to the result obtained from measurements. Furthermore both model and measurements show lack of temperature dependence in the Seebeck coefficients.

In order to be able to make better comparison between microscopic and transfer results measurements should be repeated on the same sample.

A future perspective worthy for investigation is a mobility edge, which is pushed up due to occupation of lower lying states. The shift of this mobility edge is a direct effect of the coulomb repulsion. This variable mobility edge will soften the high order terms being problematic for detailed mobility predictions.
6. Results PTAA

Poly(triarylamine) (PTAA) is an organic hole-conducting polymer. This polymer can be used in organic solar cells as the hole acceptor material in most cases alongside PCBM. It can also be used for OTFTs. One interesting feature to examine is the stabilization or even lowering of mobility for decreasing gate voltage. In order to gain understanding of the charge transport mechanism several techniques are combined: DOS extraction via SKPM, Transfer curve measurements and Seebeck measurements. We show that the best accepted transfer mechanism is unable to combine these measurements.

6.1. Experimental details

The PTAA field effect transistor is made on a heavily doped silicon substrate, with a 200nm thermally grown SiO₂ gate electrode. Golden source and drain contact are patterned using standard lithography techniques. The sample is passivated with a monolayer of HMDS and the PTAA layer is spincoated from solution on top of the structure. AFM images show it to be 4 nm thick layer. All measurements are performed in a ultra high vacuum Omicron SPM setup with a Nanonis controller. A conductive platinum coated SPM tip and a gold coated tip is used for measurements. In the vacuum system source and drain contacts are biased, where the gate contact is grounded.

The temperature dependent gate sweeps and Seebeck measurements are performed by W.C. Germs on a different device as the AFM SKPM measurements.

6.2. Results and discussion

The thickness of the layer is measured using a scratch on the material. The depth of this scratch represents the thickness of the layer. AFM pictures show the PTAA layer to be on 4 nm thick.

![AFM image of PTAA layer](image)

**Figure 23.** Typical AFM topography image of PTAA, on a linear scale. The deviation of the PTAA surface is about 2nm, it occasionally has mountains up to 12nm in height.

The topography AFM measurements are performed using both platinum and gold coated tip. The topography shows similar results: a mainly flat surface with deviation within a range of 1nm. Occasionally mountains show which reach up to 10 nm. These mountains have a diameter up to 50nm (figure 23).

There is structure in the Kelvin probe signal. About 200nm features show up. These features lose intensity when charges are accumulated. Due to trapping and noise, no real conclusions can be drawn.
from the measurements. The structure is rather similar to what is seen in pentacene and therefore we will go in depth to such features in that chapter. In the case no charges are accumulated the standard deviation is 59.3mV. When charges are accumulated this reduces to 31.6mV. PTAA traps charges faster than pentacene does. Therefore the measurements had to be flattened per line and no real conclusion can be drawn.

The density of states is measured using SKPM and gate sweeps. One of the results is shown in figure 24. As can be observed the noise on the measurements is relatively large in comparison with previous experiments. The standard deviation of the exponential fit is on average 14% of its value. With an average value of all performed measurements being 980K. The standard deviation of the uncertainty is typically 137K.

**Figure 24:** a) Kelvin probe voltage measurements verses gate bias. The solid line is the calculated Kelvin probe voltage using the exponential DOS shown in b). b) DOS calculated with the data points of figure a). The red line represents the DOS fit with exponential assumed.

In order to gain trustworthy information with the measurement set up, 57 measurements are performed. All measurements are on different location in the channel. The results of the slope of the DOS of these measurements are shown in figure 25.
Figure 25: Cumulative plot of all DOS measurements done. On the horizontal axis the slope of the DOS is plotted. The horizontal axis shows the number of counts of each interval. Total number of measurements is 57. The mean value is 980K with a standard deviation of 161K. The average slope of the DOS fitted using a Gaussian equals $T_\theta = 960$. The standard deviation of the spread of the measurements equals 154K. This is reasonably close to the 137K uncertainty found in the fitting; the spread is therefore most likely from the same source.

6.2.1. Transfer characteristics

To link the DOS found to macroscopic device characteristics the slope of the DOS is chosen to be $T_\theta = 1000K$. Gate sweeps of PTAA TFT’s are performed on different temperatures [W.C. Germs], results are shown in figure 26.

Figure 26: Transfer characteristics of a PTAA TFT. The horizontal axis shows the mobility, relative to the gate voltage on the vertical axis. The triangles represent the measurement data for the temperatures 200K, 250K, 300K and 350K in black, red, green and blue respectively. The solid lines represent the variable...
range hopping fit of the dataset. Colours coincide with temperatures of the measurements data. Parameters are extracted using the slope of the DOS found using Kelvin Probe microscopy: the localization length and conductivity are fitted. Parameters are $T_0=1000K$, $\alpha^{-1}=0.4869 \text{ nm}$ and $\sigma_0_{\text{VRH}}=7.336 \times 10^6 \text{ S/m}$. The dashed lines, with matching colours, represent the variable range hopping fit of the dataset. The parameters found for the best fit are $T_0=700K$, $\alpha^{-1}=0.4185 \text{ nm}$ and $\sigma_0_{\text{VRH}}=1.276 \times 10^6 \text{ S/m}$.

The data points are fitted using variable range hopping models. They are also fitted using mobility edge model. The mobility model fits are not shown due to a poor fit quality. The parameters extracted using the variable range hopping with the best fit are $T_0=700K$, $\alpha^{-1}=0.4185 \text{ nm}$ and $\sigma_0_{\text{VRH}}=1.276 \times 10^6 \text{ S/m}$. This slope of DOS does not match the DOS found with Kelvin probe experiments. $T_0=700K$ found for the fit assuming variable range hopping conduction does not coincide with the $T_0$ found using Kelvin probe measurements. A second fit is made using the more delocalized states, $T_0=1000K$, found using Kelvin probe measurements (figure 26). This also poorly describes the shape of the measured mobility.

From the data obtained, the Seebeck coefficient can be calculated. The Seebeck data of these experiments is typically a factor of 3-4 lower than calculated data using either the fitted data of the DOS measurements combined with the Transfer characteristics or the Transfer characteristics fitted using a free $T_0$. Both the poor fit and the theory are unable to correctly predict the Seebeck measurements, which shows that this model is insufficient to describe the transport mechanism in PTAA.

6.3. Conclusion

We compared three techniques to investigate the conduction in PTAA. These techniques are Kelvin probe DOS measurements, Variable range hopping fits of temperature dependant gate sweeps and Seebeck measurements. The DOS extracted using the Kelvin probe techniques is exponential with typical decay length of $T_0=1000 \text{ K}$. Using this to fit transfer curves with variable range hopping or mobility edge theory does not give the good shape of the curves. Letting this decay length free during fitting still does not reconstruct the shape of the transfer curves. Above all, with either fits, the Seebeck coefficient is unable to be reproduced on a factor of 4. To conclude: simple variable range hopping is unable to describe conduction in PTAA.
7. Pentacene

Pentacene is a frequently used p-type organic semiconductor in OTFT’s. Pentacene consists of five fused benzene rings. The small molecules of pentacene are likely to from polycrystalline structures with many defects and grain boundaries. This disorder leads to a broadened DOS, this broadening is also shown using UPS spectroscopy. We try to better understand the charge transport mechanism in these pentacene TFTs. A DOS measurement using Kelvin probe technique is also performed by Yogev et al. They find localized tail states and Gaussian bulk states in pentacene.

7.1. Experimental details

The pentacene field effect transistor is made on a heavily doped silicon substrate, with a 200nm thermally grown SiO$_2$ gate electrode. Golden source and drain contact are patterned using standard lithography techniques. The sample is passivated with a monolayer of HMDS and the pentacene layer is evaporated on top with a rate of 0.2 nm/s. All measurements are preformed in a ultra high vacuum Omicron SPM setup with a Nanonis controller. In the vacuum system source and drain contacts are biased, where the gate contact is grounded. The topography and potential pictures of pentacene are made using a platinum coated tip and a part of the DOS measurements are performed with a gold coated tip. Electrical characterization is done in situ with a Keithley 2636. The same sample is used for the SPM measurements as for the electrical characterization and has a width and length of 10 mm and 5 µm respectively.

7.2. Results and discussion

We start with Kelvin probe measurements to calculate the shape and size of the DOS. With this the transfer characteristics are implemented, combining both results.

7.2.1. Kelvin probe measurements

The DOS is measured as described in chapter: DOS measurements. To calculate the DOS, an average thickness of 15 nm is taken for the pentacene layer. The actual thickness. A typical result is shown in figure 27. Both a single exponential of a Gaussian fit are insufficient to describe the outcome of these experiments, therefore a double exponent is assumed. Fitting with a combination of Gaussian bulk states and exponential tail states is a possibility, which results in roughly the same lower exponential. A drawback of the Gaussian is that it has one degree of freedom more than the exponential. Therefore we stick to the double exponential fit.
Figure 27: a) Measured Kelvin probe voltage versus gate bias. The solid line is the calculated Kelvin probe voltage using the double exponential DOS shown in b). b) DOS calculated with the data points of figure a). The red line represents the DOS fit with a double exponential. The two black lines are the individual exponential fits, one with $T_0$ of 414K and the tail states with $T_0$ of 2042K.

Table 2: Fit values for the DOS of measurements. Measurements are performed at ten different locations throughout the channel. Measurement 1 to 5 is performed with a platinum coated tip, where measurement 6 to 10 with a golden tip. Measurements number 4, 5, 6, 7, 9 are performed on top of a crystal, where the other measurements are located in between crystals.

<table>
<thead>
<tr>
<th>measurement #</th>
<th>$T_{01}$ (K)</th>
<th>$T_{02}$ (K)</th>
<th>Tip</th>
<th>Location</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>566</td>
<td>2037</td>
<td>Pt</td>
<td>between crystals</td>
</tr>
<tr>
<td>2</td>
<td>588</td>
<td>2048</td>
<td>Pt</td>
<td>between crystals</td>
</tr>
<tr>
<td>3</td>
<td>856</td>
<td>2986</td>
<td>Pt</td>
<td>between crystals</td>
</tr>
<tr>
<td>4</td>
<td>502</td>
<td>1792</td>
<td>Pt</td>
<td>On crystal</td>
</tr>
<tr>
<td>5</td>
<td>414</td>
<td>2042</td>
<td>Pt</td>
<td>On crystal</td>
</tr>
<tr>
<td>6</td>
<td>665</td>
<td>2049</td>
<td>Au</td>
<td>On crystal</td>
</tr>
<tr>
<td>7</td>
<td>410</td>
<td>2208</td>
<td>Au</td>
<td>On crystal</td>
</tr>
<tr>
<td>8</td>
<td>537</td>
<td>3535</td>
<td>Au</td>
<td>between crystals</td>
</tr>
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<td>9</td>
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<tr>
<td>10</td>
<td>403</td>
<td>2520</td>
<td>Au</td>
<td>between crystals</td>
</tr>
</tbody>
</table>

Ten measurements are performed to study the reproducibility of the measurements on different locations and with a different tip. All measurements look similar as figure 26. The results of the fit values are shown in table 2, for calculations all thicknesses are assumed to be 15nm.

The measurements are nicely reproducible, since same results are found with a gold or platinum coated SPM tip. But remarkably, measurements performed on a different location don’t show a very high spread. Even though measurements are performed on top of crystals and in between crystals no correlation is observed. This is in contradiction with the assumptions that band bending should have influence. From this lack of correlation the assumption of the pentacene layer being homogeneous in DOS and electric permittivity might be invalid.
Figure 28: schematic representation of the energy throughout the pentacene layer due to inhomogeneous DOS, for three different gate voltages: zero volt (black), low gate voltage (red) and high gate voltage (green). The surface states of pentacene near the SiO₂ have high energy spread, thus high T₀. This high spread is represented with the large width of the distribution. In the bulk the spread of the local DOS is smaller. The bulk energy will follow the energy of the surface states up to the point charges are accumulated by the bulk states (green).

We find an average value of the tail states of 2372 K and 540 K of the bulk states. The measurement uncertainty in the DOS measurements makes these measurements irrelevant for detailed information about the DOS. The measurements do show a DOS with deep exponential tail states, and increasing bulk states. In the next chapter we will investigate this DOS in mobility models.

The fact that no thickness dependence is measured can be thought of it not being there. For this to happen, the states near the SiO₂ should be dominating the internal energy of the pentacene. This can be true if the delocalization of the DOS in energy of the pentacene is larger at this interface in comparison with the bulk DOS. This broadening can for instance be caused by dipoles or trapped charges in the gate dielectric or due to the interaction of the pentacene and SiO₂. The states which are highest in energy will be occupied first, and will determine the energy of the entire pentacene layer (figure 28).

7.2.2. Transfer characteristics

In order to get a better understanding of the conduction through pentacene the material is investigated by measuring the transfer characteristics. The transfer characteristic is taken from the same sample. It is shown how a double exponential shape of the DOS affects the outcome of the mobility. The DOS is questionable and I only present a mobility measurement on room temperature, this is sufficient to present the effect.
Figure 29: Mobility of pentacene verses gate voltage. Black triangles: measured transfer characteristics of the pentacene TFT. Dashed blue line: Fit using a variable range hopping model. The model assumes a single exponential DOS, fit parameters are $T_0=956K$, $\alpha^{-1}=5.1nm$ and $\sigma_{0,VRH}=9.0 \times 10^2 \text{ S/m}$. Solid green line: Fit with single exponent DOS extracted with Kelvin probe measurements $T_0=540K$. Fit parameters are $\alpha^{-1}=3.34nm$ and $\sigma_{0,VRH}=22.7 \times 10^2 \text{ S/m}$. Solid red line: double exponential DOS with $T_{01}=540K$ and $T_{02}=2372K$. Fit parameters are $\alpha^{-1}=3.74nm$ and $\sigma_{0,VRH}=17.2 \times 10^2 \text{ S/m}$ and crossing point of the two exponentials equals $3.71 \times 10^2$.

In figure 29 the measured transfer curve is plotted (blue triangles) and a fit using a VRH model (black line). The hysteresis in this device is small and therefore not taken into consideration in the analysis. The data is fitted using VRH model with an exponential DOS with an extracted width of $T_0=956K$. Temperature dependant data is necessary to extract any trustworthy values. Without such measurements the fitting parameters attribute to really specific regimes: If the localization length, $\alpha^{-1}$, is close to the hopping distance, the transfer curve bends down near high voltages. The value for the steepness of the DOS mostly accounts for the up-bending near the low voltages; this value is therefore very dependant of the chosen threshold voltage. Finally the mobility $\sigma_{0,VRH}$ changes the slope of the transfer curve. The values of these numbers are dependent on another.

The effect of the double exponential DOS is shown in figure 29 with the red line. The Tail states of the found DOS for pentacene will fill up first. Due to the relative low number of states in the tail, the conduction is low in comparison with the conduction in the bulk states. The hopping distance is very large in the tail states in comparison with the bulk states. Tail states contributions give a mobility of a few orders of magnitude lower than the mobility in the bulk. Therefore the most significant change is a shift in the threshold voltage. Besides shifting the threshold voltage the tail states take up charges which will not contribute to the conduction in the bulk. Therefore it slightly lowers the mobility with an equal gate voltage.

7.2.3. Spatial SPM

With the SPM set-up both AFM and SKPM images are constructed. In the SKPM measurements features are observed, see figure 31. In order to investigate the dependence of these features on the amount of charges present in the material multipass scanning is applied, where on each pass a different gate bias is applied. The SKPM profiles extracted can be spatially compared. Note that low scanning speed is required. One set of pictures can take up to 12 hours. The Y-scale of these pictures can be
diluted because of piezo drift. The height profile of a multi pass measurements is shown in figure 30. The different SKPM profiles at gate voltage of $+3V$, $0V$, $-2V$, $-4V$ and $-8V$ are shown in figure 31.

**Figure 30:** Non-contact mode AFM height image of pentacene. Crystals in the order of magnitude of 1μm can be observed. The typical height of the crystals is about 30nm.

<table>
<thead>
<tr>
<th>(a)</th>
<th>(d)</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1" alt="Image" /></td>
<td><img src="image2" alt="Image" /></td>
</tr>
</tbody>
</table>

**Figure 31:** SKPM images of the same location as the AFM image of figure 30. The gate is grounded where source and drain are biased with $+3V$ (a), $0V$ (b) $-2V$ (c), $-4V$ (d), $-8V$ (e). The measurements are performed using multipass scanning. The pictures have the same scale, but different offsets are used.

While moving from figure 31 a) to e), more and more charges get accumulated. While increasing the number of charges in the accumulation layer the same features are observed using SKPM, but the amplitude of the features is reduced. The correlation between the height and the potential is investigated
with use of correlation functions. Remarkably no correlation is found this shows there is no relation between thickness of the layer and the surface potential. Also no correlation is found between the visible boundaries in the topography image and the potential profile.

We qualify the decrease in visibility of these features by the spread in the values of the potential profiles. These profiles are fitted using a Gaussian. In order to gain trustworthy results the long pronounced ‘crack’ in the middle of the pictures is not used in this analysis. The results are shown in table 3. It is shown that the features are reduced. Most of the reduction occurs while the accumulation layer is just forming. After it is formed the higher amount of accumulated charges does not further reduce the spatial anisotropy.

Table 3: The average values and standard deviation of the Kelvin probe potential of figure 31.

<table>
<thead>
<tr>
<th>$V_G$ (V)</th>
<th>$V_A - &lt;V_{skpm}&gt;$ (mV)</th>
<th>$\sigma$ (mV)</th>
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</thead>
<tbody>
<tr>
<td>3</td>
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<td>71.6</td>
</tr>
<tr>
<td>0</td>
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<td>63.2</td>
</tr>
<tr>
<td>-2</td>
<td>-173</td>
<td>33.8</td>
</tr>
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<td>-4</td>
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</tr>
<tr>
<td>-8</td>
<td>-156</td>
<td>31.4</td>
</tr>
</tbody>
</table>

It is unclear, and beyond the scope of this research, what the variation in spatial potential, shown in figure 31, causes. This spatial potential profile shows equal features as the topography. As more charges get accumulated the profile persists but decreases in amplitude. A difference in surface potential, due to different faces of the crystal is ruled out. This would mean that the potential profile would persist in amplitude.

With very few charges accumulated the exact vacuum level depends on the position of a few local tail states. The delocalization of these tail states is governed by the defects in the gate dielectric, or the interaction between the SiO$_2$ and the pentacene. While increasing both source and drain voltage more charges get accumulated. The number of charges accumulated is fixed by the gate dielectric. Because of the rapidly increasing number of states to be occupied, the differences reduce but preserve shape (figure 32).

**Figure 32**, schematic representation; Local DOS have large spread in energy (gray graphs). Decreasing the gate voltage raises the local energy. The rise in energy is governed by the amount of accumulation of
holes (p) above the Fermi level. The DOS is shifted up in energy (orange graphs). Due to the rapidly increasing number of states the spatial spread is reduced.

7.2.4. Conclusion

We show by SKPM measurements that pentacene has tail states and fast increasing numbers of bulk states. Furthermore we show the importance of pentacene interface states. This conclusion can be drawn due to no observation in correlation between height profiles and potential profiles. Partial screening of the spatial potential features happens while increasing the number of accumulated charges.
8. Results ambipolar devices

Ambipolar organic semiconductor can conduct both holes and electron with comparable mobility’s. The material is useful for application ranging from light-emitting devices to logic circuits. In organic light emitting field effect transistors (OLEFET) the recombination zone can be controlled using the gate bias. For quantum efficiency it is important that light is created in the middle of the channel. We show that the stability of the recombination zone is a balance between the mobility in the device and the contact resistance. Two different materials are investigated: P17, which is a relatively good conducting light emitting polymer. In P17 we show a very unstable recombination zone. The other material is KH71; which, interestingly, shows a nice stable recombination zone for different source drain voltages. We show that the stability of this recombination zone depends on the conduction and contact resistance of the material.

Kelvin probe verses gate voltage measurements are performed on both materials, P17 and KH71 is measured. Both materials show peculiar behavior. This behavior is qualitatively described.

8.1.1. Experimental details

Both the P17 and the KH71 TFT’s are made on a heavily doped silicon substrate, with a 200nm thermally grown SiO₂ gate electrode. Golden source and drain contact are patterned using standard lithography techniques. The sample is passivated with a monolayer of HMDS and the active layer is spincoated from solution on top. The P17 is patterned with a 5μm channel length. The P17 is spincoated from chloroform with a concentration of 0.5 mg/ml and spinspeed or 7000 RPM. This results in a layer of approximately 4nm. The KH71 samples are also spincoated from solution of chloroform. The thickness of the KH71 sample 1 is measured by scratching the surface and examining the scratch with AFM. KH 71 Sample 1, on which most measurements are performed, has layer thickness of 8 nm. Sample 2 is only used to reproduce the Kelvin probe DOS measurement. The thickness is determined from a bubble in the KH 71 Layer, it has layer thickness of 40-50 nm. All samples are annealed on a temperature of 120C for 60 minutes in the vacuum system.

All measurements are preformed in an ultra high vacuum Omicron SPM setup with a Nanonis controller. In the vacuum system source and drain contacts are biased, where the gate contact is grounded All measurement are made using a platinum tip. Electrical characterization is done in situ with a Keithley 2636. The same sample is used for the SPM measurements as for the electrical characterization and has a width and length of 10 mm and 5 μm respectively.

8.1.2. Result and discussion comparison

In order to measure the potential profile along the channel of a TFT, SKPM is used. A high gradient in potential, which are unavoidable in the ambipolar regime, result in less accurate measurements. There will be high influence of the field on the SPM tip. In order to make accurate measurements the feedback controller of the Kelvin probe signal has to be slow. To capture the high gradient the scanning speed has to be low. Typical scan speed of the probe needle is close to 20 nm/s.
Figure 33: p17 Kelvin probe measurement along the channel, while the transistor is near ambipolar operation mode. The channel length equals 5μm, the flat parts on both ends are measured on top of contacts. The slightest variation in gate voltage will alter the current to be either hole (blue) or electron (red) dominated. a) blue: $V_S=3.5V \, V_D=-10V, \text{ red: } V_S=4V \, V_D=-10$. b) blue: $V_S=-30V \, V_D=+10V, \text{ red: } V_S=-28V \, V_D=+12V$.

In figure 33 it is shown that the recombination zone is unstable for the high conducting polymer P17. As can be observed there is a large potential drop near the low voltage part of the potential profile, the electron injection contact resistance is large. It is not possible for either the lower as the higher source to drain voltage to create a stable recombination zone. A gate voltage change as low as 0.3 V is plenty to switch the device from electron conducting to completely hole conducting. The ambipolar regime, setting the gate voltage in between both other regimes, is unstable. Tuning exactly on the ambipolar regime, results in shifts of the recombination zone along the channel length. Conclusion can be drawn that the recombination point shifts constantly to either one of the contacts. This shift of the recombination zone has a speed in the order of magnitude of 1 μm/s. Because of this shift scanning with a probe tip does not give a picture of one situation, and is useless. Eventually trapping makes the electron conduction favored above hole conduction.

Figure 34: KH71 Kelvin probe measurement along the channel, while the transistor is at ambipolar operation mode. The channel length equals 10μm, The contacts are just outside the rage of the SPM. a) $V_{SD}=20V$. b) $V_{SD}=40 \, V$.

The recombination zone for KH71 is stable as can be seen in figure 34. These measurements show a stable recombination zone in a range of about 3 Volt. At both source and drain contacts not the contact
resistance only drops 2 Volts, for both electron as hole injection. While increasing the source drain voltage to 40V the recombination zone gets narrower. This can be understood by considering the better conduction in the unipolar regions. The stability of the recombination zone increases slightly. The range of the gate voltage to form a recombination zone increases slightly up to 4 V.

We investigate the cause why P17 lacks a stable recombination zone in, while KH71 is stable on a range of several volts. As can be seen in figure 33 and figure 34, the voltage drop near one of the contacts of P17 is large compared to KH71. This shows the contact resistance of P17 is much more dominant than the contact resistance of KH71.

**Figure 35:** Gate sweep mobility measurements of P17 (Red) and KH 71 (Black). In both measurements $V_S=-5V$ and $V_D=+5V$. As can be observed P17 has two orders of magnitude higher mobility. (mobility is not corrected for the contact voltage drop.

Besides a higher contact resistance, P17 shows higher mobility then KH71. It is shown by C. Roelofs in a simulation that, for higher contact resistance with respect to mobility, the recombination zone shifts with lower a difference in gate voltage.
8.2. DOS P17

In order to get insight in the difference in conduction both materials are examined using SKPM. Two of
the Kelvin probe measurements of P17 are shown in figure 36. These measurements are easily
reproducible, and about a dozen are taken on different places on the substrate. Furthermore sweeps are
taken on the contacts to verify the setup. Each measurement differs slightly in offset. The sweeps shown
in figure 36 are performed on differed speeds. The sweep which takes 30 minutes shows relative high
peaks around the zero gate voltage. Where the sweep with a total time of 10 hours shows low peaks
around zero gate voltage. For the fast sweep the tangent of the slope of these peaks equals typically 0.8
\(V/V\), where for the slow sweep the tangent is close to 0.6 \(V/V\). If an active layer would not have
shielding at all the tangent would be 1 \(V/V\). The time dependence of the peaks suggest that the peaks are
not in equilibrium. These peaks are the result of high contact resistance, already shown in the previous
chapter. This high contact resistance prevents charges from being injected to shield quickly. This
contact resistance shows up around zero voltage because then few states are available near the contacts.

The down peak is significant smaller then the up peak. This is generally true for the measurements.
Although it is less pronounced, this also applies to the slow sweep. At the high positive gate voltage
electrons are accumulated, while moving alongside the down peak, electrons are pushed out of the
material, or holes are injected. The upper peak is present when going from a hole accumulated state to
the electron accumulated state. So holes are pushed out, or electrons are injected. It clearly shows that
hole injection is easier than the electron injection. This is consistent with the measurements shown in
figure 33. Where by far the largest voltage drop is present over the hole injection side.

![Figure 36: Kelvin probe voltage with respect to the gate bias. Measurements are done at steps of 1 Volt. In red, a sweep is shown that cumulatively takes 1 hour. In blue, a sweep is shown which takes cumulatively 10 hours. The measurements are performed on a different part of the sample. Both sweeps start at \(V_g=30V\), follow the lower laying line to \(V_g=-30V\). The return sweep is the upper half of the graph.](image)

The shift of the sweep in trace and retrace is due to some kind of trapping. As can be observed the
trapping mechanism which affects the screaming is relatively time independent. It is dependant to the
gate voltage; there is more stress for higher voltage. This is true for both positive as negative voltages,
in a remarkable symmetric fashion.
The current drops as a stretch exponential, at half-life of about 10 min this resembles roughly one measurement step of the slow speed scan. It also resembles about one fifth of the total measurement of the fast scan. The fast scan has speeds about the half life time of the current, where the slow scan uses a multiple of this. All features appear on the same position, this implies current drop has different origin than the stressing and this mechanism does not show in Kelvin probe measurements.

We focus on the low speed curve, for a detailed analysis. This low speed sweep is shown in figure 37. Extracting the DOS using a modified version of the program turns out very difficult, and is not shown.

![Figure 37](image)

**Figure 37:** Kelvin probe voltage vs. gate voltage. Cumulative measurement time equals 10 hours. In red the slope of the measurement is shown in the band gap, this slope equals on average 0.362V/V. Right a schematic representation of the DOS is shown.

In the case of constant equilibrium one would expect the two peaks in the middle to disappear. As can be seen the amount of screening is very poor around a gate voltage of 17V for trace, and 11V for retrace. This changes the surface potential 1.8V. The change in potential is the result of the band gap of the material. By making tangent lines we can estimate the DOS in this band gap, this slope turns out to be 0.362V/V. This slope is naively translated to a DOS using equation (27). This DOS has a value of \( g(eV) = 2.34 \times 10^{17} \text{eV}^{-1}\text{cm}^{-3} \).

The gate sweep shown in figure 35 has its minimum in between 4 and 10 Volt. It is highly peculiar that the position of the middle of the band is in between a gate voltage of 11V and 17 volt respectively for the up and down sweep. While clearly electron conduction already takes place.
Figure 38: schematic view of the energy in P17. The DOS is represented by tints of dark colour. On top of the picture the conduction band shows. On the bottom the valence band shows. The band gap is shown by the whiter area. The Red lines represent the fixed Fermi energy for different regimes.

A possible reason for this paradox to occur the possibility that something different is measured on the surface of the active layer, then what happens at the interface. While electrons accumulate at the SiO₂ interface the surface energy of the active layer still is at its former equilibrium (figure 38). Starting from a default situation where holes are accumulated. This default situation shows at the gate sweep, where the threshold voltage is positive. By increasing the voltage, holes are pushed out, and electrons are accumulated. Due to the lowered number of electrons in the band gap the energy can go all across the band gap. On the surface this will still show the hole accumulated regime. An important thing to note is that the bulk states can be filled through the materials accumulation layer. This is necessary to explain the similarity in shape of the up and down sweep.
8.3. DOS KH71

As for P17 also for KH71 Kelvin probe measurements are performed for different gate voltages. In figure 39 a typical measurement is shown. Again about a dozen measurements are performed. Because of a peculiar shape, the measurements are repeated using both a new tip and a new sample. This new sample happened to be of thickness of about 40 nm. Furthermore its surface is full of craters. The same kind of shape is found. This indicates the reproducibility of the shape. There is a variety in the Kelvin probe measurements. Especially in the exact Kelvin probe voltage, but the shape is consistent.

It is easily noted that the peaks around zero gate voltage are smaller than in the case of P17. In KH71 they do not reach more than a few volts. For the second sample, with a thicker layer these peaks are slightly lower. In comparison with the better conducting P17 the relaxation is much quicker, and both peaks are similar in height. This pleads in favor of contact resistance being the origin of the slow screening.

![Figure 39: Kelvin probe voltage with respect to the gate bias. Measurements are done at steps of 1 Volt. The sweep speed is such that cumulatively it takes 1 hour.](image)

As for the P17 material a band gap is expected, but not found. Even measuring up to a gate voltage of 75 V, no band gap is observed. A comparable slope continues while increasing the gate voltage. It remains unclear why no bandgap is observed.

It is really surprising the slope of the Kelvin probe voltage with respect to the gate voltage is negative, for negative gate voltages. As stressed above, these results are reproducible. Naively inserting a negative slope into equation (27), shows a DOS to become negative, which cannot be realistic. Something else is happening. Several things are known to happen. Charges will get accumulated near the accumulation layer. The surface lowers in electrostatic energy. The device is neutral, so the gradient of the electrostatic potential equals zero. Considering these facts, and holding on to the constant electric permittivity the most obvious potential profiles are shown in figure 40.
Figure 40: Artist impression of the suggested electrostatic energy profile with respect to the thickness of the KH71 layer. The red line is for $V_g=0\,V$. Yellow green and blue indicate higher decreasing gate voltages respectively. The solid parts on both sides of the KH71 layer are known electrostatic potential. The dotted line shows a possible electrostatic potential through the material. At the vacuum interface, the place where the measurements take place, the energy slowly decreases. Charge neutrality makes the derivative at the interface equal to zero.

How the process of the lowering in electrostatic energy in the active layer from KH71 works is unclear. A solely decreasing profile is expected. An oscillating profile is unlikely since it is found to be position and therefore thickness independent. As the electrostatic energy bands up, there must be positively charged carriers present. This means the potential lowered for an equal amount of charges. This could happen when facing a different part of the KH71 molecule. This can be due to either mobile ions or the formation and directing of dipoles. The mechanism of screening might also be responsible for the low mobility of KH71. Further explanation exceeds the scope of this research.

8.4. Conclusion

Kelvin probe measurements along the channel show the stability of the recombination zone in ambipolar regime of P17 and KH71. For the polymer P17 this recombination zone is less stable; this technique is unable to measure the balanced recombination zone. For KH71 the recombination zone is stable for a voltage difference of up to four volt gate voltage difference. This stability difference is due to the balance between conductivity and contact resistance. With the use of simulations this relation of unstable recombination zone is shown to be dependent on the contact resistance.

We measured both linear mobility and the Kelvin probe voltage with respect to the gate voltage for two types of polymers, P17 and KH71. P17 shows higher mobility than KH71 over the entire range of measurements. Around zero gate voltage high peaks show for the Kelvin probe vs. gate voltage measurements. These peaks are due to the system not being in equilibrium. Despite the higher mobility over the entire range P17 takes much longer to equilibrate than KH71. This is due to higher contact resistance.

For future perspective it would be nice to directly measure contact resistance using the TLM method. This is a rather easy and fast measurements to verify the results found.
9. Conclusion

Kelvin probe measurements are successfully used to extract the density of states (DOS) of several materials in thin film field effect transistor architecture (TFT). The technique is further developed to account for finite layer thickness. This DOS can be inserted into different mobility models, which also account for the formation of an accumulation layer. The mobility is calculated for a TFT in linear regime. These two measurements can be directly compared because the charge carriers are accumulated on the same manner.

We gained insight in the conduction properties of Gallium indium zinc oxide and could make good use of the measured DOS. The extended mobility edge model is able to describe both the transfer curves and Seebeck measurements with the measured DOS.

In the organic materials many unexplained things happen and the assumption of constant DOS and constant electrical permeability are doubtful. For pentacene it is shown that surface states at the SiO₂ play a significant role. Measurements on PTAA show relative high uncertainty. The variable range hopping and mobility edge models are unable to predict the shape of the conductivity using the measured exponential DOS.

In the ambipolar materials KH71 and P17 contact resistance shows significant contribution. And in KH71 many more effects happen which cannot be described using the assumed simple theory.

10. Outlook

In this chapter things learned from the use of Kelvin probe DOS measurements are stated. In most cases the differences and agreements of Kelvin probe measurements on the different materials. In this chapter we focus on the subjects important for the work, general notable things that confronted in measurements. There is a focus on the future work that can take this research to a higher level. Some things which are noted but not thoroughly researched will be addressed.

Most importantly for a follow up research is to investigate the influence of surface charges. As seen at both pentacene and KH71 the assumption of both a constant DOS and constant electric permittivity are not trivial. Doing Kelvin probe DOS material at different thicknesses will give insight in the surface states. With the AFM set-up in UHV this will be a time consuming task, unless it is possible to deposit different thicknesses of active layer on one sample.

Stressing is difficult to quantify, for any material investigated in the UHV set up, stress should be seen as at least two different mechanisms. One, referred to as plain stressing, is with a timescale of minutes up to hours. This directly changes the threshold voltage, and lowers the charge transport. It is reversible by grounding source, drain and gate contacts for some time. Permanent stressing lowers the conductivity and changes the threshold voltage, but does not seem to be reversible without baking. The permanent stressing is has a time span of multiple hours or days of higher gate voltage.

Only for PTAA stressing of the TFT is up to 1 volt in the time for a descent Kelvin probe measurement of around 30 minutes. For pentacene and GIZO the stressing is much slower. For these three materials permanent stressing shows after tens of sweeps. It stresses in the direction of the sweep. Stressing for ambipolar devices seems very different. The amount of stress is determined by the maximum voltage applied, and not directly on the length of time of this applied gate voltage. In ambipolar devices permanent stress reduces both the hole as the electron conducting side in mobility. This permanent stress does not change the onset voltage.

Accuracy and noise for the Kelvin probe measurements is very dependent on the material used. Measurements on the materials GIZO, P17 and pentacene, are with low noise, where for PTAA and
KH71 it is difficult to reduce the noise on the measurements. It is unclear what this difference in accuracy causes.

Temperature dependant DOS measurements can be done to measure the DOS more accurately. This might give more insight in the accuracy of the measurements. Lower temperatures are tried for PTAA TFT’s, where the amount of trapping dramatically increased while decreasing the temperature to 200K. This increase in trapping can be due to the very thin layer span where measurements with thicker layers give less problems as shown in the report. In order to be able to do thrust worthy measurements the system should be in equilibrium. For lower temperatures this equilibrium will take longer, increasing the amount of stress even more.

The simulation of the mobility through a device can be improved. A next step in improving simulations is too correct for the difference of the potential along the channel. The challenge is rewriting the program to make a grid of both the layer thickness and channel length. This would involve calculating the potential and band bending at each position in the channel length. I think it is far too ambitious to try to simulate contact resistance for different materials decently. For the ambipolar materials the contact resistance has a dominant role. Therefore transition line measurement will be a good follow up to calculate the actual sheet resistance. It is interesting to investigate the role of contact resistance of the other materials, and excluding this for the fitting.
11. References


