



**Protocol for extracting a space-charge limited mobility benchmark
from a single hole-only or electron-only current-voltage curve**
Version 2

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Protocol for extracting a space-charge limited mobility benchmark from a single hole-only or electron-only current-voltage curve

Version 2

Objective: to create a procedure for analysing single current-voltage (I-V) curves from space-charge limited electron-only or hole-only devices to give a benchmark mobility value that is reproducible when analysed by different people. More complex models can be used where multiple I-V curves are acquired (e.g. different temperatures and thicknesses).

The protocol is in three parts. The first part gives only the text of the protocol. The second part explains some of the principles behind the protocol and provides examples. Finally a complete worked example is given together with an example reporting sheet. It is recommended that users read the guidance notes and examples before applying the protocol, and use a reporting sheet based on the example provided.

1. The protocol

1) Select the data to be used for analysis:

- If positive and negative voltages are available, select either the positive voltage or negative voltage range, whichever gives the highest current. If negative voltages are selected, invert the voltage and current values so that the data can be plotted in the first quadrant of a graph.
- If the data contains voltage sweeps in two directions (increasing voltage and decreasing voltage), select data where the voltage is swept away from zero volts.
- If the voltage sweeps were repeated, choose data from the last sweep in the sequence.
- Reject any data that is clearly unstable.
- Record which data is selected.

2) Check for series resistance:

- Plot the selected data on a linear-linear scale
- If the upper part of the I-V curve is a straight line, then series resistance is a possible cause. Otherwise, go to the next step.
- Replot the data on a double-logarithmic scale. Data where series resistance is a problem will appear to level-off at high voltages. Now replace the voltage data with internal voltage using the equation:

$$V_{int} = V_{ext} - R_s I,$$

where V_{int} is the internal voltage, V_{ext} is the external voltage, R_s is an estimate of the series resistance, and I is the current. Adjust the value of R_s to make the upper part of the curve on the double logarithmic plot as straight as possible.

- If the value of R_s is reasonable given the device structure (e.g. when using an ITO electrode, sheet resistances of the order of 10 – 100 Ω/\square are typical), then continue to use the corrected data and record the value of R_s . Otherwise use the uncorrected data, and record that there might be a problem with the device.

- If correcting for series resistance, and a kink or inflection still exists in the corrected region of the data, then record the voltage at which this occurs. The data at voltages above this will be excluded from fitting.

3) Compensate for built-in voltage:

- Now replot the data to correct for built in voltage using the equation:

$$V_{int} = V_{ext} - R_s I - V_{BI},$$

where V_{BI} is an estimate of the built-in voltage. While plotting the data on a double-logarithmic scale, adjust the value of V_{BI} to straighten the I-V curve.

- If the value of V_{BI} is reasonable (typically <0.5 V depending on electrodes), record the value of V_{BI} and continue to use the corrected data.
- Compare the V_{BI} – corrected data to the uncorrected data. Make a note of the range of voltages for which the correction causes more than a factor of 10 change in the current. This data will be excluded from the fitting.
- If the value of V_{BI} needed to straighten the curve is unrealistic, do not use any built-in voltage compensation, and exclude the lower part of the curve from fitting.

4) Select data range for fitting:

- Take the logarithm (base 10) of the current and voltage data and plot these on a linear-linear scale.
- Chose a range of voltages for fitting where the curve is reasonably straight, and the data has not been excluded in the steps above. When there are several straight regions, the upper one should be chosen. Record the chosen voltage range. Only data point from within this range will be used for least-squares fitting.

5) Perform least-squares fitting:

The data are to be fitted using the Murgatroyd expression:

$$I = A\mu_0 \frac{9 V_{int}^2}{8 d^3} \varepsilon \varepsilon_0 \exp\left(0.891\gamma\sqrt{V_{int}/d}\right),$$

where d is the active layer thickness, A is the active device area, $\varepsilon \varepsilon_0$ is the permittivity of the active layer, and V_{int} is the internal voltage. μ_0 and γ are the unknown parameters that will be adjusted to get a good fit, all other parameters are fixed. μ_0 is the mobility at low electric fields, and γ is a parameter that represents the field dependence of mobility. If the permittivity of the film is unknown a relative permittivity of $\varepsilon = 3.5$ can be assumed (ε_0 is the permittivity of free space). To fit against the logarithm of the I-V curve, the fitting equation used is:

$$\text{Log}_{10}(I) = \text{Log}_{10}\left(A\mu_0 \frac{9 \varepsilon \varepsilon_0}{8 d^3}\right) + 2\text{Log}_{10}(V_{int}) + \frac{0.387\gamma}{\sqrt{d}} 10^{\text{Log}_{10}(V_{int})/2}.$$

- Use a least-squares fitting algorithm to fit the data to the above equation in the selected range.

6) Record fit parameters:

- Record the best-fit values of μ_0 and γ .
- Record the electric field ($F = V_{int}/d$) range over which the best-fit curve is a reasonable fit. A reasonable fit is defined here as being the range when the difference in $\text{Log}_{10}(I)$ from the above equation and the measured value is less than 0.1 .

7) Record mobility at specified electric field:

The Muragtrotyd expression used above assumes a field-dependent mobility of the form:

$$\mu(F) = \mu_0 \exp(\gamma \sqrt{F}).$$

- Chose a value of electric field that is representative of all devices being measured, and quote the mobility at this field for each device using the above equation.
- If the chosen electric field lies at a point where the fit is not reasonable, the mobility should not be reported or should be reported with a qualifying statement.

8) Record image of fit:

- Attach to the report an image or graph object of the data and best-fit curve for future reference.

2. Notes on the protocol

1) Select the data to be used for analysis:

- If positive and negative voltages are available, select either the positive voltage or negative voltage range, whichever gives the highest current. If negative voltages are selected, invert the voltage and current values so that the data can be plotted in the first quadrant of a graph.
- If the data contains voltage sweeps in two directions (increasing voltage and decreasing voltage), select data where the voltage is swept away from zero volts.
- If the voltage sweeps were repeated, choose data from the last sweep in the sequence.
- Reject any data that is clearly unstable.
- Record which data is selected.

When positive and negative voltages have been used, the I-V curves are normally not anti-symmetric as theory predicts they should be. This can be caused by injection-limited behaviour on one of the electrodes. The side of the curve that has the highest current should be chosen to minimise injection effects.

Depending on how the data were collected, there might be a choice of I-V curves available for analysis. For the purposes of reproducibility of benchmark mobility values, it is preferable to use data where the voltage is swept from zero volts outwards (towards positive or negative voltage), rather than the other way around. This is because bias stress can affect the shape of the curve when a high voltage is applied for some time.

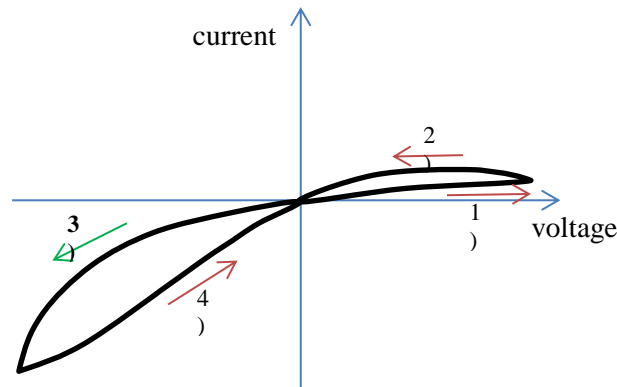
Often the first one or two I-V curves are not reproducible, but the curves become more reproducible after multiple repeated sweeps. Therefore, it is preferable to use subsequent curves if possible.

Where the measured current appears noisy, fluctuates wildly, or does not change monotonically with voltage, this is an indication of non-reproducible data that should be rejected.

Keeping a record of each step is an important part of this procedure. It can help to ensure consistency and to identify mistakes later. As the protocol requires user discretion in places, sufficient records should be kept that the result can be reproduced. An example reporting sheet is attached.

Example: A schematic I-V curve is shown with arrows indicating the direction of voltage sweep. The voltage is swept first from zero volts to a positive voltage, then to a negative voltage and then back to zero. The user first identifies that the current is higher in the negative voltage range, indicating better charge injection in this region. In many real devices, the difference between forward and

reverse bias can be orders of magnitude. Now the user has a choice between parts 3) and 4) of the data. Part 3) is selected because the voltage is being swept away from zero volts in this region.



2) Check for series resistance:

External series resistance will affect I-V curves when the current is high. The value of the series resistance is normally unknown. Experimentally, a four-point measurement is the best way to compensate for external series resistance. This part of the protocol identifies and estimates the series resistance to lessen its impact on the extracted mobility.

- **Plot the selected data on a linear-linear scale**
- **If the upper part of the I-V curve is a straight line, then series resistance is a possible cause. Otherwise, go to the next step.**

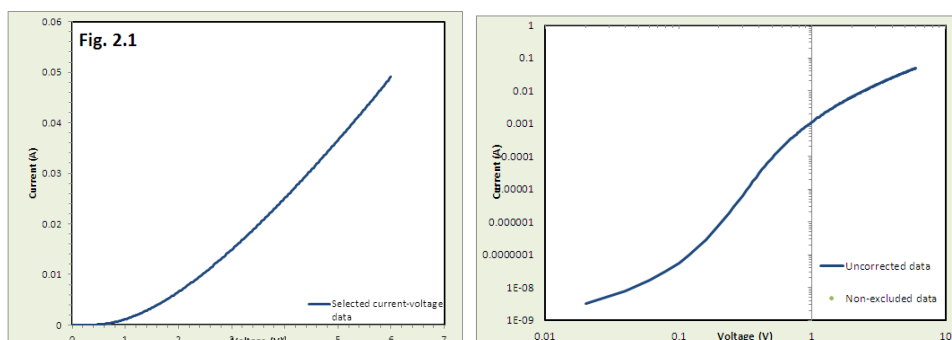
External resistances, such as thin-film electrodes, can behave like an Ohmic resistor placed in series with the device. This will cause the I-V curve, to become more linear at high currents where most of the applied voltage will be dropped across the external resistance.

- **Replot the data on a double-logarithmic scale. Data where series resistance is a problem will appear to level-off at high voltages. Now replace the voltage data with internal voltage using the equation:**

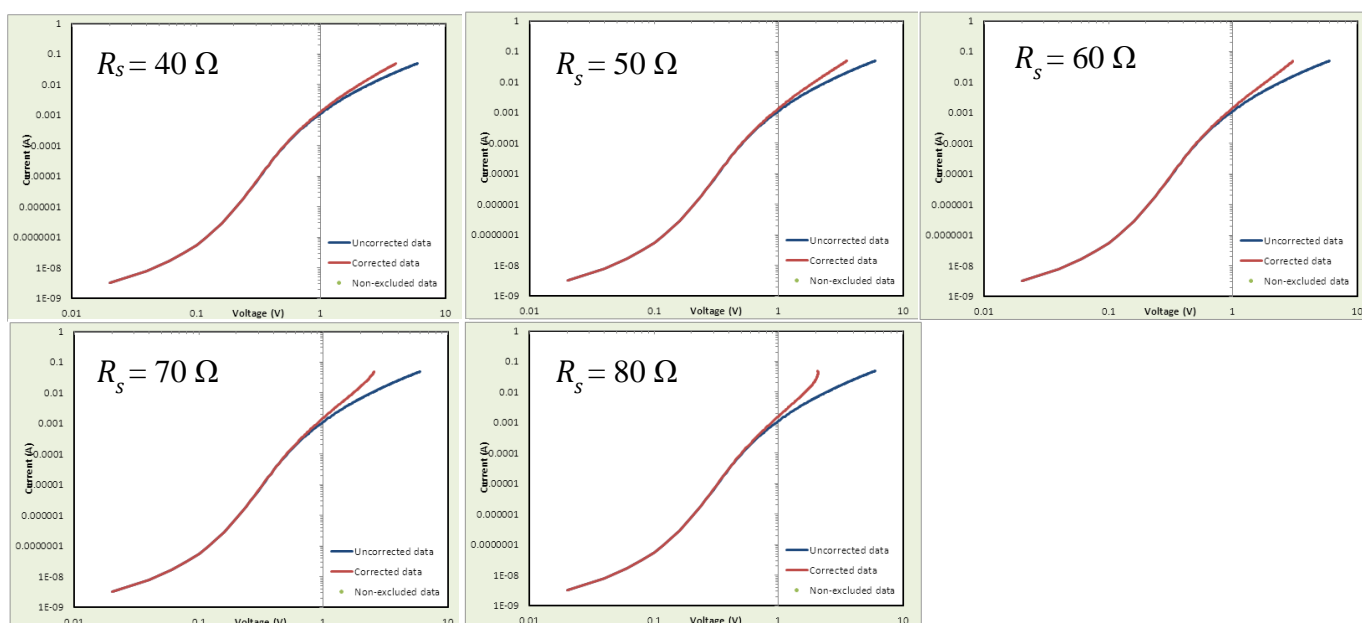
$$V_{int} = V_{ext} - R_s I,$$

where V_{int} is the internal voltage, V_{ext} is the external voltage, R_s is an estimate of the series resistance, and I is the current. Adjust the value of R_s to make the upper part of the curve on the double logarithmic plot as straight as possible.

Example: The current in this real I-V curve, shown on the left on a linear scale, increases super-linearly at low voltages, but appears to become more linear at higher voltages. This is an indication of possible series resistance. On a double-logarithmic scale (right) the gradient of the I-V curve drops off at high voltages.



The following sequence of figures shows how a built-in voltage compensated curve (red) changes on a double-logarithmic scale when a user adjusts the value of the estimated series resistance:



With R_s at 40 Ω , the gradient of the upper part of the curve still drops at high voltages. With 60 Ω , the upper part of the curve is quite straight. With higher estimated series resistance, the curve begins to increase at higher voltages. Here the user selects 60 Ω . For this data, the final extracted mobility varied almost linearly with the assume value of R_s . Different users are likely to choose values of $60 \pm 5 \Omega$ from this data, giving order $\sim 10\%$ deviation in reproducibility of extracted mobility.

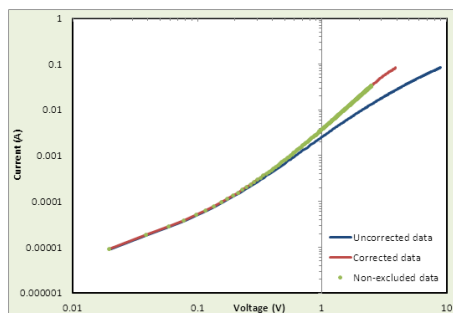
- If the value of R_s reasonable given the device structure (e.g. when using an ITO electrode, sheet resistances of the order of 10 – 100 Ω/\square are typical), then continue to use the corrected data and record the value of R_s . Otherwise use the uncorrected data, and record that there might be a problem with the device.

In the above example, an ITO electrode with a resistance of $\sim 100 \Omega/\square$ was used. The electrode was wider than the device active area, so it is very reasonable to find a series resistance of this magnitude.

- If correcting for series resistance, and a kink or inflection still exists in the corrected region of the data, then record the voltage at which this occurs. The data at voltages above this will be excluded from fitting.

Often the external series resistance is not constant throughout the experiment, and so cannot be completely compensated for. In this case the affected data should be excluded from fitting.

Example: Here a similar curve is corrected with a series resistance of 60 Ω . Despite most of the upper part of the curve being straight, there is still a downward kink visible. Applying a large correction was not able to fix this. Instead, the user decides to reject data at voltages greater than 2.5 V. When there is doubt about a series resistance correction it is best to reject the range of data that are significantly affected.



3) Compensate for built-in voltage:

- Now replot the data to correct for built in voltage using the equation:

$$V_{int} = V_{ext} - R_s I - V_{BI},$$

where V_{BI} is an estimate of the built-in voltage. While plotting the data on a double-logarithmic scale, adjust the value of V_{BI} to straighten the I-V curve.

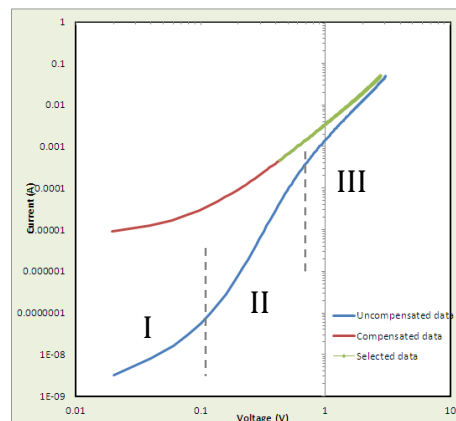
- If the value of V_{BI} is reasonable (typically <0.5 V depending on electrodes), record the value of V_{BI} and continue to use the corrected data.
- Compare the V_{BI} – corrected data to the uncorrected data. Make a note of the range of voltages for which the correction causes more than a factor of 10 change in the current. This data will be excluded from the fitting.

Sometimes I-V curves plotted on a double-logarithmic scale show a distinct middle region with a large slope. This can often be caused by built-in voltage that can be corrected for.

The amount of built-in voltage present in a device is normally unknown. It can vary depending on preparation conditions, and cannot be assumed to be the same for devices of the same type. Other effects, such as bias conditioning of electrodes, can cause similar behaviour.

Example: Here, the series-resistance corrected I-V curve above is displayed on a double-logarithmic scale (blue curve). There are three distinct regions visible in the graph. The lower region I is the Ohmic region, where conduction is by background carriers due to doping or diffusion from electrodes. The gradient is about 1 in Ohmic regions. The upper region III is where SCLC occurs. The mobility can only be extracted from regions of the curve in which SCLC is observed. The gradient is

ideally about 2 in the SCLC region, though it is frequently higher than this. Interpretation of the middle region II is more difficult. The larger gradient can be caused by injection-limited behaviour, trap filling, or built-in voltage. If either of the first two is the cause, then the region should not be used for fitting. If the cause is built-in voltage, then a correction can be used to extend the range of usable data. In the example below, the user applies a correction of $V_{BI} = 0.3$ V to extend region III until region II disappears. In this example, a change in estimated V_{BI} of 0.1 V changes the extracted mobility by about 15%. It is satisfactory to adjust V_{BI} in increments of 0.05 V.



The correction introduces uncertainty to the analysis, so data that are extremely strongly affected are to be excluded from the mobility extraction. In the above example, the difference between the corrected and uncorrected data is more than a factor of 10 for voltages below 0.5. Data from voltages below this are excluded from mobility extraction.

- **If the value of V_{BI} needed to straighten the curve is unrealistic, do not use any built-in voltage compensation, and exclude the lower part of the curve from fitting.**

Sometimes an unrealistically large built-in voltage correction can appear to straighten up the curve. In this case, there is likely another cause for different regions appearing in the I-V curves. It is safest to exclude the lower regions from fitting, and concentrate on the upper part where true SCLC is more likely to occur.

4) Select data range for fitting:

- **Take the logarithm of the current and voltage data and plot these on a linear-linear scale.**

The logarithm of the data is used to avoid problems with over-weighting of high currents when the least-squares fitting is applied later. This will produce a better looking fit and make use of more of the available data.

- Chose a range of voltages for fitting where the curve is reasonably straight, and the data has not been excluded in the steps above. When there are several straight regions, the upper one should be chosen. Record the chosen voltage range. Only data point from within this range will be used for least-squares fitting.

Theoretically, Ohmic conduction and injection-limited behaviour can occur at low voltages. If there are several distinct regions in an I-V curve, then the upper one is most likely to be the SCLC region.

In the above example, the whole of the green highlighted section is straight enough to select for fitting.

5) Perform least-squares fitting:

The data are to be fitted using the Murgatroyd expression:

$$I = A\mu_0 \frac{9 V_{int}^2}{8 d^3} \varepsilon \varepsilon_0 \exp(0.891\gamma \sqrt{V_{int}/d}),$$

where d is the active layer thickness, A is the active device area, $\varepsilon \varepsilon_0$ is the permittivity of the active layer, and V_{int} is the internal voltage. μ_0 and γ are the unknown parameters that will be adjusted to get a good fit, all other parameters are fixed. μ_0 is the mobility at low electric fields, and γ is a parameter that represents the field dependence of mobility. If the permittivity of the film is unknown a relative permittivity of $\varepsilon = 3.5$ can be assumed (ε_0 is the permittivity of free space). To fit against the logarithm of the I-V curve, the fitting equation used is:

$$\ln(I) = \ln\left(A\mu_0 \frac{9 \varepsilon \varepsilon_0}{8 d^3}\right) + 2\ln(V_{int}) + \frac{0.891\gamma}{\sqrt{d}} \exp\left[\frac{1}{2}\ln(V_{int})\right],$$

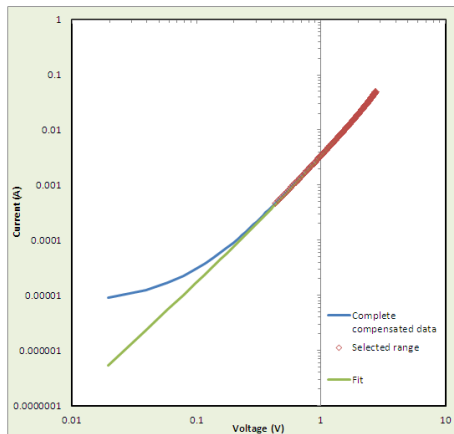
if the natural logarithm of the data are plotted, or

$$\log_{10}(I) = \log_{10}\left(A\mu_0 \frac{9 \varepsilon \varepsilon_0}{8 d^3}\right) + 2\log_{10}(V_{int}) + \frac{0.387\gamma}{\sqrt{d}} 10^{\log_{10}(V_{int})/2},$$

if the base-10 logarithm is used.

- Use a least-squares fitting algorithm to fit the data to the above equation in the selected range.

The example below shows the result when least-squares fitting is applied to minimise the difference between the above equation (green line) and the corrected data (blue line) within the selected range (red points). Only μ_0 and γ were adjusted by the program as all other parameters were fixed.



6) Record fit parameters:

- Record the best-fit values of μ_0 and γ .
- Record the electric field ($F = V_{int}/d$) range over which the best-fit curve is a reasonable fit, defined here as being the range when the difference in $\ln(I)$ from the above equation and the measured value is less than 0.25 (or 0.1 if using base 10 logarithm).

The criterion for defining a good fit corresponds to less than 25% difference between the measured data and the model curve. The use of an arbitrary definition reduces differences between different users.

7) Record mobility at specified electric field:

Above it was assumed that the mobility changes with electric field according to the relation:

$$\mu(F) = \mu_0 \exp(\gamma \sqrt{F}).$$

- Chose a value of electric field that is representative of all devices being measured, and quote the mobility at this field for each device using the above equation.
- If the chosen electric field lies at a point where the fit is not reasonable, the mobility should not be reported or should be reported with a qualifying statement.

Above we have derived two parameters that are valid within a specific range of electric fields. When making comparisons, it is usually more preferable to compare a single mobility benchmark value. Furthermore, the two parameters above are correlated. Often similar fits over a limited range can be achieved by increasing one while decreasing the other. Quoting a single value of mobility at a specified electric field is one way to improve comparability of results.

It is best to choose a value of electric field that is representative of the application for which the material is to be used, and which ideally sits within the range of good fit calculated in step 6). Mobilities from different devices, materials, formulations, etc. should be compared at the same electric field.

If comparing mobilities extracted from several devices, make a note of any cases where chosen field is outside of the range of good fit. These extrapolated mobilities have less credibility and should be used with caution.

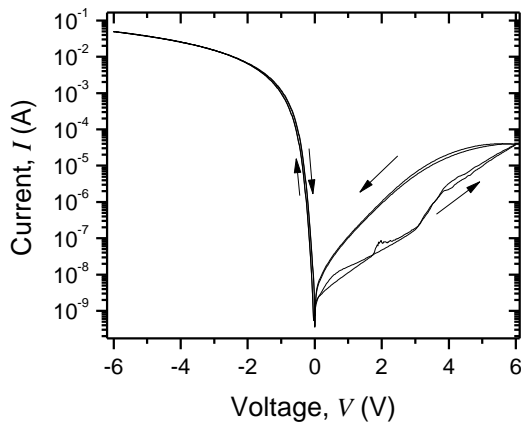
8) Record image of fit:

- **Attach to the report an image or graph object of the data and best-fit curve for future reference.**

Experience has shown that these images can later be valuable for identifying errors and checking results.

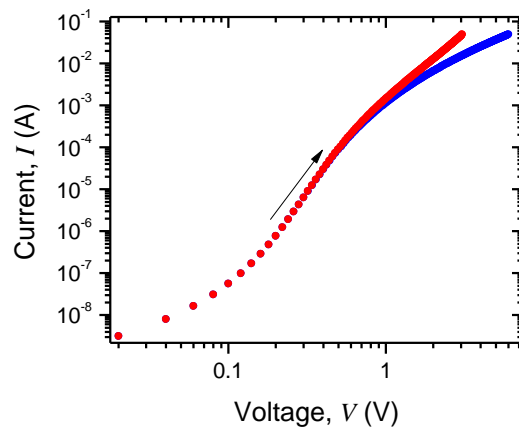
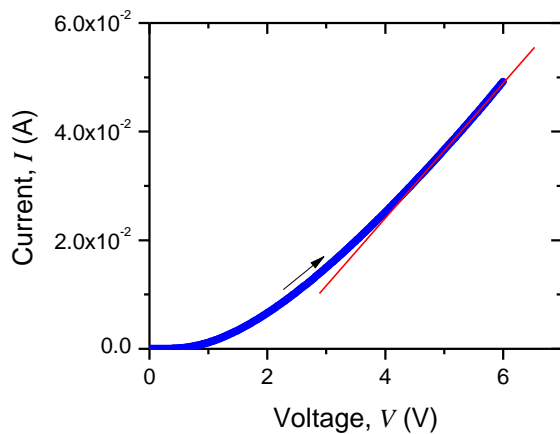
3. Complete worked example and reporting sheet:

The following I-V curve will be analysed:



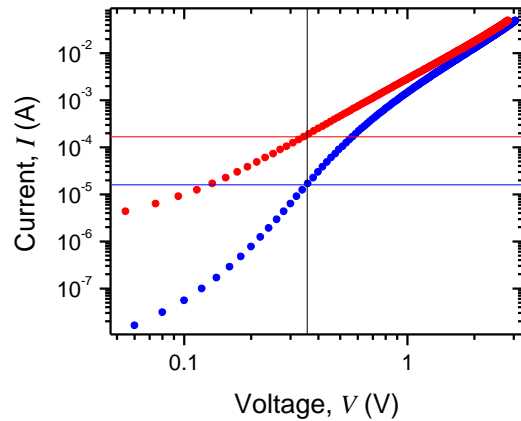
1) The I-V data include two complete cycles of sweeping voltage from zero volts to positive voltage, then to negative voltage, and then back to the origin. Clearly the current is much higher in the negative voltage region side where the hole injection is more efficient. The portion of the data in which the voltage is swept from 0 V to -6 V for the second time is selected.

2) On a linear plot, the selected part of the I-V curve becomes almost straight at high voltages. This could be due to series resistance.

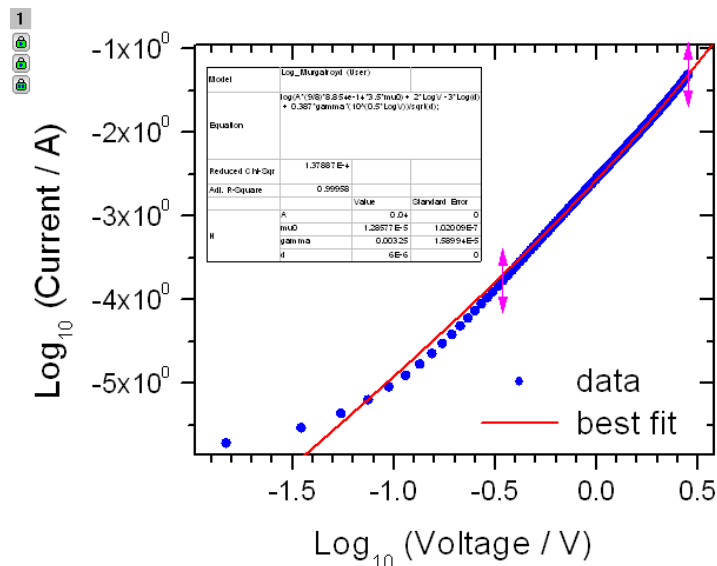


On a double logarithmic scale, the slope of the uncorrected I-V curve (blue circles) levels off at higher voltages. A series resistance correction of 60Ω is applied to straighten the upper part of the curve (red circles). There is no obvious kink or inflection in the upper part of the corrected curve, so no data are rejected.

3) The I-V curve has three distinct regions. The middle region is possibly caused by a built-in voltage. A correction of 0.225 V is applied to the internal voltage, straightening out the middle section of the I-V curve. For voltages of 0.36 V or less, the difference between the corrected and uncorrected curves is more than a factor of 10. This data range is excluded from fitting.



4) The base-10 logarithms of the data points are calculated. The data range $V > 0.36$ V are selected, as the I-V curve is quite straight in this region and points below 0.36 V have been excluded in 3) above.



5) The data are fitted using a least squares-fitting algorithm.

6) Parameters are recorded (see below). The fit is good (residual in $\text{Log}_{10}(I)$ is less than 0.1) over the range $0.31 \text{ V} < V < 2.82 \text{ V}$. This is converted to a valid electric field range by dividing by d .

7) The mobility is calculated for a representative electric field of $2.5 \times 10^5 \text{ V/cm}$.

Example reporting sheet:

Data name and device description:

TFB_60nm_Moly P4_1.txt

60nm-thick active layer of TFB with MoO₃ top electrode and PEDOT:PSS/ITO bottom electrode.

Selection of data:

Data points 1805 to 2105.

Description: Second sweep from 0 to -6 V

Series resistance:

Series resistance value used: $R_s = 60 \Omega$

Data excluded from fitting: None

Built-in voltage:

Built-in voltage value used: $V_{BI} = 0.225 \text{ V}$

Data excluded from fitting: $V_{int} < 0.36 \text{ V}$

Data fitting:

Voltage range fitted (V_{int}): $0.36 - 2.82 \text{ V}$

Fixed parameters:

$d = 6 \times 10^{-6} \text{ cm}$ $A = 0.04 \text{ cm}^2$

$\varepsilon = 3.5$

Fitted Parameters:

$\mu_0 = 1.28 \times 10^{-5} \text{ cm}^2/\text{Vs}$

$\gamma = 3.25 \times 10^{-3} \text{ cm}^{1/2}/\text{V}^{1/2}$

Good fit over voltage (V_{int}) range:

$0.31 - 2.82 \text{ V}$

Corresponding field range:

$0.5 - 4.7 \times 10^5 \text{ V/cm}$

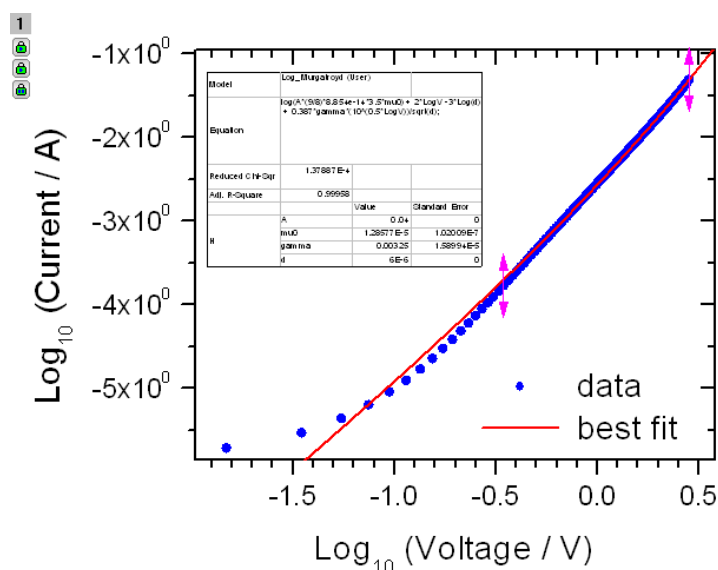
Mobility at defined field:

$\mu = 6.50 \times 10^{-5} \text{ cm}^2/\text{Vs}$

at $F = 2.5 \times 10^5 \text{ V/cm}$

Comments:

Graph of best fit:



4. Version control

Version 1, created November 2013

Initial draft version

Version 2, created January 2013

Updated following review, additional explanatory text added.

This version was used in the published interlaboratory study.

Updated March 2014; formatting changes only.