Data fusion for organic electronic material parameters

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Abstract. This paper provides a demonstration of data fusion applied to the measurement of charge mobility, an important organic electronic material parameter. It is shown that the fusion of independent data sets reduces the uncertainty associated with the charge mobility. The models used in the demonstrator are extremely simple, but the overall approach is flexible and will be applied to more complex models of organic electronic material characterization measurements in the future. The method will be used within an Open Innovation Environment for organic electronics currently under development by an EU funded project, CORNET.

1. Introduction
Organic/large area electronics (OE) is a rapidly emerging sector that will revolutionize consumer applications ranging from energy, lighting, and displays, to sensors, medicine, and wearables. OE devices are lightweight complex multilayer architectures of nanolayers (5-200nm thick) and can be manufactured cost effectively in a large area format on flexible substrates (plastics, paper, thin glass, etc.).

If the potential of OEs is to be realised fully, the materials (synthesis, thin film fabrication), materials behaviour (modelling, characterization, testing, metrology and in-line monitoring) and OE device manufacturing processes must be optimised. In order to address this need, a consortium involving academia, scientific research establishments, software and database companies, and OE manufacturers has come together to deliver a unique Open Innovation Environment for organic electronics in an EU funded project, CORNET [1].

One of the key deliverables of this project is a database that will include citable protocols for materials characterisation, modelling and processing, with the aim of making a pre-normative contribution to standards. Part of the characterisation aspect of this database will use data fusion techniques to combine data from different experiments to obtain improved estimates of material parameters and their associated uncertainties.

This paper provides a proof of concept of the approach used, using synthetic data to show how the combination of data from multiple experiments can provide better results than a single data set. The example problem is the measurement of the charge carrier mobility, a key parameter for OE systems.
2. Experiments and models

Charge carriers in OE materials can be holes or electrons, with many systems combining a hole-carrying and an electron-carrying material. The work reported here will focus on a hole-carrier system. The systems of interest generally consist of layers which are nanometres thick. During operation a potential difference of a few volts is applied in the through-thickness direction. Because the layers are thin in the direction of potential difference, the only significant charge carrier transport is in the through-thickness direction, and the system can be described by a model considering only one spatial dimension. In the absence of charge trapping, the equations governing the carrier density, \( p \), and the voltage, \( V \), in a single carrier device of thickness \( d \) are then:

\[
\begin{align*}
\frac{\partial^2 V}{\partial x^2} &= \frac{qp}{\epsilon}, \quad 0 \leq x \leq d, \\
\frac{\partial p}{\partial t} &= \frac{1}{q} \frac{\partial J}{\partial x} = \mu \left( \frac{p}{q} \frac{\partial V}{\partial x} + \frac{kT}{q} \frac{\partial p}{\partial x} \right), \quad 0 \leq x \leq d, t > 0,
\end{align*}
\]

where \( \epsilon \) is the absolute permittivity of the material, \( q \) is the charge on an electron, \( J \) is the current density, \( \mu \) is the charge mobility, \( T \) is temperature, and \( k \) is the Boltzmann constant.

The charge mobility is an important parameter, linking the voltage applied across the material to the resulting current density.

There are many ways of measuring the charge mobility. Two of the more common approaches are the steady-state space-charge limited current (SCLC) method and the dark injection transient current (DITC) method. Both of these approaches are space charge limited, meaning that an effectively infinite supply of charge carriers is available for injection into the device, and so the charge transport is governed by the characteristics of the device rather than those of the electrodes. The SCLC method applies a constant voltage to the system and measures the current density when the system reaches a steady state. It can be shown [2] that this current density is equal to

\[
J_{SCL} = \frac{9\epsilon\mu V^2}{8d^3}.
\]

Hence a line plotting \( V^2 \) against \( J_{SCL} \) for a series of experiments will have gradient \( 9\epsilon\mu/8d^3 \), and if the other parameters can be measured by other means then the charge mobility can be obtained from this gradient.

The DITC method is, as the name suggests, a transient method. A stepped voltage is applied to the system and the current density is measured over time. A typical measured current is shown in figure 1. The time at which the characteristic peak occurs, labelled \( \tau_{DI} \) in the figure, is measured. It can be shown [3] that this time is given by

\[
\tau_{DI} = \frac{2(1 - \exp(-0.5))d^2}{V\mu},
\]

and this equation can be rearranged to give \( \mu \) from the time \( \tau_{DI} \).

3. Data Fusion

Suppose that there are two measurement processes that are dependent on an unknown parameter \( \mu \), and that the measurement results from experiment 1 are \( y^{(1)} = \{y_1^{(1)}, y_2^{(1)}, \ldots, y_N^{(1)}\}^T \) with associated uncertainty \( u^{(1)} \) (taken to be the same for all measurements) and those from experiment 2 are \( y^{(2)} = \{y_1^{(2)}, y_2^{(2)}, \ldots, y_M^{(2)}\}^T \) with associated uncertainty \( u^{(2)} \). Suppose further that the function \( f^{(1)}(\mu) \) outputs results equivalent to the measured values \( y^{(1)} \) and \( f^{(2)}(\mu) \) does
the same for $y^{(2)}$. Then a data fusion approach minimises

$$S^2 = \left( \frac{1}{u^{(1)}} \right)^2 + \left( \frac{1}{u^{(2)}} \right)^2,$$

the weighted sum of squares of the differences between the model results and the measured values. The weighting by the uncertainty reflects the reliability of the measurements and makes it possible to combine measurements of different quantities. Note that this approach can be used for more than two experiments, and for more than one unknown parameter. It should also be noted that in general both the model and the data will be dependent on a control variable and a set of other experimental parameters, but these have not been explicitly included to simplify the notation. The method can also be extended by allowing uncertainties to vary within a data set.

4. A simple example

A very simple example has been developed based on the two methods for measuring charge mobility described above. A value of $\mu = 6 \times 10^{-10}$ m$^2$ V$^{-1}$ s$^{-1}$ was chosen as a reference value. A set of distribution functions for the various input parameters was defined by consulting measurement experts and previous publications [4]. The uncertainty associated with $\tau$ was chosen to make the DITC experiment of high accuracy. The distributions are listed in table 1. The mean values of $\tau_{DI}$ and $J_{SCL}$ for voltages between 1 V and 10 V were calculated using the mean values of $d$ and $\epsilon$, and a set of simulated data for each experiment was created by sampling from the distributions of $\tau_{DI}$ and $J_{SCL}$ at each voltage.

The value of $N$ (number of SCLC measurements) was kept fixed at 10, so that all of the SCLC measurements were always used, and a data fusion approach was used for values of $M$ (number of DITC measurements) between 0 and 10. A Monte Carlo simulation approach [5] was used to evaluate the uncertainties associated with the calculated value of $\mu$, based on 10,000 samples from the distributions of $V$, $d$ and $\epsilon$ listed in table 1. Figure 2 shows a plot of the calculated uncertainty associated with the charge mobility for the different numbers of added DITC measurements. It is clear that the uncertainty gets lower as more DITC data points are included, showing that the data fusion process improves the calculation process.
Table 1. Input distributions for uncertain quantities. $V_0$ is an integer voltage between 1 V and 10 V, and $J_0$ and $\tau_0$ are calculated from equations (3) and (4) respectively.

| Quantity             | Symbol | Distribution                        |
|----------------------|--------|-------------------------------------|
| Absolute permittivity| $\epsilon$ | Uniform on $[26.55, 35.4] \times 10^{-12}$ F m$^{-1}$ |
| Layer thickness      | $d$    | Normal, mean 200 nm, standard deviation 10 nm |
| Voltage              | $V$    | Uniform on $[V_0 - 0.05, V_0 + 0.05]$ V |
| Current density      | $J_{SLC}$ | Uniform on $[J_0 - 0.1, J_0 + 0.1]$ A m$^{-2}$ |
| Time of inflection   | $\tau_{DI}$ | Uniform on $[\tau_0 - 0.3, \tau_0 + 0.3]$ microseconds |

Figure 2. Calculated uncertainties associated with the charge mobility using data fusion with different numbers of DITC measurements included in the fusion.

5. Conclusions
The use of a data fusion approach to combine measurements from two independent experiments of charge mobility has lowered the associated uncertainty. Whilst the models used are very simple, the same approach will be used in future work for more complicated experiments.

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