The Extended Gaussian Disorder Model in Atlas

Preamble
In this article the various enhancements to the organic device modeling that have been implemented recently in Atlas are presented. Following the description of the carrier statistics and the new mobility and diffusion models, published data are also reproduced in the final results section.

Introduction
There has been much recent interest in organic light emitting diodes, organic solar cells, and organic field-effect transistors. The organic materials these devices are based on are disordered, significantly differentiating them from crystalline semiconductors. For example charge transport is attributed to hopping between localized sites, and the energy distribution of these sites is assumed to be Gaussian. The Extended Gaussian Disorder Model (EGDM)(1,2) calculates carrier mobility and diffusion in these organic semiconductors.

Gaussian Band Structure
In a crystalline semiconductor the band structure is usually modeled with a parabolic density of states. In organic semiconductors a Gaussian density of states is an alternative model.

When using Boltzmann statistics and a parabolic density of states, the electron density is given by:

\[ n = N_C \exp \left( \frac{\varepsilon_F - \varepsilon_C}{kT} \right) \]

When using a Gaussian density of states, the electron density is:

\[ n = \int_{-\infty}^{\infty} N(\varepsilon; N_t, \sigma, \varepsilon_C) f(\varepsilon; \varepsilon_F) \, d\varepsilon \]

where \( f(\varepsilon; \varepsilon_i) \) is the Fermi-Dirac occupation probability. This can be written as:

\[ n = N_{C,\text{eff}} G \left( \frac{\varepsilon_F - \varepsilon_C}{kT}; N_{t_\text{in}}, \sigma_n, \varepsilon_C \right) \]

where the \( G \) function must be calculated numerically. There is an equivalent expression for holes:

\[ p = N_{V,\text{eff}} G \left( \frac{\varepsilon_V - \varepsilon_C}{kT}; N_{t_\text{in}}, \sigma_p, \varepsilon_V \right) \]

The effective band edge density of states, \( N_{C,\text{eff}} \) and \( N_{V,\text{eff}} \), are chosen to ensure the expressions for the intrinsic carrier concentration and the intrinsic Fermi level have the same form as the equations for a parabolic density of states:

\[ n_{ic} = \sqrt{N_{C,\text{eff}}N_{V,\text{eff}}} \exp \left( -\frac{\varepsilon_C - \varepsilon_V}{2kT} \right) \]

\[ \varepsilon_i = \frac{\varepsilon_C + \varepsilon_V}{2} + \frac{kT}{2} \ln \left( \frac{N_{V,\text{eff}}}{N_{C,\text{eff}}} \right) \]

N\text{t}_\text{in} is the total available sites. \( \varepsilon \) is the energy. \( \varepsilon_i \) is the energy of the centre, and \( \sigma \) is the standard deviation, of the Gaussian.

![Figure 1. Band structures with parabolic and Gaussian density of states.](image-url)
For energies several \( \sigma \) below the center of the Gaussian the function \( G \) has an exponential behavior, but as \( \varepsilon \) approaches \( \varepsilon_0 \) the \( G \) curve saturates.

Various “universal” parameters associated with the Gaussian density of states are:

- \( a = \frac{N}{n} \): the average distance between sites
- \( \bar{n} = \frac{n}{N} \): the normalized carrier density
- \( \bar{\sigma} = \frac{\sigma}{\sigma_0} \): the normalized standard deviation of the Gaussian
- \( E_0 = \frac{E}{kT} \): a characteristic electric field
- \( \bar{E} = \frac{E}{E_0} \): the normalized electric field

A Gaussian band structure can be defined in Atlas in the MATERIAL command:

\[
\text{MATERIAL NTC.GAUSS}=N_{\bar{n}} \text{SIGC.GAUSS}=\sigma_{\bar{n}} \\
\text{NTV.GAUSS}=N_{\bar{\sigma}} \text{SIGV.GAUSS}=\sigma_{\bar{\sigma}}
\]

The centre of the Lowest Unoccupied Molecular Orbital (LUMO) density of states is the electron affinity below the vacuum level (so that the centre of the LUMO level is the equivalent of the conduction band edge in a parabolic band structure), and the centre of the Highest Occupied Molecular Orbital (HOMO) density of states is the band gap below the centre of the LUMO density of states (so that the centre of the HOMO level is the equivalent of the valence band edge in a parabolic band structure).

### The Pasveer Mobility

The Pasveer et al (1) mobility model has been implemented for the carrier hopping mobility in a disordered system with a Gaussian density of states. This has the following form:

\[
\mu(n, E, \sigma) = \mu_{0,300} \ g_0(\sigma) \ g_1(n, \sigma) \ g_2(E, \sigma)
\]

In this paper the first two terms are written as:

\[
\mu_0(T) = \mu_{0,300} \ c_1 \ \exp(-c_2 \bar{\sigma})
\]

However Atlas uses 300 K as the reference temperature so this is implemented as:

\[
\mu_0(T) = \mu_{0,300} \ g_0(\bar{\sigma}) = \mu_{0,300} \ \frac{\exp(-c_2 \bar{\sigma}^2)}{\exp(-c_2 \sigma_0^2)} = \mu_{0,300} \ \exp\left(-c_2 (\bar{\sigma}^2 - \sigma_0^2)\right)
\]

The expressions for the other factors are:

\[
g_1(\bar{n}, \bar{\sigma}) = \exp \left( \frac{1}{2} (\bar{\sigma}^2 - \bar{\sigma}) (2\bar{n})^2 \right)
\]

with

\[
\delta = 2 \ln(\bar{\sigma}^2 - \bar{\sigma}) - \ln(\ln(4))
\]

and

\[
g_2(\bar{E}, \bar{\sigma}) = \left(0.44 (\bar{\sigma}^{3/2} - 2.2) \left(\sqrt{1 + 0.8\bar{E}^2} - 1\right)\right)
\]

In Atlas the Pasveer mobility model can be activated for electrons with the following parameters.

\[
\text{MOBILITY PASVEER.N MUN}=\mu_{0,300} \ \text{TC2.PASV.N}=c_2 \\
\text{CCUTOFF.N}=\bar{n} \ \text{FCUTOFF.N}=\bar{E}
\]

The CCUTOFF.N parameter defines the maximum value of \( \bar{n} \) used in the calculation of \( g_1 \), and the FCUTOFF.N parameter defines the maximum value of \( \bar{E} \) used in the calculation of \( g_2 \).

This makes it relatively easy to determine the effect of the individual terms in the Pasveer mobility. By setting CCUTOFF.N=0 and FCUTOFF.N=0 the \( g_1 \) and \( g_2 \) terms are both equal to unity (their limit at \( \bar{n} = 0 \) and \( \bar{E} = 0 \), and \( g_0 \) is unity at 300 K. The following figure shows:

- \( g_0 \) as a function of \( T \) (at a fixed \( \bar{n} \) and \( \bar{E} \)) for three different values of \( c_2 \)
- \( g_1 \) as a function of \( \bar{n} \) (at a fixed \( T \) and \( \bar{E} \)) for four different values of \( \bar{\sigma} \)
- \( g_2 \) as a function of \( \bar{E} \) (at a fixed \( T \) and \( \bar{n} \)) for four different values of \( \bar{\sigma} \)
Diffusion

The diffusion coefficient is:

\[ D = \frac{\mu n}{q} \frac{1}{\frac{\partial n}{\partial x}} \frac{1}{kT} \]

With a parabolic density of states and Boltzmann probability statistics this gives:

\[ n = N_C \exp \left( \frac{\varepsilon_F - \varepsilon_C}{kT} \right); \quad \frac{\partial n}{\partial x} = N_C \exp \left( \frac{\varepsilon_F - \varepsilon_C}{kT} \right) \frac{1}{kT} = \frac{n}{kT} \]

This gives the standard Einstein diffusion coefficient:

\[ D = \frac{\mu n}{q} \frac{1}{\frac{\partial n}{\partial x}} \frac{1}{kT} = \frac{kT \mu}{q} \]

For a Gaussian density of states and Fermi-Dirac probability statistics the differential is not as simple and the diffusion coefficient is written as a correction to the Einstein value

\[ D = \frac{kT \mu}{q} g_3(\tilde{n}, \tilde{\sigma}); \quad g_3 = \frac{n}{kT} \frac{1}{\frac{\partial n}{\partial x}} \frac{1}{kT} \]

A simulation can be set up to extract the \( g_3 \) parameter. The drift-diffusion current is:

\[ J = qn\mu E + qD \frac{\partial n}{\partial x} = qn\mu E + kT \mu g_3(\tilde{n}, \tilde{\sigma}) \frac{\partial n}{\partial x} \]

If \( J=0 \) then:

\[ 0 = qn\mu E + kT \mu \frac{\partial n}{\partial x} g_3(\tilde{n}, \tilde{\sigma}); \quad g_3(\tilde{n}, \tilde{\sigma}) = -\frac{qnE}{kT \frac{\partial n}{\partial x}} \]

If \( \%\delta n = 0 \) then \( J=0 \) occurs as \( E=0 \) and this cannot be used to calculate the enhancement to the diffusion.

But if a built-in carrier gradient is introduced into the simulation, which can be performed with a graded doping, then the field required to counteract the diffusion at zero current can be used to calculate \( g_3 \).

Results

Van Mensfoort and Coehoorn (2) give the results of some simulations on simple organic devices. The symmetrical device they model is 100 nm long with Schottky contacts on either end (the Schottky boundary conditions pin the Fermi level, and therefore the carrier density, at the contact). The LUMO density of states has \( N = 8.5 \times 10^{20} \text{ cm}^{-3} \), \( \sigma = 6 \), and \( \mu_0 = 1 \times 10^{-6} \text{ cm}^{2}/\text{Vs} \). The electron concentration at the contacts is \( n = 4.25 \times 10^{20} \text{ cm}^{-3} \), this is \( N/2 \) so the work functions of the contacts are at the middle of the LUMO level. This device can be created with the commands:

```plaintext
  go atlas
mesh width=le12
  x.mesh loc=0 spac=0.25
  x.mesh loc=1 spac=0.25
  y.mesh loc=0 spac=0.001
  y.mesh loc=0.1 spac=0.005
region number=1 material=organic
electrode name=anode top
electrode name=cathode bottom
material number=1 ntc.gauss=8.5e20 \ sigc.gauss=0.155 \ eg300=3 permittivity=3 affinity=1
contact name=anode workf=1
contact name=cathode workf=1
mobility mup=1e-6 mun=1e-6 pasveer.n
```

Figure 4. The device has graded doping from the anode to the cathode, this gives a constant gradient in the electron concentration. This diffusion requires a built-in electric field to have zero current at zero bias. The middle graph is the diffusion enhancement factor, \( g_3 \), as a function of carrier density for various widths of the Gaussian density of states.
The length in the x-direction is 1\(\mu\)m, the width of the device is chosen to be 10\(^{12}\)\(\mu\)m (so that the xz-area is 1 m\(^2\) and the calculated current is equal to the current density). The affinity and the work-function of the contacts are the same value (so that the electron quasi-Fermi level at the contacts is in the middle of the LUMO level, and the resultant carrier concentration is \(N_t/2\)). The band gap is large enough that the concentration of holes is insignificant.

Conclusion

The EGDM describes the mobility with:

\[
\mu(\hat{n}, \bar{E}, \bar{\sigma}) = \mu_{0,300} \ g_0(\bar{\sigma}) \ g_1(\hat{n}, \bar{\sigma}) \ g_2(\bar{E}, \bar{\sigma})
\]

and the diffusion coefficient with:

\[
D(\hat{n}, \bar{E}, \bar{\sigma}) = \frac{kT}{q} \ \mu(\hat{n}, \bar{E}, \bar{\sigma}) \ g_3(\hat{n}, \bar{\sigma})
\]

Gaussian density of states can be activated for the LUMO/HOMO levels with the command:

```
MATERIAL NTC.GAUSS=N_{t,n} SIGC.GAUSS=\sigma_n \ 
NTV.GAUSS=N_{t,p} SIGV.GAUSS=\sigma_p
```

and the Pasveer mobility model for electrons can be activated with the command (similar parameters to activate the Pasveer model for holes):

```
MOBILITY PASVEER.N MUN=\mu_{0,300} TC2.PASV.N=C_2 \ 
CCUTOFF.N= \hat{n} FCUTOFF.N= \bar{E}
```

The \(g_3\) enhancement to the diffusion coefficient is calculated automatically due to the Gaussian density of states.

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References
