EXPLANATION OF THE MEYER-NELDEL RULE

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The Meyer-Neldel rule (MNR)[1] is observed in many processes in nature. The two main stream fields that are most affected by it are diffusion processes, where it is also known as the Compensation Effect[2], and semiconductor conduction. Areas of semiconductors where the MNR is detected include: porous and amorphous silicon[3, 4], microcrystalline silicon films[5], ionic conductivity[6], glassy materials[7] and organic materials[8] in various devices such as charge-coupled devices[9], thin-film transistors[4] and even superconductors[10]. The Meyer-Neldel rule for conduction processes states that the activation energy for conduction can depend on various parameters ranging from the (partial) pressure[11] to the bias. It is the latter, the dependence on bias, that we observe frequently in our organic thin-film field-effect transistors and therefore focus on these materials and devices in the current work. The above listed materials all have in common an abundant density of traps in a less-than perfect crystalline structure. We will show that exactly this feature causes the observation of the Meyer-Neldel rule. Recently we have proven that conduction in α-sexithiophene (T6) is governed by the traps[12] and with the current work we demonstrate the direct link between the traps and the MNR.

The Arrhenius behavior of conduction states that the conductivity is depending on the temperature in an exponential way:

$$\sigma = \sigma_0 \exp\left(-E_A/kT\right), \tag{1}$$

with E_A the activation energy, k the Boltzmann constant and T the absolute temperature. The empiric Meyer-Neldel rule states that the pre-factor σ_0 depends on the activation energy[8, 13]

$$\sigma_0 = \sigma_{00} \exp\left(E_A/kT_{\mathrm{MN}}\right), \tag{2}$$

with σ_{00} a true constant and T_{MN} the iso-kinetic temperature. This implies that 1) The activation energy of current or carrier mobility depends on for instance the bias conditions but 2) There exists a temperature, T_{MN}, where the dependence on bias disappears. In an

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Arrhenius plot, the curves of current or mobility are straight lines that pass through or converge to a common point not coinciding with infinite temperature. Using the theory of Shur and Hack[14, 15] we will now show that an exponential distribution of trap states results in an observation of the MNR.

Modern FETs differ from the standard inversion channel devices presented in textbooks in that they are often accumulation channel devices (the channel carriers are the same as the bulk carriers) and they are thin films. Moreover, standard theory assumes a low density of trap states. However, to define the effective mobility of carriers, the standard equation is often used as a guideline. The field-effect mobility is defined via the derivative of a transfer curve (I_{ds} vs. V_{g}). The found values can thus substantially deviate from mobilities measured by other techniques such as time-of-flight or Hall effect. Moreover, it can depend on the bias conditions and the temperature. It is not uncommon to find non-linear transfer curves. Experimentally it has been found[12] that deviations from standard theory can be expressed in the form

$$I_{\mathrm{ds}} = \frac{W}{L}\mu C_{\mathrm{ox}} V_{\mathrm{ds}} (V_{\mathrm{g}} - V_t)^{\alpha}. \tag{3}$$

Here W and L are the source and drain electrode length and distance respectively, C_{ox} is the oxide capacitance density, V_{ds} and V_{g} the drain-source and gate-source bias respectively, and α an empirical factor which is equal to 1 for standard theory. V_t is the bias needed to open the channel. The above equation makes the as-measured mobility depending on the gate-bias, $\mu \propto (V_{\mathrm{g}} - V_t)^{\alpha-1}$. Qualitatively it is not difficult to see how the mobility can be gate-dependent and the currents supra-linear. We have to bear in mind that the mobility is a weighed average over all the states. Whereas the band states have high mobility, carriers trapped on deep states do not contribute to the current and have therefore mobility equal to zero. Because the gate bias can change the ratio of trapped-to-free carriers, the mobility becomes gate-bias dependent. Specific models take this a step further and quantitatively predict the value of α. These models such as Poole-Frenkel[16, 17] and the similar multi-trap-and-release[18] or variable-range-hopping[19] all include trap states. In a recent publication we have shown that the Poole-Frenkel model of conduction is very adequate for describing the T6-FETs, thus showing the importance of trap states in these materials. For amorphous-silicon thin-film transistors, Shur and Hack[14] developed a theory incorporating an exponential distribution of trap states, $N_T(E) \propto \exp(-E/kT_2)$, with T_2 a parameter describing the distribution. Their model dictates that the drain-source current is of the form (Equation 53 of Ref.[14])

$$I_{\mathrm{ds}} = \frac{q\mu_0 W}{L} f\left(T, T_2\right)\left[C_{\mathrm{ox}}\left(|V_{\mathrm{g}} - V_t|\right)\right]^{\left(\frac{2T_2}{T}-1\right)} V_{\mathrm{ds}}, \tag{4}$$

with

$$f(T, T_2) = N_{\mathrm{V}} \exp\left(\frac{-E_{F0}}{kT}\right) \frac{kT\epsilon}{q} \left(\frac{\sin(\pi T/T_2)}{2\pi\epsilon T_2 kT g_{F0}}\right)^{T_2/T}. \tag{5}$$

Here N_V is the effective density of band states which is considered independent of temperature (assuming a more accurate slowly-varying function, such as $N_V \propto T^{3/2}$ [16], does not change the analysis). g_{F0} is the density of deep localized states at the Fermi level E_{F0}, which can be as large as N_V. μ_0 is the band mobility, ϵ the semiconductor permittivity, q the elementary charge and k the Boltzmann constant. Note that a factor q has been removed from the last term of the original form of Eq. 5 in order to make the units correct. The dependence of the mobility on the gate-bias is immediately evident because for a general temperature $\alpha = 2T_2/T - 1 \neq 1$. Equation 4 also directly predicts the second part of the Meyer-Neldel observation, namely there exists a temperature where the current doesn't depend on the gate voltage, $T_{\mathrm{MN}} = 2T_2$. In other words, the Meyer-Neldel temperature is a direct measure of the distribution of deep trap states and this temperature can rapidly be determined by taking temperature-scanned-current curves at different biases and thus becomes a figure-of-merit for the quality of the material used in the FET.

The above equations also predict the first part of the Meyer-Neldel rule: For temperatures well below T_2, the approximation $\sin(\pi T/T_2) \approx \pi T/T_2$ can be made and, together with the relation $a^x = \exp(x\ln(a))$, it is easily shown that the Arrhenius plots of current are linear and the effective activation energy depends on the gate bias:

$$E_A = E_{F0} - kT_2\left[\ln\left(\frac{1}{2\epsilon(kT_2)^2 g_{F0}}\right) - 2\ln\left(C_{\mathrm{ox}}\left(|V_{\mathrm{g}} - V_t|\right)\right)\right]. \tag{6}$$

Note that this activation energy can thus substantially deviate from the depth of the traps at the Fermi level, E_{F0}. In view of this and the linearity of the Arrhenius plots, one can easily make the mistake of assuming a single discrete trap level to be responsible for the activation of the current.

Figure 1 shows a simulation of a temperature-dependent-current of a system with deep traps with the parameters as of Table 1. Note that the as-measured mobility is much smaller than the band conduction mobility μ_0. As an example, for the parameters of Table 1 and $|V_\mathrm{g} - V_t| = 6$ V and $T = 300$ K, the measured mobility is 8.0 x 10^{-3} cm^2/Vs - 3 orders of magnitude below the band mobility μ_0.

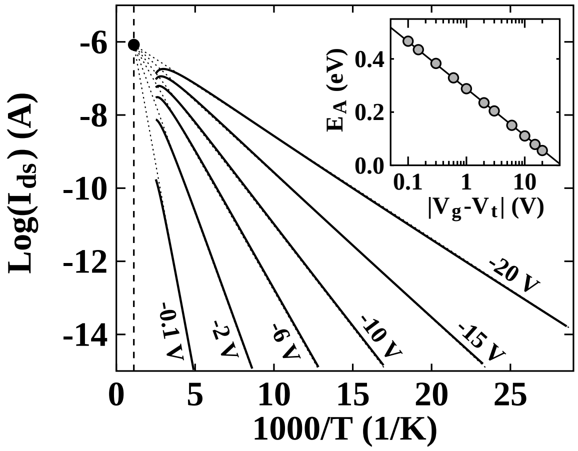

Figure 1: *Simulation of temperature-dependent currents (I-T) based on parameters of Table 1, with gate biases from 0.1 V to 20 V as indicated. The solid dot (●) represents the Meyer-Neldel point (T_MN,I_MN). The inset shows the effective activation energy as a function of bias.*

Table I: *Simulation parameters used to generate Figure 1.*

Parameter	value	unit
N_V	10^{19}	cm^{-3}
C_ox	1.92 10^{-4}	F/m^2
E_{F0}	484	meV
V_ds	-0.1	V
g_{F0}	10^{16}	cm^{-3}eV^{-1}
T_2	450	K
W	1	cm
L	30	μm
μ_0	3	cm^{2}V^{-1}s^{-1}
ϵ	$5\epsilon_0$	

For a specific α-sexithiophene p-channel FET, with geometric parameters W, L and C_ox as given in Table 1, I-T scans were made for various bias conditions[12]. An example of an I-T curve for V_g = -10.5 V and V_ds = -0.5 V, together with a simulation on basis of Equation 4 is shown in Figure 2. A summary of the measured activation energies of current as a function of gate bias is given in Figure 3. In these experiments, the scanning had to be limited to below 210 K to avoid the phenomenon known as stress[20, 21], substantial shifts of the threshold voltage V_t upon application of gate bias. This is especially pertinent because the effect of bias on the measured activation energy is expected to be largest for V_g close to V_t, as predicted by Equation 6. Thus, small changes of V_t influence the results dramatically.

One final thing to note is that for temperature approaching T_2 Equations 4 and 5 don't yield a real value for the current. Interesting in this respect is the lack of presented results in literature for measurements at the iso-kinetic temperature. In all cases the Meyer-Neldel point is found by extrapolation of the curves.

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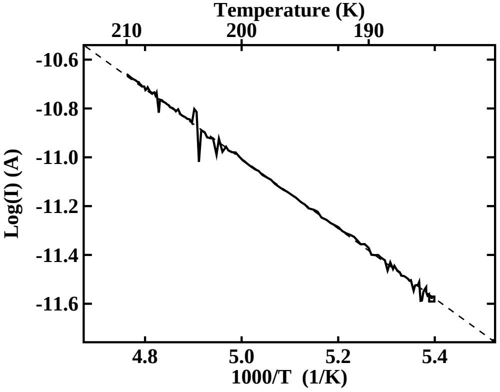

Figure 2: *Arrhenius plot of the current of an FET based on T6 with bias* V_{ds} = *-0.5 V and* V_{g} = *-10.5 V. The dashed line shows a simulation with* E_{F0} = *535 meV*, N_V = *1.7 x* $10^{19}/cm^3$, $V_{\mathrm{g}} - V_t$ = *-2 V and other parameters as of Table 1. The slope of the curve yields an effective activation energy of 296 meV.*

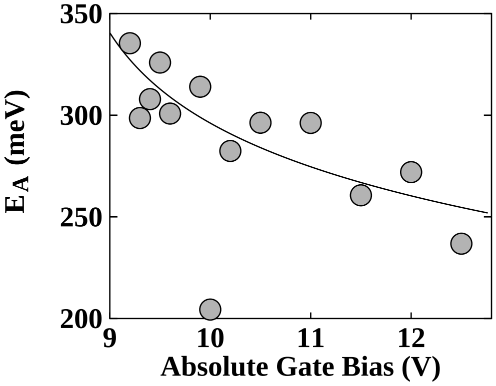

Figure 3: *Measured activation energy as a function of bias of an FET based on sexithiophene. The solid line is a fit to the data yielding* T_2 = *250 ± 200 K and* V_t = *-8.5 ± 1.4 V. To avoid systematic error, the measurements were carried out in random order. Each point represents a curve such as shown in Figure 2.*

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