Appendix A

Algebraic Description of the Multiple Trapping Model

Dispersive transport is a characteristic observed in many disordered semiconductors and can be described by simple models of trap-controlled charge carrier transport (see e.g. [97, 185] for a review). Within this section, the special case of multiple trapping in an exponentially decaying band-tail is described analytically. The calculations are adopted from Schiff [186], while the algebra is based on the "TROK" approximations established by Tiedje, Rose, Orenstein and Kastner [187, 188]. The model assumes that states in the valance band-tail are separated by an mobility edge E_V, where transport takes place only in the extended states located below E_V. Charge carriers trapped in states above E_V are totally immobile. In this section, an approximate expression for the experimentally accessible value of the displacement/electric field ratio L/F is given. For an exponentially decaying distribution of traps the density of states g(E) in the valence band-tail can be written as

$$g(E) = g_0 \cdot \exp\left(-\frac{E}{\Delta E_V}\right), \tag{A.1}$$

where g_0 is the density of states at the mobility edge E_V (note that E is defined as the zero of energy, which increases in the direction of the bandgap) and ΔE_V the width of the valance band-tail. One "TROK" approximation assumes that the capture cross section of the localized states is energy independent and states above E_V will initially be populated uniformly by carriers which are trapped following the excitation. Somewhat later, charge carriers in shallow states will be released thermally, while trapping processes remains random. The demarcation level $E_D(t)$ can be defined as the energy which separates those states who are so deep that charge carriers trapped in them have not yet been thermally excited even once, from those who are in thermal equilibrium with the conducting states. E_d can be written as

$$E_d(t) = E_V + kT \ln(\nu t), \tag{A.2}$$

where kT is the temperature in energy units and ν an attempt-to-escape frequency. It has been shown by Tiedje, Rose, Orenstein, and Kastner that at any time prior to the transit time and in the absence of recombination the carrier distribution is determined by the demarcation energy as

$$N = F(t) \int_{-\infty}^{+\infty} \frac{g_0 \cdot \exp\left(-\frac{E}{\Delta E_V}\right)}{1 + \exp\left(\frac{E - E_d}{kT}\right)} dE. \tag{A.3}$$

where $F(t)$ is an occupation factor which acts to conserve the excitation density N. For the occupancy factor $F(t)$ one derives

$$F(t) = \frac{N}{kT_0 g_0} \frac{sin(\alpha\pi)}{\alpha\pi} (\nu t)^{\alpha}, \tag{A.4}$$

where $\alpha = kT/\Delta E_V$, while the time dependent drift mobility can be written as

$$\mu(t) \equiv \mu_0 \frac{n(t)}{N} = \mu_0 \frac{N_V}{kT_0 g_0} \cdot \frac{sin(\alpha\pi)}{\alpha\pi} (\nu t)^{-1+\alpha}, \tag{A.5}$$

where N_V is the effective density of states at the mobility edge, $n(t)$ is the density of mobile charge carriers, and μ_0 is their mobility. Since $\mu(t)$ is defined as

$$\mu(t) = \frac{\bar{\mathrm{v}}(t)}{F}, \tag{A.6}$$

where v(t) is the mean drift-velocity and F is the electric field, one can find the displacement L(t) by integration:

$$\frac{L(t)}{F} = \frac{N_V}{kT g_0} \cdot \frac{sin(\alpha\pi)}{\alpha\pi} \left(\frac{\mu_0}{\nu}\right) (\nu t)^{\alpha} \tag{A.7}$$

Using Eq. A.1, the effective DOS in the valence band can be written as

$$N_V = \int_{-\infty}^{0} g(E) \cdot \exp\left(\frac{E}{kT}\right) \tag{A.8}$$

For $kT < \Delta E_V$ and assuming that the integral is dominated by an exponential region of $g(E)$ below E_V one obtains for N_V

$$N_V = \frac{kT g_0}{1 - \frac{kT}{\Delta E_V}}. \tag{A.9}$$

Eq. A.7 then becomes

$$\frac{L(t)}{F} = \frac{sin(\alpha\pi)}{\alpha\pi(1-\alpha)}\left(\frac{\mu_0}{\nu}\right)(\nu t)^{\alpha} \qquad \text{with} \qquad \alpha = \frac{kT}{\Delta E_V}. \tag{A.10}$$

Using this equation the displacement/field ratio only depends on three parameters, the width of the exponential band-tail ΔE_V, the band mobility μ_0 describing the mobility of charge carriers in extended states and the attempt to escape frequency ν, all describing crucial properties of band-tail.

The analysis of the multiple trapping model presented above is based on the (plausible) assumption that a Fermi-Dirac type of distribution applies to the carriers in traps [186, 128, 188]. This ”TROK” approximation has been shown by Monte-Carlo calculations to be quite good for exponential band-tails, and can be shown to be exact for the special case $\alpha = 1/2$ [189]. For non-exponential densities-of-states, the TROK approximation is unreliable.

Appendix B

List of Samples

Table B.1: Parameters of intrinsic μc-Si:H prepared using a HWCVD process. The filament temperature was T_F = 1650°C, while the deposition pressure was p = 3.5 Pa, except for samples 02C261-02C297 with p = 5 Pa.

	Sample	[SiH$_4$]	m [mg]	σ_D [S/cm]	I_C^{RS}	N_S	g-value
185°C	01c297	5.0	34.8	5.21×10^{-08}	0.6	$4.70\times10^{+15}$	2.0046
	01c298	5.7	35.8	4.40×10^{-09}	0.51	$5.10\times10^{+15}$	2.0046
	01c299	5.7	37.5	5.38×10^{-07}	0.4	$4.30\times10^{+15}$	2.0045
	02C261	5.0	54.6		0.63	$1.67\times10^{+16}$	2.0047
	02C260	6.3	63.3			$7.57\times10^{+15}$	2.0048
	02C287	5.5	31.1		0.58	$7.01\times10^{+15}$	2.0043
	02C288	4.7	16.4		0.67	$9.79\times10^{+15}$	2.0048
	02C292	6.0	15.7		0	$1.66\times10^{+16}$	2.0047
	02C291	7.0	20.7		0.23	$8.29\times10^{+15}$	2.0048
	02C297	9.0	13.9		0	$1.03\times10^{+16}$	2.0049
250°C	02c128	3.0	34.8		0.74	$8.82\times10^{+16}$	2.0047
	02c117	4.0	45.5		0.7	$3.18\times10^{+16}$	2.0049
	02c125	5.0	41.3		0.63	$1.98\times10^{+16}$	2.0049
	02c113	6.0	41.5		0.59	$7.76\times10^{+15}$	2.0046
	02c121	7.0	56.3		0.5	$8.87\times10^{+15}$	2.0047
	02c134	9.0	46.3		0	$1.17\times10^{+16}$	2.0052

Table B.2: Parameters of intrinsic μc-Si:H prepared using a HWCVD process. The filament temperature was T_F = 1750°C for samples prepared at T_S = 450°C and T_F = 1650°C for the other. The pressure was p = 5 Pa.

	Sample	[SiH$_4$]	m [mg]	σ_D [S/cm]	I_C^{RS}	N_S	g-value
285°C	01c050	3.0	23.0	1.38×10^{-06}	0.77	$2.13\times10^{+17}$	2.0480
	01c045	5.0	24.0	2.42×10^{-06}	0.65	$1.36\times10^{+16}$	2.0050
	01c052	6.3	22.1	1.12×10^{-05}	0.54	$8.67\times10^{+15}$	2.0048
	01c047	7.5	15.3	1.03×10^{-06}	0.4	$2.28\times10^{+16}$	2.0052
	01c051	8.8	15.0	6.69×10^{-07}	0.29	$1.46\times10^{+16}$	2.0051
	01c048	10.0	14.1	1.05×10^{-10}	0	$4.84\times10^{+16}$	2.0050
	01c074	10.0	29.3		0.1	$1.42\times10^{+16}$	2.0049
	01c077	11.3	24.8		0	$1.18\times10^{+16}$	2.0050
	01c075	12.5	28.9		0	$1.23\times10^{+16}$	2.0049
330°C	01c067	5.0	31.6	2.74×10^{-07}		$2.60\times10^{+17}$	2.0050
	01c073	5.0	35.6	2.74×10^{-07}	0.63	$2.84\times10^{+17}$	2.0050
	01c064	7.5	25.6	1.15×10^{-05}	0.58	$1.29\times10^{+17}$	2.0053
	01c066	10.0	28.1	1.13×10^{-06}	0.42	$7.70\times10^{+16}$	2.0053
	01c072	11.3	27.1	5.13×10^{-08}	0.31	$3.08\times10^{+16}$	2.0051
	01c068	12.5	29.5	9.38×10^{-12}	0.15	$4.37\times10^{+16}$	2.0053
	01c065	15.0	17.9	1.95×10^{-11}	0	$1.40\times10^{+17}$	2.0038
	01c070	19.0	19.5		0	$8.30\times10^{+16}$	2.0051
450°C	00C247	5.0		2.38×10^{-07}	0.76	$4.80\times10^{+18}$	2.0050
	00C235	7.5		6.94×10^{-07}	0.66	$1.70\times10^{+18}$	2.0048
	00C264	10.0		5.01×10^{-07}	0.75	$4.30\times10^{+18}$	2.0056
	00C241	12.5		3.30×10^{-07}	0.69	$1.00\times10^{+18}$	2.0053
	00C258	15.6		3.05×10^{-07}	0.74	$8.10\times10^{+17}$	2.0050
	00C266	15.6		2.46×10^{-08}	0.48	$1.30\times10^{+18}$	
	00C242	18.8		7.64×10^{-08}	0.58	$5.20\times10^{+17}$	2.0050
	00C256	21.9		1.59×10^{-08}	0.55	$1.00\times10^{+18}$	2.0053
	00C261	25.0		7.09×10^{-11}	0.1	$9.00\times10^{+16}$	2.0057

Table B.3: Parameters of n-type μc-Si:H prepared using VHF-PECVD. The process parameters were T_S = 200°C, the pressure was p = 40 Pa and the plasma power density P = 0.07 W/cm^2.

Sample	[SiH$_4$]	m [mg]	σ_D [S/cm]	I_C^{RS} (glass)	I_C^{RS} (Al)	N_S
1 ppm						
01B467	2.0	72.2	3.11×10^{-05}	0.81	0.82	$2.36\times10^{+16}$
01B363	4.0	69.3	6.78×10^{-04}	0.71	0.77	$4.12\times10^{+16}$
01B357	5.0	78.5	6.04×10^{-04}	0.66	0.7	$5.17\times10^{+16}$
01B399	6.0	91.9	1.66×10^{-04}	0.33	0.45	$4.24\times10^{+16}$
01B361	7.0	67.2	1.49×10^{-10}	0	0.03	$6.87\times10^{+15}$
01B466	8.0	91.1	3.76×10^{-10}	0	0	$4.44\times10^{+15}$
5 ppm						
01B390	2.0	42.0	2.11×10^{-04}	0.83	0.84	$4.71\times10^{+16}$
01B364	4.0	44.0	6.19×10^{-03}	0.78	0.78	$1.69\times10^{+17}$
01B385	6.0	83.4	4.24×10^{-04}	0.12	0.4	$1.38\times10^{+17}$
01B391	7.0	81.2	2.94×10^{-08}	0	0.05	$2.56\times10^{+17}$
01B468	8.0	93.3	1.90×10^{-08}	0	0	$7.74\times10^{+15}$
10 ppm						
01B415	2.0	79.0	2.87×10^{-03}	0.82	0.83	$1.20\times10^{+17}$
01B402	4.0	60.0	2.06×10^{-02}	0.74	0.76	$2.52\times10^{+17}$
01B410	6.0	83.0	1.12×10^{-02}	0.38	0.51	$2.72\times10^{+17}$
01B413	7.0	109.0	1.45×10^{-06}	0	0.08	$1.33\times10^{+17}$
01B472	8.0	87.7	1.72×10^{-07}	0	0	$8.71\times10^{+15}$

Table B.4: Parameters of intrinsic μc-Si:H prepared using a PECVD process. The process parameters were T_S = 200°C, the pressure was p = 300 mTorr, and the was plasma power density P = 0.07 W/cm^2.

	Sample	[SiH$_4$]	m [mg]	σ_D [S/cm]	I_C^{RS}	N_S	g-value
VHF	00B501	2.0	75.0	5.09×10^{-06}	0.78	$7.20\times10^{+16}$	2.0046
	00B493	3.0	70.0	3.47×10^{-06}	0.68	$2.50\times10^{+16}$	2.0044
	00B489	4.0	80.0	1.34×10^{-06}	0.61	$2.15\times10^{+16}$	2.0044
	00B483	5.0	58.0	2.40×10^{-06}	0.53	$2.00\times10^{+16}$	2.0044
	00B487	6.0	80.0	6.81×10^{-08}	0.43	$1.30\times10^{+16}$	2.0046
	01B098	6.0	104.0		0.39	$8.50\times10^{+15}$	2.0046
	01B103	7.0	88.0		0.16	$2.80\times10^{+15}$	2.0047
	00B497	7.0	91.0	1.50×10^{-10}	0	$2.66\times10^{+15}$	2.0047
	00B509	8.0	81.0	2.45×10^{-11}	0	$3.20\times10^{+15}$	2.0048
	01B096	9.0	123.7		0	$3.60\times10^{+15}$	2.0050
	00B512	9.0	93.0	2.00×10^{-11}	0	$2.00\times10^{+15}$	2.0047
	03B274	20.0	67.4		0	$3.80\times10^{+15}$	2.0053
	03B275	30.0	92.9		0	$5.00\times10^{+15}$	2.0054
	01B163	50.0	158.0		0	$7.00\times10^{+15}$	2.0054
	03B277	100.0	65.5		0	$9.50\times10^{+15}$	2.0054

Appendix C

Abbreviations, Physical Constants and Symbols

Abbreviations

a-Si:H	Hydrogenated amorphous silicon
c-Si	Crystalline silicon
CE	Conduction electron
D^+	Positively charged dangling bond defect
D^0	Neutral dangling bond defect
D^-	Negatively charged dangling bond defect
DB	Dangling Bond
db_1	ESR line at g=2.0043
db_2	ESR line at g=2.0052
DOS	Density of states
ESR	Electron spin resonance
HWCVD	Hot-wire chemical vapor deposition
IR	Infrared spectroscopy
μc-Si:H	Hydrogenated microcrystalline silicon
MT	Multiple trapping
PECVD	Plasma enhanced chemical vapor deposition
SWE	Staebler-Wronski-Effect
TCO	Transparent conductive oxide
TEM	Transmission electron microscopy
TOF	Time-of-flight
XRD	X-ray diffraction

Symbols

α	Dispersion parameter
A	Contact area
b	Electrode spacing
B_0	Flux density
C	Capacitance
D	Diffusion constant
d	Thickness
d_i	Thickness of the i-layer
d_w	Depletion layer width
ΔE_C	Conduction band-tail width
ΔE_V	Valence band-tail width
Δg	g-tensor
ΔH_{pp}	Peak to Peak line width
η	Energy conversion efficiency
E	Band gap
E_A	Activation energy
E_B	Barrier hight
E_0	Energy of the groundstate
E_C	Conduction band mobility edge
E_F	Fermi level
E_G	Energy band gap
E_{Tr}	Energy of the transport path
E_V	Valence band mobility edge
ε	Relative dielectic constant
F	Electric Field
g	Electronic g-value
g_0	Electronic g-value of the free electron
$g(E)$	Density of states
$\mathbf{L}$	Orbital angular moment
I	Current
η	Solar cell efficiency
$\mathcal{H}$	Hamilton operator
I_C^{RS}	Raman intensity ratio
J_{SC}	Short circuit current density
l	width of electrode
L	Displacement
L_D	Debye screening length
λ	excitation wavelength
μ_0	Band mobility

μ_d	Drift mobility
$\mu_{d,h}$	Hole drift mobility
$\mu\tau_{h,t}$	Deep trapping mobility-lifetime product
N_{CE}	Spin density of CE resonance
N_D	Number of active donors
N_{DB}	Spin density of DB resonance (N_{db_1}+N_{db_2})
N_{db_1}	Spin density of db$_1$ resonance
N_{db_2}	Spin density of db$_2$ resonance
N_P	Phosphorous doping concentration
N_T	Concentration trapped charge carrier
N_S	Spin density
ν	”Attempt-to-escape” frequency
p	Pressure
PC	Phosphorous doping concentration
q	Charge density
Q_0	Photoinjected charge
$Q(t)$	Transient photocharge
$Q(\infty)$	Collected Photocharge
r, R	Separation
$\bar{R}$	Mean intersite distance
R_0	Localization Radius
σ	Conductivity
σ_D	Dark conductivity
$\mathbf{S}$	Spin operator
T	Temperature
T_S	Substrate temperature
t	Time
t_{ann}	annealing period
T_1	Spin-lattice relaxation time
T_2	Spin-spin relaxation time
t_τ	Transit time
T_S	Substrate temperature
τ	Lifetime
τ_D	Deep trapping life time
τ_{rel}	Dielectric relaxation time
U_{corr}	Correlation energy
U_{relax}	Relaxation energy
U_{eff}	Effective correlation energy
V	Applied voltage

V_{int}	Internal voltage
v_d	Drift velocity
ω	Lamor frequency
w	Dispersion

Physical Constants

e	1.602×10^{-19}	C	Elementary charge
ε_0	8.8542×10^{-12}	A s V^{-1} m^{-1}	Dielectric constant
k	1.38066×10^{-23}	J K^{-1}	Boltzmann's constant
μ_B	9.274×10^{-24}	J T^{-1}	Bohr Magneton