This way $C(t)$ is separated into the constant term $C \propto \sqrt{N_{eff}}$ and the time dependent part $\Delta C \propto n_T(t)$.

Because the capture of electrons in the SCR can be neglected, the decrease of the number of occupied traps in the SCR is governed by the emission time constant $\tau_{e,n} = (e_n)^{-1}$ (see eqs. 2.42 and 2.43), it is

$$n_T(t) = n_{T,0} \exp\left(\frac{-t}{\tau_{e,n}}\right). \tag{4.15}$$

Hence also the capacitance depends exponentially on the time :

$$\Delta C(t) = C_E \frac{n_{T,0}}{2N_{eff}} \exp\left(\frac{-t}{\tau_{e,n}}\right). \tag{4.16}$$

If the capacitance is measured at two times t_1 and t_2, after the filling pulse a difference

$$\Delta C_{1,2} = C(t_2) - C(t_1) \tag{4.17}$$

can be calculated. In a conventional DLT-spectrum the measured values of $\Delta C_{1,2}$ are plotted versus temperature. Since $\tau_{n,p} = 1/e_{n,p}$, it follows from eqs. 2.42 to 2.45:

$$\tau = \frac{1}{\sigma N_{C,V} v_{th,n,p}} \exp\left(\frac{\Delta E_T}{k_B T}\right), \tag{4.18}$$

where ΔE_T is the energy difference between the trap level and valence or conduction band respectively. Therefore, in the case of low temperature, the time constant is long ($\tau \gg t_2$) and the measured difference is small. The same result occurs at high temperatures, when the emission time constant is very short and the value of steady-state is already reached at $t < t_1$. Between these extreme values $\Delta C_{1,2}$ behaves as shown in fig. 4.7. The maximum value of $\Delta C_{1,2}$ is gained, if the time constant obeys the following relation

$$\tau_m = \frac{t_2 - t_1}{\ln(\frac{t_2}{t_1})}, \tag{4.19}$$

which can be deduced from eqs. 4.16 and 4.17. Thus a time constant can be related to the temperature at which the maximum $\Delta C_{1,2}$ occurs. For a different time window (t_1', t_2') the maximum $\Delta C_{1,2}'$ will occur at a different temperature T' and another pair τ', T' is found. If several time windows are used $\tau(T)$ can be determined. The energy level ΔE_T and the cross section σ of the defect can be obtained using the Arrhenius-relation :

$$\ln \tau T^2 = \ln\left(\frac{1}{F\sigma}\right) + \left(\frac{\Delta E_T}{kT}\right), \tag{4.20}$$

which can be deduced from eq. 4.18, if $F = N_{C,V} v_{th,e,h}/T^2$ is taken into account. ΔE_T is the slope of the straight line and σ follows from the extrapolation $T \to \infty$. The trap concentration follows from eq. 4.16 :

$$n_{T,0} = 2\frac{\Delta C_0}{C_E} N_{eff}, \tag{4.21}$$

where $\Delta C_0 = \Delta C(t = 0)$. A significant disadvantage of this method is the use of only two points or the average of a few measured values close to t_1, t_2 respectively.

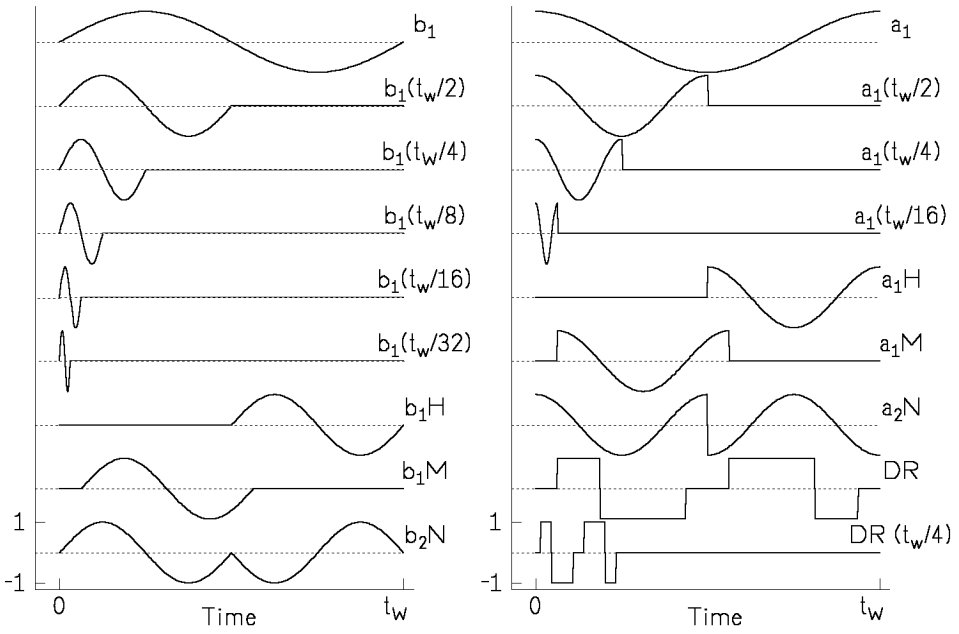

Figure 4.8: Correlator functions used for analysis of maxima. The period of the sine and cosine functions is shortened systematically by a factor of two in order to cover also short transients. DR and $DR_{t_w/4}$ are sophisticated box-car functions.

An improvement is achieved by folding the measured transient with a correlator function, e.g. a sinus. This way the complete transient can be used for the further analysis. The folding of the function $f(t) = \exp(-t/\tau)$ with a sinus is shown in fig. 4.7. The result is a correlator

$$b_1 = \frac{2}{t_w} \int_0^{t_w} \exp\left(\frac{-t}{\tau}\right) \sin(\frac{2\pi}{t_w} t)\, dt, \tag{4.22}$$

with t_w being the *time window*. As $\Delta C_{1,2}$ also b_1 depends on the temperature (see fig. 4.7) and a peak will occur, if b_1 is plotted versus temperature. The peak maximum is reached, if the time constant and the time window have the following ratio : [3]

$$\tau_m / t_w = 0.43.$$

This way the time constant can be related to the corresponding temperature.

In total, 18 different correlator functions were used. They are shown in fig. 4.8. The temperature dependence of two of the correlators a_1 and b_1 is shown in fig. 4.9. It can be seen that the peak maximum occurs at different temperatures for each correlator in combination with a certain time window. The specific ratios τ_m/t_w can be used for the determination of further pairs τ,T. Thus by applying different

[3]Because the measured transient is not a continuous signal and the folding is a numerical procedure, the ratio depends on the time binning. The given ratio corresponds to a transient of 512 bins.

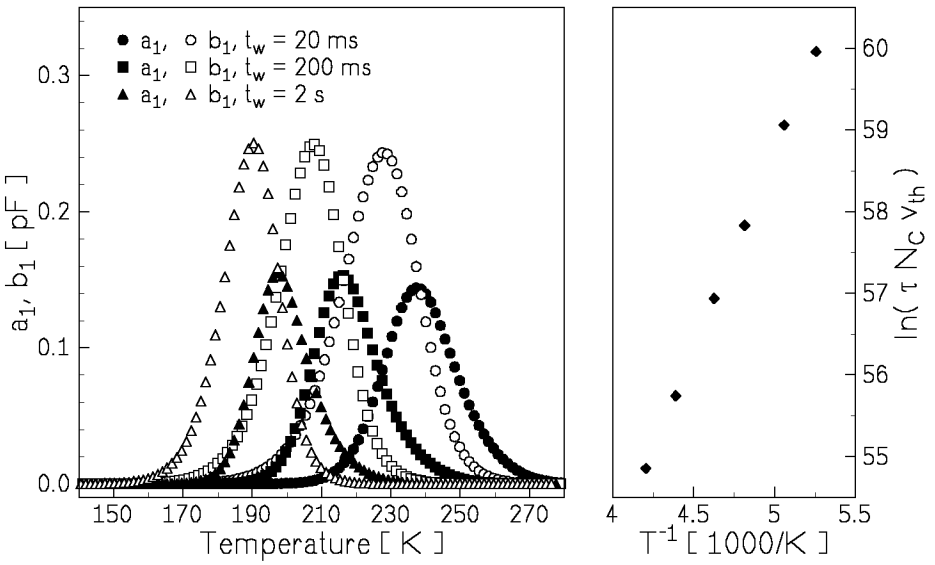

Figure 4.9: Analysis of maxima : 6 peaks occur due to 2 different correlator functions which were applied on the transients measured with 3 different time windows t_w. Each maximum provides a point in the Arrhenius-plot.
(Simulation : $\Delta E_T = 0.42$ eV, $\sigma = 1.2{\cdot}10^{-15}$ cm^2)

correlator functions and/or varying t_w various peak maxima occurring at different temperatures can be obtained and the dependence of the time constant on the temperature can be determined by finding the maxima. This method will be called hereafter *Analysis of maxima*. Usually three different time windows were used : $t_{w,1} = 20$ ms, $t_{w,2} = 200$ ms, and $t_{w,3} = 2$ s. If e.g. 2 correlator functions were used in combination with the above given time windows, 6 pairs τ,T would be obtained. The corresponding Arrhenius plot is shown in fig. 4.9.

It has to be emphasised that the analysis of maxima provides no tool which allows the verification of whether the measured transients are exponential and temperature dependent according to eq. 4.18 or not. The only possibility to prove the results for consistency is to recalculate the measured peak with the obtained parameters and compare calculation and measurement.

4.2.2 Application of the Fourier transformation

A function $f(t)$ with a periodic time t_w and a frequency $\omega_0 = \frac{2\pi}{t_w}$ can be written as an infinite sum of harmonic functions :

$$f(t) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos(n\omega_0 t) + \sum_{n=1}^{\infty} b_n \sin(n\omega_0 t) \tag{4.23}$$

with a_n, b_n being the Fourier coefficients :

$$a_n = \frac{2}{t_w} \int_0^{t_w} f(t) \cos(n\omega_0 t)\, dt, n \geq 0 \tag{4.24}$$

$$b_n = \frac{2}{t_w}\int_0^{t_w} f(t)\sin(n\omega_0 t)\,dt, n \geq 1 \tag{4.25}$$

A comparison with eq. 4.22 shows that a_n and b_n can be interpreted as a set of correlators. Note, that the coefficients (as the correlators) are calculated without assuming a specific function $f(t)$. For an exponential function

$$f(t) = \mathcal{A}\exp\left(-\frac{t+t_o}{\tau}\right) + \mathcal{B}, \tag{4.26}$$

where $\mathcal{A}$ is the amplitude, $\mathcal{B}$ is the offset and τ is the time constant, the Fourier coefficients are the following :

$$a_0 = \frac{2\mathcal{A}}{t_w}\exp(-t_0/\tau)\left(1-\exp(-t_w/\tau)\right)\tau + 2\mathcal{B} \tag{4.27}$$

$$a_n = \frac{2\mathcal{A}}{t_w}\exp(-t_0/\tau)\left(1-\exp(-t_w/\tau)\right)\frac{1/\tau}{(1/\tau^2)+n^2\omega_0^2} \tag{4.28}$$

$$b_n = \frac{2\mathcal{A}}{t_w}\exp(-t_0/\tau)\left(1-\exp(-t_w/\tau)\right)\frac{n\omega_0}{(1/\tau^2)+n^2\omega_0^2} \tag{4.29}$$

and the following relations can be deduced :

$$a_k < a_n < \frac{k^2}{n^2}a_k \qquad \text{if} \qquad n < k, \tag{4.30}$$

$$\frac{n}{k}b_k < b_n < \frac{k}{n}b_k \qquad \text{if} \qquad n < k, \quad \text{and} \tag{4.31}$$

$$\frac{b_n a_k}{a_n b_k} = \frac{n}{k}. \tag{4.32}$$

The time constant can be determined in three different ways from two coefficients :

$$1) \qquad \tau(a_n, a_k) = \frac{1}{\omega_0}\sqrt{\frac{a_n - a_k}{k^2 a_k - n^2 a_n}}, \tag{4.33}$$

$$2) \qquad \tau(b_n, b_k) = \frac{1}{\omega_0}\sqrt{\frac{kb_n - nb_k}{k^2 nb_k - n^2 kb_n}}, \tag{4.34}$$

$$3) \qquad \tau(a_n, b_n) = \frac{1}{n\omega_0}\frac{b_n}{a_n}. \tag{4.35}$$

Note that the time constants as given above (eqs. 4.33 to 4.35) depend only on the coefficients, but neither on the amplitude $\mathcal{A}$ nor on the offset $\mathcal{B}$! The amplitude can be calculated by solving eqs. 4.28 or 4.29 [4]. For capacitance-DLTS it is $\mathcal{A} \equiv \Delta C$ and the trap concentration can be calculated using eq. 4.21.

In contrast to the analysis of maxima, eqs. 4.33 to 4.35 allow the calculation of the time constant from all recorded transients in the entire temperature range covered by the peak, as long as the two coefficients chosen to calculate τ are not zero.

[4] b_1 has been used without exception. Further details on trap concentration determination are discussed in the next section.

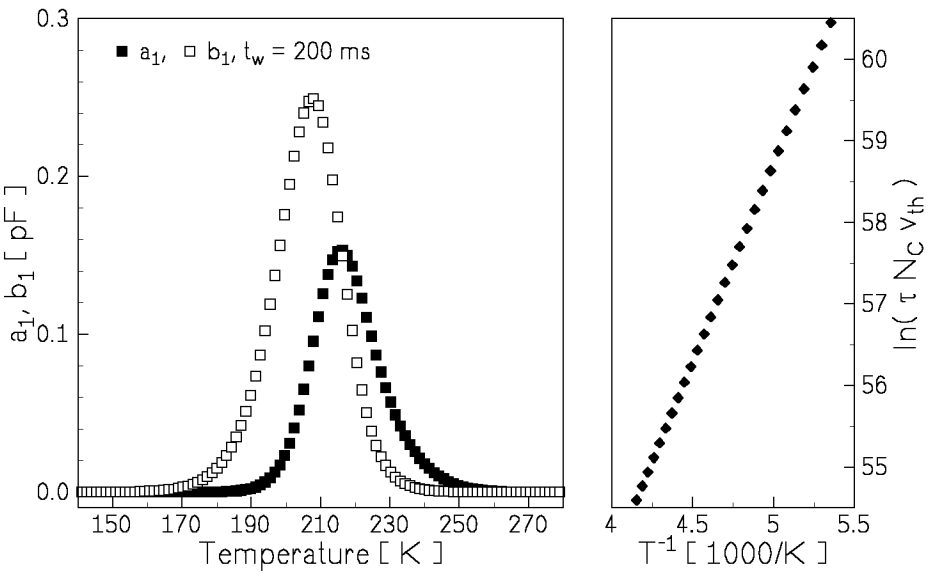

Figure 4.10: Direct analysis : 2 peaks occur due to 2 correlators applied to the transient recorded with 1 time window t_w. The data are the same as shown in fig. 4.9. But for each recorded transient a time constant can be calculated from eqs. 4.33 to 4.35. The number of points in the Arrhenius-plot is drastically increased although only 2 instead of 6 peaks were analysed.
(Simulation : $\Delta E_T = 0.42$ eV, $\sigma = 1.2{\cdot}10^{-15}$ cm^2)

The application of one of eqs. 4.33 to 4.35 will be called the *direct analysis*. An Arrhenius plot resulting from the direct analysis is shown in fig. 4.10. The data are the same as used for fig. 4.9. Although only a_1 and b_1 from the $t_w = 200$ ms - peak are analysed many more points are obtained for the Arrhenius-plot. The temperature range can be widened significantly if additionally different time windows are used as already proposed in the preceding section.

However, it is more consistent to use an optimum time window for each temperature. The optimum time window $t_{w,o}$ is given if the amplitude of the transient signal covers the full range of the ADC. [5] Because τ depends on the temperature, the time window has to be adjusted to changes in temperature. If the signal measured at temperature T is analysed immediately by the controlling computer, that is the determination of the time constant, the time constant expected at the following temperature $T + \Delta T$ can be calculated from eq. 4.18. [6] and thus also the optimum time window $t_{w,o}$. Measurements made in this mode are said to be made with a *variable time window* as opposed to those made with a *constant time window*. Since τ and t_w always have the same ratio no spectrum can be seen.

The superiority of the direct analysis based on the Fourier-coefficients over the analysis of maxima is given by the possibility of checking whether the measured transient obeys the assumed exponential law. Only if the relations eqs. 4.30 to 4.32

[5] For details see Weiss [85] p.55.

[6] After a few time constants are determined it is also possible to calculate the value of ΔE_T, but for the start of the procedure a value has to be set.

are fulfilled is the measured signal proven to be exponential. Non-exponential transients will be excluded from the direct analysis. The reason for a non-exponential behaviour is given if e.g. the transient signal is the sum of two exponential functions with a long and a short component or if the measurement has been disturbed.

Furthermore it is possible to analyse parts of the transient signal. If e.g. the first and the second half of an exponential signal are analysed independently the results of a Fourier analysis should be the same for both of them. But if the signal is a sum of two exponential functions, with a short and a long component, the results will differ indicating the presence of two levels.

4.2.3 Accuracy and Limits

The accuracy in determining the energy level ΔE_T, the cross section σ and the trap concentration n_T is limited due to the following objections. The analysis of ΔE_T and σ requires an exact temperature measurement. But the accuracy of the temperature measurement is already limited by the thermometer device (see sec. 5.4) and additionally experimental effects could cause further uncertainty. Hence the influence of an error in temperature on the determination of ΔE_T and σ shall be discussed briefly now, although the same consideration also yields for the TSC-method (see sec. 4.3) and the evaluation of activation energies from heat treatments (see sec. 4.4).

According to the Arrhenius-relation (eq. 4.20) ΔE_T is determined by the following expression :

$$\frac{d\ \ln(\tau N_{C,V} v_{th,e,h})}{d\,1/T} = \frac{\Delta E_T}{k_B}, \tag{4.36}$$

which is found if the temperature dependence of $(N_{C,V} v_{th,e,h})$ is neglected due to $(\ln(T^2) \approx \ln(T+\Delta T)^2)$. In case of a temperature shift ΔT between the true sample temperature T and the thermometer temperature T_{meas} the following expression has to be derived

$$\ln(\tau N_{C,V} v_{th,e,h}) = \ln\frac{1}{\sigma} + \frac{\Delta E_T}{k_B(T_{true}+\Delta T)}, \tag{4.37}$$

and one obtains

$$\frac{d\ \ln(\tau N_{C,V} v_{th,e,h})}{d\,1/T} = \frac{\Delta E_T}{k_B} + \frac{2\Delta E_T \Delta T}{k_B T} = \frac{\Delta E'_T}{k_B}. \tag{4.38}$$

Thus instead of ΔE_T a different energy

$$\Delta E'_T = \Delta E_T + \frac{2\Delta E_T}{T}\Delta T \tag{4.39}$$

results from the analysis. Eq. 4.39 shows that the deviation from the correct value of ΔE_T is proportional to ΔT. The error in σ can be approximated by

$$\frac{\sigma'}{\sigma} = \exp\left(\frac{\Delta E_T}{k_B T}\frac{\Delta T}{T}\right), \tag{4.40}$$

as it is shown in sec. 9, eqs. 9.1 to 9.5. From eq. 4.40 an expression corresponding to eq. 4.39 can be formed :

$$\ln\sigma' = \ln\sigma + \frac{\Delta E_T}{k_B T^2}\Delta T. \tag{4.41}$$

Note that the deviation from the correct value of σ also grows in proportion to ΔT. Thus σ' is correlated linearly with $\Delta E_T'$. If the measured temperature is higher than the sample temperature $\Delta E_T'$ and σ' will be overestimated, otherwise both parameters will be underestimated.

The determination of the energy level E_T can be affected also by the influence of the electric field [4], either by lowering the emission barrier (*Poole-Frenkel effect*) or by tunnelling. But none of these effects contributes significantly, since in most cases the electrical field is not stron enough.

The technique of DLTS has been introduced in sec. 4.2.1 in a very straightforward way in order to focus on the essentials. In the following a more detailed insight on the charge distribution during the emission process is given and the effect on the evaluation of the trap concentration is considered. The situation right after the filling pulse is shown in an energy band diagram (fig. 4.11).

Three regions with different charge concentrations exist. The first region is $0 < x < L_P$, wherein the energy levels are not filled, because during the filling pulse the depletion region was reduced to $L_P \neq 0$ by the filling voltage $V_f > 0$. The charge concentration in this range is N_{eff}. In the second region $L_P < x < L_R$ the energy levels are filled by the filling pulse. Because they are above the Fermi-level now, the trapped electrons will be detrapped into the conduction band and thus the charge concentration is $N_{eff} - n_T(t)$. In the transition region $L_R < x < W$ (see sec. 2.4) the energy levels can not change the charge state, because they are below the Fermi-level. The charge concentration is $N_{eff} - n_T$. The distance $W - L_R = \lambda$ can be found from the following equation [19] :

$$\lambda = \sqrt{\frac{2\epsilon_S}{q^2 n}(E_T - E_F)}. \tag{4.42}$$

Note that λ does not depend on an external voltage. From Poissons equation one gets the potential difference between 0 and W :

$$\Phi(W) - \Phi(0) = V = \frac{q_o}{2\epsilon_S}\Big(W^2(N_{eff} - n_T(t)) - 2W\lambda(n_{T,0} - n_T(t)) + \lambda^2(n_{T,0} - n_T(t)) + L_P^2 n_T(t)\Big) \tag{4.43}$$

which can be resolved to $W(V,t)$ [7] :

$$W(V,t) = \lambda\frac{n_{T,0} - n_T(t)}{N_{eff} - n_T(t)} \pm \sqrt{\lambda^2\frac{(n_{T,0} - n_T(t))^2}{(N_{eff} - n_T(t))^2} + \frac{\mathcal{X}}{(N_{eff} - n_T(t))}},$$
$$\text{with} \quad \mathcal{X} = \frac{2V\epsilon_S}{q_o} - \lambda^2(n_{T,0} - n_T(t)) - L_P^2 n_T(t). \tag{4.44}$$

The capacitance can be deduced now according to eq. 2.32 :

$$C = \frac{dQ}{dW}\frac{dW}{dV}. \tag{4.45}$$

[7] The built-in voltage is neglected here.

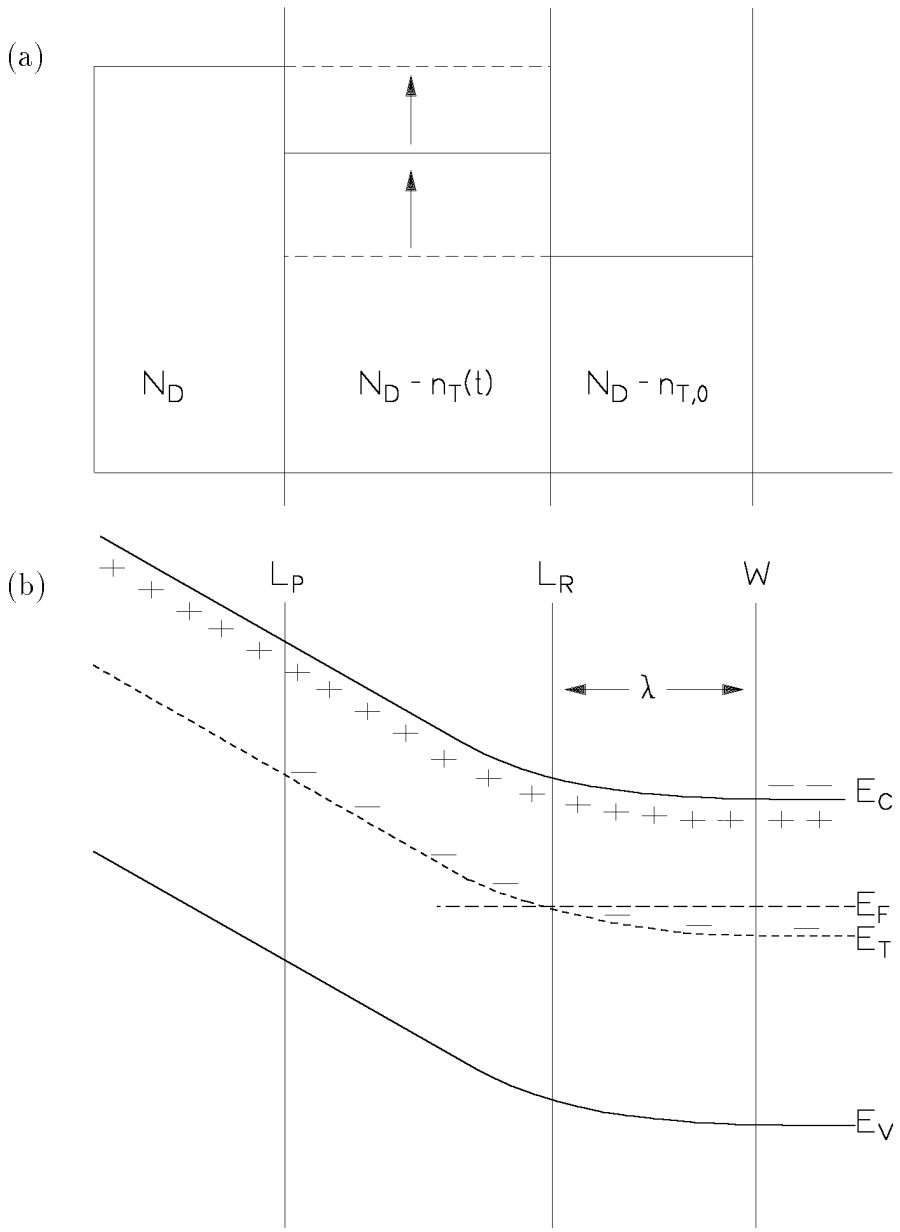

Figure 4.11: Charge distribution after the filling pulse.

It is

$$Q = qA\left(N_{eff}L_P + (N_{eff} - n_T(t))(W - \lambda - L_P) + (N_{eff} - n_{T,0})\lambda\right) \tag{4.46}$$

and hence

$$\frac{dQ}{dW} = qA(N_{eff} - n_T(t)). \tag{4.47}$$

Furthermore it is

$$\frac{dW}{dV} = \frac{\epsilon_S}{q_o(N_{eff} - n_T(t))}\sqrt{\frac{(N_{eff} - n_T(t))}{\lambda^2\frac{(n_{T,0} - n_T(t))^2}{(N_{eff} - n_T(t))} + \mathcal{X}}}. \tag{4.48}$$

In case of $\lambda = L_P = 0$ eq. 4.48 corresponds (as expected) to eq. 2.31. Finally the exact expression of the capacitance as function of time after the filling pulse is found to be :

$$C(t) = \epsilon_S A\sqrt{\frac{(N_{eff} - n_T(t))}{\lambda^2\frac{(n_{T,0} - n_T(t))^2}{(N_{eff} - n_T(t))} + 2V\frac{\epsilon_S}{q_o} - \lambda^2(n_{T,0} - n_T(t)) - L_P^2 n_T(t)}}. \tag{4.49}$$

From eq. 4.49 it is not evident if it is possible to approximate $C(t)$ the same way as in eq. 4.14, because not only the numerator but also the denominator depends on time. However, it can be shown (see sec. 9, eqs. 9.7 to 9.10) that the denominator in eq. 4.49 is dominated by $2V\frac{\epsilon_S}{q_o}$ and hence the change of the capacitance after the filling pulse can still be described by an exponential function as long as $N_{eff} \gg n_{T,0}$.

The question remains as to how the determination of the trap concentration is concerned if $\lambda \neq 0$ and $L_P \neq 0$. $n_{T,0}$ depends on the ratio $\Delta C/C_E$ (see eq. 4.21) and ΔC is defined as $C_E - C_0$, (C_0=$C(t = 0)$). From eq. 4.49 one can obtain both C_0 and C_E. If $t = 0$ it is $n_T(t) = n_{T,0}$ and it follows :

$$C_0 = \epsilon_S A\sqrt{\frac{(N_{eff} - n_{T,0})}{2V\frac{\epsilon_S}{q_o} - L_P^2 n_{T,0}}}. \tag{4.50}$$

If $t \to \infty$ it is $n_T(t) = 0$ and hence :

$$C_E = \epsilon_S A\sqrt{\frac{N_{eff}}{2V\frac{\epsilon_S}{q_o} + \lambda^2 n_{T,0}(\frac{n_{T,0}}{N_{eff}} - 1)}}. \tag{4.51}$$

Note that due to the presence of deep levels C_E is no longer given by the simple expression of eq. 2.32. The difference $C_E - C_0$ can be approximated (see sec. 9, eqs. 9.11 to 9.16) by :

$$\Delta C = \frac{\epsilon_S A}{W}\frac{n_{T,0}}{2N_{eff}}\frac{W^2 + \lambda^2 - L_P^2}{W^2}, \tag{4.52}$$

where W is the width of the SCR corresponding to C_E and $t \to \infty$. Thus the exact expression for the trap concentration according to eq. 4.21 is the following :

$$n_{T,0} = 2\frac{W}{\epsilon_S A}N_{eff}\frac{W^2}{W^2 + \lambda^2 - L_P^2}. \tag{4.53}$$

In order to estimate the minimum trap concentration which can be detected, it is reasonable to apply eq. 4.21 again. Due to the resolution of the capacitance bridge ($C_{res} \approx 0.1$ fF, see sec. 5.3) the minimum value of ΔC_0 should be about 5 fF. Typical values of C_E are about 20 pF in the case of high resistivity material ($N_{eff} > 5{\cdot}10^{11}$ cm^{-3}). Using eq. 4.21 it follows that the smallest value of trap concentration is $n_T \approx 2{\cdot}10^8$ cm^{-3}. The smallest ratio N_T/N_{eff} is in the range of some 10^{-4} .

4.3 Thermally Stimulated Current (TSC)

Already in 1972 the TSC-method has been used by Buehler to determine the emission parameters and concentration of impurity centres [87]. The theory and parts of the sections about the analysis of TSC-measurements, (sec. 4.3.2.1, method of delayed heating and sec. 4.3.2.4, variation of the heating rate) follow this paper.

For a TSC-measurement, the sample is cooled to a low temperature at which the energy levels are filled by applying a forward voltage which leads to a current injection.

After the filling pulse, a reverse bias is applied and instead of keeping the temperature constant as in the DLTS-method, the sample is heated and the emission of charge carriers is measured as function of temperature. Also, in contrast to the DLTS-method, TSC is not restricted to a small N_T/N_{eff} ratio, because the technique of TSC directly measures the emitted charges, and a minimum of free charges to measure the capacitance as required for C-DLTS is not necessary. It is shown in the following that the TSC-signal will be even more pronounced in case of high defect concentration.

4.3.1 Basic Equations and Determination of Trap Concentration

The thermally stimulated current consists of two parts, namely the emission current I_{emis} and the displacement current I_{disp} :

$$I_{TSC} = I_{disp} + I_{emis}. \tag{4.54}$$

The emission current can be written as product of the volume of the SCR and change of occupied traps :

$$I_{emis} = -qAW\frac{dn_T}{dt}. \tag{4.55}$$

The displacement current which occurs due to change of charge in the SCR is given by

$$I_{disp} = A\epsilon_S\frac{d\mathcal{E}}{dt}. \tag{4.56}$$

Applying $V > V_{fd}$ and using eqs. 2.61 and 2.26 the electrical field can be written as :

$$\mathcal{E}(x) = \frac{V}{d} + \frac{q_o(N_{eff} - n_T)}{2\epsilon_S}(d - 2x). \tag{4.57}$$