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Deep-Level Transient-Spectroscopy for Localized States at Extended Defects in Semiconductors

H. Hedemann (*) and W. Schröter

Universität Göttingen, IV. Physikalisches Institut, Bunsenstraße 13, 37073 Göttingen, Germany

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(superlattices, quantum well structures and multilayers)

Abstract. — We prove that for localized states at extended defects the high-temperature sides of deep-level transient spectra can be written as a product of an amplitude function depending on the pulse length and a shape function depending on temperature. By this property localized states can be distinguished experimentally from bandlike states. Simulations of deep level transient spectra for localized and bandlike states using the same density of states function and parameter values illustrate the differences and show the failures of conventional analysis in both cases.

1. Introduction

Spatially extended defects in silicon like dislocations, grain boundaries, or precipitates are generally associated with a distribution of electronic states, \( N_D(E) \), which can be roughly classified according to their origin into three groups: (1) bandlike states which are split off from the valence and conduction band by the action of the long-range strain field of the defect, (2) bandlike states originating from the internal and interfacial bond structure of the defect, and (3) localized states resulting from the interaction of the defect with point defects or from local imperfections of its core structure.

While shallow states at extended defects can be described with conventional theoretical methods [1, 2], the interplay between atomic and bond structure and the electron-electron-correlation at extended defects are still limits for a quantitative theoretical evaluation of their deep bandlike states. Experimentally shallow states give rise to various low-temperature effects like photoluminescence, optical absorption, double spin resonance, microwave conductivity, and electric dipole spin resonance [3], but have no significant effect on the room-temperature properties in silicon.

Deep electronic states at extended defects, especially at dislocations and metal silicide particles are known to have strong effects on bulk properties like mobility [4] and lifetime [5, 6], and to create detrimental effects in microelectronic and solar cell technology [7]. To understand these effects, numerous investigations have been performed, but have brought forth data, which could not be analyzed and interpreted unambiguously. One main difficulty is the appropriate

(*) Author for correspondence (e-mail: hedemann@physik4.gwdg.de)

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consideration of electrostatic effects on the distribution of levels with their occupation. Thus the determination of origin and distribution of deep-lying states at extended defects remained an open problem of semiconductor physics for about forty years [8].

Using Deep Level Transient Spectroscopic (DLTS) data of 60°-dislocations and of small NiSi2-platelets and simulation of DLTS, it has been shown recently, that deep electronic states at extended defects can be classified as bandlike or localized, when electron equilibration at the defect is taken into account [9].

Furthermore it has been demonstrated using DLTS-data of NiSi2-platelets and simulation of DLTS, that the parameters of a given bandlike density of states, its occupation in the neutral state, the occupation-dependent capture barrier, which is built up by long-range electrostatic fields, and the capture cross section may be obtained from the fitting of the rate equation for fast internal equilibration to the DLTS-data [10].

To distinguish bandlike and localized states at extended defects, the internal equilibration time $\Gamma_\text{i}$ associated with the extended defect has to be compared with the inverse carrier emission rate, $R_\text{e}^{-1}$, and the inverse carrier capture rate, $R_\text{c}^{-1}$, of the defect (Fig. 1, [9]). The case, that $\Gamma_\text{i}$ is the smaller time, should hold for bandlike states, which are extended at the defect, while the case, that $\Gamma_\text{i}$ is the larger time, should hold for localized states of point defect clouds. The distinction between bandlike and localized states can be made from the qualitative features of the DLT-spectra. For bandlike states, it has been proven that the high-temperature sides of DLTS-lines are mainly independent of the filling pulse length $t_\text{p}$ [10] (cf. Fig. 2a). On the other hand, simulations performed for localized states introduced by dense point defect clouds in the vicinity of a dislocation suggested, that the high-T-sides of DLTS-lines with different $t_\text{p}$ coincide after normalization with respect to their maxima [9]. Similar results have been obtained for simulations considering other distributions of energy levels [11].

In this paper we describe in more detail DLTS on extended defects with localized electronic states. We show that the high-T-sides of DLTS-lines of localized states can be written as a product of an amplitude function depending on the filling pulse length $t_\text{p}$ and a shape function depending on temperature. As a fingerprint for localized states we therefore conclude that the high-T-sides of DLTS-lines in general coincide after normalizing with respect to any point of the high-T-side, e.g. the maximum of the lines (cf. Fig. 2b). A direct comparison of simulations for bandlike and localized states using the same defect parameters demonstrate the differences between the models and the failures of conventional analysis (Arrhenius-plots) of extended defects for both models.
Fig. 2 — Simulated DLTS spectra for bandlike states (a) and for localized states (b) at an extended defect with varying filling pulse length $t_p$ from $10^{-6}$ s to $10^{-3}$ s; for further parameters see Table I.

2. High-T-Sides of DLTS for Localized States

We summarize the model for localized states as proposed previously [9]. The rate equations for localized states represent a system of coupled differential equations for the occupation probabilities $f_E$ of the defect state at energy $E$:

$$\frac{df_E}{dt} = c_n n e^{-\frac{E_E}{kT}} (1 - f_E) - e_E f_E$$

(1)

with the density of free electrons $n$, the capture coefficient $c_n := \langle v_{th} \rangle \sigma_n$ given as the product of the average thermal velocity of electrons $\langle v_{th} \rangle$ and the capture cross section $\sigma_n$. The emission
rate $e_E$ of the level with energy $E$ is determined through the principle of detailed balance. The system (1) is coupled if there is a capture barrier $\delta E_c$ depending on the occupation $F(t)$ of the defect as a whole. This total occupation is related to the values of $f_E$ via

$$ F(t) = \sum_E \rho_E f_E; \quad \sum_E \rho_E = 1, \quad (2) $$

where $\rho_E$ is the normalized weight of the $E$-th state according to the distribution of levels.

As an example, we consider a dense point defect cloud of donor-type and charge exchange with the conduction band. We assume $\delta E_c$ to be proportional to the total occupation, $\delta E_c = \alpha F$, with the capture barrier coefficient $\alpha$. The capture barrier representing a contribution to the total enthalpy of the defect should not be confused with the activation energy for point defects, whose occupation is coupled to a lattice relaxation. Unlike this activation energy, $\delta E_c$ does not influence the emission rates $e_E$.

It has been demonstrated by simulations for point defect clouds surrounding edge-type dislocations [9] that the high-T sides of DLTS-spectra for different $t_p$ coincide after normalization with respect to the line maxima. We have obtained the same behaviour e.g. in the simulations presented in Figure 2b. In what follows we will explain why this effect in general holds for localized states.

We note, that DLTS-lines of different $t_p$ coincide after normalization with respect e.g. to the line maxima, if the signal can be written as

$$ \Delta C = A(t_p)S(T), \quad (3) $$

with an amplitude function $A(t_p)$ independent of the temperature $T$ and a shape function $S(T)$ independent of the pulse length $t_p$. The trivial case of a completely filled defect, where the DLTS-signal does not depend on $t_p$ at all, will be excluded in our further considerations.

Let us now examine the ionization kinetics during the emission phase in more detail. Unlike for a simple point defect the transients for extended defects are non-exponential. While for bandlike states the emission process of different levels contributing to the defect is never independent due to internal charge exchange [10], for localized states, the only coupling of the ionization kinetics stems from the common capture barrier. Therefore, during the emission phase and in the space charge region, where no free carriers are available, the emission of the states is independent, and (neglecting effects of the Debye-tail) the occupation can be written as

$$ t \in [t_p, t_e]: \quad F(t) = \sum_E f_E(t_p)\rho_E e^{-e_E(t-t_p)}, \quad (4) $$

where the sum runs over the distribution of states. Based on this expression, the concept of “rate windows” in DLTS-measurements, developed for exponential transients, remains valid. The experimentally given repetition frequency $t_e^{-1}$ and correlation mode define an interval of rates $R$, the rate window, such that the DLTS-signal arises only from a subset of levels with emission rates falling in this window. Therefore, we write (4) as

$$ t \in [t_p, t_e]: \quad F(t) = \sum_{E: e_E \in R} f_E(t_p)\rho_E e^{-e_E(t-t_p)} + r(t; t_p, T), \quad (5) $$

where $E: e_E \in R$ denotes the summation over energies such that the corresponding emission rates enter the rate window. The function $r(t; t_p, T)$ does not influence the DLTS-signal. The subset of levels entering the rate window strongly depends on temperature. At the high-T side of the DLTS-line the subset consists of the deeper part of the distribution of states. As a
consequence, at the end of the emission phase all states in the space charge region are empty at the high-T side of the lines. For periodic conditions, this means that the initial values $f_E(0)$ of the capture phase approach zero.

Now we have to consider the ionization kinetics during the capture phase, where capture takes place. In general, emission during the pulse phase plays a role in the capture kinetics. For states falling in the rate window, however, $e_E t_e \sim 1$ within one to two orders of magnitude holds. For a typical DLTS experiment the pulse length $t_p$ is some orders of magnitude lower than $t_e$, hence we have $e_n t_p \sim t_p/t_e \ll 1$, such that emission of these states during the capture phase is negligible. In other words, the capture kinetics of states in the rate window does not depend on the level anymore:

$$E : e_E \in R : \frac{df_E}{dt} = c_n n e^{-\frac{\alpha E(t)}{kT}}(1 - f_E),$$

and $f_E(t_p) = f_R(t_p)$ is independent of $E$ [12].

Using this result, (5) writes

$$t \in [t_p, t_e] : F(t) = f_R(t_p) \sum_{E \in E_R} \rho_{EE} e^{-\frac{\epsilon E(t-t_p)}{kT}} + r(t; t_p, T),$$

such that the part of the transient influencing the DLTS - signal factorizes in a part with only slight T-dependence ($f_R(t_p)$) and a part with only slight $t_p$-dependence, as long as we have $t_e \gg t_p$ and $f_R(0) = 0$. The last condition and therefore (3) holds for the high-T side, which had to be shown.

The proof given here is based on the properties of the spectral distribution of the occupation probabilities at the end of the filling pulse, $f_E(t_p)$, and on the rate window concept. Figure 3 shows a typical example of the function $f_E(t_p)$ obtained for a point in the middle of the space charge region. We derived the factorization (7) using the assumptions $t_e \gg t_p$ and $f_E(0) = 0$, valid for the high-T sides of typical DLTS-lines. Within Figure 3 this corresponds to the idea, that the states entering the rate window for higher temperatures are states of the middle region (II), where $f_E(t_p)$ does not depend on $E$.

3. DLTS – Simulations for Bandlike and Localized States: Conventional Analysis

Within DLTS experiments, simple point defects are known to provide exponential transients. The emission rate at the temperature of the line maximum is therefore proportional to the pulse repetition frequency, and the electronic parameters (ionization enthalpy $\Delta H$, capture cross section $\sigma^*$ including the entropy factor) are conventionally obtained from a linear regression of Arrhenius-plots of the $T^2$-corrected emission rates $e_n/T^2$. There have been many attempts in literature to apply this conventional analysis also in the case of defects with non-exponential transients (e.g. [13-16]). Omling et al. [13] considered an assembly of isolated point defects with a Gaussian shaped distribution of levels. They could explain symmetrically broadened DLTS lines and stated that the ionization enthalpy obtained from the conventional analysis of the line maxima for different pulse repetition frequencies refers to the mean level of the distribution. For extended defects, however, a common capture barrier occurs which is not included in the model of Omling. Our proposed model for localized states at extended defects can be seen as a direct extension of the model of Omling including a capture barrier. Experimentally, from the application of the conventional analysis on extended defects a broad variety of values for the ionization enthalpy were obtained. An example is the dislocation related so-called C-line observed in plastically deformed n-type silicon [14,16], which has been analyzed to be due to localized states [9].
Fig. 3. — Occupation probabilities at the end of the capture phase, \(f_E(t_p)\), and at the end of the emission phase, \(f_E(t_e)\), for the DLTS-line with \(t_p = 10^{-5}\) s from Figure 2b at \(T = 240\) K and a point in the middle of the space charge region. Note, that the abscissa \(\log(e_E t_e)\) (emission-rate/pulse repetition frequency) is proportional to energy of the states: \(\log(e_E t_e) \sim -(E_F - E)/kT\). We distinguish three regions: (I) For the deepest states, the emission is not sufficient to empty the states during the emission phase. The initial values \(f_E(t_e) = f_E(0)\) and therefore \(f_E(t_p)\) increase with falling E (falling \(e_E\)). (II) The emission is strong enough as to empty the states completely during the emission phase, \(f_E(0) = 0\). The capture kinetics of the states does not depend on E, \(f_E(t_p) = \) const. (III) For shallow states emission during the capture phase takes place \(f_E(t_p)\) decreases with E. The rate window (centre indicated with arrow) is generally located in the regions (I) and (II). For higher temperatures, even the deepest states are emptied during the emission phase, and the region (I) vanishes. This means, that the initial values \(f_E(t_p) := f_R(t_p)\) for states in the rate window \(R\) are independent of E for high temperatures. In this regime, the transients factorize in an amplitude function depending on the pulse length \(\nu a f_R(t_p)\) and a shape function depending on the temperature (see text).

We will demonstrate how a conventional analysis would work on extended defects caused by bandlike and localized states.

Since a closed solution for the differential equation (I) is not at hand, the rate equations have to be treated numerically to simulate the DLTS-experiment [17]. The values of the parameters and the density of state function have been chosen equal for bandlike and localized states (see Tab. I).

For the simulations we assumed \(N_0 \gg N_D|F(t_p)|\) with \(N_0\), \(N_D\) being the concentrations of the shallow dopant and the deep levels, respectively. This condition has been checked to hold for our simulations. A full integration over the space charge region including the Debye-tails has been performed [18], and we solved the rate equations with periodic conditions for the transients, i.e. the values of the vector \(f_E(t = 0)\) at the begin of the capture phase have been chosen to be the values at the end of the emission phase, \(f_E(t_e)\).

For bandlike states (Fig. 2a), the high-T sides of the lines coincide, and the maximum temperatures of the lines decrease with increasing \(t_p\). It has been stated already, that these properties are typical for DLT spectra of bandlike states [9,10]. Figure 2b shows the results for localized states. It turns out, that the high-T sides of the spectra coincide after normalizing them with respect to the maxima (see Fig. 2b, insert, and Sect. 2). Compared to the spectra for bandlike states (Fig. 2a), there is only a very slight change in the temperatures of the maxima with different \(t_p\). These two properties are characteristic for localized states.
Table I. — *Parameter values used for simulations.*

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>material</td>
<td>n-type Si</td>
</tr>
<tr>
<td>doping level $N_0$</td>
<td>$10^{16}$ cm$^{-3}$</td>
</tr>
<tr>
<td>capacitance meas.</td>
<td></td>
</tr>
<tr>
<td>correlation</td>
<td></td>
</tr>
<tr>
<td>bias voltage</td>
<td>$-4.0$ V</td>
</tr>
<tr>
<td>pulse voltage</td>
<td>$0.0$ V</td>
</tr>
<tr>
<td>gate time</td>
<td>$1 \times 10^{-4}$ s</td>
</tr>
<tr>
<td>pulse repetition frequency</td>
<td>$17$ s$^{-1}$</td>
</tr>
<tr>
<td>output</td>
<td>$\Delta C/C_0$</td>
</tr>
<tr>
<td>density of states</td>
<td>box-like</td>
</tr>
<tr>
<td>capture barrier coefficient $\alpha$</td>
<td>$0.60$ eV</td>
</tr>
<tr>
<td>upper level enthalpy $\Delta H_2$</td>
<td>$0.20$ eV</td>
</tr>
<tr>
<td>lower level enthalpy $\Delta H_1$</td>
<td>$0.50$ eV</td>
</tr>
<tr>
<td>capture cross section $\sigma$</td>
<td>$5.0 \times 10^{-16}$ cm$^2$</td>
</tr>
<tr>
<td>ionization entropy</td>
<td>$0.0$</td>
</tr>
<tr>
<td>number of states $N_D$</td>
<td>$10^{15}$ cm$^{-3}$</td>
</tr>
<tr>
<td>neutral occupation $F^{(N)}$</td>
<td>$0.0$</td>
</tr>
</tbody>
</table>

Table II. — *Apparent values of emission enthalpies $\Delta H$ and capture cross sections $\sigma^*$ (including the entropy factor), dependent on filling pulse length $t_p$, as obtained from simulations and conventional analysis. The points do not precisely form a line in an Arrhenius-plot. The errors given here are an effect of this curvature.*

<table>
<thead>
<tr>
<th>$t_p$ [s]</th>
<th>$\Delta H$ [eV]</th>
<th>$\sigma^*$ [10$^{-16}$ cm$^2$]</th>
<th>$\Delta H$ [eV]</th>
<th>$\sigma^*$ [10$^{-16}$ cm$^2$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^{-6}$</td>
<td>$0.492 \pm 0.003$</td>
<td>$120 \pm 30$</td>
<td>$0.475 \pm 0.003$</td>
<td>$15 \pm 2$</td>
</tr>
<tr>
<td>$10^{-5}$</td>
<td>$0.506 \pm 0.006$</td>
<td>$380 \pm 150$</td>
<td>$0.473 \pm 0.003$</td>
<td>$13 \pm 2$</td>
</tr>
<tr>
<td>$10^{-4}$</td>
<td>$0.534 \pm 0.005$</td>
<td>$2900 \pm 1000$</td>
<td>$0.520 \pm 0.010$</td>
<td>$150 \pm 80$</td>
</tr>
<tr>
<td>$5 \times 10^{-4}$</td>
<td>$0.465 \pm 0.010$</td>
<td>$120 \pm 100$</td>
<td>$0.610 \pm 0.020$</td>
<td>$13000 \pm 10000$</td>
</tr>
<tr>
<td>$10^{-3}$</td>
<td>$0.409 \pm 0.010$</td>
<td>$6.7 \pm 0.4$</td>
<td>$0.540 \pm 0.020$</td>
<td>$500 \pm 500$</td>
</tr>
</tbody>
</table>

The results of a conventional analysis of the spectra for bandlike states are given in Figure 4a and Table II. The choice of pulse repetition frequencies is typical for a practical experiment. As can be seen, the Arrhenius-plots for different $t_p$ differ significantly. While in the region of lower $t_p$ the main effect is a shift of the lines, for higher $t_p$ also the slope changes strongly. Similar results have been obtained experimentally by Grillot et al. [19]. The simulated Arrhenius-plots showed slight curvatures, which have been used to calculate the errors in Table II. However, the curvature would hardly be detectable in a real experiment.

For localized states (Fig. 4b, Tab. II) there is a shift of the lines for small $t_p$ in the reverse direction than for bandlike states. Both parameters, the apparent ionization enthalpy and the
apparent capture cross section, change non-monotonically. The apparent activation energies even exceed the limits of the original distribution. Figure 5 summarizes the results for the apparent ionization enthalpies.

In general, it can be seen that the use of Arrhenius-plots is only of limited use for extended defects. They may be seen as a possibility of a condensed presentation of DLT-spectra for different pulse repetition frequencies, provided that all parameters of the measurement including the pulse length are given, but the interpretation of the obtained parameters is far from clear. For bandlike states, the defect parameters can be determined via fitting of experimental
Fig. 5 — Apparent ionization enthalpies from Arrhenius plots of simulated DLT spectra for localized and bandlike states as a function of the filling pulse length $t_p$. For the parameter values of the simulations see Table I, for the results presented here see also Table II.

DLTS-data [10]. We will demonstrate in a forthcoming paper, that it is also possible to fit parameter values to DLTS-spectra in the case of localized states.

4. Summary

We have examined the implications of a model for localized states at extended defects on DLT spectra. It has been shown that within this model the high-T-sides of DLTS lines for different pulse length coincide after normalization with respect to a point of the high-T-side, e.g. the maxima of the lines. This result holds for any distribution of levels which make up an extended defect and can be seen as a criterion to distinguish localized states from bandlike states.

The results of a conventional analysis applied on simulated DLT spectra for extended defects have been shown. It has been demonstrated for both bandlike and localized states, that the apparent values of parameters obtained from this analysis depend on the pulse length and can not be simply ascribed to some 'average' values for the distribution of levels. Therefore, the presentation of Arrhenius-plots for extended defects should be seen only as a condensed presentation of experimental data, provided that the parameters of the measurement, namely the pulse length, are reported.

Acknowledgments

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Dedicated to the memory of Prof. Dr. Peter Haasen.
References

[12] (6) does not imply that the emission during the capture phase is completely neglected, since the capture barrier \( \alpha F(t) \) depends also on the shallow states of the distribution which might emit strongly during the capture phase. The point here is that \( F(t) \) is common to all states, i.e. it does not depend on \( E \). In other words, (6) says that emission during the capture phase affects all states entering the rate window in the same way.