

Interpretation of lifetime and defect spectroscopy measurements by generalized rate equations

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Abstract We introduce a new approach for modeling the dynamics of charge carrier interactions with defects in semiconductors starting from nearly first principles. A system of generalized rate equations was developed whose numerical solutions account for many details of experimental results also in the case of complex defect models. The theoretical model is neither restricted by the number nor by the type of defects under consideration. Details of simulations are presented for different experimental results. The influence of traps on lifetime measurements with different experimental methods is analyzed in detail and the Application to determine iron concentrations from lifetime measurements are shown.

1 Introduction

In the last years, lifetime measurements are well established as a sensitive and easy to use method for investigations of defects in semiconductors. The most commonly used methods for contact-less and non-destructive measurement of the minority carrier lifetime are QSSPC (Quasi Steady State Photo Conductivity), μ -PCD (Microwave detected Photo Conductance Decay) and the new developed MDP (Microwave Detected Photoconductivity) [1]. The outstanding sensitivity of the MDP method enables the time

dependent detection of photoconductivity signals in a large injection range ($\Delta n = 10^{11} \dots 10^{17} \text{ cm}^{-3}$) [2]. In nearly all cases the interpretation of lifetime measurements is based on the well-known Shockley-Read-Hall (SRH) model in its various forms or on rather simple trapping models [3–5]. Due to the simplifications inherent with these models, they are of limited value for applications in more complex defect situations as usually found in most practical cases [6]. One of the strongest restrictions of the SRH model arises by neglecting trapping effects. The MD-PICTS (Microwave Detected Photo Induced Current Transient Spectroscopy) method uses such trapping effects to obtain DLTS Deep Level Transient Spectroscopy-like defect spectra from the temperature dependent measurement of the photoconductivity. The classical PICTS theory [7] is derived under the assumption of a constant and very short minority carrier lifetime τ . Moreover the lifetime has to be independent from trap occupation and re-emission of trapped carriers into the band. These prerequisites are clearly not fulfilled in defect-rich material like solar grade mc-Si.

In the following a possible way is shown for describing both injection dependent lifetime (IDL) and (MD)-PICTS measurements using one defect model.

2 Theory

In our approach we use a generalized rate equation system (RES) which describes carrier dynamics in the bands and defect states of a semiconductor using as few simplifications as possible. Fig. 1 shows all principal transitions of a simple single-defect model. Every possible transition of a charge carrier (electron) between two energy levels (or the bands) is modeled by an appropriate transition rate. The terms of the transition rates are written in the most general

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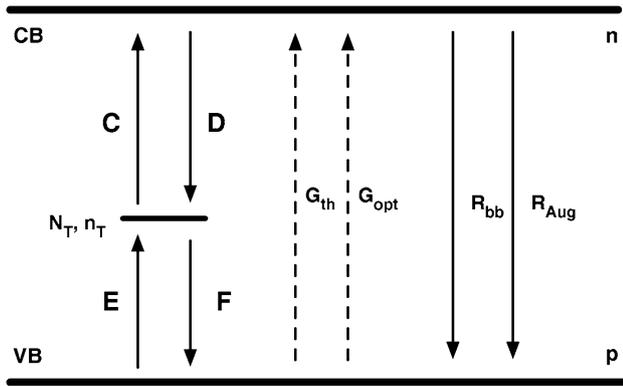


Fig. 1 Schematic diagram of a defect level in the band gap of a semiconductor. All relevant processes for the RES are marked by arrows (details see text)

form $N_s^c \times r \times N_t^p$ (N_s^c := source level electron concentration, r := transition parameter, N_t^p := concentration of free places at target level). The complete RES for the simple defect model in Fig. 1 is:

$$\dot{n} = G_{th} + G_{opt} - R_{bb} - R_{Aug} + C - D \quad (1)$$

$$\dot{p} = G_{th} + G_{opt} - R_{bb} - R_{Aug} + F - E \quad (2)$$

$$\dot{n}_T = E - F - C + D. \quad (3)$$

We take into account optical (G_{opt}) and thermal (G_{th}) band-band generation as well as direct band-band and Auger recombination (R_{bb} , R_{Aug}). All defects (recombination centers, traps, donors, acceptors) are treated as a general defect whose microscopic properties (energy, capture cross sections, concentration, charge state) determine its role in the RES. It should be noted that no lifetime parameter is present in the RES. Individual thermal rates have the usual form (e.g. for defect-CB interaction):

$$C = n_T(t) \sigma_n v_n \exp(-[E_C - E_T]/kT) [N_C - n(t)] \quad (4)$$

$$D = n(t) \sigma_n v_n [N_T - n_T(t)]. \quad (5)$$

Other terms are equivalent. Every additional defect in the model leads to one additional equation and four extra terms in \dot{n} and \dot{p} . The RES is solved numerically for pulse (illumination, $G_{opt} > 0$) and the transient decay (dark $G_{opt} = 0$) using an adaptive-step-size routine. As results the electron and hole concentrations within the bands and the (time dependent) occupation of *all* defect levels are obtained. In all common lifetime measurement methods the photo conductivity $\Delta\sigma(t)$ is measured and not e.g. $n(t)$ that why $\Delta\sigma(t) = e(\Delta n(t)\mu_n + \Delta p(t)\mu_p)$ is calculated. Therefore we use the excess electron and hole concentrations from the RES solution and an appropriate mobility model [8]. Afterwards we apply the usual evaluation techniques (linear regression, $1/e$ lifetime, two-gate-technique) to $\Delta\sigma(t)$ for obtaining lifetime values or (MD)-PICTS spectra.

3 Applications

In Fig. 2 the minority carrier lifetime τ_{eff} calculated using $\Delta\sigma(t)$ for a simple defect model (M1) containing only one RC (Fe-interstitial) is shown. In this simple case the results of our simulation agree exactly with the SRH theory. Like expected the influence of Auger recombination at high injection levels is modeled correctly. The results of a more complex defect model (M2) are shown in Fig. 3. Additional to the RC from M1 a pure electron trap was added. The same data evaluation as for the M1 simulation was performed. The additional electron trap leads to an apparent higher τ_{eff} at low injections (see Fig. 3a), whereas the trap has no effect at high injection levels. The low injection results agree well with the trapping model proposed in [9]. In contrast to the model in [9] we are able to calculate the lifetime over the whole injection range. Auxiliary we obtained the (MD)-PICTS spectra for model M2 by applying the well known two-gate-technique to the defect part of the calculated conductivity signals. Different trap concentrations results in the MD-PICTS spectra which are shown in Fig. 3b.

Another distinctive feature of the presented simulation system is the possibility of a detailed analysis of the different measurement techniques. The main difference between QSSPC and MDP on the one hand and μ -PCD on the other hand are the illumination conditions. QSSPC and MDP use illumination times long enough to achieve true steady state conditions whereas μ -PCD uses a very short

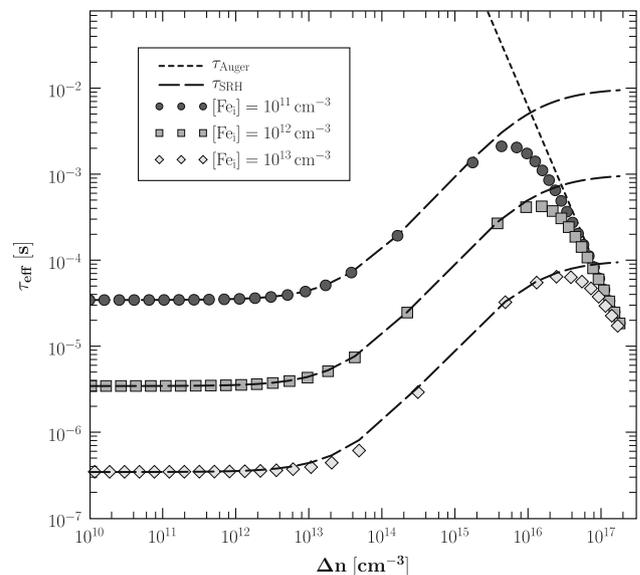


Fig. 2 Simulation results (symbols) of model M1 (one RC, Fe) compared to SRH and Auger lifetime calculations of the same model. Simulation parameters were typical for MDP measurements (p-Si, $T = 273$ K, $N_A = 1 \times 10^{16}$ cm $^{-3}$, Photopulse = 10 ms, Transient = 30 ms)

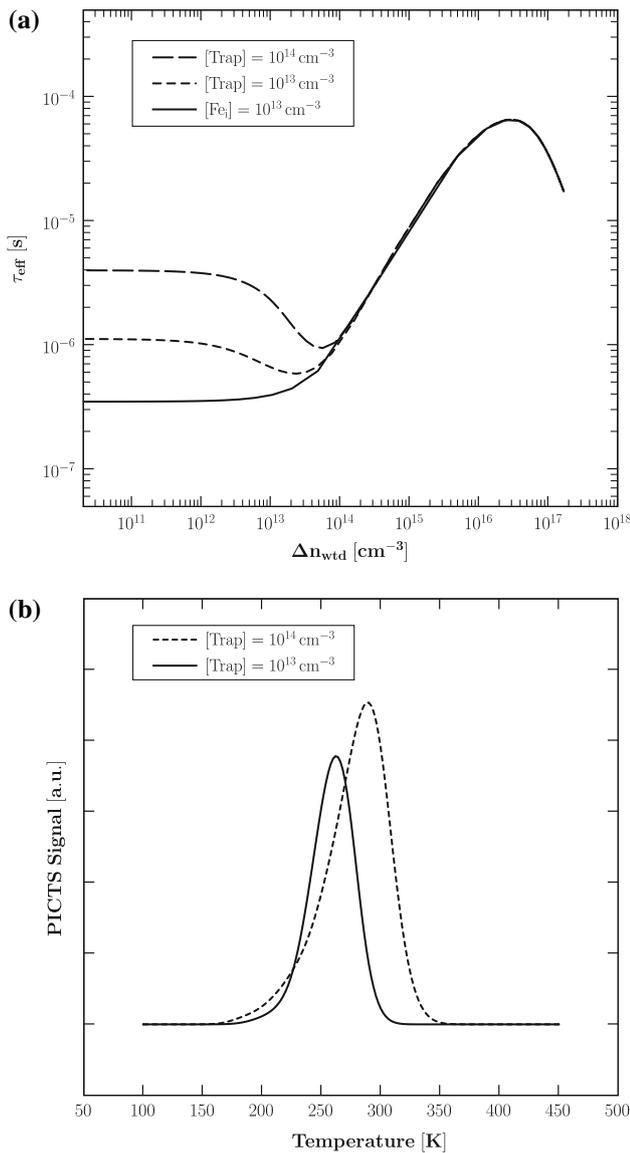


Fig. 3 Simulation results for model M2 (p-Si, $T = 273 \text{ K}$, $N_A = 1 \times 10^{16} \text{ cm}^{-3}$) having different electron trap concentrations. Trap parameters: $E_C - E_T = 0.4 \text{ eV}$, $\sigma_n = 10^{-16} \text{ cm}^2$. **(a)** Measured lifetime as function of injection for different trap concentrations (steady state illumination). **(b)** (MD)-PICTS spectra calculated by two-gate technique from model M2

(200 ns) and intense light flash. Figure 4a shows a comparison of injection dependent lifetimes calculated for typical MDP and μ -PCD illumination conditions using model M2. If there are no traps present ($N_t = 0 \text{ cm}^{-3}$) we expect both methods to measure the same values for the minority carrier lifetime τ_n . However, if the trap concentration increases, the μ -PCD method measures a decreased lifetime over nearly the complete injection range. As like we have seen before, the MDP (or QSSPC) method measures an apparent higher lifetime with increasing trap concentrations at low injections. The analysis of the time

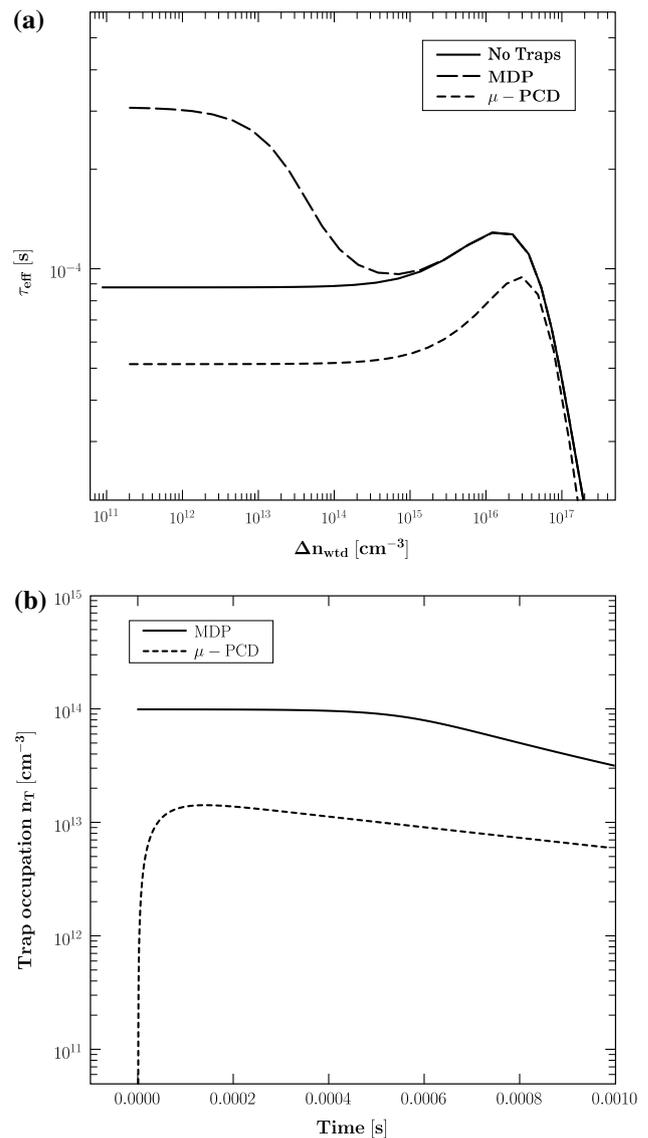


Fig. 4 Comparison of calculated injection dependence of the lifetime for **(a)** MDP (or QSSPC) illumination conditions and for typical μ -PCD illumination (200 ns flash). In any case $\sigma(t)$ was used to obtain the lifetime from the simulation data. **(b)** Calculated time dependence of the concentration of trapped electrons. Light is switched off at $t = 0 \text{ s}$

dependence of the trap occupation for both measurement conditions explains this behavior (see Fig. 4). Whereas MDP conditions leads to a monotonic decreasing concentration of trapped electrons after the light is switched off ($t = 0 \text{ s}$), the short light flash of the μ -PCD method induces the filling of trap states after the light pulse (at least for a short period of time). The additional flow of electrons into the trap state decreases the measured effective lifetime. The MDP method has to deal with the opposite effect. Thermal reemission of trapped electrons increases the measured lifetime. Furthermore it should be noted, that

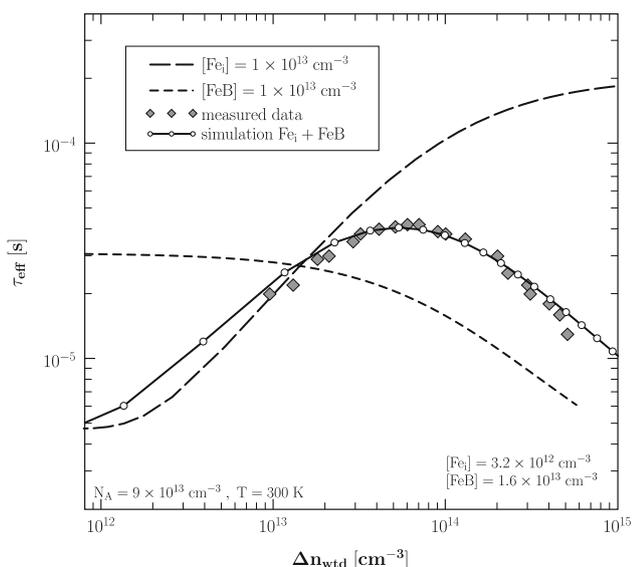


Fig. 5 QSSPC lifetime data (closed symbols) and the results of a fit with a FeB and Fe-interstitial as RC's (solid curve). Also shown are the lifetime curves calculated for either FeB or Fe-interstitial (dashed lines)

μ -PCD illumination is not able to fill up the trap states with electrons. The maximum trap occupation is approximately one order of magnitude lower than in the steady state (MDP) case.

A common problem related to lifetime simulations is the absence or uncertainty of one or more defect parameters. For instance the only information available about a specific recombination center may be its energy level E_t and the ratio $k = \sigma_n/\sigma_p$ of the capture cross sections for electrons/holes, but the absolute values of σ_n and σ_p are unknown. In such cases we are able to predict the defect systems behavior by systematical varying the uncertain parameters over a wide range of possible values. The comparison with experimental results enables us to determine the uncertain values. With today's computer technology the calculation of hundreds or thousands of injection dependent lifetime curves per second is possible. The calculation speed depends on the complexity of the defect model. By using appropriate algorithms together with a proper defect model we can determine unknown parameters with a "least-square-fit". An example for this

approach is shown in Fig. 5. QSSPC-measured lifetime data of an intentional Fe contaminated mc-Si sample are shown. The Fe recombination center in silicon may occur as iron-boron pair (FeB) or as interstitial iron (Fe_i). In the case shown here, it was not possible to fit the measured lifetime data with neither FeB or Fe-interstitial as the recombination center in the defect model. The fit succeeded only if a model with the two recombination centers FeB and Fe-interstitial was used. We were able to estimate the iron concentrations like shown in Fig. 5 using the concentrations of FeB and Fe-interstitial as free parameters for the fit.

4 Summary

Using a generalized RES enabled the calculation of injection dependent lifetimes and (MD-)PCTS spectra using a single defect model. A detailed analysis of the influence of traps on QSSPC, MDP and μ -PCD lifetime measurements was performed. It was shown that the different illumination conditions of these methods results in qualitative different behavior of lifetime measurements if traps are present. The concentrations of FeB and Fe-interstitial in an Fe-contaminated sample were determined by direct fitting of a model containing the both recombination centers to measured QSSPC data.

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