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To cite this article before publication: Johan Lauwaert 2021 *J. Phys. D: Appl. Phys.* in press <https://doi.org/10.1088/1361-6463/ac34ad>

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Technology computer aided design based deep level transient
spectra: Simulation of high-purity germanium crystals

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(Dated: October 29, 2021)

Abstract

Very often Deep Level Transient Spectroscopy (DLTS) specimens deviate from ideal textbook examples making the interpretation of spectra a huge challenge. This challenge introduces inaccurate estimates of the emission signatures and the lack of appropriate estimates for the concentrations of the observed trap levels. In this work it is shown with the example of high-purity germanium that Technology computer aided design including symbolic differentiation provides the necessary numerical stability over a wide temperature range to model DLTS spectra. Moreover this high-purity germanium is a quasi intrinsic semiconductor for which it is well-known that the original small signal theory can introduce strong errors. It is furthermore shown that the parasitic impact of fractional filling and high resistivity material can be modelled and that these modelled spectra can in the future assist the interpretation of experimental results.

PACS numbers:

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I. INTRODUCTION

Device Technology Computer Aided Design (TCAD) simulations are used extensively to describe the working principle of devices under conditions they will be used during operation.[1] This allows to predict their behavior in a circuit, performance or stability. Moreover these simulations can clearly help in the understanding of the working principle or the occurrence of failure. Consequently these TCAD simulations are nowadays not only used to calculate the operational behavior but also to help interpreting experiments, which are often performed at a temperature, a reverse bias, illumination that are not the typical operational conditions.

A typical example, which will be discussed in this paper, is Deep Level Transient Spectroscopy (DLTS)[2–4]. DLTS is probably the most sensitive technique to observe the presence of deep levels in semiconductors, and this has been used extensively to identify many defect levels in semiconductor materials[5]. This identification in group IV semiconductors as for example germanium often relies on fabrication of dedicated specimens[7, 8]. Such a fabrication of specimens becomes a difficult challenge for thin film technologies for which ideal constants are technologically not available [9] and nearly intrinsic material for which series resistance from the neutral part is unavoidable. Consequently DLTS experiments are performed on the final devices, with the main advantage that the observed features are originating from effects that are present in the final product. But this has a major drawback that the observed signals are more difficult to interpret, due to the presence of these parasitic effects[6].

Device TCAD can therefore help to interpret these observed capacitance transients. However the calculation of the defect transient, which is often only a small variation on the quiescent capacitance i.e. transients with an amplitude of 10^{-4} times the reverse capacitance are detectable, demands a high numerical accuracy. Moreover these transients occurs at different temperatures, which due to the Boltzmann factor have a big effect on the semiconductor equations and calculating a DLTS spectrum therefore explicitly requires convergence for all these temperatures.

In this work it will be shown that with the Open Source TCAD package DeVSIM[10, 11], which includes a symbolic differentiation of algebraic expressions with Python and Tcl interface (DiffSym) can be used to obtain the necessary numerical stability and accuracy

to simulate DLTS spectra. In this work the DevSim software package is used to simulate the DLTS spectra of n-type and p-type high-purity germanium for which it is well-known that the parasitic effects of the nearly intrinsic material has its influence on the spectrum. The simulation of the conventional and optical DLTS spectra of high-purity germanium containing substitutional copper and copper-related complexes is therefore a good example to evaluate the potential of such numerical calculations. Moreover these Cu-related traps have been extensively studied in the past, including studies with dedicated specimens [12–14], leading to a well-established assignment of the emission peaks and a hands-on procedure to calculate the trap concentration for conventional[15, 16] and optical[17, 18] DLTS. This methodology will be used on the simulated spectra to demonstrate the added value of TCAD to interpret spectra with fractional filling and strong impact of the series resistance (Q-effect).

II. SIMULATION

The python scripting interface of DevSim[11] is used to implement a uniform germanium bulk crystal in a one-dimensional model with thickness between 1.2mm and 5.0mm. The devices have a metal contact on top having a metal work function resulting in a Schottky barrier and a back contact which results in flat band conditions. Both p-type and n-type models have a shallow doping concentration with a concentration of 10^{10}cm^{-3} . This shallow doping is included as a fixed uniform charge in the device, therefore the freeze-out of these shallow levels is not included, since no impact on the carrier concentration in the temperature range $T_{min} = 18\text{K}$ to $T_{max} = 200\text{K}$ used in this work is expected. The temperatures for which the transient will be calculated T_i are chosen using the following formulae:

$$T_i = T_{max} \cdot \exp\left(\frac{\ln\left(\frac{T_{min}}{T_{max}}\right)i}{N_{points} - 1}\right)$$

with the number of point $N_{points} = 100$. Such similar sequence of points is often chosen for DLTS experiments, because the typical Boltzmann factor dependence of the emission on temperature renders the peaks at lower temperature narrower. Figure 1 shows the deep levels of Cu_s and the Copper-Hydrogen (Cu,H), Copper-Lithium (Cu,Li) and Copper-Lithium-Hydrogen (Cu,Li,H) complexes that are included in the simulation. These levels are

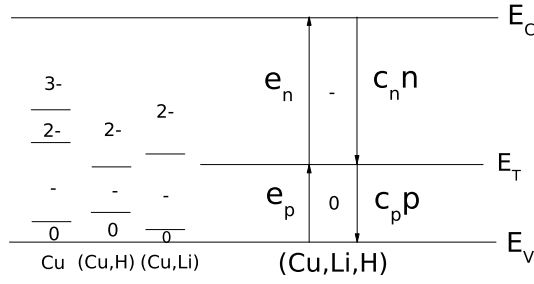


FIG. 1: Typical deep levels observed in high-purity germanium that are also included in the simulations in this work. The arrows from the bands to the (Cu,Li,H) neutral to negatively charged transition show the transitions of the electron that are incorporated in the model.

described as individual levels, each with transition rates to the conduction and valence bands as indicated with arrows on the (Cu,Li,H) level. These arrows shown in figure 1 represent the electron transitions for electron emission (e_n), electron capture ($c_n n$), hole emission (e_p) and hole capture ($c_p p$). The transitions rates (e_p , $c_p p$, e_n , $c_n n$) are temperature dependent and can be written as:

$$e_p = \sigma_p v_{th,p} N_V \exp\left(\frac{\Delta S_p}{k_B}\right) \exp\left(-\frac{\Delta H_p}{k_B T}\right) \quad (1)$$

$$c_p p = \sigma_p v_{th,p} p \quad (2)$$

$$e_n = \sigma_n v_{th,n} N_C \exp\left(\frac{\Delta S_n}{k_B}\right) \exp\left(-\frac{\Delta H_n}{k_B T}\right) \quad (3)$$

$$c_n n = \sigma_n v_{th,n} n \quad (4)$$

with k_B and T the Boltzmann constant and the temperature respectively. $v_{th,p}$, $v_{th,n}$, N_V , N_C are the thermal velocities for holes and electrons and the density of states for the valence band and conduction band respectively for which the typical $T^{1/2}$ and $T^{3/2}$ temperature dependency is included. The defect specific parameters are therefore the capture cross sections for electrons (σ_n) and holes (σ_p) and the entropy change ($\Delta S_{p/n}$) and enthalpy change ($\Delta H_{p/n}$) corresponding with the emission of a carrier (index p hole, index n electron). For a hole trap like the (Cu, Li, H) $^{0/-}$ level the parameters for the transitions including the valence band are taken from Simoen et al.[13]: $\sigma_p = 5 \times 10^{-14} \text{cm}^2$, $\Delta H_p = 160.4 \text{meV}$, including the observed apparent capture cross section for hole emission results in an entropy change

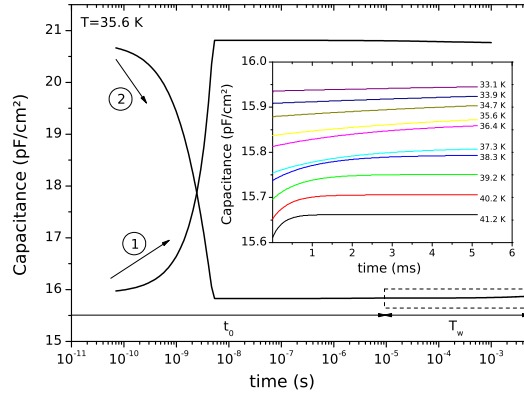


FIG. 2: Time dependence of the capacitance during pulse (V_p , 1) and reverse bias (V_r , 2). The inset shows a zoom of the window for different temperatures to demonstrate how the DLTS is generated.

of $\Delta S = 2.06k_B$. The parameters describing the transitions for this hole trap including the conduction band are more difficult to obtain. As enthalpy change is taken $\Delta H_n = E_G - \Delta H_p$ with E_G the temperature dependent band gap energy which for germanium[5]:

$$E_G = 0.742\text{eV} - \frac{4.8 \times 10^{-4} \frac{\text{eV}}{\text{K}} \cdot T^2}{T + 235\text{K}} \quad (5)$$

But the electron capture cross-section for this (Cu,Li,H)-complex is unknown. Due to the acceptor nature of this defect it is expected that the electron capture cross section to be significantly smaller than the hole capture cross-section, therefore $\sigma_n = 10^{-15} \text{cm}^{-2}$ is implemented. No entropy change for the emission of electrons ΔS_n is included for these hole traps. For the $\text{Cu}^{2-/3-}$, which is an electron trap also the thermal activated electron capture cross section is included[14], while for all the other levels the carrier capture cross sections are temperature independent. Moreover since this level is an electron trap the enthalpy change for emission is measured relative to the conduction band. This third copper-level is not observed in conventional DLTS spectra on p-type Ge, but but its signature appears in our simulations of n-type Ge, in line with experiments. [14]. Equations 1, 2, 3 and 4 introduce a time-dependence of the fractional occupation of each of the defect levels f_T , which are coupled equations with the semiconductor equations and therefore needs to be solved simultaneously for each time step. Although the constitutive equations are in these simulations not directly dependent on the time, since the time constant for relaxation of

the mobile carriers is much faster than the observed transients in this situation, these constitutive equation becomes time dependent via the changes in recombination rate which is directly dependent on the fractional occupation f_T of these defect levels. Moreover the recombination for electrons and holes is different because the charge collected on the defect is dependent on time. For each time step the capacitance is calculated by adding a small-signal AC source to the circuit voltage source. The frequency of this AC-signal is set to 1 MHz, corresponding with typical capacitance bridges used in DLTS[19]. Figure 2 shows the calculated time dependence at a temperature of 35.6 K, calculated for a germanium specimen with a thickness of 1.2mm and a substitutional copper concentration $[Cu_s]$ of $2 \times 10^8 \text{cm}^{-3}$. The change of the bias in the circuit voltage source is implemented with a ramp-time of $5ns$, which can be seen on the curve with label (1) and label (2) describing the capacitance during the pulse $V_p = -2V$ and reverse bias $V_r = -4V$ respectively. The pulse length is chosen $t_p = 1ms$, the dead time $t_0 = 10\mu s$ and the window time is $T_w = 5.12ms$ shown in figure 2. The inset of figure 2 shows the capacitance transient simulated during the window time interval $[t_0 = 10^{-5}s, T_w + t_0 = 5.13ms]$ on a linear time-scale, to demonstrate the effect of the emission of holes from the $Cu_s^{0/-}$ level.

III. RESULTS AND DISCUSSION

The challenge in modelling DLTS spectra is to include an accurate evolution of the occupation of each trap and calculate the impact of this small variation in charge density on the capacitance of the device. These simulated spectra should have an excellent agreement with what will be observed in the experiment. In other words the amplitude of the transient ΔC and the time-constant τ should be calculated accurate enough, i.e. within the experimental acceptable uncertainty.

To evaluate the accuracy of modelled capacitance transients (amplitude ΔC and time-constant τ), the simulated spectra for high purity germanium ($N_A = 10^{10} \text{cm}^{-3}$) containing Cu will be simulated and compared with the analytical calculated Fourier components. Figure 3 shows a comparison of the analytically calculated Fourier components as proposed by Weiss et al. [20]:

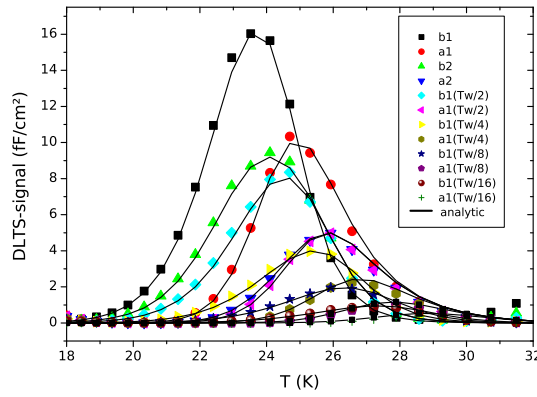


FIG. 3: Comparison of the DLTS signal originating from the $\text{Cu}_s^{0/-}$ level and the analytically calculated Fourier components based on the analytical calculated emission signature of this level full line.

$$b_n = \frac{2\Delta C}{T_w} \cdot \exp\left(-\frac{t_0}{\tau}\right) \left[1 - \exp\left(-\frac{T_w}{\tau}\right)\right] \frac{n \frac{2\pi}{T_w}}{\frac{1}{\tau^2} + n^2 \left(\frac{2\pi}{T_w}\right)^2}$$

$$a_n = \frac{2\Delta C}{T_w} \cdot \exp\left(-\frac{t_0}{\tau}\right) \left[1 - \exp\left(-\frac{T_w}{\tau}\right)\right] \frac{\frac{1}{\tau}}{\frac{1}{\tau^2} + n^2 \left(\frac{2\pi}{T_w}\right)^2}$$

for $n = 1$ window times T_w , $\frac{T_w}{2}$, $\frac{T_w}{4}$, $\frac{T_w}{8}$ and $\frac{T_w}{16}$ and $n = 2$ for T_w . The excellent agreement between the analytic calculated Fourier components with the signature of the $\text{Cu}^{0/-}$ level [13] shows that even for such low temperatures sufficient accuracy can be obtained for the variation in the capacitance as a function of time. Moreover simulation tests for germanium specimens with doping levels for which one would not expect parasitic anomalies in the spectrum (i.e. $N_A > 10^{14} \text{cm}^{-3}$) have also an excellent agreement with the analytic calculations. To evaluate the accuracy of the calculated amplitude of the transient ΔC the simulated Copper concentration is reduced. Figure 4 shows the numerically calculated DLTS spectrum for Cu in p-Ge with different trap concentrations. DLTS is a sensitive technique with a rule of thumb based on signal to noise ratio in typical capacitance meters that only 10^{-4} of relative trap concentrations $\frac{N_T}{N_S}$ can be detected which might become also a numerical challenge for the accuracy of the modelled capacitance. From this demonstration it can be seen that even a Cu concentration of only $2 \times 10^4 \text{cm}^{-3}$ can be easily observed in the simulated spectrum, therefore it is clear that the numerical detection limit is lower than the

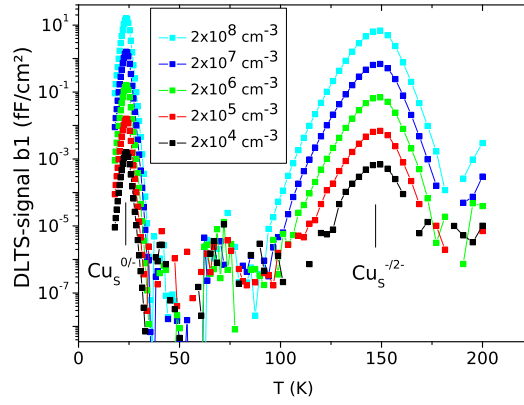


FIG. 4: Simulated DLTS spectra for the $\text{Cu}^{2-/-}$ and $\text{Cu}^{-/0}$ levels for different Cu concentrations.

actual experimental detection limit. These numerical tests are convincing and show that the necessary accuracy is obtained to use these simulations to assist the interpretation of spectra which contains anomalous effects as in high-purity germanium for which it is not always experimentally possible to reduce the impact of the series resistance of the neutral zone, the fractional filling of the traps and to have an accurate estimate of the quiescent capacitance. These processes are included in the model and the modeled spectra will be used to calculate the trap concentration with the general trap concentration formulae proposed by Simoen et al. [15]:

$$\frac{N_T}{N_S} = \frac{\Delta C}{C} \frac{[2 - \frac{\Delta C}{C}] - V_r + V_{bi}}{[1 - \frac{\Delta C}{C}]^2 V_p - V_r} \quad (6)$$

with a typical Q-correction for the amplitude of the transient observed experimentally $(\frac{\Delta C}{C})_{exp}$:

$$\frac{\Delta C}{C} = \frac{1 + Q^2}{1 - Q^2} \left(\frac{\Delta C}{C} \right)_{exp} \quad (7)$$

Figure 5 shows the simulated DLTS spectra including the typical trap levels shown in figure 2 with each a concentration of $2 \times 10^8 \text{ cm}^{-3}$. The corresponding quiescent capacitance (C) is shown in figure 6. The Q-effect induced by the series resistance of the neutral zone can clearly be observed in the spectra and as expected this effect is much stronger for the specimens with the largest thickness. Figure 7 shows the calculated relative concentration based on equations 6 and 7, the temperature dependence of Q herein is calculated from the reduction

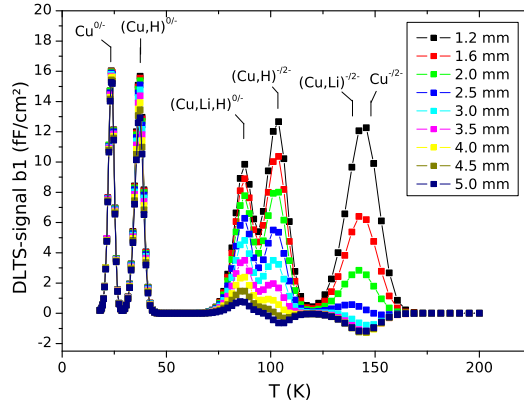


FIG. 5: Conventional Capacitance DLTS spectra of p-type high-purity Germanium specimens with different thickness'.

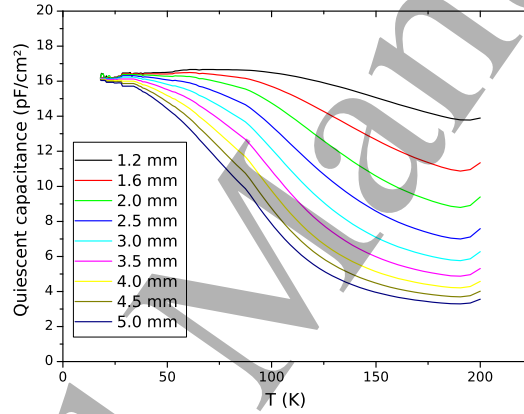


FIG. 6: Quiescent capacitance calculated at V_r for the p-type high-purity germanium specimens with different thickness.

of the measured capacitance (C) with respect to the constant depletion capacitance C_w :

$$C = \frac{C_w}{1 + Q^2} \quad (8)$$

The C_w is estimated as the maximum of the capacitance curve as a function of temperature, assuming that the thickness of the depletion layer has no strong temperature dependence. This assumption is typically used experimentally[15], by inspecting the calculated free carrier profiles it can be seen that this is not a strong assumption even over the wide temperature range of 200K to 18K. This allows to determine the necessary Q-correction (Eq. 6) as a

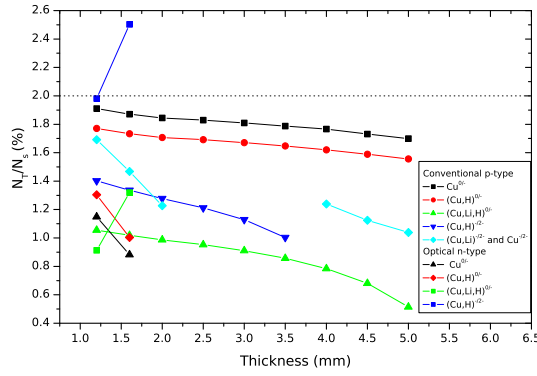


FIG. 7: Classical calculation of fraction N_T/N_S for the defect levels observed in conventional p-type and optical n-type simulated spectra as a function of the thickness of the device. Dotted line at 2% corresponds with the concentration implemented in the model.

function of temperature. From the calculated concentration as a function of thickness of the specimen in figure 7 it can be seen that even with this valuable correction proposed by Simoen et al.[15] the trap concentration can be seriously underestimated. Moreover in the temperature region with $Q \approx 1$ close to peak reversal this formulae does not result in an accurate (within 10%) estimate of the concentration. Nonetheless as already was proposed in many publications one has too try to minimize the impact of the Q effect by selecting high reverse voltages and by adjusting the thickness of the specimens. In this case the impact of the correction is limited and a fair estimate of the concentration can be made with the analytic formulae (Eqn. 6, 7 and 8). In this paper it is shown that when it is experimentally unavoidable to stay in this "ideal" regime, the spectrum can be modelled and concentrations can be derived by comparing experimental and simulated spectra. This might become even more important when: (i) traps are only fractionally filled as is the case for the $(\text{Cu}, \text{Li}, \text{H})^{0/-}$ level and (ii) emission peaks overlap as is the case for the $(\text{Cu}, \text{Li})^{-/2-}$ and $\text{Cu}^{-/2-}$ levels. For those peaks that the analytic estimate has intrinsically a strong uncertainty. The peaks for which the Q -correction is larger than 5 are not included in figure 7 since for those peaks the relative concentration had a strong deviation with the expected 2% shown as a dotted line. Moreover in this situation it is not expected that the analytic amplitude correction is still valid.

In this work the possibility to optically generate carriers is also included in the TCAD

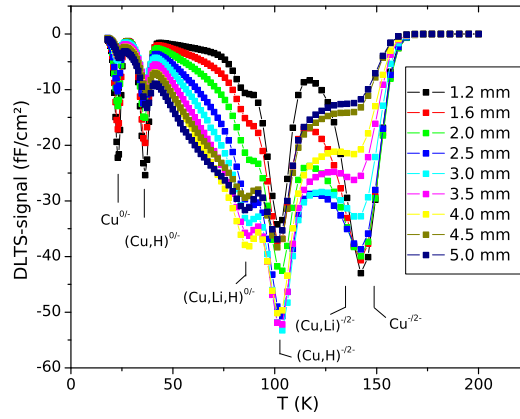


FIG. 8: Optical capacitance DLTS spectra of n-type high-purity germanium for specimens with different thickness'.

scripting, which makes it possible to model optical DLTS spectra with excitation through the back contact as proposed by Blondeel et al. [17]. Figure 8 shows optical DLTS spectra for n-type specimens with different thickness'. The generation of carriers during the pulse occurs by a monochromatic source with wavelength of 900nm and intensity $I_0 = 8\text{mW/cm}^2$. For this wavelength Germanium has an absorption coefficient of $\alpha = 5 \times 10^4\text{cm}^{-1}$, which for simplicity of the example shown here is kept independent of temperature. With these properties the generation profile during the pulse time $t_p = 10\text{ms}$ as a function of position (x) relative to front contact can be written as:

$$I_0 \alpha \exp(\alpha(x - t)) \quad (9)$$

with t the thickness of the specimen.

During the optical excitation and the observation of the emission the bias is kept constant at $V_r = -4\text{V}$. With the assumption that the peak amplitude is saturated Blondeel et al. [18] proposed an analytical methodology to correct the observed amplitude useful to estimate the concentration of the hole traps. We have included this estimate for the two thinnest specimens $t = 1.2\text{mm}$ and 1.6mm . These data points are included in figure 7. For the specimen with larger thickness this extra neutral zone introduces a broad background on top of the spectra which is also observed experimentally [17]. Moreover based on the variation of the amplitude of the signal originating from the $\text{Cu}^{-/0}$ level for different specimen thickness it might not be expected that the saturation criterion

is fulfilled. Nevertheless even for these thin specimens the estimate has an unavoidable large uncertainty, which might be improved by comparing the experiment with the TCAD modelled spectrum.

IV. CONCLUSIONS

In this paper it is shown via the example of high-purity germanium DLTS spectra that TCAD simulations can be used to calculate DLTS spectra. The symbolic differentiation enhances the numerical stability for a wide range of temperatures to have the necessary accuracy to calculate capacitance transients with a small relative amplitude ($< 10^{-4}C_r$). Moreover to describe the parasitic impact of series resistance and fractional filling of traps on the DLTS peak amplitude and shape, simulations might be necessary. Moreover in the situation where the impact cannot be minimized experimentally due to the quality of the device these simulations can help to make an estimate of the trap concentration.

Acknowledgments

The author would like to thank the fruitful discussions with H. Vrielinck.

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