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# Discussions on the Numerical Solutions of Schön-Klasens Model: Trapping and Recombination Probability

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**Abstract:** Theoretical and numerical viewpoints of the Schön-Klasens model were discussed. The brief information about mathematical principals of the model was given. Expressions that controlled charge carrier traffic were derived. Some numerical solutions of the model were performed by using variable $A_{te}$, $A_{th}$, Are and $A_{rh}$ parameters. This study has concluded that the glow curve is affected by both charge carriers according to relationship between ($n_c$.m.$A_{re}$) and ($n_v$.n.$A_{rh}$).

**Key words**: thermoluminescence, numeric solutions, Schön-Klasens model.

## INTRODUCTION

Since applying thermoluminescence (TL) for radiation dosimetry purposes a very great deal of efforts have been made in the scientific community to explain the mechanism of TL. Since then much research has been carried out for a better understanding and improvement of the TL emitting mechanism[1-2]. Although the first theoretical explanations of TL there are no general theoretical models up to now to explain the exact characteristics of TL emitting mechanism. The theoretical explanation of TL is based on the electron band theory of an insulating or semiconducting solid. It consists of a set of localized energy levels in the forbidden band, which arises due the presence of impurities and other point defects. These acts as traps and recombination centres in the TL process[1-5]. All TL phenomena are governed by the process of the electron hole recombination. It should be noted that rather complex processes are taking place in the traffic of charge carrier between trapping states and luminescent recombination centres during the heating of the TL material. Almost all of thermoluminescence (TL) models have been based on the consideration of charge release from electron trap only. In this paper Schön–Klasens type a more complex model has been discussed. This model introduced originally by Schön and colleagues[6-7] and used by Klasens[8]. Schön-Klasens model suggests that not only electrons but also holes are mobile in the same temperature interval. In this case, holes also contribute to TL emitting like electrons. Figure 1 show that energy levels, charge carrier transitions and related parameters suggested by the Schön-Klasens model.

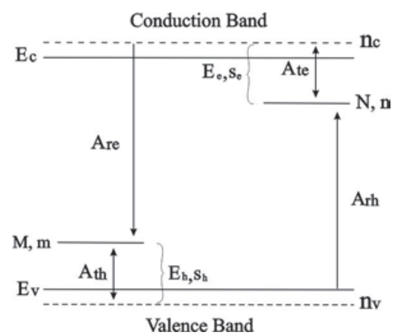


**Figure 1**: Generalized energy levels scheme and allowed transitions (thermal excitation, re-trapping and recombination) for Schön-Klasens model.

According to Schön-Klasens model charge carrier concentrations in the trap levels are given in Eq.1-4. These 4 equations also describe the simultaneous release of holes during the thermal stimulation of the trapped electrons[1-4].

$$\frac{dn}{dt} = -s_e.n.\exp\left(-\frac{E_e}{k.T}\right) + A_{te}.n_c.(N-n) - A_{rh}.n_v.n \qquad [1]$$

$$\frac{dn_c}{dt} = s_e.n.\exp\left(-\frac{E_e}{k.T}\right) - A_{te}.n_c.(N-n) - A_{re}.n_c.m \qquad [2]$$

$$\frac{dm}{dt} = -s_h.m.\exp\left(-\frac{E_h}{k.T}\right) + A_{th}.n_v.(M-m) - A_{re}.n_c.m \qquad [3]$$

$$\frac{dn_v}{dt} = s_h.m.\exp\left(-\frac{E_h}{k.T}\right) - A_{th}.n_v.(M-m) - A_{rh}.n_v.n \qquad [4]$$

This set of equations deals with the traffic of charge carrier during the heating of the sample, when one trapping state and one kind of recombination centre are involved. In here, the instantaneous concentration of electrons in the conduction band is denoted by $n_c(m^{-3})$ and that of holes in the valence band by $n_v(m^{-3})$ respectively. $N(m^{-3})$ denotes here the total concentration of electron trapping states which is a constant and $n(m^{-3})$ the instantaneous concentration of filled electrons trap which is a variable. $E_e(eV)$ and $s_e(s^{-1})$ are the activation energy and frequency factor of the electron trap, respectively, k is the Boltzmann constant $(eV.K^{-1})$ and $A_{te}(m^3.s^{-1})$ is the trapping (re-trapping during heating) probability of electrons from the conduction band. $M(m^{-3})$ denotes here the total concentration of hole trapping states which is a constant and $m(m^{-3})$ the instantaneous concentration of filled holes trap which is a variable. $E_h(eV)$ and $s_h(s^{-1})$ are the activation energy and frequency factor of the hole trap, respectively. $A_{th}(m^3.s^{-1})$ is the probability of capturing hole in M, whereas $A_{re}(m^3.s^{-1})$ is the recombination probability of free electrons with captured holes. $A_{rh}(m^3.s^{-1})$ is the recombination probability of free holes with captured electrons in electron trap. At the same time, these four equations to keep to the right neutralization condition expressed in Eq 5.

$$\frac{dn}{dt}+\frac{dn_c}{dt}=\frac{dm}{dt}+\frac{dn_v}{dt} \qquad [5]$$

If we assumed that all recombination events are radiative and therefore produce photons and all photons are detected by detector. Under these assumptions TL glow curve is expressed by Eq.6[1-4].

$$I_{TL}=I_{TLn}+I_{TLp} \qquad [6]$$

For these equations set approximate solutions were given by Bräunlich and Scharmann[9]. These authors considered four extreme cases, involving the rates of electron and hole retrapping and their comparison with the corresponding recombination rates. The model also solved numerically by Mckeever *et.al.*[10] without any of the assumptions of the Bräunlich and Scharmann and reached the same conclusions. But exact numerical solutions of these rate equations for this model have not been published and it is not yet possible to discuss further the precise effect of the various assumptions introduced the analysis.

## METHODOLOGY

In this study, we assumed that material irradiated before heating stage and has electrons in electron trap ($n_o$) and holes in hole trap ($m_o$). In this case it is important assumption that there are not any charge carriers in the conduction and valence bands. This is followed by a heating stage. During this stage M and N are assumed to be rather far from the valence band and conduction band, respectively. Electrons from N may be thermally released into the conduction band and then either re-trap in N or recombine with holes in M. At the same time holes from M may be thermally released into the valence band and then either re-trap in M or recombine with electrons in N. For a given set of trapping parameters, differential equations governing the process during the excitation stage were numerically solved by using a special code in the Mathematica 8.0 computer program. During the solutions temperature was changing with a constant heating rate (β) and therefore instantaneous temperature is expressed by Eq. 7.

$$T=T_0+\beta.t \qquad [7]$$

Where $T_o$ is the initial temperature at the beginning of heating stage and t is the time (s). Both recombination into N and M are considered to be radiative, but separable. Thus, the intensity in photons per $m^3$ per second of one spectral component of TL is proportional to the rate of change of N, i.e. Eq. 1 and the second spectral component is assumed to be proportional to the rate of change of M, namely, Eq. 3. The shape, position and intensity of the glow curve are related to a various trapping parameters of the trapping states responsible for the TL emission. Constant trapping parameters using in the simulation are given in Table 1.

**Table 1:** Constant parameters used in the simulation

| **Parameter** | **Values** |
|---|---|
| $E_e$-$E_h$ ( eV ) | 1.00 |
| $S_e$, $S_h$ ( $s^{-1}$ ) | $10^{12}$ |
| N=M ($cm^{-3}$) | $10^{10}$ |
| β ( °C/s ) | 1 |
| $n_o$=$m_o$ ($cm^{-3}$) | $10^{10}$ |

## RESULTS

First of all, to show that Schön-Klasens model gives the same glow curves as FOK-SOK model, specially designed simulation parameters were chosen and Eq.1-6 were solved numerically. For this purpose, electron and hole trap depth were chosen different. Calculated glow curves for different trapping probability of electron ($A_{te}$) are shown in Fig. 2. From the Fig.2 one can be seen that Schön-Klasens model gives the same glow curves as FOK model for $A_{te}$=$A_{th}$=$10^{-9}$ and other appropriate trapping parameters. Four points should be emphasized here. Firstly, if $A_{te}$≥$A_{th}$ and Ate=$10^{-9}$, the model gives the same glow curves as FOK model. Secondly, if $A_{te}$≥$A_{th}$ and $A_{te}$=$10^{-7}$, the model gives the same glow curves as SOK model. Thirdly, while $A_{te}$≥$A_{th}$, the model gives the same glow curves as FOK or SOK model depending on only the values of the $A_{te}$. Fourth, the results of above are always true when the difference between $E_e$ and $E_h$ is greater than ~0.25eV ($E_h$>$E_e$). In this case, the values of the $A_{th}$ are not important.

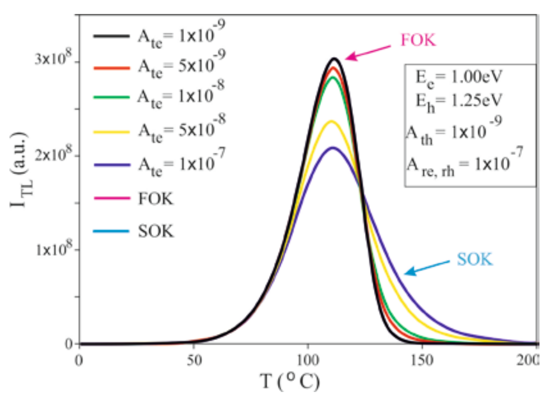


**Figure 2:** Glow curves for different $A_{te}$.

Fig.3 show glow curves calculated for different trapping probability of electron ($A_{re}$). Schön-Klasens model gives the same glow curves as FOK model for $A_{re}$=$A_{rh}$=$10^{-7}$ and other appropriate trapping parameters. Four points also should be emphasized here. Firstly, if $A_{re}$≥$A_{rh}$ and $A_{re}$=$10^{-7}$, the model gives the same glow curves as FOK model. Secondly, if $A_{re}$≥$A_{rh}$ and $Ar_{te}$=$10^{-9}$, the model gives the same glow curves as SOK model. Thirdly, while $A_{re}$≥$A_{rh}$, the model gives the same glow curves as FOK or SOK model depending on only the values of the $A_{re}$. Fourth, the results of above are always true when the difference between $E_e$ and $E_h$ is greater than ~0.25eV ($E_h$>$E_e$). In this case, the values of the $A_{rh}$ are not important.

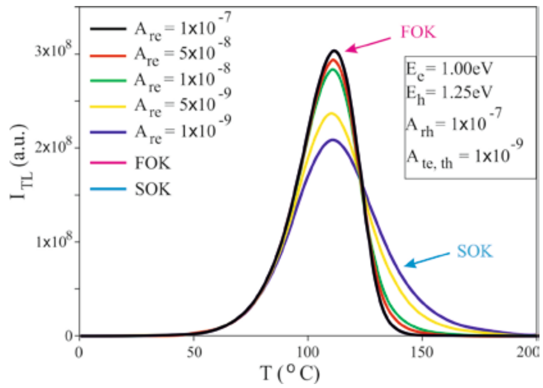


**Figure 3** Glow curves for different $A_{re}$

Using different $A_{te}$ and $A_{th}$ probabilities, both electron and hole movement effect on glow curves were investigated. Figure 4 show glow curves calculated for different $A_{te}/A_{th}$ ratios. In Fig.4 one can be seen that glow curve is a superposition of two satellite peaks came from electron and hole movement. In the case of $A_{te}$=$A_{th}$, the glow curve is affected both electron and hole movement at the same ratios. On the other hand, when $A_{te}$ >> $A_{th}$, hole movement can be negligible and the model gives the same glow curves as FOK model. When $A_{te}$ << $A_{th}$, electron movement can be negligible and the model gives the same glow curves as SOK model.

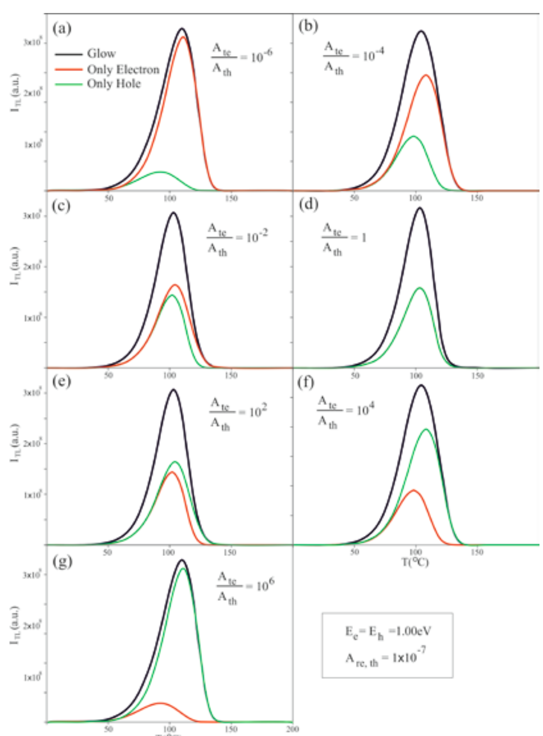


**Figure 4:** Glow curves for different $A_{te}/A_{th}$ ratios

Figure 5 show glow curves calculated for different $A_{te}/A_{th}$ ratios and $E_e \neq E_h$. In this case, above discussions are valid. It is the important to point out that, when $A_{te}=A_{th}$, the glow curve is affected both electron and hole movement at the different ratios.

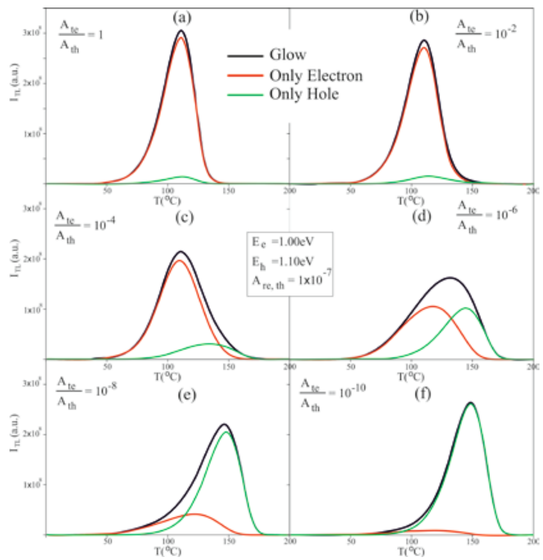


**Figure 5:** Glow curves for different $A_{te}/A_{th}$ ratios and $E_e \neq E_h$

The effect of $A_{re}$ and $A_{rh}$ on glow curves are show in Fig. 6 and 7

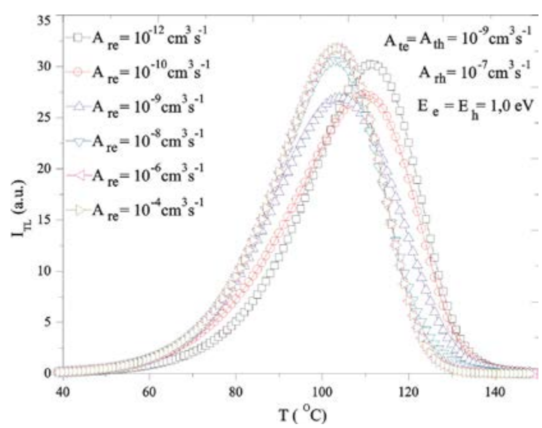


**Figure 6:** Schematic comparison of TL glow curves computed the different values of the electron recombination probabilities, $A_{re}$.

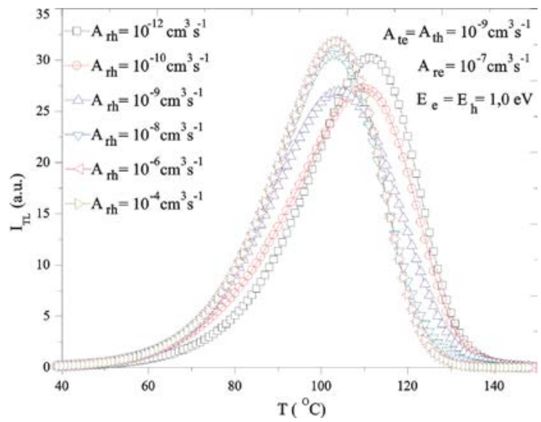


**Figure 7:** Schematic comparison of TL glow curves computed the different values of the hole recombination probabilities, $A_{rh}$.

Figure 6 and 7 have the same characteristics; because their thermoluminescence trap parameters were chosen the same and their luminescence mechanisms are similar. Hence, figure 7 can be obtained by swapping $A_{re}$ to $A_{rh}$ and electron to hole. In figure 4a one can see easily that up to $A_{re} = A_{rh}$, glow curve is shaped by holes and $I_m$ and $T_m$ are determined by holes. Beyond this point, $A_{rh}<A_{re}$, glow curve is shaped by electrons and $I_m$ and $T_m$ are determined by electrons. As a parameter $A_{re}$ is increased and $A_{rh}$ is kept constant, recombination probability of electron increases, and therefore total recombination probability also increases. Because $n_o$ and $m_o$ are kept constant, area under glow curve does not change. While $A_{re}$ is being increased, peak maximum temperature ($T_m$) moves to lower temperature. In addition to this, hole concentration in traps is decreased by increasing of electron recombination and is thus, peak maximum height ($I_m$) decreases. In figure 4b one can see easily that up to $A_{rh} = A_{re}$, glow curve is shaped by electrons and $I_m$ and $T_m$ are determined by electrons. Beyond this point, $A_{re}<A_{rh}$, glow curve is shaped by holes and $I_m$ and $T_m$ are determined by holes. As a parameter $A_{rh}$ is increased and $A_{re}$ is kept constant, previous interpretations can be valid by swapping $A_{re}$ to $A_{rh}$ and electron to hole. By the same way, contributions of charge carriers on glow curve for various recombination probabilities $A_{re}$ and $A_{rh}$ can be seen in Fig.8 and Fig.9, separately.

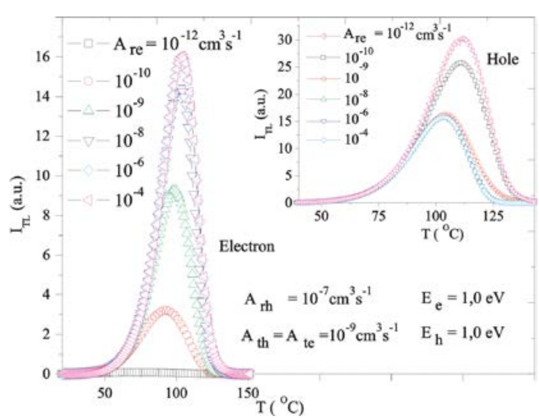


**Figure 8:** Effect of recombination probability of electron, $A_{re}$, on glow curve for different values. Contributions of both charge carriers on glow curve are given separately.

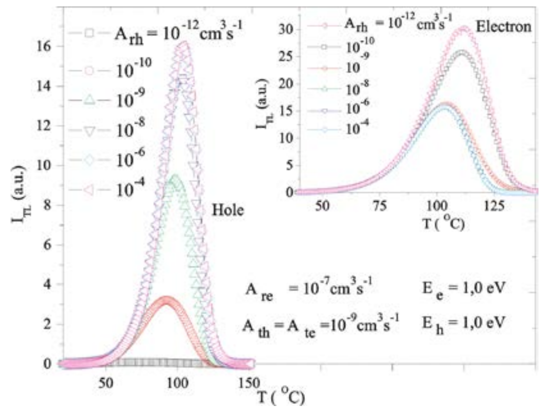


**Figure 9:** Effect of recombination probability of hole, $A_{rh}$, on glow curve for different values. Contributions of both charge carriers on glow curve are given separately.

In Fig.8, one can see that as a parameter $A_{re}$ is increased, contribution of electrons on glow curve increases or, it is decreased, contribution of holes on glow curve increases. By contrast, it can be seen in Fig.9 9 $A_{rh}$ is increased, contribution of holes on glow curve increases or, it is decreased, contribution of electrons on glow curve increases.Fig.10–Fig.11 and Fig.12– Fig.13 show that changes occurred peak maximum temperature ($T_m$) and peak maximum height ($I_m$) for different $A_{re}$ and $A_{rh}$ values, respectively.

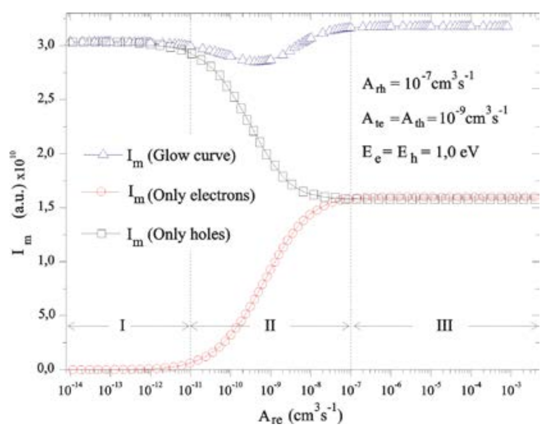


**Figure 10:** Changes occur on $I_m$ for different $A_{re}$ values. Contribution of both charge carriers on $I_m$ are given separately.

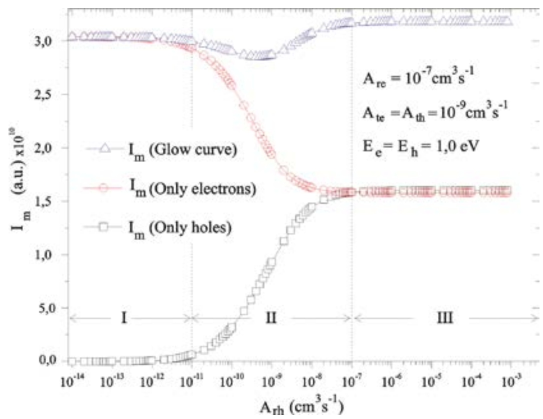


**Figure 11:** Changes occur on $I_m$ for different $A_{rh}$ values. Contribution of both charge carriers on $I_m$ are given separately.

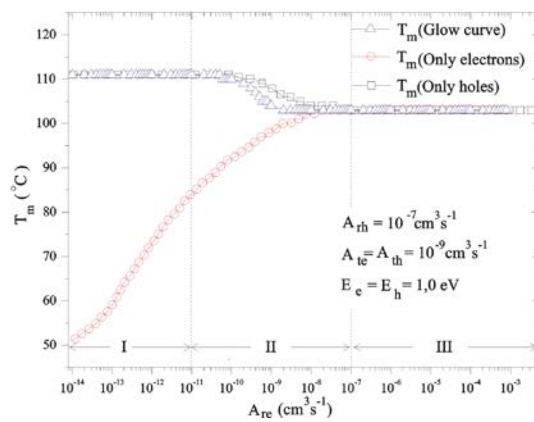


**Figure 12:** Changes occur on $T_m$ for different $A_{re}$ values. Contribution of both charge carriers on $T_m$ are given separately.

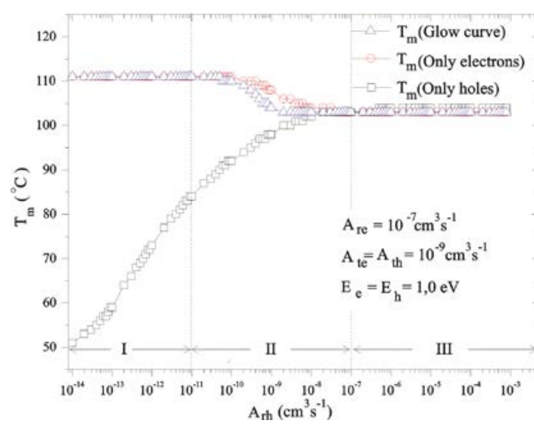


**Figure 13** Changes occur on $T_m$ for different $A_{rh}$ values. Contribution of both charge carriers on $T_m$ are given separately.

If we take into account Fig.10 and Fig.12, three regions can thus be defined; (i) $A_{re} << A_{rh}$ (ii) $A_{re} \sim A_{rh}$ (iii) $A_{re} >> A_{rh,\ te}$. For each of these three regions the assumptions of $A_{rh}=10^{-7}$ $cm^3/s$, $A_{te}=10^{-9}$ $cm^3/s$ and

$A_{th}$=$10^{-9}$ $cm^3$/s are also made. It is important point that when Fig.12 and 13 are being interpreted, Fig.10 and 11 must be taken into account. Using these assumptions we can be reached following results; In region (i) $I_m$ and $T_m$ are determined by recombination rate of hole (see Fig.8 and Fig.9) and they are both approximately constant; nevertheless, contribution of electron is rather small. Because $A_{rh}$, $A_{te}$ and $A_{th}$ are constant and $A_{re}$ << $A_{rh}$, variation rate of charge carrier concentrations in traps are approximately constant. Therefore, recombination rate of electron may be neglected and recombination rate of hole is approximately constant. In region (ii) $I_m$ and $T_m$ are affected by both electron and hole movements (see Fig.8 and Fig.9). At the beginning of this region, recombination rate of hole is bigger than electron; even so, recombination rate of electron progressively increases. But recombination rate of hole is still bigger than electron. Therefore, $I_m$ determined by hole recombination rate but, increment of $A_{re}$ values, recombination rate of electron increases. This increment keeps on which recombination rate of electron reaches to recombination rate of hole at the end of this region (when $A_{re}$ = $A_{rh}$,). In this case, electron recombination rate can be effective on glow curves as well as hole recombination rate. Furthermore, in this region, total recombination probability progressively increases and electron recombine with hole into hole traps at lower temperatures is thus, $T_m$ shifts to lower temperatures. In region (iii) $I_m$ and $T_m$ are determined by recombination rate of both charge carriers (see Fig.8 and Fig.9). Because of $A_{rh}$, $A_{te}$ and $A_{th}$ are constant, recombination rate of electron and hole are approximately constant. Due to the fact that recombination rates of charge carriers are constant, $I_m$ and $T_m$ reach saturation. At the saturation region, because total recombination probability is bigger than the other regions, $I_m$ reaches the highest value; however, $T_m$ reaches the minimum value. Fig. 11 and Fig. 13 taken into account, three region can thus be defined; (i) $A_{rh}$ << $A_{re}$ (ii) $A_{rh}$ ~ $A_{re}$ (iii) $A_{rh}$ >> $A_{re}$. For each of these regions the assumptions of $A_{re}$=$10^{-7}$ $cm^3$/s, $A_{te}$=$10^{-9}$ $cm^3$/s and $A_{th}$=$10^{-9}$ $cm^3$/s are also made. Using these assumptions for all of these regions, previous interpretations can be valid by swapping $A_{re}$ to $A_{rh}$ and electrons to holes. In Figure 14 and 15 depict the effect of re-trapping probability of electron, $A_{te}$, and hole, $A_{th}$, on glow curves, respectively.

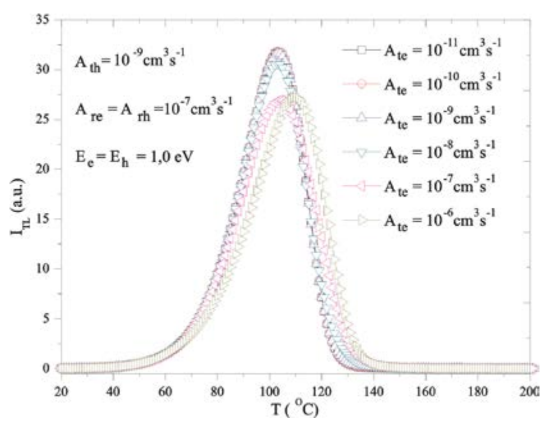


**Figure 14:** Effect of changes of the re-trapping probability of electron ($A_{te}$) on glow curve.

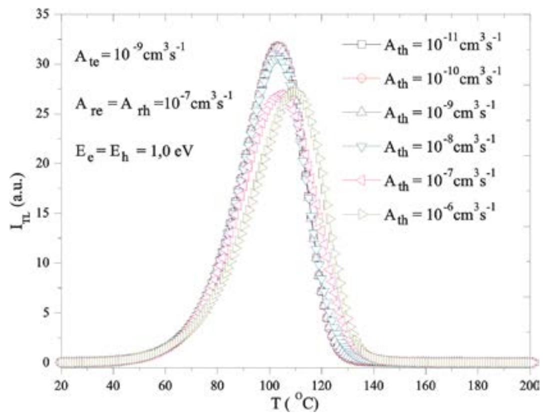


**Figure 15:** Effect of changes of the re-trapping probability of hole ($A_{th}$) on glow curve.

Fig.14 and Fig.15 have the same characteristics because their thermoluminescence trap parameters were chosen approximately same. In Fig.14 and Fig.15, one can see easily that as a parameter $A_{te}$ is increased or $A_{th}$ is decreased and other parameters are kept constant, recombination probability of electron decreases. In addition to this, electron concentration in traps increases and therefore, hole recombination probability increases. All in all, $A_{te}$ is increased, contribution of electron on glow curve decreases and contribution of hole on glow curve increases. Because $n_o$, $m_o$ and $A_{th}$ are kept constant, area under glow curve does not change and therefore total recombination probability decreases up to $A_{te}=A_{th}$. Hence, $A_{te}$ is increased, $I_m$ decreases and $T_m$ is shifted to upper temperatures. Incidentally, Fig.16 and Fig.17 show that contributions of charge carriers on glow curves for various re-trapping probabilities, $A_{te}$ and $A_{th}$, separately.

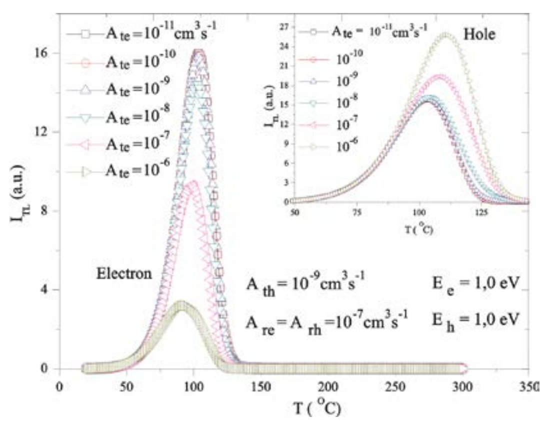


**Figure 16:** Contribution of electron and hole on glow curve for different $A_{te}$ values.

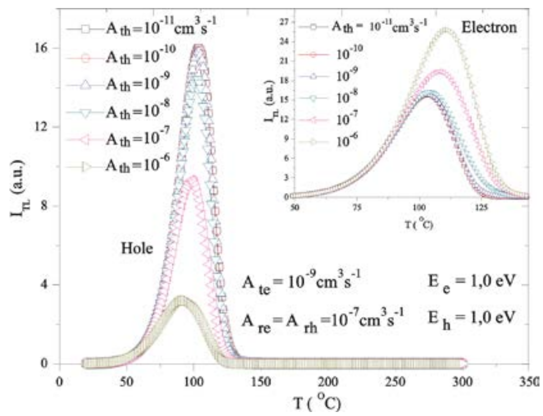


**Figure 17:** Contribution of electron and hole on glow curve for different $A_{th}$ values.

In Fig.16 and Fig.17 show that $A_{te}$ is increased or $A_{th}$ is decreased, contribution of electron on glow curve decreases and contribution of hole on glow curve increases. It is important point that hole recombination probability is determined by amount of trapped electrons and electron recombination probability is determined by amount of trapped holes. Fig.18, Fig.19 and Fig.20, Fig.21 show that changes occurred peak maximum temperature and peak maximum height for various re-trapping probabilities, $A_{te}$ and $A_{th}$, separately.

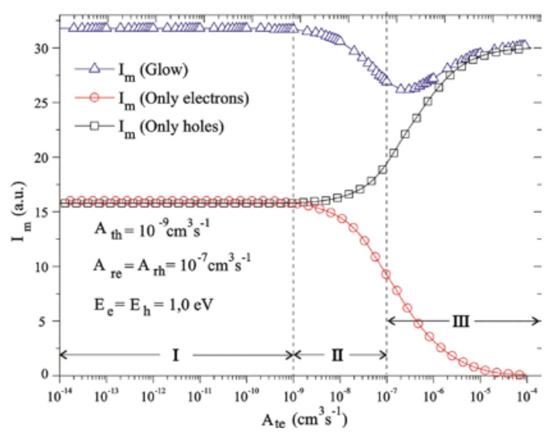


**Figure 18:** Change occurs on $I_m$ for different $A_{te}$ values. Contributions of both charge carriers on $I_m$ are given separately.

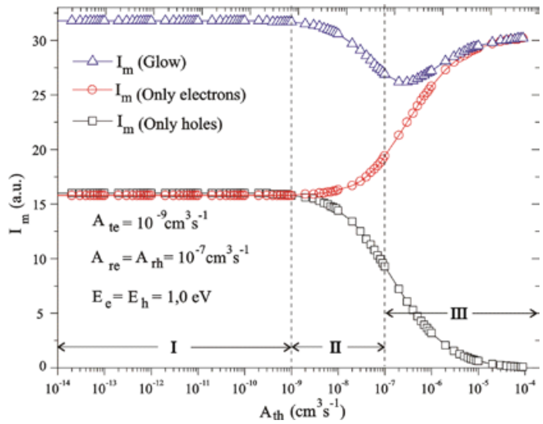


**Figure 19:** Change occurs on $I_m$ for different $A_{th}$ values. Contributions of both charge carriers on $I_m$ are given separately.

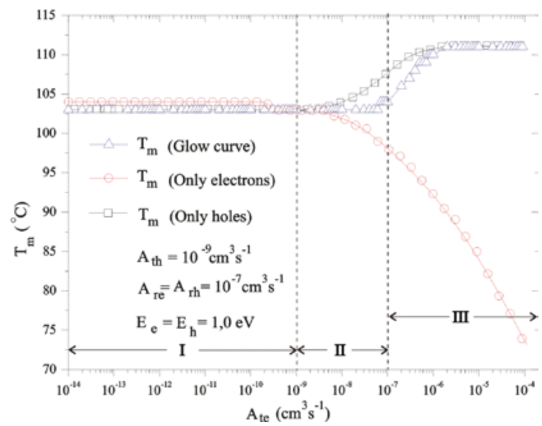


**Figure 20:** Change occurs on $T_m$ for different $A_{te}$ values. Contributions of both charge carriers on $T_m$ are given separately.

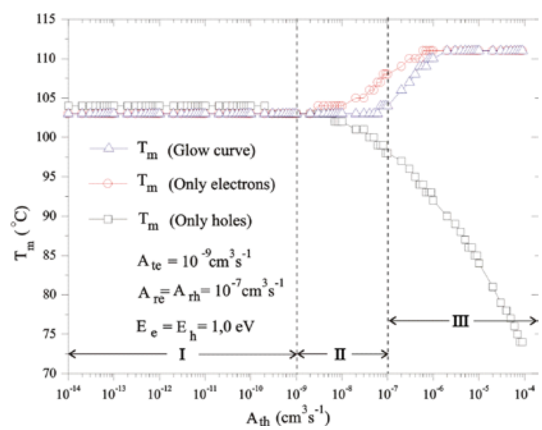


**Figure 21:** Change occurs on $T_m$ for different $A_{th}$ values. Contributions of both charge carriers on $T_m$ are given separately.

If we take into account Fig.18 and Fig.20, three region can thus be defined; (i) $A_{te} << A_{th}$ (ii) $A_{te} \sim A_{th}$ (iii) $A_{te} >> A_{th}$. For each of these regions the assumptions of $A_{re} = A_{rh}=10^{-7}$ cm$^3$/s and $A_{th}=10^{-9}$ cm$^3$/s are also made. Using these assumptions we may reach following results; In region (i) $I_m$ and $T_m$ are controlled by recombination rates of both electron and hole and they are approximately constant. Because $A_{re}$, $A_{rh}$ and $A_{th}$ are constant and $A_{te} << A_{th}$, variation rate of charge carrier concentrations in traps are approximately constant. Therefore, recombination rate of hole is equal to recombination rate of electron. In region (ii) $I_m$ and $T_m$ are affected by both electron and hole movements. At the beginning of this region, recombination rate of electron is still effective on $I_m$ and $T_m$ but contribution of it decreases. At the same time recombination rate of hole progressively increases. Therefore, $I_m$ is controlled by hole but, recombination rate of electron is decreased by increment of $A_{te}$ values. Furthermore, in this region, total recombination probability progressively decreases and electrons recombine with holes into hole trap at high temperatures and are thus, $T_m$ shifts to high temperatures.In region (iii), $A_{te}$ is progressively increased and is thus, contribution of electron on glow curves decreases and hole recombination can be effective on glow curves. $A_{re}$, $A_{rh}$ and $A_{th}$ are constant and $A_{te}$ is progressively increased, as a consequence recombination rates of charge carriers also decrease. When $A_{te}$ has become $A_{te} >> A_{th}$ electron recombination rate can be neglected. Due to the fact that recombination rate of hole is dominant and constant, $I_m$ and $T_m$ reach saturation. Fig. 19 and Fig. 21 taken into account, three region can thus be defined; (i) $A_{th} << A_{te}$ (ii) $A_{th} \sim A_{te}$ (iii) $A_{th} >> A_{te}$. For each of these regions the assumptions of $A_{re} = A_{rh}=10^{-7}$ cm$^3$/s and $A_{te}=10^{-9}$ cm$^3$/s are also made. Using these assumptions for all of these regions, previous interpretations can be valid by swapping $A_{te}$ to $A_{th}$ and electrons to holes.

## CONCLUSIONS

In this study Schön-Klasens model has been solved by numerically. In the solutions we have just mentioned the magnitudes $A_{tr}$ and $A_{th}$ namely, two independent parameters. By using these parameters, which determine the shape of a glow curve, Eq.1 to Eq.6 are solved by numerically but no simplifying assumptions had been made. In the simulations for $A_{tr}$ and $A_{th}$ a complex dependence on the traps depth of charge carriers in broad ranges is found. Simulations show that according to Schön-Klasens model, in which electron and hole can be released by thermally, thermoluminescence glow curve is shaped by charge carrier movement resulting recombination. This process is different from the other models' process because, now hole is not a stable charge carrier. By taking into account of all numerical simulations the following results can be reached;

(i) Characteristics of the glow curve is mainly governed by recombination rate of free electrons when $S_e.\exp[-E_e/kT] >> S_h.\exp[-E_h/kT]$ or $(n_c.m.A_{re}) >> (n_v.n.A_{rh})$.

(ii) Characteristics of the glow curve is mainly governed by recombination rate of free holes when $S_h.\exp[-E_h/kT] >> S_e.\exp[-E_e/kT]$ or $(n_c.m.A_{re}) << (n_v.n.A_{rh})$.

(iii) Characteristics of the glow curve is governed by both type of charge carriers when $S_e.\exp[-E_e/kT] \sim S_h.\exp[-E_h/kT]$ or $(n_c.m.A_{re}) \sim (n_v.n.A_{rh})$.

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