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DISCUSSIONS ON THE NUMERICAL SOLUTIONS OF SCHÖN-KLASENS MODEL: CHARGE CARRIER TRAPS DEPTH

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ABSTRACT

Non-radiative transitions are one of the important problems for the thermoluminescence event. One of the models offered to explain non-radiative transition is Schön-Klasens. In this paper, the Schön-Klasens model was discussed both from theoretical and numerical viewpoints. The brief information about mathematical principals of the model was given and differential equations that controlled charge carrier traffic were derived. Some numerical solutions of the model were performed by using variable E_e and E_h parameters. This study has concluded that the glow curve is affected by both charge carriers according to relationship between E_e and E_h parameters.
Keywords: Thermoluminescence, numeric solutions, Schön-Klasens model.

SCHÖN-KLASENS MODELİNİN SAYISAL ÇÖZÜMLERİ ÜZERİNE TARTIŞMALAR: YÜK TAŞIYICI TUZAKLARI

ÖZ

Işınımsız geçişler termolüminesans olayın en önemli sorunlarından bir tanesidir. Bu etkiyi açıklayabilmek için ileri sürülen modellerden bir tanesi de Schön-Klasens'dir. Bu çalışmada Schön-Klasens modeli teorik ve sayısal bakış açılarından incelenmiştir. Öncelikle, modelin matematiksel prensipleri hakkında kısa bir ön bilgi verilmiş ve yük taşıyıcı trafiğini kontrol eden diferansiyel denklemler türetilmiştir. E_e ve E_h parametreleri kullanılarak modelin sayısal çözümleri yapılmıştır. Bu çalışmada ışıldama eğrisinin, E_e ve E_h parametrelerine bağlı olarak her iki yük taşıyıcısından da etkilendiği sonucuna ulaşılmıştır.
Anahtar Sözcükler: Termolüminesans, sayısal çözümler, Schön-Klasens model.

1. 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

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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. They 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 TL models have been based on the consideration of charge release from electron trap only. In this paper, Schön – Klasens model has been discussed. The model introduced originally by Schön and colleagues [6,7] and used by Klasens [8]. The 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 model [4].

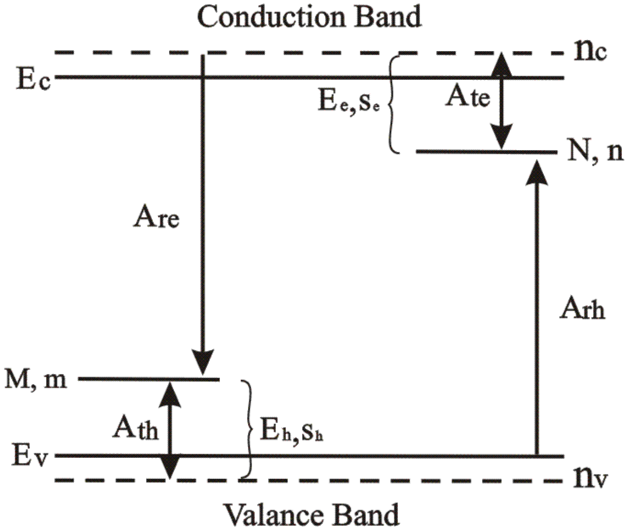

Figure 1. Generalized energy levels scheme and allowed transitions for Schön - Klasens model [4]

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

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

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

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

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

The 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) rate 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 rate of free electrons with captured holes. A_{rh} (m^3 s^{-1}) is the recombination rate of free holes with captured electrons in electron trap.

At the same time, the equations to keep to the right neutralization condition expressed in Eq 5.

$$\frac{dn}{dt}+\frac{dn_c}{dt}=\frac{dm}{dt}+\frac{dn_v}{dt} \tag{5}$$

If all recombination events are radiative and produce photons and all photons are detected, TL glow curve is expressed by Eq.6. [1-4].

$$I_{TL}=I_{TLn}+I_{TLp} \tag{6}$$

For the equations set of 1-6, approximate solutions were given by Bräunlich and Scharmann [9]. The 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.

2. METHODOLOGY

In this study, it is assumed that material is irradiated before heating stage and has electrons in electron trap (n_o) and holes in hole trap (m_o). It is important to point out that there are not any charge carriers in the conduction and valence bands. It is followed by a heating stage. During the 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 of 1-6 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.

$$T=T_0+\beta.t \tag{7}$$

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.

3. RESULTS

Calculated glow curves for different hole trap depths (E_h) are shown in Figure 2 and trap parameter are given in Table 1. Schön-Klasens model gives the same glow curves as FOK model for sufficiently bigger E_h and other appropriate trapping parameters. When E_h is constant (E_h=1eV) and electron trap depths (E_e) are changed, the same glow curves are calculated.

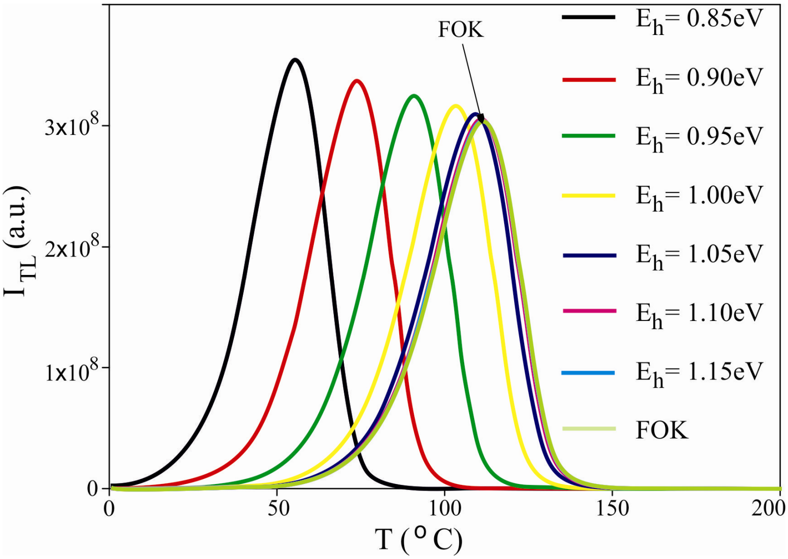

Figure 2. Glow curves for different E_h parameters

Table 1. Parameters used in the E_h simulation

Parameter	Value
E_e (eV)	1.00
E_h (eV)	0.85-1.15
S_e (s^{-1})	10^{12}
S_h (s^{-1})	10^{12}
$A_{te} - A_{th}$ ($cm^3\ s^{-1}$)	10^{-9}
$A_{re} - A_{rh}$ ($cm^3\ s^{-1}$)	10^{-7}
N=M (cm^{-3})	10^{10}
β (°C/s)	1
n_o=m_o (cm^{-3})	10^{10}

The effect of charge carrier trap depths (E_e, E_h) on I_m and T_m can be seen in Figure 3 and Figure 4, respectively. Parameters used in the simulation are presented in Table 2.

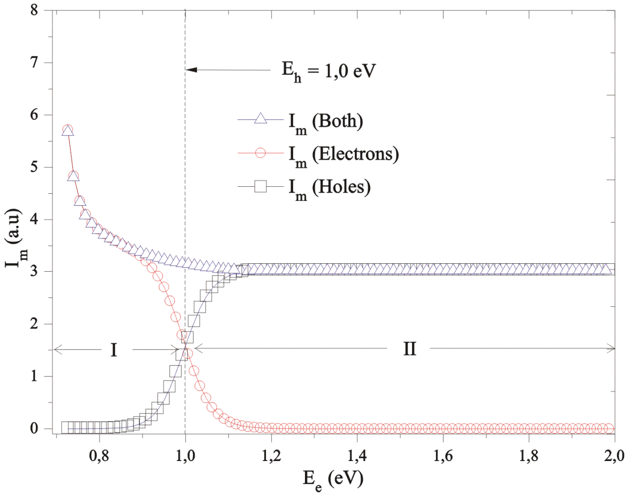

Figure 3. The relationship between charge carrier trap depths and I_m

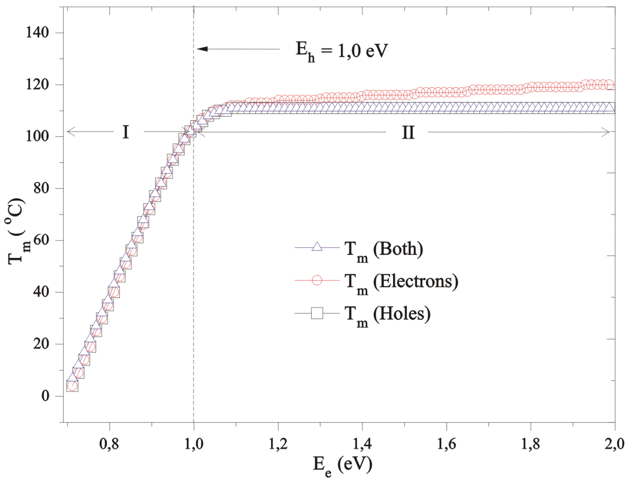

Figure 4. The relationship between charge carrier trap depths and T_m

Table 2. Parameters used in the trap depths (E_e, E_h) simulation

Parameter	Value
E_e (eV)	*0.70-2.00*
E_h (eV)	1.00
S_e (s^{-1})	10^{12}
S_h (s^{-1})	10^{12}
$A_{te} - A_{th}$ (cm^3 s^{-1})	10^{-9}
$A_{re} - A_{rh}$ (cm^3 s^{-1})	10^{-7}
N=M (cm^{-3})	10^{12}
β (°C/s)	1
n_o=m_o (cm^{-3})	10^{12}

By taking into account of Figure 3 and Figure 4, two separable regions can be determined; (i) $E_e < E_h$ and (ii) $E_e > E_h$. In the first region, $E_e < E_h$ and E_h is constant; holes need to more thermal energy than electrons to release from traps and electrons can be released from electron traps before holes at the same temperature interval and glow curve are shaped by electrons. Hence, in region i, I_m and T_m are determined by electron movement. By the same way, in the second region, I_m and T_m are determined by hole movement.

On the other hand, when $E_e = E_h$, contributions of electrons and holes on I_m and T_m are the same. Moreover, while E_e is deepened and E_h is kept constant, total recombination probability also decreases. Thus, in a unit of time, less recombination takes place and I_m decreases but T_m moves to high temperatures.

4. CONCLUSIONS

In this study, Schön-Klasens model has been solved by numerically. The solutions of the model were performed by using variable E_e and E_h parameters. By using the 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 E_e and E_h a complex dependence on the traps depth of charge carriers in broad ranges is found. The role of the traps depth of trapped charge carriers is that able to few parameters E_e and E_h found as the total area under the glow curve.

Simulations show that according to Schön-Klasens model 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 and also contribute to TL emitting like electrons.

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