Semiconductor Physics, Quantum Electronics & Optoelectronics, 2024. V. 27, No 4. P. 450-456

Optics

Sensory properties of dosimetric materials under conditions of parameter fluctuations: Monte Carlo method

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Abstract. The results of *ab initio* calculations of the thermoluminescent and phosphorescent characteristics of semiconductors used in dosimetric studies, free from any approximations, are presented. A scaling procedure is proposed to model the sensing capabilities of dosimeters of different types. This makes it possible to establish the scope of various approximations used in practical dosimetry to explain similar experimental data. For the first time, the role of statistical factors determining the range of changes in the energy and kinetic parameters of luminescent processes of actual dosimetric materials in forming their sensory characteristics was investigated. The proposed approach can complement the computerized glow curve deconvolution (CGCD) technique, widely used to assess the structure of energy levels and kinetic coefficients of actual dosimetric materials. The capabilities of the new method are implemented in the Lumini calculation package.

Keywords: dosimetric materials, phosphorescence, thermoluminescence, kinetic equations, Monte Carlo method, Lumini package.

https://doi.org/10.15407/spqeo27.04.450
PACS 21.60.Ka, 78.55.Hx, 78.60.Kn, 87.53.Bn

Manuscript received 20.08.24; revised version received 04.09.24; accepted for publication 13.11.24; published online 06.12.24.

1. Introduction

Dosimetry of ionizing radiation is one of the directions of sensor technologies that allows recording the effect of ionizing radiation on the object of study by a system of active centers of dosimeters based on the wide-bandgap optical materials. The absorbed dose can be evaluated by studying the amount of energy stored by the dosimeter during interaction with nuclear particles [1–8].

As a rule, information about the amount of stored energy is obtained from the spectra of light emission stimulated by heating (thermally stimulated luminescence dosimeter or TL dosimeter) or after exposure to optical radiation (optically stimulated luminescence dosimeter or OSL dosimeter). Studying the luminescent characteristics of irradiated samples also allows us to investigate the structure of energy levels in the band gap and the frequency parameters that determine the transition kinetics. The corresponding energy structure is formed in dosimetric materials by their doping or due to structural defects [9]. It plays an important role in radiation dose accumulation, sensitivity, and delivery. Given the statistical nature of the distribution of local energy levels in the bounded band and kinetic parameters, these factors should be considered using dosimeters as radiation sensors.

However, usually, the modeling of their characteristics is based on a one-level model [2, 3]. In this case, a group of energy levels is represented by only one of them and analytical expressions are obtained using various approximations that do not always adequately describe the physics of dosimetric processes. Some authors have pointed out the need to go beyond it (see [10]).

This paper presents the results of first-principles calculations of the luminescent characteristics of dosimetric materials without restrictions in the values of the model parameters that describe the kinetics of excitation of the electron-hole system of these materials, the degree of filling of charge carrier traps, level-band transitions, and their recombination. The influence of statistical factors that cause the blurring of the energy spectrum of local levels in the forbidden energy gap of the dosimeter material and fluctuations in the values of kinetic coefficients on the temperature and time evolution of its recombination characteristics is also investigated.

2. Scaling method in the theory of luminescence: package Lumini

The sensing characteristics of dosimetric materials are determined by the energy spectrum of local levels in the forbidden band, which act as the capture and recombination centers. The physics of processes in dosimetric measurements based on the one-level model assumes the presence of electron traps with a concentration of N and

an activation energy of ε, the filling of which corresponds to the amount of absorbed radiation energy by the dosimeter material.

The ionizing radiation causes the transition of electrons from the valence band to the conduction band. During and after irradiation, these charge carriers are redistributed due to their capture by traps: in the conduction band, the electron concentration becomes equal to n_1, while at the trap levels, respectively, it is n_2. The number of holes, h, formed in the valence band equals to the number of electrons at the trap levels, and in the conduction band, $h = n_3 = n_1 + n_2$. The annihilation of the electron-hole pair at the recombination level of the electron leads to generating a quantum of light. In this paper, we consider dosimetric materials based on *n*-type semiconductors. The structure of the energy levels of such materials, first proposed in [11], and the scheme of transitions between them are shown in Fig. 1.

To consider the physics of the processes of activation of excitation centers under the influence of radiation, trapping of charge carriers in the forbidden band temperature, as well as electron-hole recombination with light radiation one can use the following well-known equations.

$$\frac{dn_1(t)}{dt} = -\frac{dn_2(t)}{dt} + \frac{dn_3(t)}{dt},$$
$$\frac{dn_2(t)}{dt} = k_1 \cdot n_1(t) \cdot \left(N - n_2(t)\right) - k_2 \cdot n_2(t) \cdot \exp\left(-\varepsilon/kT\right), \qquad (1)$$
$$\frac{dn_3(t)}{dt} = k_3 \cdot n_1(t) \cdot n_3(t).$$

The description of the parameters k_i, $i = 1 - 4$, n_j, $j = 1 - 3$ is given in the text of the article.

Although the accurate picture implies the presence of shallow and deep charge carrier traps, as well as the interaction between them, often for many practical applications, the problem is reduced to the analysis of transformations of the electron-hole system within the framework of the one-level model shown in Fig. 1.

Moreover, the one-level model is now widely used within the framework of the computerized glow curve deconvolution (CGCD) technique to determine the order of the TSL kinetics, the energy structure of dosimetric materials, and frequency coefficients.

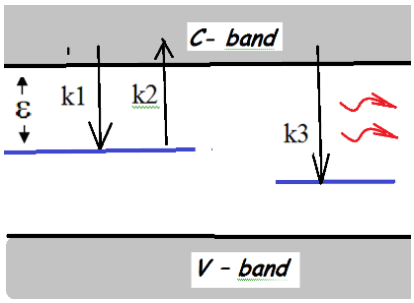

Fig. 1. Energy diagram describing the kinetics of charge carrier transitions in dosimetric materials for a one-level model.

The differential equations (1) contain the following frequency parameters: k_1 is the intensity of charge carrier trapping, k_2 is the frequency of their release into the conduction band due to thermal emission, k_3 is the intensity of electron-hole recombination with light emission and the concentration of trapping levels N. Despite the simplicity of this system of differential equations, there are no examples of its *ab initio* solutions in the literature. It is due to the values of the parameters involved ~ 10^{13-15}, which makes it unrealistic to use the available computational capabilities. Therefore, the modern theory of dosimetric processes uses numerous approximations, namely $n_1 << n_2$, different ratios of the coefficients $k_1 - k_4$, and the assumption that $n_2 << N$. One of the consequences of using these approximations is the assumption that it is possible to estimate the luminescence intensity of dosimeters I not through the integral index $I_3 = -dn_3(t)/dt$ but through the rate of change in the electron concentration of trap levels $I_2 = -dn_2(t)/dt$.

This approximation is widely used in practical dosimetry and allows the development of theoretical methods for estimating the energy level position and kinetic parameters of dosimetric materials. However, it is still actual to carry out *ab initio* studies of the kinetics of electron-hole transformations and estimate the limitations of these approximations. Such studies can be performed after the scaling procedure using a large-scale transformation of physical quantities [13–16]. It can be done by the following transformations of the parameters of the kinetic equations (1), here, $i = 1 - 4$:

$$n_i^*(t) = \frac{n_i(t)}{n_1^0 + n_2^0} \cdot A, \qquad k_1^* = k_1 \cdot N, \qquad k_2^* = k_2,$$
$$k_3^* = k_3 \cdot \frac{n_1^0 + n_2^0}{A}, \qquad k_4^* = \frac{n_1^0 + n_2^0}{A \cdot N}. \qquad (2)$$

Here, n_1^0, n_2^0 are the initial values $n_1(t)$, $n_2(t)$, $n_1^0 = n_1(0)$, $n_2^0 = n_2(0)$, $n_1^0 + n_2^0 = n_3(0)$, the scaling factor A can have different values, taking into account the order of magnitude of the initial parameters n_1^0, n_2^0. It is easy to see that the renormalized initial values $n_1^*(t), n_2^*(t)$ of the quantities satisfy the following equations:

$$n_1^*(0) = \frac{n_1^0}{n_1^0 + n_2^0} \cdot A, \qquad n_2^*(0) = \frac{n_2^0}{n_1^0 + n_2^0} \cdot A, \qquad (3)$$
$$n_1^*(0) + n_2^*(0) = A, \; T = b_1 + \alpha b_2 t, \quad b_1 = kT_0, \quad b_2 = k,$$

where k is the Boltzmann constant. Considering the methods of thermally stimulated dosimetry, the temperature T in (3) is taken as linearly dependent on time t, $T = T_0 + \alpha b_2 t$, where α has the meaning of heating rate, deg./s. When the activation energy ε is measured in units of eV, and the initial temperature T_0 corresponds to 293 K, the expression for T gives the values $b_1 = 2.5 \cdot 10^{-2}$ eV, $b_2 = 8.6 \cdot 10^{-5}$ eV/s. In the case of modeling the phosphorescence problems, $\alpha = 0$, and the subject of study may be the time dependence $I_3 = -dn_3(t)/dt$.

Taking into account the scaling conditions (2) and (3), the modified system of kinetic equations is as follows:

$$\frac{dn_1^*(t)}{dt} = -\frac{dn_2^*(t)}{dt} + \frac{dn_3^*(t)}{dt},$$

$$\frac{dn_2^*(t)}{dt} = k_1^* \cdot n_1^*(t) \cdot \left(1 - k_4^* n_2^*(t)\right) - k_2 \cdot n_2^*(t) \cdot \exp\left(-\frac{\varepsilon}{b_1 + \alpha b_2 t}\right),$$

$$\frac{dn_3^*(t)}{dt} = k_3^* \cdot n_1^*(t) \cdot n_3^*(t). \qquad (4)$$

The compact form of the kinetic equations (4), with the account of the scaling conditions (2) and (3), allows numerical simulations for arbitrary ratios of model values and a method of going beyond the one-level approximation.

These possibilities were implemented in the Lumini package that contains a well-known algorithm for solving the system (4) by the Runge–Kutta method of the 4th order with automatic selection of the integration step [17] at the initial values $n_1^*(0) = w_1, n_2^*(0) = w_2$, $w_1 + w_2 = A$.

The Lumini program for studying the conditions of dosimetric experiments consists of three packages: thermoluminescence, phosphorescence, and partial luminescence. The C# programming language was used to write the program as a component.

The program contains two components – a graphical display of the results and a logical part that performs the basic calculations of the system of equations (4) to solve the problems of TSL or phosphorescence. Another part of the complex displays the obtained data graphically.

Both parts are written in C# programming language, using the Net Framework. Switching between modes of operation is performed using the TabControl of Windows Forms. This control is used to display tabs similar to dividers in a notebook or labels in a set of folders in a file cabinet, see [18–20]. The Windows Forms text boxes are used to receive input from the user. The TextBox control is usually used for editable text, although it also can be set to read-only permissions. The TextBox control allows you to use a single format for text displayed or entered in the control. The Windows Forms Button control starts a calculation process, allowing the user to click the control to act. The Button control displays the text "Start", which is clicked to start the calculation.

The Chart class is used to display a graph with the received data. Two important class properties are the Series capabilities and Chart Areas, which are used to store both the data to be displayed and their attributes. After setting all the necessary values in the interface console and activating the "Start" window, the program starts, the output coefficients of the Lumini interface are written to the input file of the program, they are read, the calculation process is performed, and the resulting data is written to the output file. After the calculations are completed, the Lumini program graphically displays the data from the output file. One feature of this software package is the ability to use the Monte Carlo method [21, 22] to account for the statistical nature of the distribution of parameters of capture levels in the restricted area of the dosimetric material. This allows one to be free from the one-level kinetic model of thermoluminescence and go beyond different approximations.

3. *Ab initio* modeling of thermoluminescent processes

The proposed scaling method allows us to study the system of kinetic equations (4) for arbitrary values of parameters using the Lumini package. In particular, to go beyond proximity $n_2(t) \approx n_3(t)$ the possible assumptions under the suggestion of a small number of accumulated charge carriers in the conduction band $n_1(t) << n_3(t)$ should be used. The *ab initio* modeling capabilities allow us to perform a set of studies on the influence of kinetic coefficients on the characteristics of TSL semiconductors. Such studies are essential for solving the first stage of the task of using the CGCD technique to determine the energy structure and kinetic parameters of dosimetric materials based on the TSL characteristics: the position and intensity of the luminescence maxima, as well as their heating rate.

The following calculations are illustrative for a model dosimetric material containing one level of electron traps with an activation energy of 0.8 eV, initial values of the concentrations of electrons trapped at the trap level: $n_1^0 = 10^{12}\,\mathrm{cm}^{-3}$, $n_2^0 = 10^{15}\,\mathrm{cm}^{-3}$, $N = 10^{18}\,\mathrm{cm}^{-3}$, the condition is met $n_1^0 << n_2^0$, which is generally used in practical calculations. Three options for choosing the kinetic coefficients for model calculations are considered: I – {$k_2 = 1.0\cdot10^8\ \mathrm{s}^{-1}$; $k_3 = 10^{-16}\ \mathrm{cm}^3\cdot\mathrm{s}^{-1}$}, II – {$k_2 = 5.0\cdot10^8\ \mathrm{s}^{-1}$; $k_3 = 10^{-16}\ \mathrm{cm}^3\cdot\mathrm{s}^{-1}$}, and III – {$k_2 = 5.0\cdot10^8\ \mathrm{s}^{-1}$; $k_3 = 10^{-7}\ \mathrm{cm}^3\cdot\mathrm{s}^{-1}$}. The values of the coefficients $k_1 = 5.0\cdot10^{-20}\ \mathrm{cm}^3\cdot\mathrm{s}^{-1}$ and $k_4 = 200$ are common to these sets.

The results shown in Fig. 2 demonstrate both the time evolution of current carrier concentrations in the conduction band, trap levels, $n_1(t)$, $n_2(t)$, and their sum, $n_3(t)$, in (a), (b), and (c). In this figure, the electron concentration in the conduction band (a) – blue curves, (d), (e), and (f) – thermal luminescence intensity curves $I_2 = -dn_2(t)/dt$, black curves, $I_3 = -dn_3(t)/dt$, red curves, and $I_1 = -dn_1(t)/dt$, blue curves, obtained by numerical differentiation of the corresponding dependences (a), (b), (c). The condition $n_1^0 << n_2^0$ is satisfied.

The value of $n_3(t)$ equals the concentration of holes at the recombination levels. Figs 2d, 2e, and 2f show the results of their numerical differentiation in (d), (e), and (f), given for the temperature scale in T, K.

The latter parameters are essential for estimating the intensity of the dosimeter illumination, which is calculated by the rule $I_3 = -dn_3(t)/dt$. For comparison, the figure shows the value $I_2 = -dn_2(t)/dt$ commonly used in practical dosimetry. Such comparison is important for analyzing the validity of such approximations.

Figs 2a and 2d show the time changes of all concentration parameters of the model $n_1(t)$, $n_2(t)$, and $n_3(t)$ calculated for the variant I of the choice of kinetic coefficients. It demonstrates the complex nature of the behavior of $n_1(t)$, in particular, the possibility of a local increase in its value under the influence of kinetic parameters $k_1 - k_4$, which can lead to a violation of rule $n_1(t) << n_2(t)$ even under the initial condition $n_1^0 << n_2^0$. Another interesting fact is that the maximums of the derivatives of all concentration indicators are

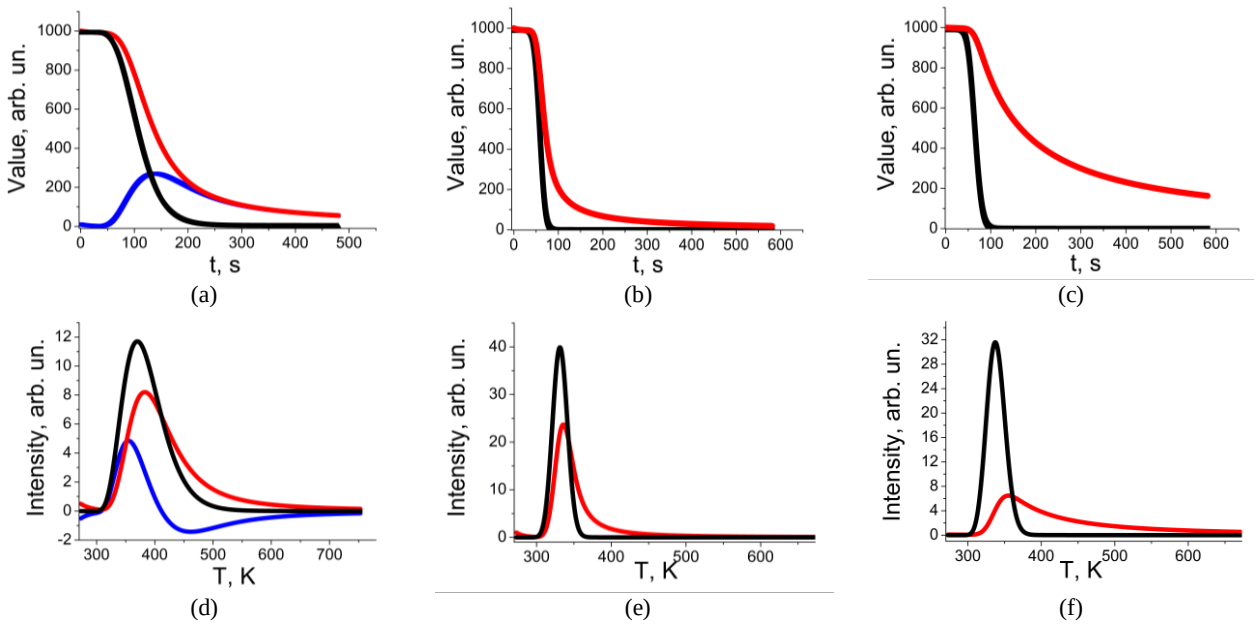

Fig. 2. (a), (b), and (c) – time dependence of the electron population at the trap levels $n_2(t)$ (black curves), the total concentration $n_3(t)$ (red curves – for different sets, I, II, and III, of the kinetic coefficients (3), the values of which are given in the text). The electron concentration in the conduction band, on (a) – blue curves, on d), e), and f) – thermal luminescence intensity curves I_2 (black curves), I_3 (red curves), and I_1 (blue curves). For interpretation of the colors in the figures, the reader is referred to the web version of this article.

concentrated near the dosimetric peak $I_3 = -dn_3(t)/dt$ and the kinetics of "band-level" and "level-band" transitions determine their specific position.

This fact is illustrated in the mentioned above graphs by the behavior of the parameters $n_2(t)$ and $n_3(t)$ alone. Thus, the results shown in Figs 2b and 2e are obtained for variant II when the frequency factor k_2 is five times larger than in variant I. This causes a sharper dependence of the dosimetric peak I_3 as I_2, and their shift to the low-temperature range. The case shown in Figs 2c and 2f and obtained for option III, when an order of magnitude reduces the value of k_3 with the same frequency factor k_2 as in the previous case k_2, demonstrates the possibility of a significant difference in the temperature positions of the peaks I_3 and I_2. The latter indicates the need for more careful use of the indicator I_2 instead of I_3 in practical dosimetry. According to Fig. 2, the parameter I_2 over-estimates the TSL results compared to the *ab initio* calculations for I_3.

4. Monte Carlo method in dosimetric studies

Along with analyzing the approximations accompanying the theory of dosimetric measurements, it is essential to investigate the material sensing capabilities, considering the statistical nature of the distribution of energy states of trap levels and the associated kinetic coefficients. This makes it possible to go beyond the one-level model (Fig. 1a) when a single energy value approximates the set of energy states in the forbidden band, ε, and the use of fixed values of their kinetic coefficients k_1 – k_4. This possibility is provided by the Monte Carlo method, which allows the consideration of the statistical nature of the distribution of energy and kinetic parameters when studying the luminescence intensity of a model dosimetric material, I_3 for the problems of TSL and phosphorescence. This work was done within the framework of statistical tests for material with initial values of the kinetic coefficients of set *I* (Figs 2a, 2d) and capture levels with an activation energy of 0.8 eV.

The Lumini package performed the calculation, and the blurring was realized symmetrically concerning the initial parameters ε and the coefficients k_1 – k_4, which satisfy set *I*. The software Lumini package allows us to separately study the effect of the degree of fluctuations of kinetic and energy parameters on the luminescent characteristics. The statistical test results are shown in Fig. 3 for the TSL problem, considering the blurring of only the coefficients k_1 – k_4, (a), the energy ε (b), and their combined effect (c).

First, it should be noted that even the symmetric nature of the blurring of these parameters, which is assumed to be symmetric, leads to asymmetry of the TSL characteristics, with the output intensity being more sensitive to fluctuations in energy parameters than to the characteristics of transition kinetics.

This may be due to the thermal excitation nonlinearity processes $k_2 \exp\left(-\frac{\varepsilon}{b_1 + \alpha b_2 t}\right)$ concerning symmetric fluctuations by the value of $\pm\Delta\varepsilon$. These data illustrate that the kinetic coefficients $k_1 - k_4$ determine the dispersion and the value of the maximum TSL and, therefore, provide criteria for the search for promising dosimetric materials with high sensing capabilities.

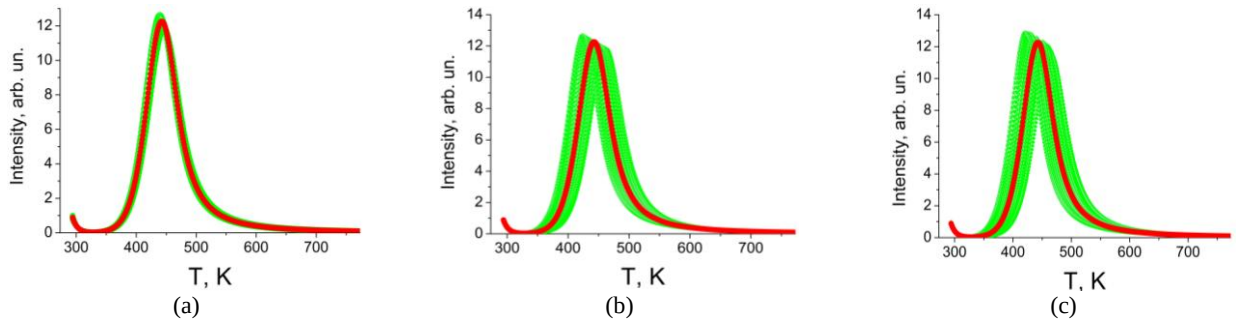

Fig. 3. Temperature dependence of TSL intensity obtained by Monte Carlo simulation: a) with only the kinetic coefficients blurred by 30%, b) with 10% of ε, trap energy, blurring, and c) their combined effect of 10 and 30% blurring. The red line in these graphs shows the initial TSL value before statistical testing. Everywhere, the effect of blurring the TSL curves is highlighted in green.

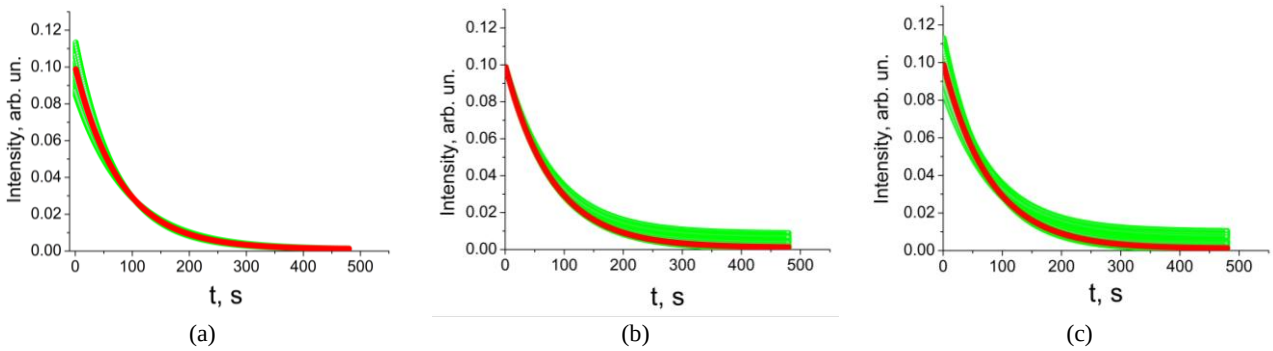

Fig. 4. Phosphorescence decay obtained by the Monte Carlo method: a) considering the blurring of kinetic coefficients within 30%, b) 15% energy ε blurring, c) their combined effect of 15 and 30%. The red line in these graphs represents the initial value of the phosphorescence dependence before statistical testing; the effect of Monte Carlo testing on phosphorescence curves marked by green color.

Fig. 4 shows the results of similar studies of the phosphorescence process – spontaneous illumination of dosimetric material immediately after its irradiation over time. This is a relatively new effect in dosimetric studies. Its feature is the dependence of luminescence on the irradiation intensity, which has less impact on the characteristics of the TSL [9, 23] and can supplement information on irradiation conditions. Interest in the study of phosphorescence arose after using solid-state dosimetry in fields of intense radiation from high-energy nuclear particles, which occur in radiation technologies and nuclear power.

Generally, phosphorescence is associated with small energy levels of capture. It is not considered in the practice of tissue-equivalent dosimetry of low-intensity radiation fluxes, where it has a weak effect on TSL. The results show a peculiarity of the influence of statistical energy fluctuations ε (Fig. 4), and the kinetic coefficients of the model on the time dependences I_3. In the last case, the fluctuations lead to more significant blurring at the initial stages of the decay I_3, which can be explained by the peculiarities of the behavior of the conduction band $n_1(t)$ electrons under the influence of temperature excitation (Fig. 2a). Only statistical fluctuations of the activation energy (Fig. 4b) cause changes in the following parts of the time evolution I_3, which the nonlinearity of the thermal excitation term can explain. As shown in Fig. 4c, the statistical fluctuations of the energy and kinetic parameters harmonize the decay curve I_3 along the blurring interval over the entire time interval.

The obtained results can be used to process experimental data of TSL and dosimetric materials for their energetic and frequency characteristics parameterization. Currently, the CGCD technique is widely used in these studies [24–27]. Its limitations lie in using several assumptions, such as a one-level model of TSL, preliminary selection of the order of phosphorescence kinetics, *etc.* These results can complement the capabilities of the CGCD methodology and provide more information about the energy structure and kinetic coefficients of dosimetric materials.

5. Conclusions

Thus, the scaling procedure was applied for the first time to conduct an *ab initio* study of the luminescent characteristics of dosimetric materials free of approximations. The obtained results will enable us to visualize the pattern of changes in the concentration of charge carriers formed during the collection of radiation energy by the dosimeter. It is shown that their time and temperature evolution can violate the conditions of approximations used in applied dosimetry. Another essential task solved in this work is to consider the statistical nature of the formation of the energy spectrum of dosimetric materials during their doping and to go beyond the one-level approximation that is dominant in the theory of dosimetry.

These studies make it possible to determine how the degree of disorder can affect the sensory capabilities of materials for different conditions of collection of the absorbed radiation dose. As a first stage of these studies, the paper presents the results of numerical simulation of the luminescent characteristics of dosimeters within the model that considers fluctuations in their energy and kinetic parameters within 10–20%. In the future, the proposed model can complement the capabilities of the computerized glow curve deconvolution (CGCD) technique for assessing the structure of energy levels and kinetic coefficients of actual dosimetric materials: LiF:Mg, Ti; LiF:Mg, Cu, P; Al_2O_3:C [1–4].

The capabilities, compactness, and visibility of the proposed *ab initio* method became the basis of the Lumini package for studying TSL, phosphorescence, and partial light emission in dosimetric studies.

The work was presented at the conference of young scientists in semiconductor physics "Lashkaryov Readings – 2024".

Funding

The work was partially carried out within the framework of the project supported by the National Research Foundation of Ukraine. State registration number – 2023.04/0083.

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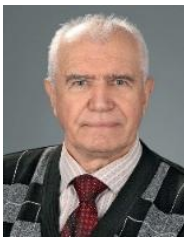

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Сенсорні властивості дозиметричних матеріалів в умовах зміни параметрів: метод Монте-Карло

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Анотація. Наведено результати *ab initio* розрахунків термолюмінесцентних і фосфоресцентних характеристик напівпровідників, що використовуються в дозиметричних дослідженнях, вільних від будь-яких наближень. Для моделювання сенсорної здатності дозиметрів різних типів запропоновано процедуру скейлінгу. Це дозволяє встановити сферу застосування різних наближень, які використовуються в практичній дозиметрії для пояснення подібних експериментальних даних. Уперше досліджено роль статистичних факторів, що визначають діапазон зміни енергетичних і кінетичних параметрів люмінесцентних процесів реальних дозиметричних матеріалів у формуванні їх сенсорних характеристик. Запропонований підхід може доповнити техніку комп'ютеризованої деконволюції кривої світіння (CGCD), яка широко використовується для оцінки структури енергетичних рівнів і кінетичних коефіцієнтів реальних дозиметричних матеріалів. Можливості нового методу реалізовані в розрахунковому пакеті Lumini.

Ключові слова: дозиметричні матеріали, фосфоресценція, термолюмінесценція, кінетичні рівняння, метод Монте-Карло, пакет Lumini.