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LUMINI PACKAGE FOR AB INITIO MODELING OF DOSIMETRIC EXPERIMENTS

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The paper presents the capabilities of the new Lumini code for ab initio modeling of dosimeter efficiency parameters. It is based on a scaling method that allows unifying the parameters of the kinetic model of the dosimeter without the numerous approximations used to interpret experimental results of thermal-, phosphorescence, and partial illumination of irradiated semiconductors. For the first time, the Monte Carlo method was used to consider the influence of statistical fluctuations in the energy and kinetic parameters of the model on the dosimetric parameters of typical dosimeters. As a first step, the data of Lumini's interpretation of the experimental TLD spectra of 500K dosimeters irradiated on the M-30 microtron was discussed.

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INTRODUCTION

Solid-state dosimetry (SD) is an effective method of fixing and accumulating the energy of nuclear radiation, in some cases even simulating its effect on biological objects [1, 2]. The modern theory of dosimetry uses the concept of accumulation of nuclear energy by luminescence centers in dosimetric materials, which are released by the stimulated release of charge carriers and their annihilation when interacting with charges of opposite signs. Due to their high sensitivity, accuracy, and reliability, such dosimeters effectively monitor radiation levels, which is critical to ensuring the safety of people, the environment, and radiation technology regimes [3].

Constant monitoring of radiation levels allows timely detection of deviations from the norm and taking necessary measures to prevent accidents at nuclear power facilities. Currently, SD-based radiation monitoring systems can be integrated with other security systems, such as access control, emergency warning, and protection systems, which allows for the creation of integrated solutions to ensure radiation safety.

Modern conditions pose new challenges for SDs since intense high-energy nuclear radiation fields when structural damage to dosimetric materials is possible, have become the areas of absorbed dose recording and radiation monitoring [4]. Under these conditions, new approaches are needed, starting with the search and implementation of radiation-resistant materials for SDs [5, 6] and the development of new methods to improve the accuracy and sensitivity of measurements, expand the range of measured doses, miniaturize devices, and integrate them with other dosimetric systems. This will help improve radiation safety in various fields, including medicine, industry, and nuclear power, where nuclear radiation of various types, including neutron, gamma, and electron radiation, and intense mixed radiation fields, is widely used.

Solving these problems requires a new stage of scientific research, modeling the conditions of a dosimetric experiment, which consists of fixing the absorbed energy of nuclear radiation and its release by heating the sample [2, 7] or by optical methods [8–10]. The current situation in practical dosimetry uses numerous approximations to obtain methods for fixing the dose. Such an approach needs to consider the statistical factors that accompany the formation of the energy structure of dosimetric materials and the kinetics of luminescent processes of irradiated materials under thermal or optical excitation. There is a need for ab initio modeling of such processes to establish the optimal structure of energy levels of wide-bandgap semiconductors to improve their sensing properties.

This paper presents the capabilities of the Lumini mathematical package for solving these problems. It is shown that the scaling method allows us to operate with parameters of kinetic equations with an order of magnitude $10^{13}…10^{15}$ and to obtain the first-principle results of their luminescent characteristics, which is essential for dosimetry practice. The structure and capabilities of the package are discussed, in particular, to take into account the natural conditions of a radiation experiment.

1. THEORY BASES OF THE LUMINI PACKAGE

SD is based on wide-bandgap semiconductors in the bandgap of which a particular set of local energy levels is formed. The physics of processes in dosimetric studies within the one-trap-one-recombination center model (OTOR) considers several stages: absorption of nuclear radiation energy; excitation of valence band (VB) electrons to the conduction band (CB) in amounts proportional to the irradiation energy, the same number of holes, m, remains in the VB; redistribution of free CB electrons: n_2 electrons are captured at the level of traps, their number n2 remains in the CZ; neutrality condition $m= n_3= n_1+n_2$.

The kinetics of the processes is determined by the following coefficients: electron capture by traps k1 ($s^{-1}\cdot cm^3$) and their thermal emission in the SC according to the Boltzmann term $k2\cdot\exp(-\varepsilon/(kT))$, k2 is a frequency factor (s^{-1}), ε contains the activation energy of the trap levels in eV and is determined by the difference between the trap level and the bottom of the SC, k is the Boltzmann constant ($8.62\cdot10^{-5}$ eV/T).

Heating of the sample leads to thermal excitation of the trapped electrons and their transfer to the QD, where they can interact with holes at recombination levels, emitting a quantum of light. Although the real picture implies the presence of shallow and deep charge carrier traps and the need to consider the interaction between them, for many practical applications, the problem is reduced to analyzing the transformations of the electron-hole system within a one-level model. Graphically, the situation for OTOR is shown in Fig. 1,a with the zone-level, level-zone transitions, and the kinetic coefficients k1, k2, s that determine their intensity.

However, for real dosimeters, the picture should consider the statistical distribution of trap energy values and frequency coefficients, modeled by the Monte Carlo method (see Fig. 1,b).

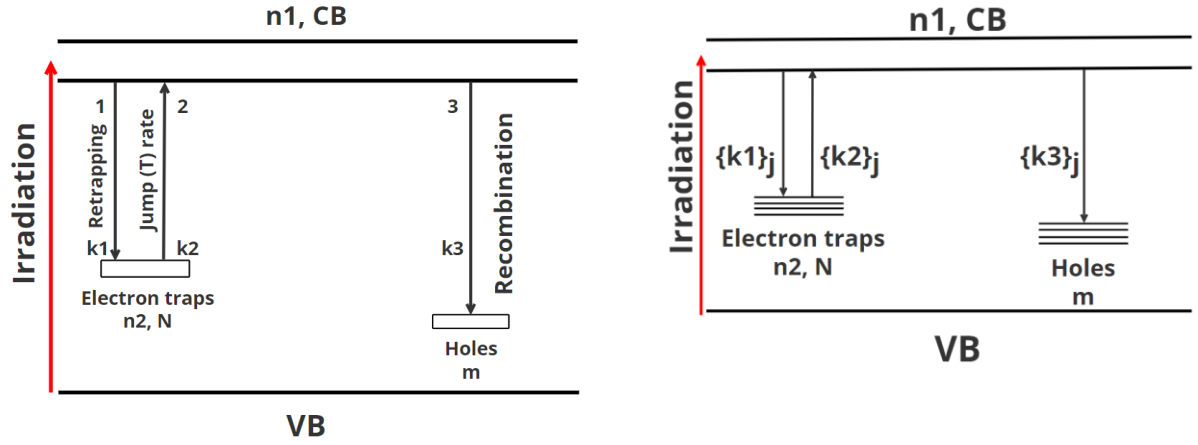


Fig. 1. Energy diagram and structure of electron transitions during the accumulation and release of nuclear energy by thermally stimulated luminescence: a – OTOR model and b – realistic model of dosimetric material considering the statistical disorder of trap energy values and kinetic coefficients

The equations describing the kinetics of transitions for such a model, called OTOR [11] Fig. 1, were first proposed in [12] to explain the phenomenon of phosphorescence. They are as follows:

$$dn_1(t)/dt = -dn_2(t)/dt + dn_3(t)/dt, \quad (1)$$

$$dn_2(t)/dt = k_1 * n_1(t) * (N - n_2(t)) - s * n_2(t) * \exp(-\varepsilon/kT),$$

$$dn_3(t)/dt = k_2 * n_1(t) * n_3(t).$$

Here, N is the meaning of trap concentration. The solution to (1) is sought at the initial conditions $n_1(0) = n_1^0, n_2(0) = n_2^0$. It is interesting to consider the order of the quantities appearing in (1). Thus, the frequency factor s is associated with the frequency characteristics of the semiconductor lattice, setting the range of its change to $10^8 \ldots 10^{14}$ s^{-1}. The concentration of trap N is determined by the degree of doping or defectiveness of the material and can be estimated in the $10^{17} \ldots 10^{20}$ cm^{-3} range. Finally, the concentration of metastable states, h = n_3, formed during irradiation of the dosimeter can be estimated in the range of $10^{16} \ldots 10^{18}$ cm^{-3}, depending on the conditions of the radiation experiment. This fact explains the complexity of the numerical integration of equations (1), so the success of their use for dosimetry problems is associated with works [13–15] that introduced several approximations for their solution and use for TLD problems. In this paper, a scaling procedure is introduced to solve (1): The following transformations of the parameters of the kinetic equations (1) are carried out, here $i = 1 \ldots 3$:

$$n_i^*(t) = \frac{n_i(t)}{n_1^0 + n_2^0} * A, \; k_i^* = k_1 * N \;,$$

$$k_2^* = k_2 * \frac{n_1^0 + n_2^0}{A} \quad \boldsymbol{k_3^*(t) = \frac{n_2(t)}{N}}. \quad (2)$$

The scaling factor A can have different values depending on the order of the initial parameters n_1^0, n_2^0. It is easy to see that the renormalized initial values of the quantities $n_1^*(t), n_2^*(t)$ satisfy the equations:

$$n_1^*(0) = \frac{n_1^0}{n_1^0 + n_2^0} * A, \qquad n_2^*(0) = \frac{n_2^0}{n_1^0 + n_2^0} * A, \quad (3)$$

$$n_1^*(0) + n_2^*(0) = A, \qquad T = b1 + \alpha * b2 * t.$$

Here the meaning of the heating rate is deg/s. When the activation energy, ε, is measured in eV, and the initial temperature T_0 corresponds to 20 ^{0}C, the expression for T gives the values for b1=2.5E-2 eV, b2 =8.6E-5 eV/s. Taking into account the scaling conditions (2), (3), the modified system of kinetic equations is as follows:

$$dn_1^*(t)/dt = -dn_2^*(t)/dt + dn_3^*(t)/dt,$$

$$dn_2^*(t)/dt = k_1^* * n_1^*(t) * (1 - n_2^*/N^*) - s * n_2^*(t) * \exp(-\frac{\varepsilon}{b1 + \alpha * b2 * t}), \quad (4)$$

$$dn_3^*(t)/dt = k_2^* * n_1^*(t) * n_3^*(t).$$

The compact form of the kinetic equations (4), taking into account the scaling conditions (2) and (3), allows for numerical modeling for arbitrary conditions of the dosimetric experiment, as well as proposes a method of going beyond the one-level approximation. Such possibilities were implemented in the Lumini

package, which is based on the algorithm for solving system (4) by the Runge-Kutta method of the 4th order [16] with automatic selection of the integration step at the initial values $n_1^*(0) = n_1^0, n_2^*(0) = n_2^0$.

2. THE CODE STRUCTURE AND FEATURES OF THE LUMINI PACKAGE

The C# programming language and Windows Forms technology were used to create the Lumini software package. The programming tools used are convenient for developing applications in the Windows environment. Thus, C# provides significant opportunities for object-oriented programming, and Windows Forms represents the capabilities of the graphical library for creating applications in the Windows environment, which is part of the .NET platform. The basis of the package is the code for integrating the system (4), using the fourth-order Runge-Kutta method, which allows for ab initio studies of the kinetic processes of irradiated dosimetric materials, according to (1) and (4). Its main idea is to calculate the weighted average of the derivatives at intermediate points within a single integration step. The adaptive algorithm of this method estimates the error at each step and adjusts the integration step. This allows you to use more significant steps in areas with smooth changes and smaller steps where the function changes are more abrupt. Intermediate values are calculated using the Kutt function, which implements the necessary steps for the Runge-Kutta method. Error estimation and appropriate step adjustment ensure the solution's stability and accuracy at each integration stage.

The Lumini program for dosimetric experiments consists of three pages for modeling the phenomenon of thermoluminescence, phosphorescence, and partial emission under a stepwise change in heating temperature, T. The program algorithm is shown in Fig. 2. As can be seen, the software product contains several essential components, each of which performs specific functions to ensure accurate and reliable numerical integration of Eq. At the beginning of the program, the variables are initialized, and the parameters are set, which are necessary for performing numerical integration. This includes declaring constants and variables, initializing arrays, and setting initial conditions. The settings ensure that all variables have the correct initial values, which is critical for the correct operation of the algorithm. The software product consists of two subroutines – one for the graphical display of data and the other for fixing it in a numerical format for further use. The user is presented with the initial program window when the program starts. In the initial window, the "Thermally Stimulated Luminescence" mode is open; the user can stay in this mode or select other modes (Phosphorescence or Partial Luminescence). After selecting the mode, the user must fill in all the necessary fields by entering the initial values of the coefficients. Also, the user can enter the value of the blurring of the activation energy values of the trap levels, or the kinetic coefficients k1-k4 (see Fig. 1,b), using the Monte Carlo statistical test method [17].

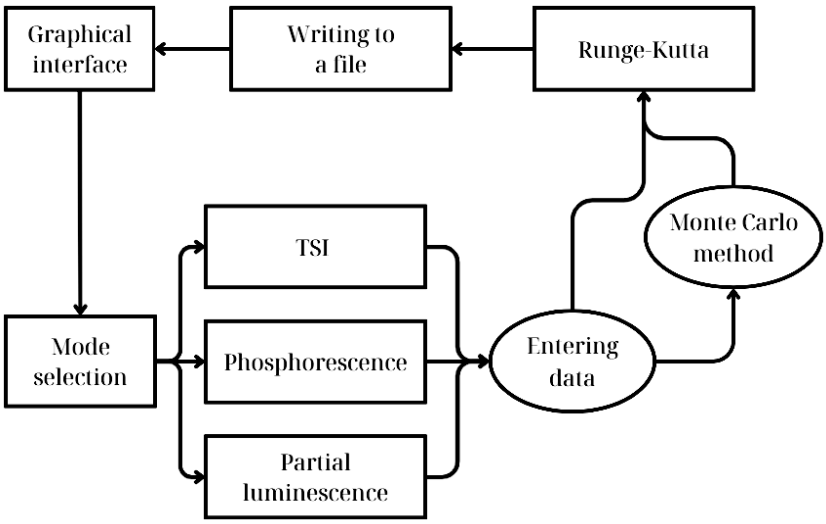


Fig. 2. Flowchart of the Lumini software product operation

After clicking the "Start" button, the coefficients entered are written in the input file. The created input file is processed by an internal program to solve differential equations using the Runge-Kutta method. The solutions obtained are written in the output file, allowing you to save the data for further analysis and use them as a graph on the screen. The program includes several criteria and stop conditions, allowing you to stop the integration when the specified conditions are met (4). The graphical interface of the Lumini package is shown in Fig. 3, which illustrate the result of determining the luminescent characteristics of a model dosimeter with a TSL peak in the vicinity of 150 °C, the initial number of electrons in the conduction band is 10^{13} cm^{-3}, and at the trap levels – $9.9 \cdot 10^{14}$ cm^{-3}.

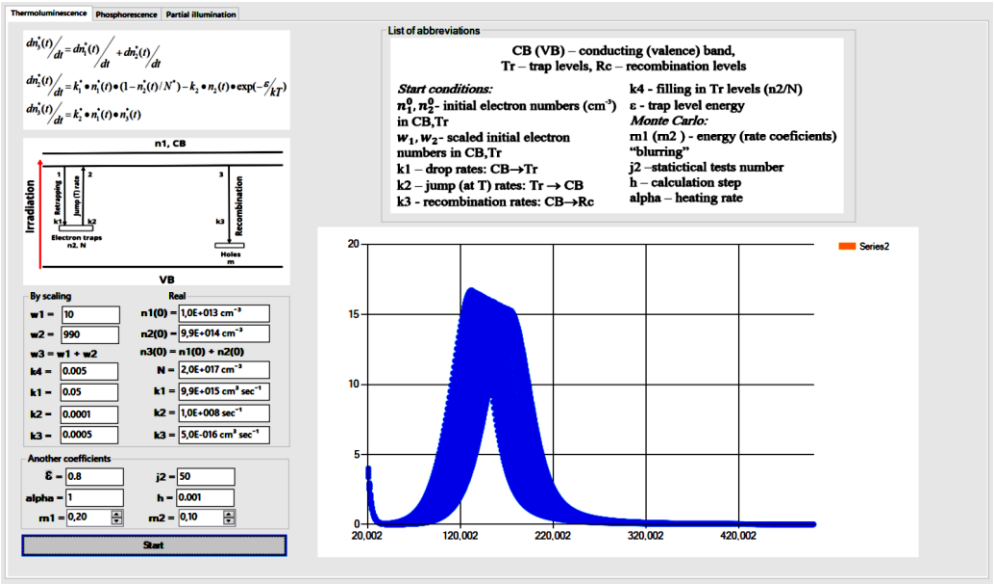


Fig. 3. The initial window of the program product

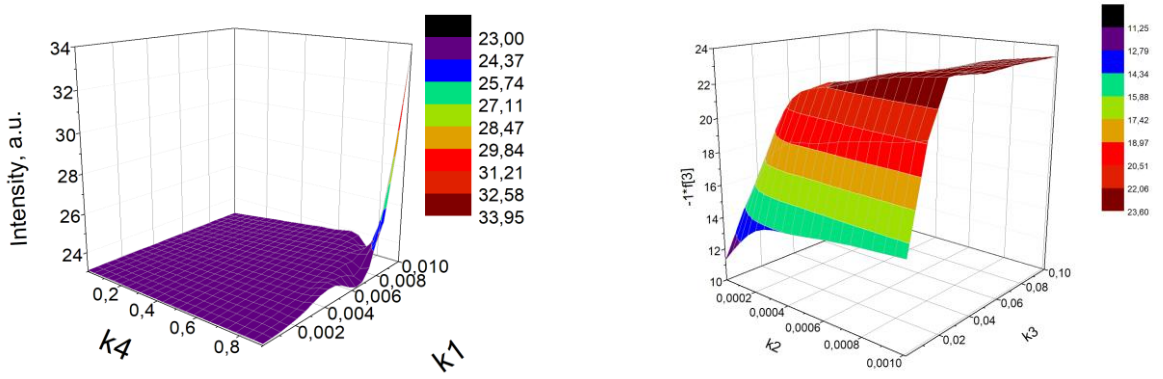
As can be seen, the calculation considered fluctuations in the energy characteristics within 10 and kinetic coefficients of 20%. A feature of the developed Lumini virtual console is that it contains information on scaled and real values of the model dosimeter parameters. As can be seen, the data shown in Fig. 3 are obtained from the numerical integration of equations (4) for the scaling constant A = 1000, i.e., the model parameters vary within $0 \le n_1^*(t), n_2^*(t) \le A$. For real experimental conditions, this corresponds to the values $0 \le n_1(t), n_2(t) \le 10^{15}$ cm^{-3}. By changing the degree of filling of the trap levels with charge carriers through the parameter k4, the Lumini program allows us to estimate their concentration N, which for the data of Fig. 3 is equal to $2 \cdot 10^{17}$ cm^{-3}. The same can be said for the values of the kinetic coefficients k1 and k3 (see Fig. 3). The base part of the coefficient k2 is assumed to be 10^{12} s^{-1}, and by changing its value within the range of 10^{-3} and 10^{3}, it is possible to adjust the value of the frequency factor from 10^{9} to 10^{15} s^{-1}. The k4 coefficient is a dimensionless value and does not change its value during the scaling procedure.

This applies to using the Lumini package to model phosphorescence curves and partial illumination of dosimetric materials. The software allows adjusting the model parameters' values for fitting the experimental TSL and phosphorescence curves using the FOM (Figure of merit) criterion [18], ignoring the concept of first- or second-order luminescence kinetics. This makes it possible to find the energy parameters of a real dosimetric material and the entire array of kinetic coefficients – {k1 – k4}.

3. MODELING OF DOSIMETRIC CHARACTERISTICS WITH THE LUMINI PACKAGE

The resulting Lumini package allows modeling the thermoluminescent characteristics of dosimetric materials for arbitrary values of energy levels and kinetic parameters k1 – k4. This fact, in particular, makes it possible to estimate the errors allowed by the dosimetric theory under the widely used assumption $n_2(t) \approx n_3(t)$, which is permitted under the assumption of a small number of accumulated charge carriers in the conduction zone: $n_1(t) << n_3(t)$. The *ab initio* modeling capabilities of the Lumini package allow us to conduct a set of studies of the influence of the kinetic coefficients on the luminescent characteristics of semiconductors and to use the TSL experimental data to establish the energy structure and kinetic parameters: the position and intensity of the luminescence maxima, as well as their heating rate.

For such studies, a model dosimetric material containing one level of traps for electrons with an activation energy of 0.8 eV was chosen; the initial values of the concentrations of electrons trapped at the trap level are: $n_1^0 = 10^{13}\text{cm}^{-3}, n_2^0 = 10^{15}\text{cm}^{-3}$, the concentration of traps is given by equation $N = n_3^0 / k4$ cm^{-3}. Fig. 4 shows the results of modeling the efficiency of such a dosimetric material, i.e., the value of the TSL signal $I = -dn_3(t)/dt$ depending on the values of the model kinetic coefficients, which are chosen in a dimensionless scaled form (4). Equation (1) and transformation (2) should be performed to obtain the initial values of these coefficients. The dependence of Fig. 4,a demonstrates the value of the TSL signal *I=I(k1, k4)*, i.e., on the rate of fall of charge carriers from the conduction zone (CZ) at the level of traps, k1, depending on the degree of their filling, k4, at fixed values of the real coefficients k2=10^{9} s^{-1}, k3 = 10^{-14} cm^{3}·s^{-1}. It can be seen that a significant luminous power of TSL is achieved at a considerable degree of filling of the trap levels and high rates of their filling with electrons of the WP, and this effect is local for a given set of parameters {k1 – k4}. Fig. 4,b shows the same dependence of TSL *I=I(k2, k3)*, i.e., on the frequency factor of thermal emission of trap levels in the ZP k2 and the rate of annihilation of ZP electrons in the interaction with valence band holes, k3, at fixed initial values of k1=10^{13} cm^{3}·s^{-1} and a significant degree of filling of the trap levels, k4 = 0.9.

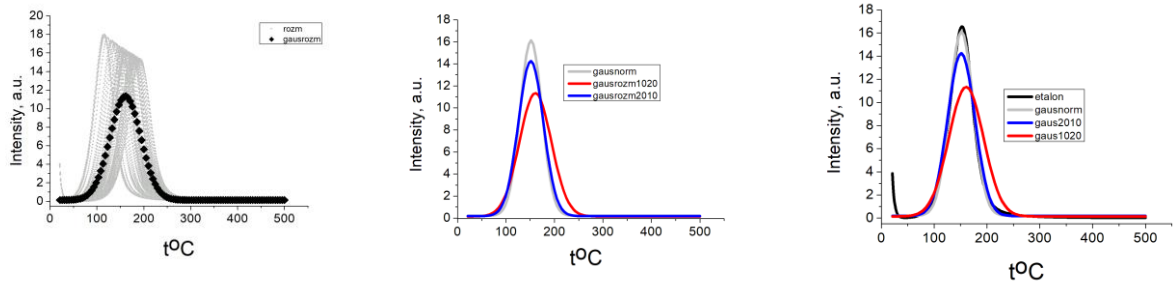


a *b*

Fig. 4. Dependences of intensity, I, TSL of dosimetric material on the degree of filling of trap levels and values of kinetic coefficients of luminescent processes: a – dependence I=I(k1, k4) at fixed parameters k2, k3; b – the same dependence I=I(k2, k3). The data were obtained with the Lumini package

For this set of parameters, the height of the maximum TSL peak is only 0.7 of the same value obtained in Fig. 4,a. The results presented in Fig. 4 indicate the methodology for the targeted selection of dosimetric materials according to their efficiency for radiation measurements.

Although practical dosimetry is based on the one-level model shown in Fig. 1, the proposed Lumini package allows us to go beyond these approximations and take into account the statistical nature of the distribution of trap levels $\varepsilon \rightarrow \{\varepsilon_i\}$ and kinetic coefficients $k_j \rightarrow \{k_j\}_i$, j = 1, 4 using the Monte Carlo method. Fig. 5 shows the results of the calculation intensity of the dosimeter material, taking into account the method of statistical tests and different degrees of "blurring" of the energy and kinetic parameters of the model.



a *b* *c*

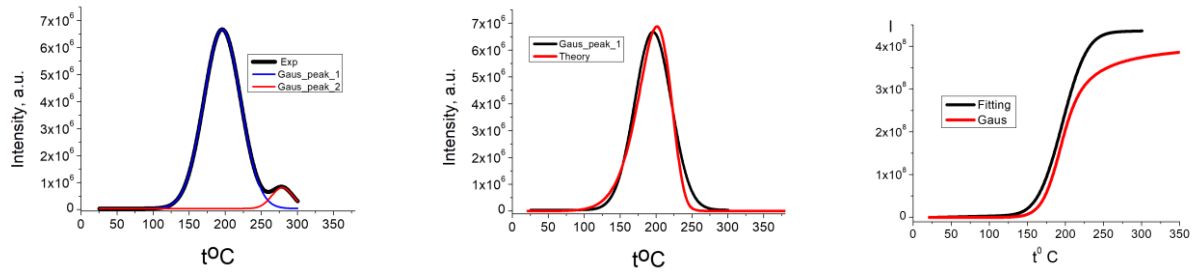
Fig. 5. Data of statistical modeling of the Lumini package of the effect of fluctuations in the energy and kinetic parameters of dosimeters on their efficiency Here a – TSL curves taking into account fluctuations of the arrays $\{\varepsilon_i\}$ within 5% and $\{k\}_{ji}$, – 10%, the solid line is the result of Gaussian filtration; b – the values of the original TSL and Gaussians approximating the TSL arrays with blurring of energy and kinetic parameters, respectively, within 10, 20% and 20, 10%

The calculations were performed with the following parameters of the energy structure of the dosimeter: $n_1^0 = 1.0 \cdot 10^{13}\,\text{cm}^{-3}, n_2^0 = 9.9 \cdot 10^{14}\,\text{cm}^{-3}$, $N = 2.0 \cdot 10^{16}\,\text{cm}^{-3}$, $k1 = 9.9 \cdot 10^{-16}\,\text{cm}^3 \cdot \text{s}^{-1}$; $k2 = 1.0 \cdot 10^{8}\,\text{s}^{-1}$; $k3 = 5.0 \cdot 10^{-12}\,\text{cm}^3 \cdot \text{s}^{-1}$; k4 = 0.05. Fig. 5,a demonstrates the nature of such a blurring of the TSL signal and the approximation of the resulting array of values by the Gaussian function. Figs. 5,b and c show how the choice of intervals of "blurring" of energy and kinetic parameters affects the efficiency of the TSL technique for dosimetry.

Finally, Fig. 6 shows the results of using the Lumini package to fit the experimental data of the TLD 500K dosimeter based on leucosarphyrin Al_2O_3:C irradiated in an electron beam with an energy of 18.5 MeV [19]. The accuracy of the fit was evaluated using the Figure Of Merit (FOM) criterion [18]:

$$FOM = \frac{\sum_i | Y^i_{\text{exp}} - Y^i_{fit} |}{S}. \qquad (5)$$

Here Y^i_{exp} та Y^i_{fit} – are the i-values of the experimental and fitted TSL curve obtained by the Lumini package, i=1, N; S is the area of the curve under the experimental TSL curve.



a *b* *c*

Fig. 6. Stages of fitting the experimental and theoretical TSL dependence with the Lumini package. Here a – the procedure for deconvolution of the experimental TSL dependence by two Gaussians; b – fitting the obtained Gaussian with the Lumini package; c – estimation of the fitting accuracy through the areas of the experimental and fitted TSLs, the FOM value is 11.2 %

The approximating curve in Fig. 6,b is obtained with the following values of the Lumini package coefficients: $n_1(0) = 1.0 \cdot 10^{15}$ cm^{-3}, $n_2(0) = 4.2 \cdot 10^{20}$ cm^{-3}, $k_4 = 0.039$ cm^{-3}, $N = 1.1 \cdot 10^{22}$ cm^{-3}, $k_1 = 5.3 \cdot 10^{13}$cm$^3 \cdot$s^{-1}, $k_2 = 1.0 \cdot 10^{13}$ s^{-1}, $k_3 = 4.8 \cdot 10^{18}$ cm$^3 \cdot$s^{-1} $\varepsilon = 1.31$ eV, which corresponds well to the values obtained in [16]. Using the formula (5) to determine the FOM and the data in Fig. 6,c, we estimate the approximation accuracy to be 11.2%.

CONCLUSIONS

Thus, the proposed Lumini package allows us to go beyond the OTOR model when evaluating typical dosimetric materials' TSL and phosphorescence phenomena. The data obtained in this case belong to the ab initio class since they are free from restrictions on the coefficients of luminescent transitions in the substance. The scaling methodology, which is the basis of this package and allows unifying the parameters of the kinetic model of the dosimeter and going beyond the numerous approximations used in practical nuclear radiation dosimetry, is discussed. Data on the algorithm, structure, and services of the Lumini package are presented, which allows us to evaluate the class of problems that can be solved within its framework. For the first time, it is possible to consider the influence of statistical fluctuations of energy and kinetic parameters on dosimetric parameters of practical studies. The prospects of using the Lumini package for modeling and predicting the efficiency of real dosimeters, highlighting the critical model parameters responsible for the sensitivity and reliability of dosimetric measurements, are shown. In the example of data from TLD 500K dosimeters, the theoretical dependences obtained by the Lumini package were fitted to the experimental spectra of TSL obtained on the M-30 microtron.

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ПАКЕТ LUMINI ДЛЯ AB INITIO-МОДЕЛЮВАННЯ ДОЗИМЕТРИЧНИХ ЕКСПЕРИМЕНТІВ

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Представлено можливості нового коду Lumini для ab initio-моделювання параметрів ефективності дозиметрів. В його основі лежить метод масштабування, який дозволяє уніфікувати параметри кінетичної моделі дозиметра без використання численних наближень, що використовуються для інтерпретації експериментальних результатів термо-, фосфоресценції та часткового висвітлення опромінених напівпровідників. Вперше застосовано метод Монте-Карло для розгляду впливу статистичних флуктуацій енергетичних і кінетичних параметрів моделі на дозиметричні параметри типових дозиметрів. Як перший крок обговорено дані інтерпретації за допомогою Lumini експериментальних спектрів TLD-дозиметрів 500K, опромінених на мікротроні М-30.