Information-measuring methods for controlling physical parameters as information system building element

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Abstract. A method for measuring the parameters of photostimulated processes in an ion-covalent crystal is considered. An information measurement model for AgCl and CdS:Ag crystals was built. A correlation-regression model for describing the process of cluster formation in luminescent crystals was developed. An algorithm for using the information-measuring model as part of the information-measuring complex for controlling technological processes by the method of photostimulated luminescent flash is presented.

1. Introduction
Automation of production technology control is an urgent task of modern production. In particular, the problem of developing and improving information-measuring methods for monitoring the physical parameters of objects with a size of several nanometers remains relevant. Photostimulated processes play an important role in semiconductor systems [1,2]. The method of a photostimulated flash of luminescence was successfully used to determine the qualitative changes in objects on the surface of luminescent wide-gap solids [3]. An information-measuring model for assessing the physical characteristics of luminescent condensed media is considered in this article.

2. Main part
When a new phase is formed, objects of several angstroms in size do not manifest themselves in the absorption and electrical conductivity spectra. This is due to the low concentration of such objects. To study them, special methods are required. The method of a photostimulated flash of luminescence makes it possible to receive a signal from objects whose dimensions are only a few nanometers. Moreover, without destroying unstable low-atomic clusters [4].

The development of information-measuring methods is of practical interest. The construction of a mathematical model allows us to propose algorithms for the application of new methods for controlling the processes of nucleation or modification of centers with the participation of ions or atoms of the metal Men in crystals with ion-covalent bonds.

To build the models, kinetic modeling of nonequilibrium processes was used. To measure the parameters of the observed processes, we used the method of photostimulated luminescence flash (PSLF) [4].
The PSLF method consists in the fact that if there are deep traps of nonequilibrium charges in the band gap of the condensed medium, the concentration of such traps can be fixed by scanning the band gap of the crystals with resonance radiation [5]. A luminescence flash appears as a result of the capture of a quantum of light by an electron, which is localized in a deep trap.

A band diagram of crystallophosphorus having local levels (electron traps) is shown in figure 1, where \( N_i \) is the concentration of electron traps of type \( i \); \( n_i \) is the concentration of type \( i \) traps that capture an electron; \( \delta_i \) and \( \omega_i \) are the probabilities of electron capture into the trap and ionization of the trap, respectively; \( N \) is the concentration of glow centers; \( n \) is the concentration of ionized emission centers; \( \beta \) is the probability of recombination of a free electron with a center of emission.

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\begin{align*}
\gamma & \quad \delta_1, \omega_1 \quad N \quad n_1 \\
\beta & \quad \delta_2, \omega_2 \quad N_2 \quad n_2 \\
& \quad \vdots \quad \vdots \\
\end{align*}
\]

**Figure 1.** The band diagram of crystallophosphorus in the presence of deep electron traps after excitation of the sample with UV

For the PSLF method, the main registration method is the photon counting method. The signal-to-noise ratio is more than 10. Therefore, the number of deep traps in the band gap of a solid can be measured.

Adsorbed metal clusters (\( N < 10 \)) form deep traps. As a result of irradiation of the sample with ultraviolet light, the traps become filled. Then the sample is irradiated with infrared light. From the conditions of the experiment, we can assume that \( \omega_1 = 0 \). For \( j \) traps \( 0 = 0 \) for \( i = 1, \ldots, k; i \neq j \). Taking into account the approximations, the system of kinetic equations is written as follows:
In the approximation of the absence of re-capture of nonequilibrium carriers, we have the following solution of the system:

$$I(t) = \sigma_j I_0 \exp \left( -\sigma_j t \right)$$  \hspace{1cm} (2)

$$S_0 = I(0) = \sigma_j I_0$$  \hspace{1cm} (3)

$$K_k = \frac{S_0}{S_{\infty}} = \sigma_j I - \sigma_j (1 - \text{const})$$  \hspace{1cm} (4)

$S_0$ is the amplitude of the PSLF, and $S_{\infty}$ is the total accumulated light sum.

The PSLF method is a universal method that allows you to measure the number of centers of localization of nonequilibrium charges in crystallophosphorus. This method determines the effective cross section for the absorption of IR light by the localization center, which is proportional to their size [8].

For most luminescent crystals with an ion-covalent bond, a decrease in the luminescence intensity under the action of high doses of UV occurs due to the formation of metal particles on the surface of the crystals ($\text{Me}_n$, $n > 2$).

To describe the process of formation of metal clusters on the crystal surface, one can use the model of mutual transformation of two types of centers [8]. We use the following notation: $x_0$ is the initial concentration of metal adatoms on the crystal surface, and $X$ is the concentration of places on the crystal surface where adsorption of adatoms is possible. $y$ is the concentration of low-atomic metal clusters, and $Y$ is the concentration of meth adsorption. For low-atom clusters, the approximation $x_0 \ll X$ and $y \ll Y$ will be performed. At the initial time, only adsorbed metal atoms are on the surface of the crystal:

$$\begin{cases}
\frac{dy}{dt} = A \cdot x - B \cdot y \\
\frac{dx}{dt} = B \cdot y - A \cdot x \\
x_0 - x = m \cdot y
\end{cases}$$  \hspace{1cm} (5)

In the last equation of system (5), the coefficient $m$ determines the average number of centers of type $x$ in $y$. Solving (4), we obtain:
Metal atoms and low-atomic metal clusters adsorbed on the surface of crystals have a set of energy levels in the band gap of the crystal [6], therefore, they will manifest themselves in PSLF [5,6].

By measuring the parameters of PSLF, it is possible to estimate the size of the formed centers by the formula $\frac{S_x^\infty}{S_y^\infty}$.

The presented model of the process of formation of low-atomic metal clusters shows that using the PSLF method it is possible to control the size of small metal clusters [7].

It is proposed to use the method of correlation and regression analysis to assess the feasibility of using the PSLF method to control the parameters of surface processes in luminescent condensed media with a mixed type of bonds.

The data on the change in the PSLF parameters for the AgCl crystal led to the conclusion that there is a correlation between the PSLF parameters [8]. The data shown in figure 2 were analyzed. It was possible to construct a correlation-regression model for the relationship between the kinetics coefficient $K_k$ and the total accumulated light sum $S$. The result is shown in figure 3. The coefficient $R^2$ does not change depending on the excitation energy and is 0.91. The regression equation is represented by the formula (7).

$$y = 1.07x + 1.13$$

This correlation-regression model confirms the possibility of using the PSLF method to assess the formation of low-atomic clusters in crystals in ion-covalent crystals AgCl and AgBr. For a CdS: Ag crystal, the correlation coefficient is $R^2 = 0.78$. A change in the value of $R^2$ indicates that the processes of cluster formation in crystals with an A$^II$ B$^{VI}$ lattice are more complex than in AgCl [9].

The obtained regression model (7) clearly indicates that with an increase in the concentration of the treatment solutions, the number of clusters decreases and the cluster size increases.

![Figure 3. Graph of correlation between S and Kk for AgCl.](image-url)
The algorithm for applying the PSLF method to control the technological process, taking into account the application of the criterion for determining the parameters $K_k$ and $S_\infty$ upon receipt of the calibration table.

The value of the correlation coefficient $R^2$ is a condition for assessing the applicability of the model.

Based on the proposed measurement technique, an algorithm was built. This algorithm can be applied in the development of equipment for the control of technological processes involving luminescent condensed media with a mixed type of coupling.

Firstly, a calibration table of PSLF parameters is compiled (the right branch of the algorithm). If there are calibration tables in the database that are similar to the working process conditions, the process of controlling the manufacturing technology by the PSLF method (the left branch of the algorithm) is started.

3. Conclusion

The results of the studies allow us to conclude that it is possible to use the PSLF method to control the concentration of localization centers of nonequilibrium carriers provided that there is a correlation between the PSLF kinetics coefficient and the total stored light sum.

Consideration of model crystals to test the criteria for using the PSLF method within the framework of the cluster formation model and taking into account the possibility of estimating cluster sizes showed that the PSLF method works well for AgCl crystals. In this case, the determination coefficient is about 1. For CdS and ZnS crystals, the values $R^2$ of the determination coefficient allow us to speak about the possibility of using the PSLF model (value 0.8). Therefore, it is necessary to conduct additional studies depending on the structure of the studied objects and chemical composition.

The method of controlling the concentration and degree of dispersion of adsorbed metal clusters, based on the PSLF method, allows us to select conditions for controlling the formation of low-atomic clusters and the formation of metal clusters of specified sizes on the surface of luminescent condensed media on the basis of regression analysis.

This model can be extended to a wider class of condensed matter having levels of localization of nonequilibrium charges in the band gap and exhibiting luminescent properties.

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