

## **MODELLING OF RAPID STAGE DECAY OF SIGNAL OF OPTICAL SENSOR BASED ON HETEROSTRUCTURE CdS-Cu<sub>2</sub>S**

Odessa I. I. Mechnikov National University,  
2, Dvoryanskaya str., Odessa, 65082, Ukraine

Phone: +380(48)7266356, Fax: +380(48)7233461, e-mail: borschak\_va@mail.ru

The work is devoted to modeling and calculation of the spatial distribution of the concentration of charge localized in the space charge region (SCR) heterojunction, this distribution changes with time at different initial filling of deep traps centers nonequilibrium holes. Within the framework described model the theoretical calculation of two characteristic stages of relaxation current, compliance with the calculated and experimentally obtained dependencies was demonstrated.

### **Samples obtaining procedure**

Technology of the Cu<sub>2</sub>S layer formation is briefly discussed above. The semiconductor grade purity of used CdS powder was checked and controlled by XPS technique (X-ray photoelectron spectroscopy) at respective production facilities. Cartridge with CdS films after cooling to room temperature were transferred to the next vacuum chamber department, where evaporation of CuCl was carried. The graphite mask was used for CuCl film configuration. It was found out technologically that complete evaporation of CuCl powder in an amount of 0.3 g at evaporator temperature 650 ° C during 7-10 min leads to creation of CuCl layer of desired thickness  $\approx 1$   $\mu$ m. Substrate temperature during evaporation of CuCl changed within 180 - 240 ° C.

Then, the cassette with CdS-CuCl layer structure samples was moved into the third section of the vacuum chamber was set to the heater - a flat metallic stove, parallel to the sample surface on 1 cm distance. For 10 - 15 sec sample temperature reached 200 ° C and further maintained constant throughout the process of heterojunctions formation. As a result of such heat treatment the substitution reaction proceeded in CdS-CuCl layer system by the scheme:  $\text{CdS} + 2\text{CuCl} \rightarrow \text{Cu}_2\text{S} + \text{CdCl}_2$ .

CuCl film thickness and annealing time were chosen experimentally so that all of copper chloride could react with the upper layer of CdS (near 1  $\mu$ m thickness, this is the value of CdS layer loss). The best results were obtained with heat treatment time  $\approx 3$  minutes. Cu<sub>2</sub>S thickness directly determined by the initial thickness of the initial layer of CuCl. Thus, the use of different modes, in which time evaporation varied from 4 to 12 min, allowed to receive Cu<sub>2</sub>S layer thickness in the range from 200 to 1000 nm. The optimal parameters (temperature and time of formation) to maximize the reaction completeness were obtained experimentally by checking the value of the open circuit voltage and short circuit current through heterojunctions, obtained by using these or other processing parameters. Uniformity of Cu<sub>2</sub>S layer was determined by initial CuCl film uniformity and was controlled by using microscopic techniques.

Homogeneous Cu<sub>2</sub>S film is formed throughout the sample area, despite local differences in the rate of growth. A prerequisite for this is a complete depletion of copper chloride during the reaction. The formation of a homogeneous film thickness is due to the fact that each part of a copper chloride layer can react only with its adjoining part of the CdS layer.

During the reaction two Cu<sup>+</sup> ions and one Cd<sup>2+</sup> ion must diffuse in opposite directions through the constantly growing films of copper sulfide and cadmium chloride. Sulfur atoms must stay on one side, and the chlorine atoms - on the other side. As a result of this process, the entire surface is covered with a layer of cadmium chloride, which is easily removed by distilled water. But several phases of Cu<sub>x</sub>S, such as Cu<sub>1.96</sub>S Cu<sub>1.92</sub>S and other can be formed during the substitution reaction due to different diffusion velocities of the reaction components and lack of Cu<sup>+</sup> ions in reaction zone as a result. Other observed phases of copper sulphide appear because of sample time degradation (copper atoms diffusion from Cu<sub>x</sub>S to CdS layer).

### Charge distribution modeling

Consistent with the experimental data model of the processes responsible for the kinetics of decline in short-circuit current CdS-Cu<sub>2</sub>S, based on the description of thermal and tunneling mechanisms to release localized charge in the absence of photoexcitation, ie case descending relaxation was developed. Kinetics of non-equilibrium concentration of holes in traps in this case is described by the equation [1-3]:

$$\frac{dp_t}{dt} = -p_t \bar{v} S_{pt} P_v \exp\left(-\frac{E_t}{kT}\right) - p_t \bar{v} S_{pt} P_v D_1(x) - p_t \bar{v} S_{nt} n_0 D_2(x) \quad (1)$$

where  $\bar{v}$  – carriers thermal velocity,  $S_{pt}$  and  $S_{nt}$  – capture cross section for electrons and holes,  $n_0$  – free electrons concentration in CdS,  $D_1(x)$  and  $D_2(x)$  – tunnel transparency coefficients.

Each of the terms describing the devastation traps through a mechanism - thermal emission, tunneling of trapped holes in the valence band electron tunneling Cu<sub>2</sub>S and CdS conduction band with subsequent recombination in the SCR. Evaluation of the contribution of tunneling in the process of relaxation of the trapped charge is made by calculating the second and third terms of the right side of equation (3), while the probability of tunneling transmission coefficient determined by the values corresponding barriers D1 (x) and D2 (x), which strongly depend on the coordinates

[2]. To determine the transmission coefficient for tunnel junctions used semiclassical approximation. This takes into account that in the real case the form of the barrier, and with it the transparency coefficients tunnel (respectively the concentration of trapped holes) change over time. That is, the kinetic equation (1) there are values that explicitly depend on time.

The concentration of trapped positive charge  $p_t(x, t)$  in the real case depends on the coordinates and the time directly determines the shape of the potential barrier structure. A building in the course is associated with the intensity of tunnel junctions as coefficients tunnel transparency is dependent on the profile  $\varphi(x)$  of the barrier [4, 5]. Values are coefficients tunnel transparency, in turn, are present in the expression describing the kinetics of changes in the concentration of trapped holes

$\frac{dp_t}{dt}$ . Thus, to describe the real situation of  $p_t(x, t)$  distribution the self-consistent equations were derived from the scheme:

$$p_t(x, t) \rightarrow \frac{d^2 \varphi}{dx^2} \rightarrow \varphi(x, t) \rightarrow D_{1,2}(x, t) \rightarrow \frac{dp_t}{dt} \quad (2)$$

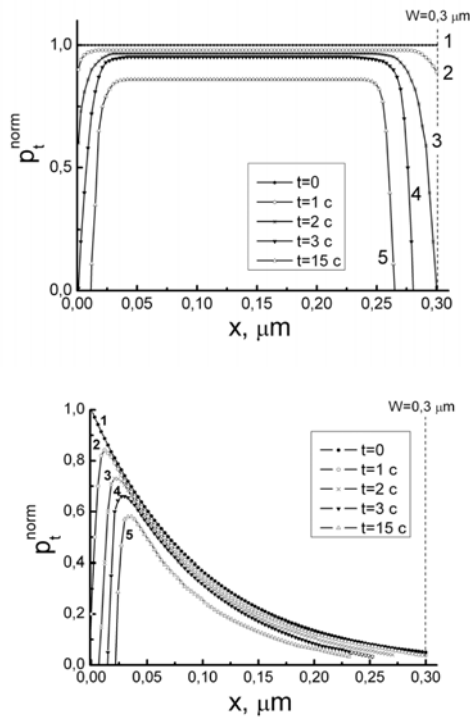
Described model with thermal release mechanism allows for tunnel release trapped holes in the traps, which prevails in the initial phases of changes in the concentration of space charge. This gained in photoexcited charge is actually the optical information carrier, fixed sensor, so the devastation traps determines the memory effect and re-reading sensor signal.

The results of modeling calculations and nonequilibrium charge distribution localized in the barrier HJ based tunneling charge transport mechanisms. Within The model used in the calculation of two cases of initial concentration distribution of trapped holes at  $t = 0$ : the case of complete filling centers traps, exponential distribution and concentration of positive charge (Fig. 1).

For numerical calculation solution program used MathLab and Octave, where computer-implemented Dormand method Prince (Runge-Kutt variation), which is widely used for finding

the solution of ordinary differential equations. The initial set barrier width  $W$  of the coordinate  $x$  was divided into 100 points, and the value of  $\Delta t$  was set equal to 0.1 sec. These steps were selected partition for reasons of compliance accuracy further building are calculated from recession photocurrent accuracy of the experimental curves.

The simulation results of the process to reduce the concentration of trapped charge-trap centers in the SCR GP presented in Figure 1. Calculated data are presented as a set of normalized ( $p_t(x,0) = N_t \equiv 1$ ) curves of the spatial distribution of concentration  $p_t^{norm}$  at certain values of time  $t$ , elapsed after photoexcitation termination (at  $t = 0$ ).



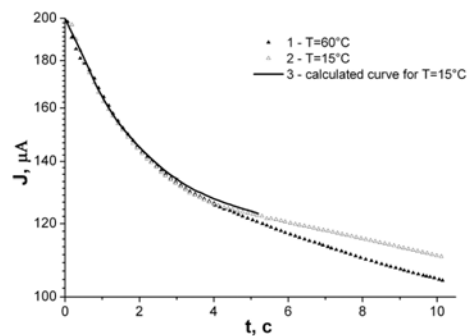
**Fig. 1. Calculated dependence of  $p_t$  concentration distribution profiles of holes captured in the traps in the initial full (a) and exponential (b) distribution of concentration. Profiles are normalized.**

The results of modeling dependencies sensor signal decline after cessation of photoexcitation and comparing them with the experimentally obtained relaxation curves were obtained. The analytical expressions that show the connection of nonequilibrium charge distribution in the

SCR, the shape of the potential barrier and heterojunction with a value of short-circuit current through the sample. The principal difference between the proposed and the method used process modeling short circuit photocurrent relaxation (ie, sensor signal) from the previously described are not only taking into account a change in the distribution of quadratic potential barrier near heteroborder on the exponential of the latter CdS, but also quantitatively account tunneling effects [6, 7]. Thus, the model takes into account the demonstrated dramatic change in the transparency of the tunnel barrier and subsequent relaxation effects concentration of trapped non-equilibrium charge and current through GP after termination of photoexcitation [7].

It was found that the best matching relaxation curves calculated short-circuit current of the experimentally obtained values achieved using exponential terms in the modeling of the spatial distribution of the initial concentration of trapped holes in deep traps, which act as carriers of captured optical information in the studied sensor structure.

Within the framework described model the theoretical calculation of two characteristic stages of relaxation of current when first performed this calculation depends on the concentration of trapped deep trap charge with time for a quick relaxation phase, which is caused by the process of tunnel release charge (Fig. 2).



**Fig. 2. Experimental (individual points) and calculated (solid curve) short-circuit current dependences in case of initial exponential filling of traps by nonequilibrium holes at the stage of fast relaxation.**

## Conclusion

It is shown that the experimentally obtained dependence is modeled using only one type of traps involved in the accumulation of charge in the SCR. The settlement established by the energy position  $E_t$ , capture cross section  $S_{pt}$  and concentration  $N_t$  trap centers involved in the processes of capture of nonequilibrium holes whose values held to agreement between experimental and theoretical curves of obtained short-circuit current recession:  $E_t = 0.32$  eV,  $S_{pt} = 3 \cdot 10^{-14}$  cm<sup>2</sup>,  $N_t = 1.4 \cdot 10^{17}$  cm<sup>-3</sup>. This value is the energy depth of the trap is in accordance with the experimentally obtained changes in research capacity barrier heterojunction.

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*V. A. Borschak, V. A. Smyntyna, Ie. V. Brytavskiy*

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**Key words:** nonideal heterojunction, image sensor, deep traps, tunneling.