INVESIGATION OF THE BEHAVIOR OF POINT DEFECTS IN CdS_xSe_{1-x} SEMICONDUCTOR NANOCRYSTALS

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1. Introduction

A new branch of the semiconductor physics is related to the study of the optical and electric properties of the smallest semiconductor crystals with size of several nanometers [1,2]. Recent interest in the semiconductor nanocrystals in silicate glass has been driven by the applications in optoelectronic devices, fluorescent labels in bioengineering, and window materials in solar cells [3,4].

In comparison with bulk semiconductors, nanocrystals exhibit limitation on the motion of electrons and hence energy quantization. The positions of discrete energy levels depend on the size and shape of nanocrystals [5, 6]. The calculations of the energy spectra are normally performed with allowance for the distribution of the periodic energy potential and limitations on the motion of electrons in the presence of a periodic field. However the electron microscopy [7,8] shows imperfect crystal lattice at the initial stage of the nucleation in nanocrystals. Thus, nanocrystals exhibit both periodic and random potentials that contribute to the formation of the band structure.

In this work, we study the effect of structural defects on the optical properties of the CdS_xSe_{1-x} semiconductor nanocrystals in silicate glass.

2. Experiment

The CdS_xSe_{1-x} nanocrystals in silicate glass were fabricated using the procedure of [9]. The samples differ from each other by mean sizes of nanocrystals and degrees of perfection of crystal lattice. Two types of samples were investigated: in the first series`T of samples the formation of semiconducting nanocrystals corresponded to a thermal treatment temperature of $530^0$C and the second series` A of samples of 510^0C.The temperature of the heat treatment is reached over one hour, then the samples are stored at a constanat temperature (sample T_1 is not thermally processed and the processing times of samples T_2 –T_8 at a temperature of 530^0C are t_2=5 min, t_3=15 min, t_4=35 min, t_5=65 min, t_6=125 min, t_7=245 min and t_8=425 min, sample A_1 is not thermally processed and the processing times of samples A_2 –A_{15} at a temperature of 510^0C are t_2=10 min, t_3=15 min,t_4=30 min, t_5=80 min, t_6=120 min, t_7=180 min, t_8=270 min, t_9=420 min, t_{10}=510 min, t_{11}=630 min, t_{12}=810 min, t_{13}=1050 min, t_{14}=1410 min,and t_{15}=1890 min.).

The transmission spectra studied in the wavelength interval 300-900 nm using Ocean optics USB-4000 spectrometers.

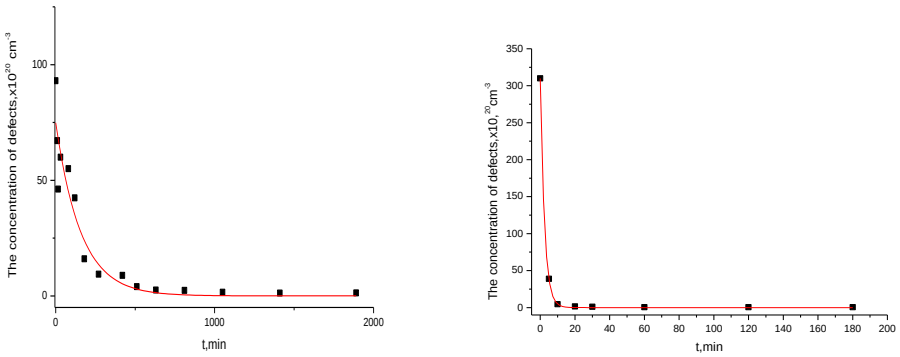
In this work, through the study of the optical transmission spectra to determine the behavior of point defects in the $CdSxSe_{1-x}$ nanocrystals, which are in various stages of formation.The spectral dependence of absorption coefficient the studied samples of the range where the absorption is weak $\alpha = f(h\nu)$ has an exponential. This dependence in non-crystalline materials, known as the Urbach`s "tail". The main mechanism explaining the exponential dependence is associated with the presence of disorder at the atomic level in these structures.The exponential part of the dependence $\alpha = f(h\nu)$ obeys the Urbach rule:

$$\alpha = \alpha_0 \exp\frac{(E_g - h\nu)}{E_0}, \qquad (1)$$

where E_g is the band gap, $h\nu$ is the energy of the incident photon, E_0– is the characteristic energy that characterizes the edge steepness and carries information about the standard deviation of interatomic distances. For the characteristic energy in [10] obtained a formula.

$$E_0 = 2.2W_B(N_t a_B^3)^{2/5}, \qquad (2)$$

where $W_B = e^2/2\varepsilon a_B$, a_B is an exciton Bohr radius, Ɛ-dielectric constant, N_t-the effective concentration of charged centers. Figure 1 a and b shows dependence of the effective concentration of defects on the heat treatment time, which was defined using formula (2), for samples T and A series, at temperature 530^{0}C and 510^{0}C.



a) b)

Fig. 1. Dependence of the effective concentration of defects on the heat treatment time. a) for samples T and b) for samples A.

Law changes in the concentration of defects is well described by the formula $N = N_0 e^{-\frac{t}{\tau}}$, where N_0 is the defect concentration in the samples before heat treatment, and τ is the relaxation time of defects. At a temperature of 510^{0}C defects relaxation time was 158 min., and at 530^{0}C 2.4min. Such a strong dependence of the relaxation time of the heat treatment temperature recalls that the recovery process of defects has a thermal activation character.In such cases, the connection between the relaxation time and the diffusion activation energy can be written in the form

$$\tau = \tau_0 \exp(\frac{E_{diff}}{kT}), \qquad (3)$$

where E_{diff} is a diffusion activation energy.Taking into account values of the relaxation times, the activation energy of diffusion of molecules dissolved in the silicate glass was determined, which is about 8eV.

The presence of defects in the nanocrystals from the energy viewpoint is equivalent to the formationof discrete levels in the band gap. Absorption at these levels is the cause of the Urbach tail. Decrease the concentration of defects should lead to a reduction in the width of the Urbach tail. Fig. 2 shows the dependence of the width of the exponential region of the heat treatment time for the sample series A.

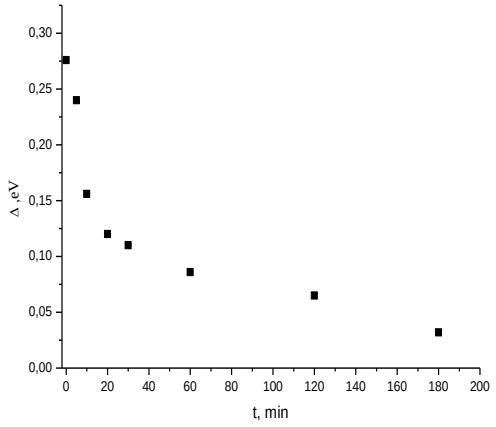


Fig.2. Dependence of the width of the exponential region of th treatment time for the sample series A.

The obtained dependences confirm the assumptions made, that is: the larger the heat treatment temperature, the faster the formation of crystal lattice in nanocrystals

3.Conclusions

Thus, by means of optical transmission spectra investigated dependence of the concentration of point defects in nanocrystals of heat treatment time. It is shown that the recovery process of defects has thermal activation character. It estimates the activation energy of diffusion.

References

1. ***Zh.I. Alferov***.Rev. Mod. Phys., v. 73(3), 767 (2001).
2. ***X. Peng, L.Manna , W.Yang , J. Wickham***. Nature, v. 404, 59 (2000).
3. ***Y.Masumoto, T.Takagahara***. Semiconductor Quantum Dots. Springer. Berlin, (2002).
4. ***N. Y. Morgan, C.A Leatherdale, M.Drndic***. Phys. Rev. B, v.66, 075339(2002) .
5. ***A. I. Ekimov, A. L. Efros***.Phys.status solidi. 1988. v. B150, 627(1988).
6. ***I. P. Suzdalev***. Nanotechnology:Physics and Chemistry of nanoclasters, nanostructures, and nanomaterials, Moscow, 2006.
7. ***L. E. Brus***. Nanosttruct. Mater., v. 1, 71(1992).
8. ***S. A.Gyrevich, A. L. Ekimov, I. A Kudryavcev***.Semiconductor,v. 28,830(1994).
9. ***L.Grigoryan, P. Petrosyan ,S. Petrosyan , V. Bellani***. Eur. Phys. J.,v. B 34, 415(2003).
10. ***V.L.Bonch-Bruevich***.Physics-Uspekhi,v.140,583(1983).