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MODIFICATION OF BAND-GAP IN SURFACE LAYER OF CdZnTe BY YAG:ND^{+3} LASER RADIATION

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ABSTRACT

According to the effect, the interstitial atoms of Cd (Cd_i) in $Cd_{1-x}Zn_xTe$ move along the temperature gradient while the Cd vacancies (V_{Cd}) and Zn atoms – in the opposite direction, into the bulk of the semiconductor where temperature is lower. Photoluminescence spectra studied at 5 K show that concentration of Cd atoms increases, but concentration of Zn atoms decreases at the surface due to redistribution atoms in temperature gradient of field. Formation of a graded band gap in $Cd_{1-x}Zn_xTe$ crystal at irradiation by the second harmonic of Nd:YAG laser is found.

"1. INTRODUCTION"

One of the most promising methods of semiconductor processing providing high locality and cleaner "technology", speed of processing by updated electric and recombination properties is laser processing. The most important electronics problem at semiconductor laser processing is the change of the material structure [1] and occurrence barrier structures [2].

CdTe and its solid solutions are the basic materials used in modern optoelectronics for manufacturing solar cells and semiconductor detectors of X-ray and γ- radiations. Various point defects generated at laser processing of CdTe are redistributed under conditions of temperature gradient [1]. For example, A-centre and interstitial Cd in CdTe (Cl) generated by laser irradiation [2]. A number of studies [3-9] have been devoted to effects of laser radiation on the structure and semiconductor properties. Particular theoretical calculations have been made [3] assuming enrichment of $Cd_xHg_{1-x}Te$ with Hg near the surface caused by "phonon wind" arising at laser irradiation. However, the calculations do not allow to make an unequivocal conclusion concerning the mechanisms of mass transfer. For example, the increase of duration of the radiation pulse within the range of microseconds increases efficiency of the "phonon wind" impact. On the other hand, reduction of the temperature gradient minimizes efficiency of "phonon wind" impact contradicting earlier conclusions.

Tauc, the first point at possible TGE for electron-hole pairs, has created his theory [10]. In [11] the authors have showed theoretically the essential difference of laser induced impurity diffusion on an example GaAs on a comparison with isothermal process. A theory of the phenomenon in a general case has been developed in [12]. According to the TGE theory [11], the interstitial Cd atoms (Cd_i) move in the direction of temperature gradient. Accordingly, Cd vacancies (V_{Cd}) move in the opposite direction, i.e. – to lower temperature. The purpose of the presented work is a further study of processes occurring near the surface of $Cd_{1-x}Zn_xTe$ at laser radiation.

“2. EXPERIMENTAL DETAILS”

Photoluminescence (PL) was employed as the main investigation tool. The PL method allows investigating the energy spectrum and concentration of luminescence centre. Single crystals of $Cd_{1-x}Zn_xTe$ (x=0.06), grown from melt by modified Bridgman method under overpressure of Cd, were used in our experiments. Irradiation was carried out at room temperature and atmospheric pressure. The samples were irradiated by the second harmonic of the YAG:Nd laser (λ = 532 nm, τ=15ns) in Q-modulation with the intensity from 0,2 MW/cm^2 to 2 MW/cm^2 to provide a high grad T. The irradiated surface of the crystal was covered with a 0,3µm thick layer of SiO_2 to avoid material evaporation at laser heating. The SiO_2 layer was transparent for laser radiation. PL spectra were excited by Ar+ laser (514 nm) at powers of less than 200mW and measured at 5 K. The samples were of size 10x10x2 mm^3.

“3. RESULTS AND DISCUSSION”

To obtain the best resolution the PL spectra were measured at 5K in the range of 1.35 to 1.63 eV. The PL spectra before irradiation are presented in Fig.1. The initial PL spectrum contains an intense line (A^0, X) at 1.6139 eV ascribed to excitons bound to shallow acceptors (Cd vacancies - V_{Cd}) and a weaker line (D°, X) of excitons bound to shallow donors at 1.6186 eV. The PL band around 1.55 eV is caused by recombination of donor-acceptor pairs (DAP) and consists of the zero-phonon line (ZPL) at 1.592 eV and its LO-phonon replicas. After laser irradiation of the $Cd_{1-x}Zn_xTe$ crystal of intensity 0.2 MW/cm^2 all the lines of PL spectra shift to lower energy (red shift). The shift of A°X line at this intensity was 9 meV. In turn, spectral shift of the A°X line at maximal laser intensity I=2MW/cm^2 was 41meV (Fig.2.).

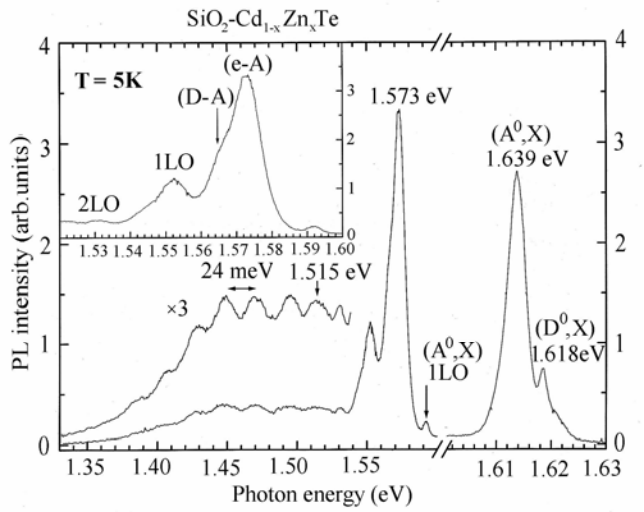

Fig.1. PL spectra of a $Cd_{1-x}Zn_xTe$ sample measured before irradiation.

After laser treatment at intensities over 0,2 MW/cm^2 all the lines of PL spectra shift to lower energies, for example, A^0X (Fig.2). Such a laser treatment of the semiconductor leads to generation of additional point defects at the interface, first of all V_{Cd} and Cd_I. In a recent study [13] a significant reduction of cadmium vacancies in the structure of a mixed crystal has been shown to result from incorporation of Zn into the CdTe lattice. The movement of A^0X can be explaining by redistribution of Zn atoms and V_{Cd}.

Calculation of the distribution of Zn atoms and Cd_I in the presence of temperature gradient (grad T) in the direction of laser beam propagation has shown that concentration of Zn atoms increases in the bulk of the semiconductor [12].

It follows that concentration of V_{Cd} increases in the same place where concentration of Zn atoms. As a result the situation in the bulk of semiconductor becomes favorable for recombination of V_{Cd} with Zn atoms.

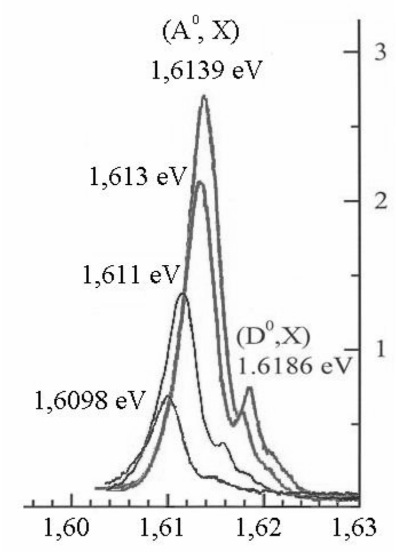

Fig.2. Photoluminescence spectra of $Cd_{1-x}Zn_xTe$ crystals after laser radiation (1 -nonirradiated, 2-I_1=0,2 MW/cm^2, 3-I_2=1,6MW/cm^2, 4-I_3=2 MW/cm^2) with causes change of composition **x**

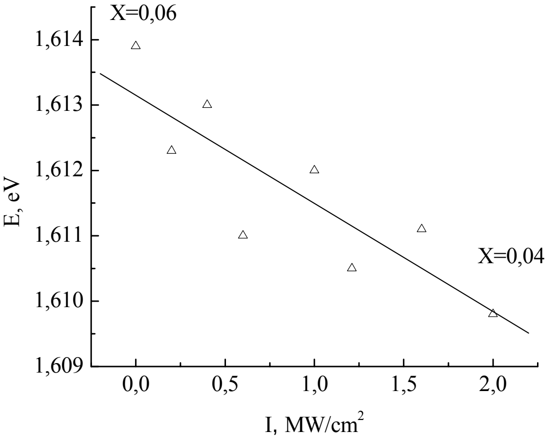

Fig.3. Evolution of energetic position of the 1.6139 eV exciton band as a function of laser intensity

In the ternary the decrease of Zn atom concentration leads to a corresponding decrease of the $Cd_{1-x}Zn_xTe$ [14] band gap near the irradiated surface. As it follows from Fig.3 Zn concentration near the irradiated surface decreases by 2%.

The change of Zn atoms concentration from X=0,06 to X=0,04 (Fig. 3) in direction to bulk of the sample is assumed to change the band-gap in $Cd_{1-x}Zn_xTe$. The monotonous change of band-gap with coordinate in the bulk of the sample leads to creation of a graded band-gap in the bulk of the sample.

Intensities of the exciton luminescence peaks decrease appreciably due to increasing of absorption of PL and its excitation light as deepening of the exciting layer. The peaks shift to lower energies due to a decrease of the energy gap that is well seen from fig 2. The change of the position of the A^0X exciton recombination band (experimental) can be explained by decrease of the band-gap width of the semiconductor.

The change of the band gap structure after laser irradiation can be explained using TGE model which is illustrated schematically on Fig. 4.

After laser irradiation the band gap value has changed as shown in this figure due to the Zn atoms drift toward the bulk of the sample and the Cd_I atoms drift to the surface. As a result of such atom drift the band gap value has been changed in the following manner: at the surface it is decreased but in the bulk of the sample - increased.

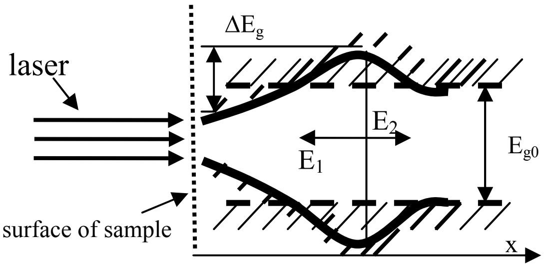

Fig.4. The scheme of band gap change after semiconductor irradiation by laser caused by the redistribution of Zn and Cd atoms due to presence of TGE. E_1, E_2 are quasi electrical fields; E_{g0} is band gap of semiconductor and ΔE_g is its change.

The maximum of the band gap is situated at the place where the concentration of Zn atoms has a maximum. Beyond this maximum the band gap decreases due to decrease of the Zn atom concentration. Two electrical fields (E_1, E_2) are created in the bulk of the sample.

According to the given model in near-surface a layer of the semiconductor thickness 1μm creates the built in electric field due to presence of a gradient of width of the band gap. The near-surface of the semiconductor is characterized by the big concentration of electron-hole pairs in comparison with not irradiated surface because of smaller band-gap width. It leads to occurrence on a surface of the semiconductor of a layer (channel) with increased conductivity, in comparison with conductivity in the field of the maximal width of the band-gap in depth of the semiconductor. Other application graded band-gap structures of CdZnTe its use as optical window where radiation providing more effective transformation in wider band of frequencies, for example, in solar batteries, in photo detectors can be given.

“4. CONCLUSIONS”

The TGE plays the main role in redistribution of Zn atoms at the irradiated surface of $Cd_{1-x}Zn_xTe$. Formation of a graded band - gap in $Cd_{1-x}Zn_xTe$ crystal is shown to be possible under second harmonic irradiation of Nd: YAG laser.

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