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Features of the origin and propagation of a shock wave in semiconductors during nanosecond laser irradiation

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In this paper, the mechanisms of mass transfer to In/CdTe systems under nanosecond pulsed laser irradiation, which are due to nonstationarity, nonequilibrium, physical and geometric nonlinearity, high speed and simultaneity of various physical processes; in particular, it is a change in the physical state of a solid body, the generation of elastic and shock waves, significant temperature and stress gradients, defect formation, diffusion, and others. The dominant mechanisms and regularities of indium mass transfer in CdTe during nanosecond laser irradiation of the In-CdTe structure were established, taking into account the factors of shock wave origin and propagation, temperature and pressure.
Keywords: CdTe, In/CdTe, pulsed laser irradiation, shock wave, doping.

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Introduction

Recently, the methods of pulsed laser processing and modification of near-surface layers are increasingly used for the formation of inversion and varizon layers of solid solutions based on CdTe, in particular $Cd_{1-x}(Mn, Zn, Hg)_xTe$, creation of ohmic and barrier contacts, solid-phase and liquid-phase alloying in the manufacture of structures and devices based on them for photo- and opto-electronics, sensor electronics, and especially IR and ionizing radiation detectors based on CdTe and Cd(Hg, Zn)Te [1-4]. By varying the component composition x during pulsed laser irradiation, it is possible to change the band gap of the near-surface layers of solid solutions and, accordingly, the spectral sensitivity, as well as other parameters.

Laser-induced doping of CdTe and solid solutions with the formation of inversion layers is carried out by irradiating the In/CdTe(CdMeTe) film structure with nanosecond pulses and is accompanied by the simultaneous flow of various physical processes at high speed. A particularly important phenomenon in this case is the occurrence and propagation of a shock wave in a solid body [4], which is a significantly nonlinear process and leads to a change in the defective semiconductor system and mass transfer (diffusion). This, in turn, leads to a change in the functional electrical and optical parameters of structures based on CdTe and solid solutions.

The influence of the occurrence and propagation of the shock wave, as well as the ultrafast generation of temperature and pressure during pulsed laser irradiation on the structural, electrical, and, especially, photovoltaic characteristics of CdTe and solid solutions has not been sufficiently studied.

I. Experimental results and discussion

To find out the mechanisms of shock wave generation and propagation, p-CdTe crystals of size 5x5x0.5..3 mm^3 with specific resistance $(2\text{-}4)\cdot 10^9\ \Omega\cdot cm$, orientation (111), compensated by Cl were used. The surface of the crystals (the studied samples) was subjected to mechanical treatment (cutting, grinding, polishing), followed by chemical treatment (washing, etching, rinsing) and drying of the samples. The In film of a given thickness (30-400 nm) was applied by thermal sputtering in a vacuum at a pressure of 10^{-5} atm. At the next stage, the samples were subjected to laser treatment, namely, the surface of the crystal was uniformly irradiated at room temperature (T = 300 K) with single pulses of Nd:YAG laser radiation (λ = 535 nm) of nanosecond duration (τ = 5-6 ns) in the interval energies of 10-500 mJ/cm^2.

During powerful nanosecond laser irradiation of metal(In)/p-CdTe (CdMeTe) structures in the semiconductor, an inversion near-surface layer is formed, that is, a layer of n-type conductivity (relative to p-type conductivity) due to the processes of diffusion (mass transfer) of indium (In) atoms , who act as donors. With nanosecond irradiation, mass transfer – by definition, it is fast diffusion, since this process lasts tens to hundreds of nanoseconds – occurs due to mechanisms of a different physical nature. In particular, this is such a mechanism as the occurrence and propagation of a shock wave, which leads to the generation, change and redistribution of a system of point and long defects [5-6]. As well as the mechanism of generation and relaxation of sharp spatial gradients and rates of temperature increase and, accordingly, thermal stresses (pressure) (dT/dx, dP/dx, dT/dt, dP/dt), since during laser irradiation with a nanosecond pulse duration, the rate of heat transfer to the near-surface layer (that is, to the depth of the optical skin layer and to the depth $\sqrt{\chi\tau}$) is very significant in relation to the speed of heat propagation in the volume due to heat and temperature conductivity. The process of generating thermal stresses (which are the cause of barodiffusion) and their propagation is a significantly non-linear and non-stationary process, which subsequently, during the evolution (propagation of the pressure pulse), leads to the emergence of a shock wave. Recently, the method of laser-induced doping of the near-surface layer of CdTe crystals and solid solutions based on it, previously coated with an In film, has been widely used in the creation of barrier structures for ionizing radiation detectors. Therefore, it is relevant to calculate the depth of shock wave formation in order to control the diffusion process, as well as to find out the peculiarities of the occurrence and propagation of the shock wave in semiconductors and structures during pulsed laser irradiation.

A shock wave is a discontinuity surface, at the intersection of which the pressure, density, and temperature increase sharply, and the rate of propagation of the disturbance in the medium decreases sharply. A shock wave is an example of a normal hydrodynamic discontinuity, and a flow of matter flows through it (unlike a tangential discontinuity, through which matter does not flow). From a macroscopic point of view, a shock wave is an imaginary surface on which the thermodynamic values of the environment (which, as a rule, change continuously in space) have finite jumps. When passing through the front of a shock wave, the pressure, temperature, density of matter, entropy of the medium, as well as the speed of its movement (oscillating speed) relative to the front of the shock wave change. Here, by a shock wave, we will understand a wave with an "overturned" profile (front) according to [6] surface of a break in the continuity of thermodynamic quantities in a substance. Shock waves do not have the property of additivity in the sense that the thermodynamic state of the medium, which occurs after the passage of one shock wave, cannot be obtained by the successive passage of two shock waves of lower intensity. Acoustic waves are fluctuations in the density of the medium propagating in space. The equation of state of ordinary media is such that in the region of increased pressure, the speed of acoustic oscillations (that is, the speed of propagation of disturbances) increases (in fact, the acoustic wave is a nonlinear wave). During propagation, this nonlinearity inevitably leads mathematically to "overturning of solutions", which generate shock waves. Due to this mechanism, a shock wave in a normal environment is always a compression wave. However, in those systems in which the rate of propagation of disturbances decreases with increasing density, a rarefaction shock wave will be observed. Rapid conversion of the density fluctuation into a shock wave requires strong initial deviations from equilibrium. This can be achieved by creating an acoustic wave of very high intensity during pulsed laser irradiation.

The length of the shock wave front in a semiconductor of the order of interatomic distances. A characteristic difference between a shock wave and a stress wave is that the transfer of momentum from a substance compressed by a shock wave to an unexcited part is not a collective movement of atoms, but individual collisions.

An acoustic pulse in a solid body due to physical nonlinearity is a nonlinear [7]. By physical nonlinearity, we mean the difference (continuous change) of the modulus of the elastic constant C_{ijkl} and the density along the coordinate in the direction of wave propagation at each pulse point. In other words, it is the dependence of C_{ijkl} and ρ on deformation, deviation from Hooke's law. The speed of sound in a solid body $\upsilon = \sqrt{\frac{C_{ijkl}}{\rho}}$, respectively, an increase in speed due to changes in elasticity and density $d\upsilon = \sqrt{\left(\frac{dC_{ijkl}}{d\rho}\right)}$ (Fig. 1). Therefore, the "faster" components (harmonics) of the pulse will catch up with the "slower" ones. This corresponds to the transfer of energy from low-frequency harmonics to higher-frequency harmonics – accordingly, the pulse profile will be distorted, twisted. Steepening the profile of the sound wave leads to several effects. First, before the formation of gaps, so that with the passage of time, the initially sinusoidal wave will turn into a sawtooth wave. In addition, the steepening of the profile, leaving the movement of the wave periodic, significantly changes the spectral composition of the wave. In the initial monochromatic wave with frequency ω, high-frequency harmonics increase as it propagates. Moreover, high overtones nω with a larger n reach a maximum at the place of the greatest steepness. At the same time, there is a continuous transfer of energy from the fundamental harmonic to high overtones. Since the attenuation of sound is approximately proportional to the square of the frequency, this leads to a stronger attenuation of the wave, i.e. an increase in the high-frequency amplitude leads to an increase in attenuation, the attenuation coefficient $\alpha_{acoust} \sim f^n$, f is the frequency, n = 2...2.3, accordingly, the energy will be more dissipated. The tightening of the wave front will occur until it is stabilized by dissipative processes. Thus, the wave profile depends on the ratio of nonlinear and dissipative effects and its intensity. If the amplitude of the wave is large enough, nonlinear effects dominate and the wave profile eventually "overturns" and a shock wave is formed. Otherwise, due to dissipation, the wave has time to die out before nonlinear effects accumulate in it [6].

It should be noted that for a solid body there is no complete equation of state, which complicates the theoretical description of the occurrence and propagation of the ular wave. Therefore, the gas model for which this equation is known is more often used. At the same time, in a solid, the analog of the adiabatic index is the isentropy index [4].

In a homogeneous isotropic gas with equilibrium values of P_0, density ρ_0, in a nonlinear wave, small perturbations of pressure P', density ρ', will add u (u << a_0), $\bar{u}$ = 0 to the propagation speed a_0. The speed of sound is equal to $a = \sqrt{(\partial P/\partial\rho)_S}$. In the linear, acoustic approximation, u = 0 and all points of the sound wave profile propagate with the same speed a_0. In the next, first approximation for the velocity υ displacement of the points of the sound wave profile in an ideal gas $\upsilon = a_0 + \frac{\partial u}{\partial\rho}(\rho_0)\rho' = a_0 + \frac{\gamma+1}{2}u$, γ – adiabatic exponent. Therefore, with the passage of time, the profile of the traveling wave will be twisted and a break will be formed, overturning (dissipation not taken into account). In the case of the evolution of a planar harmonic sound wave excited in an ideal gas by a plane at x = 0, i.e. $u = u_0 \sin\omega t$ at x = 0, the solution for the time and coordinates of the formation of a gap, or overturning of the profile will be $t_s = \frac{\lambda}{u_0}\frac{1}{\pi(\gamma+1)}$, $x_s = \frac{a_0}{u_0}\frac{\lambda}{\pi(\gamma+1)}$, where $\lambda = 2\pi a_0/\omega$. [8]. More complete, but very complicated, expressions for the time and coordinates of the formation of a shock wave in a solid body are given in [9].

Figure 1 shows a crystal lattice during the propagation of an acoustic wave in it - there are areas of compression and areas of tension, and also the profile of a nonlinear acoustic wave is given, on which three areas are distinguished – the peak (maximum speed of propagation of a disturbance, υ_1), the border of an undisturbed area (minimum speed perturbation propagation, υ_3), and in the middle (υ_2). Such a scheme, together with the above, explains the formation of a shock wave.

It can be seen from Figure 2 that during the propagation of a nonlinear acoustic wave after pulsed laser irradiation of a solid body, energy is pumped from low-frequency harmonics to high-frequency ones, due to which the profile is stiffened. The depth of shock wave formation in indium and CdTe when a laser pulse is applied to their surface can be calculated using the expression from work [6, 7].

$$l_{YX} = \frac{2c_l^2\tau}{\zeta(m+1)}\left[\frac{2\rho}{\bar{\chi}(\gamma-1)(1-R)E\alpha_h}\right]^{1/2} \quad (1)$$

where c_l is the velocity of the longitudinal acoustic wave, τ is the duration of the laser pulse, ρ is the density, ζ is the parameter of the acceleration of the surface layer, m is the isentropy index, $\bar{\chi}$ the effective value of the pulse front twist coefficient, γ is the adiabatic index, R is the optical reflection coefficient, E is the energy density of the laser pulse, α_λ is the optical absorption coefficient. As in [10],

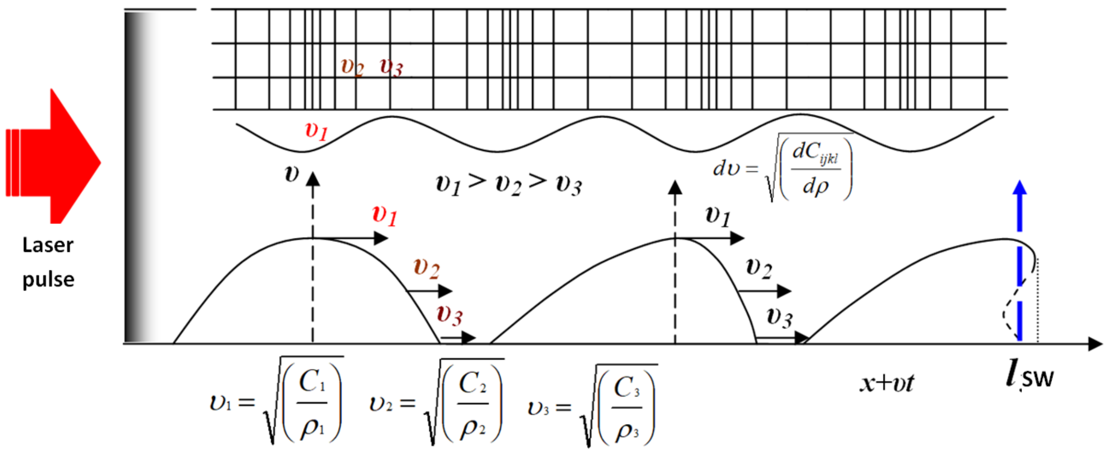

Fig. 1. – Scheme of formation of a shock wave during pulsed laser irradiation of a solid body.

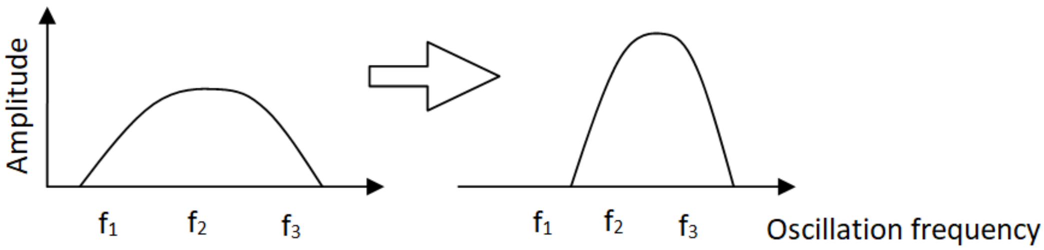

Fig. 2. – Scheme of energy transfer from low-frequency to high-frequency harmonics during the propagation of a nonlinear acoustic wave after pulsed laser irradiation of a solid body.

we take $\bar{\chi} = 1$, $\zeta = 1$, $m = 3$, $\gamma = 5/3$. Consider that, according to [11], in metals, the value of the speed of propagation of pressure pulses during nanosecond pulsed laser irradiation is 15-30% higher than the longitudinal speed of sound.

In fig. 3 shows the calculation of the depth of shock wave formation (SW) in indium and CdTe depending on the intensity density of the laser pulse ($I = E/\tau$) in a wide range of intensities; this result is important in the analysis of mass transfer in In/CdTe(CdMeTe) with the formation of inversion and varizon layers.

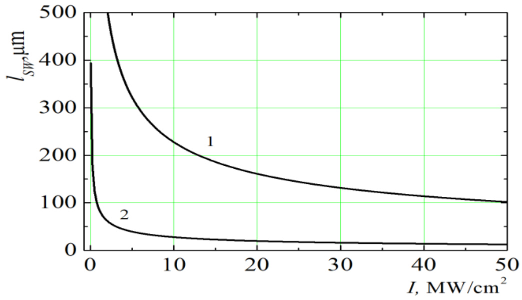

Fig. 3. - The depth of shock wave formation in CdTe (1) and In (2) depending on the intensity of the ruby laser pulse. τ_{imp} = 20 ns. For CdTe R = 0.43, for In R = 0.9.

According to the graph in Fig. 3, by choosing the thickness of CdTe, it is possible to avoid the formation of a shock wave in the volume, and it is also possible to locally influence the defective subsystem at different depths of the semiconductor. Since it is practically important from the point of view of creating p-n structures by the method of laser-induced doping, consideration of two-layer structures of a metal film (indium) – a semiconductor (CdTe, CdMeTe), the above fundamental consideration and calculation of the depth of shock wave formation makes it possible to predict the place of origin of the shock wave – in the deposited film or in the semiconductor. It should be noted that significant film thicknesses are necessary for the occurrence of a shock wave in the alloying film, since at very high intensities of pulsed laser irradiation, the mechanism of intense melting and evaporation is activated. If the thickness of the film In l is such that the depth of formation of the shock wave $x < l$, then it is formed in it and contributes to the mass transfer. If $x > l$, then a shock wave is not formed in it, but the mass transfer mechanism operates due to (spatial and temporal) temperature and pressure gradients. The case when $x = l$ is very interesting, in this case all the energy of the newly formed shock wave actually goes to mass transfer, interesting effects are possible here, as, for example, in [12].

Consider the criterion for the formation of a shock wave during single-pulse irradiation. The left part of inequality (2) is a dimensionless combination of values characterizing the parameters of the radiation and absorbing solid body. In (3), on the left are the values characterizing laser radiation, on the right - the absorbing medium.

$$\frac{\bar{\chi} l^2 (1-R) E a_\lambda}{c_l^4 \tau^2 \rho} > \frac{8}{\xi^2 (m+1)^2 (\gamma-1)} \qquad (2)$$

or

$$\frac{Q}{\tau^2} > \frac{c_l^4 \rho}{a_\lambda} \qquad (3)$$

Here l is a characteristic size, which is the smaller value of 2 values – the thickness of the crystal and the radius of the radiation beam. $Q = E \cdot S$ – laser radiation energy, S – irradiation area, τ = 20 ns. Table 1 shows the physical parameters of CdTe and In.

Table 1.

Mate-rial	c_l, m/s	ρ, kg/m^3	$\alpha_{\lambda=0,694}$ 1/m	R	T_{ml} °C
CdTe	3300	5860	$2.94 \cdot 10^6$	0.43	1092
In	1400	7310	$5.4 \cdot 10^7$	0.8…0.9	157

According to criterion (2), for a CdTe crystal with a thickness of 2 mm, the inequality is fulfilled up to the energy density E = 6 mJ/cm$_2$ (I = 0.3 MW/cm^2), for indium of the same thickness - 0.1 mJ/cm^2 (I = 5 MW/cm^2).

At the same time, the melting threshold of CdTe is, according to various data, 2...6 MW/cm^2, and calculations of the maximum heating temperature of the surface of CdTe and In, made according to the expression $\Delta T = \frac{2AI}{\lambda}\sqrt{\frac{\chi\tau}{\pi}}$, indicate that at such energy densities, melting radiation, and even more evaporation from the surface of indium will not happen. Moreover, it is possible to clamp the surface by applying a material transparent to radiation or by placing it in a transparent liquid. Then there will be no discharge wave, ablation will begin at higher I. Here τ is the pulse duration (20 ns), A is the optical absorption coefficient, λ is the thermal conductivity coefficient, χ is the thermal conductivity coefficient.

In Fig. 4 the dependence of the surface temperature of CdTe and In upon nanosecond laser irradiation is given.

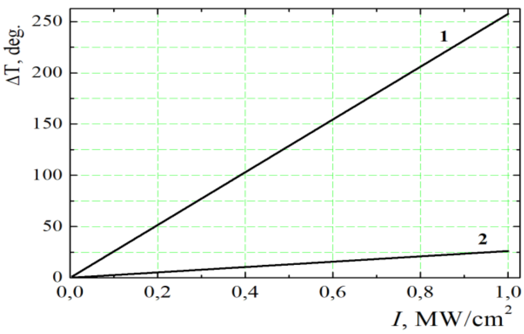

Fig. 4. – Theoretical dependence of the maximum surface temperature of CdTe (1) and In (2) on the intensity of pulsed laser radiation.

In Fig. 5 an accurate calculation of the dependence of the maximum surface temperature of CdTe on the intensity during irradiation with a ruby laser at τimp = 20 ns is given, taking into account the typical experimentally obtained thermophysical, electronic and optical parameters of CdTe. The calculation was made according to the complete approach [13]. The non-linearity of the graph is explained by the dependence of heat capacity and thermal conductivity on temperature, which is not taken into account in the calculations in Fig. 4

according to a simpler expression, since the error is small when I is small. From the comparison of Fig. 4 and Fig. 5, it can be seen that such a dependence on the temperature of the thermal parameters gives a growing deviation as the laser intensity increases.

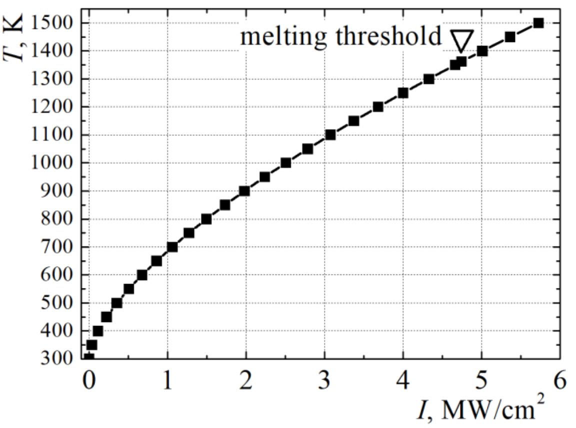

Fig. 5. – Theoretical dependence of the maximum temperature of the CdTe surface on the intensity during irradiation with a ruby laser at τ_{imp} = 20 ns.

When irradiating In/CdTe(CdMeTe) structures to create ionizing radiation detectors, the right-hand part of criterion (3) is equal to $9{\cdot}10^8$ J/s^2 for indium. At S = 16 mm^2, the minimum energy density required to fulfill this criterion is 0.003 mJ/cm^2 (150 W/cm^2). At the same time from fig.4. it is clear that melting, let alone evaporation from the surface, will not occur. The same is true for CdTe (Figs. 4 and 5). That is, these inequalities are performed with a larger margin (below T_{melt} by approximately 1000 orders of magnitude).

The calculation of the depth of the formation of the shock wave lX indicates that such a wave at optimal irradiation regimes E = 10-500 mJ/cm^2 (0.5-25 MW/cm^2) does not arise in a thin film of indium and is formed already in the volume of the CdTe crystal at a distance much greater than the penetration depth of indium lIn during nanosecond pulsed laser irradiation [4].

The most intensive generation of defects occurs precisely in the region of the front of the shock wave at the moment of its formation and the beginning of movement, where the maximum concentration of structural [6] and point defects is observed, as well as the maximum of microhardness, which indicates local mass transfer. The shock wave also causes hardening in the material (metal) and changes the yield strength and the course of phase transformations [7] The characteristic attenuation length of the incident wave at E ≈ 10-16 J/cm^2 is approximately 60-100 μm [6, 7]. Calculations according to expression (1) showed that a shock wave at I = 100 MW/cm^2 will form at a depth of 72 μm.

The pressure gradient in the nonlinear wave increases as it propagates in depth, reaching a maximum in the region of the formation of the shock wave front. Both matrix atoms and defects (scattering centers) acquire the impulse of the shock wave during transmission. An increase in the energy of the laser pulse leads to a shift of the maximum of defects closer to the surface, that is, the effect of the pressure gradient of the nonlinear wave and the location of the formation of the shock wave front are revealed. Thus, the experimental results indicate the formation of dislocations in CdTe as the gradient of a significantly nonlinear wave and the formation of a shock wave increase. With shock waves of high intensity, the pressures in the front are so high that the shear hardness of the material is not manifested, the atoms leave the correct arrangement in the crystal layers (cleavage plane), the crystalline body temporarily acquires the properties of an amorphous, vitreous, liquid body. Such waves, in contrast to waves that preserve the crystalline properties of the body, are called plastic [7].

Conclusions

Using the example of CdTe, it is shown that a shock wave in a solid during its formation and propagation, as well as before its occurrence – due to a gradual increase in the pressure gradient – leads to the formation of dislocations. At the same time, the density of dislocations increases with depth and is maximum at the place of formation of the shock wave.

It is shown that evaporation (and/or ablation) of the near-surface layer of a semiconductor during nanosecond laser irradiation is not an exact (general) criterion for the formation of a shock wave. The general criterion is the dominance of the accumulation of nonlinear effects over the dissipation processes of the acoustic nonlinear pulse during its propagation.

The depth of shock wave formation in CdTe and indium doping film during their nanosecond laser irradiation with the formation of inversion and varizon layers is calculated.

It was established that the shock wave can locally affect the defective subsystem at different depths of the CdTe crystal and solid solutions based on it.

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Особливості виникнення та поширення ударної хвилі в напівпровідниках при наносекундному лазерному опроміненні

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В даній роботі розглянуто механізми масопереносу в системи In/CdTe при наносекундному імпульсному лазерному опроміненні, які обумовлена нестаціонарністю, нерівноважністю, фізичною та геометричною нелінійністю, високою швидкістю і одночасністю протікання різних фізичних процесів; зокрема це зміна агрегатного стану твердого тіла, генерація пружних та ударних хвиль, значних градієнтів температур і напруг, дефектоутворення, дифузія та ін. Встановлено домінуючі механізми та закономірності масопереносу індію в CdTe при наносекундному лазерному опроміненні структури In-CdTe з урахуванням факторів виникнення та поширення ударної хвилі, температури та тиску.

Ключові слова: CdTe, In/CdTe, імпульсне лазерне опромінення, ударна хвиля, легування.