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Features of a shock wave in CdTe by pulsed laser irradiation

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Abstract. Analyzed on the example of CdTe are formation and propagation of shock waves during pulsed laser irradiation of a solid surface. It is shown that before the appearance of a shock wave in a solid, a gradual increase in pressure gradient leads to formation of dislocations, density of which increases with depth. The dislocation density is maximum at the place of shock wave formation.

Keywords: pulsed laser irradiation, CdTe, dislocation density.

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1. Introduction

Up to date, the method of pulsed laser processing and modification of subsurface layers has been increasingly used to form inverse and graded layers in semiconductors, to create ohmic and barrier contacts, for solid and liquid phase doping when manufacturing the structures and devices based on them in photo- and optoelectronics, sensor electronics, and especially ionizing radiation detectors based on CdTe and CdZnTe [1].

Pulsed laser doping the samples of CdTe is produced using nanosecond irradiation of the structure In/CdTe and accompanied by the simultaneous occurrence of various physical processes at a high velocity. In this case, particularly important phenomenon is the emergence and spread of a shock wave (SW) in solid [1-7], which is essentially a nonlinear process and leads, in particular, to changes in the defect system of semiconductor [2-4]. This, in its turn, leads to changes in electrical and optical parameters of devices based on CdTe.

Therefore, the purpose of this study was to determine the characteristics of the shock wave in the structure of CdTe and In/CdTe after nanosecond laser irradiation.

2. Some properties of shock waves

The shock wave is a discontinuity surface at the intersection where the pressure, density and temperature

increase dramatically, and the velocity of operating medium motion is dramatically reduced. The shock wave is an example of normal hydrodynamic discontinuity, and through it a flow of matter goes (as opposed to a tangential discontinuity, through which the substance does not flow). From the macroscopic point of view, the shock wave is an imaginary surface on which the thermodynamic quantities of the medium (which tend to vary continuously in space) make finite jumps. When passing through a shock front, changed are pressure, temperature, density of matter, entropy environment, and its velocity relatively to the shock front. Here, as the shock wave we mean the “inverted” profile (front) according to [8-10], which moves in the material surface of discontinuity of the thermodynamic quantities. Shock waves do not possess the additivity property in the sense that the thermodynamic state of the environment that occurs after the passage of a shock wave is impossible to get with a consistent passing of two shock waves with lower intensities. Acoustic waves are oscillations of the density of the medium, which propagate in space. The equation of state of ordinary matter is that in the high-pressure velocity of acoustic waves (i.e., the speed of perturbation spread) increases (it means that the acoustic wave is the nonlinear one). When spreading, it inevitably leads to the phenomenon of overturning solutions that give rise to shock waves. By this mechanism, the shock wave in normal environment is always a wave of compression. However, in those systems where the speed of perturbation spread decreases with increasing the density, rarefaction shock

wave is observed. For the rapid transformation of the density oscillations to the shock wave, it requires strong initial deviations from equilibrium. This can be achieved by creation of acoustic waves with a very high intensity provided, for example, by pulsed laser irradiation (PLI).

The length of the shock front in semiconductors is of the order of interatomic distances. The characteristic difference between the shock and stress waves is that the transfer of momentum from the shock compressed matter to a non-excited its part has a character of individual collisions and not a collective atomic motion.

Acoustic pulse in a solid, due to physical nonlinearity, is the nonlinear wave [5]. As the physical nonlinearity, we mean the difference modules of the elastic constants and density C_{ijkl} along the coordinate of wave propagation at each point of pulse. In other words, there arises the dependence of C_{ijkl} and ρ on the strain, i.e., Gooke's law violation. The speed of sound in solids

is commonly expressed as $v = \sqrt{\frac{C_{ijkl}}{\rho}}$, the velocity increment due to changes in elasticity and density is as

$$\text{follows } dv = \sqrt{\left(\frac{dC_{ijkl}}{d\rho}\right)}.$$

Therefore, a more "fast" component of the pulse will catch the more "slow" ones. This corresponds to the energy transfer from the low-frequency harmonics to the higher frequency ones. Respectively, the pulse profile will be distorted and more sharp. Profile distortion of the sound wave leads to several effects. First, steepening the profile may lead to the formation of gaps, so the initial sine wave becomes a sawtooth wave with time. Moreover, steepening the profile, leaving the movement in a wave to be periodic, alters the spectral composition of the wave. In the original monochromatic wave with the frequency ω , both distribution and distortion of the profile are related with increasing high-frequency harmonics. Moreover, high overtones $n\omega$ with larger n reach a maximum in the place of the greatest slope. Thus, there is a continuous transfer of energy from the fundamental harmonic to the high overtones. Since the attenuation of sound is proportional to the square of frequency, this leads to stronger damping. Steepening the wave front will take place until it stabilizes the dissipative processes. Thus, the wave profile depends on the ratio of non-linear and dissipative effects, and its intensity. If the wave amplitude is sufficiently high non-linear effects dominate, and the wave profile in the end is "turned over", which generates a shock wave. Otherwise, the wave due to dissipation is damped out earlier than it accumulates non-linear effects [10].

It should be noted that the equation of state for solids is absent, which hinders the theoretical description of occurrence and propagation of SW. Therefore, it seems reasonable to use the model of gas for which it is known. In the solid state, analogue of the adiabatic exponent is the index of isentropy [6, 7].

In homogeneous isotropic gas with equilibrium values of the pressure P_0 and density ρ_0 , in a non-linear wave, small perturbations of pressure P' and density ρ' will give a small increment a_0 to the propagation velocity u ($u \ll a_0$), $\bar{u} = 0$. The speed of sound is $a = \sqrt{(\partial P / \partial \rho)_s}$. In the linear acoustic approximation $u = 0$, and all points of the sound wave profile spread at the same speed a_0 . In the following first approximation for the rate of displacement of points v in the sound wave profile in ideal gas

$$v = a_0 + \frac{\partial u}{\partial \rho}(\rho_0)\rho' = a_0 + \frac{\gamma + 1}{2}u,$$

γ – adiabatic exponent. Therefore, over time, the profile of running wave will be distorted, and formation of the gap, rollover will take place (without account of dissipation). In the case of evolution of a plane harmonic acoustic wave excited in ideal gas for the plane at $x = 0$, i.e., $u = u_0 \sin \omega t$ at $x = 0$ the solution for the time and coordinates of the discontinuity, or turnover of the profile will be

$$t_s = \frac{\lambda}{u_0} \frac{1}{\pi(\gamma + 1)}, \quad x_s = \frac{a_0}{u_0} \frac{\lambda}{\pi(\gamma + 1)},$$

where $\lambda = 2\pi a_0 / \omega$ [10]. Common, but more complicated expressions for the time and coordinate of SW formation in a solid are given in [9].

3. Results and discussion

The depth of shock wave formation in indium and CdTe exposed on their surface by the laser pulse can be calculated using the expression from [6, 7]

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

where c_l is the velocity of the longitudinal acoustic wave, τ – laser pulse duration, ρ – density, ζ – setting the value of acceleration of the surface layer, m – isentropic index, $\bar{\chi}$ – the effective value of the distortion coefficient for the pulse front, γ – adiabatic exponent, R – coefficient of optical reflection, E – energy density of the laser pulse, α_λ – optical absorption coefficient. As in [6], we take $\bar{\chi} = 1$, $\zeta = 1$, $m = 3$, $\gamma = 5/3$. Taking into account that according to [11] in metals, the value of propagation velocity for pressure pulses in the nanosecond pulsed laser irradiation is 15-30% higher than the longitudinal speed of sound.

Fig. 1 shows the results of calculation for the depth of SW formation in In and CdTe as dependent on the density of laser pulse intensity ($I = E / \tau$).

Following the plot in Fig. 1, selection of the CdTe thickness allows to avoid formation of SW in the bulk, and to locally influence the defect subsystem at various depths of semiconductor.

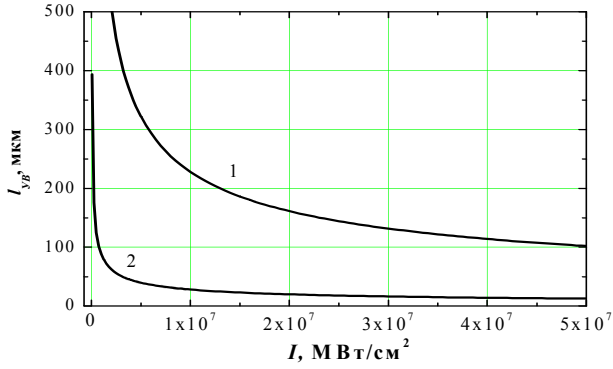


Fig. 1. The depth of shock wave formation in CdTe (1) and In (2) versus the intensity of ruby laser pulse. For CdTe $R = 0.43$, for indium $R = 0.9$.

Consider the criterion of SW formation under single-pulse irradiation. The left-hand side of (2) is a dimensionless combination of variables that characterize the parameters of radiation-absorbing body. On the left in (3), there are values that characterize the laser radiation, on the right – those of absorbing medium

$$\frac{\chi l^2 (1-R) E \alpha_\lambda}{c_l^4 \tau^2 \rho} > \frac{8}{\xi^2 (m+1)^2 (\gamma-1)} [7], \quad (2)$$

$$\text{or } \frac{Q}{\tau^2} > \frac{c_l^4}{\alpha_\lambda} [6]. \quad (3)$$

Here, l is the characteristic size that is lower than the values of 2 variables – the crystal thickness and radius of the radiation beam. $Q = E \cdot S$ is the laser radiation energy, S – irradiated area, $\tau = 20$ ns. Table 1 shows the physical parameters of CdTe and In.

According to the criterion (2) for the CdTe crystal 2-mm thick, the inequality holds up to the energy density $E = 6$ mJ/cm² ($I = 0.3$ MW/cm²), for In of the same thickness – 0.1 mJ/cm² ($I = 5$ kW/cm²). At the same time, the melting threshold of CdTe is 2...6 MW/cm² in accord with various data, while calculations of the maximum heating temperature for the surface of CdTe and In, made using the expression

Table 1.

Material	$c_l, \text{m} \cdot \text{s}^{-1}$	$\rho, \text{kg} \cdot \text{m}^{-3}$	$\alpha_{\lambda=0.694}, \text{m}^{-1}$	R	$T_{\text{melt}}, \text{°C}$
CdTe	3300	5860	$2.94 \cdot 10^6$	0.43	1092
In	1400	7310	$5.4 \cdot 10^7$	0.9	157

$$\Delta T = \frac{2IA}{\lambda} \sqrt{\frac{\chi \tau}{\pi}} [12]$$

(here, χ – coefficient of thermal diffusivity, τ – pulse duration (20 ns), λ – heat conductivity, A – optical absorption coefficient), indicate that this energy density

melting and, moreover, evaporation from the In surface does not take place. Especially, since you can clamp the surface by depositing a transparent material to radiation or place it in transparent liquid. Then there will be no unloading wave. Fig. 2 shows the surface temperature of CdTe and In after nanosecond laser irradiation.

When irradiating structures In/CdTe to create detectors of ionizing radiation, the right-hand side of criterion (3) is $9 \cdot 10^{18}$ J/s² for In. For $S = 16$ mm², the minimum energy density required to implement this criterion is 0.003 mJ/cm² (150 W/cm²). Fig. 2 shows that melting and, moreover, evaporation from the surface will not occur. The same is valid for CdTe (Fig. 2). I.e., these inequalities are performed in a wide range (below T_{melt} within approximately three orders).

Thus, according to the criteria (2) and (3) [6, 7], SW appears at energy densities up to melting and evaporation of the surface layer. At the same time, there [6, 7] used is the model of evaporation of the skin layer to assess the depth of the shock wave, but nevertheless, evaporation is not necessary and/or sufficient condition for the emergence of the shock wave. This is such a model, which assumes that the skin layer is evaporated. The fact that it is convenient to use gas (but not solid) in the model of SW formation, because there is no equation of state for solids and the speed of sound as dependent on the internal energy. There is a simple relationship for ideal gas, but for a rigid body it is very complex. Respectively, calculation is very complicated, in particular, the index of isentropy – analogue of heat should be used. By their values for gas and solid, these quantities are almost identical (3 and 4). In principle, “gas” model is satisfactory for estimating the depth of the shock wave in solid, but gives large uncertainties in the problem of laser exposure (as indicated in [6]). The theory of formation and propagation for shock waves in gases is well developed [10].

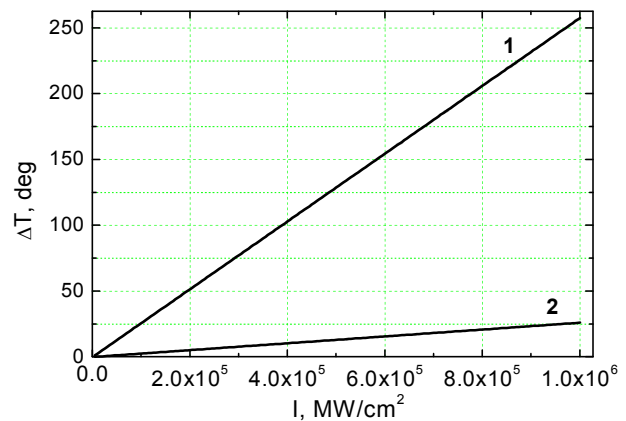


Fig. 2. Theoretical dependence of the surface temperature of CdTe (1) and In (2) on the intensity of pulsed laser radiation.

At the same time, the general condition of the shock wave appearance is accumulation of non-linear effects that dominate over the processes of dissipation of acoustic nonlinear pulse during its propagation after laser irradiation of solids. The first makes the pulse front sharper, while the second is broadens it. Especially because there can be 4 causes (joint) of SW formation in a solid during PLI, in general. I.e., shock deformation and, accordingly, generation of compression pulse by nanosecond laser irradiation is due to:

1. Very fast, within 20 ns, heating (thermal shock) and, accordingly, deformation at a high rate of it.
2. Fast (with the shock velocity) phase transition at the solid-liquid interface.
3. Rapid evaporation from the surface and thus generation of the recoil pressure of non-equilibrium vapor.
4. Optical breakdown and plasma formation in vapor – there is the emergence and rapid expansion of the plasma under absorption of radiation, then ionization and breakdown.

The most intense defect generation takes place in the area of the shock wave front in the instant of its formation and the beginning of movement, when there arises a maximum concentration of point defects in the structure (Fig. 3 and [2, 3]), as well as the maximum microhardness [13], indicating the local mass transfer. SW also causes hardening the material and alters the yield [14]. The characteristic decay length of the shock wave at $E \approx 10-16 \text{ J/cm}^2$ is approximately $60-100 \mu\text{m}$ [3, 13]. Calculations based on the expression (1) showed that SW for $I = 100 \text{ MW/cm}^2$ is formed at the depth of $72 \mu\text{m}$, which is consistent with Fig. 3, where the dislocation density is the highest one. Dislocation network after the passage of the shock wave was also observed in [15].

The pressure gradient increases in a nonlinear wave, as the latter propagates inside the bulk, reaching a maximum in the points of the shock wave front. The shock wave momentum is transferred both to matrix atoms and defects (scattering centers). Increasing the laser pulse energy results in a shift of the concentration maximum of defects closer to the surface, i.e., we deal with the influence of the pressure gradient of the nonlinear wave and its front location. Thus, experimental results indicate formation of dislocations in CdTe by increasing the gradient of the non-linear wave and formation of SW (Fig. 3b). Fig. 3 shows that in the place of SW formation one can observe the maximum concentration of dislocations. This is also consistent with previous results [2, 3].

When shock waves possess a high intensity, the pressure in the front is so high that the shear stiffness of the material does not manifest itself, the atoms leave the correct location in the crystalline layers (cleavage), a crystalline body temporarily acquires the properties of amorphous (glassy, liquid) body. These waves, in contrast to the waves preserving the crystalline properties of the body, are called as the plastic ones [8].

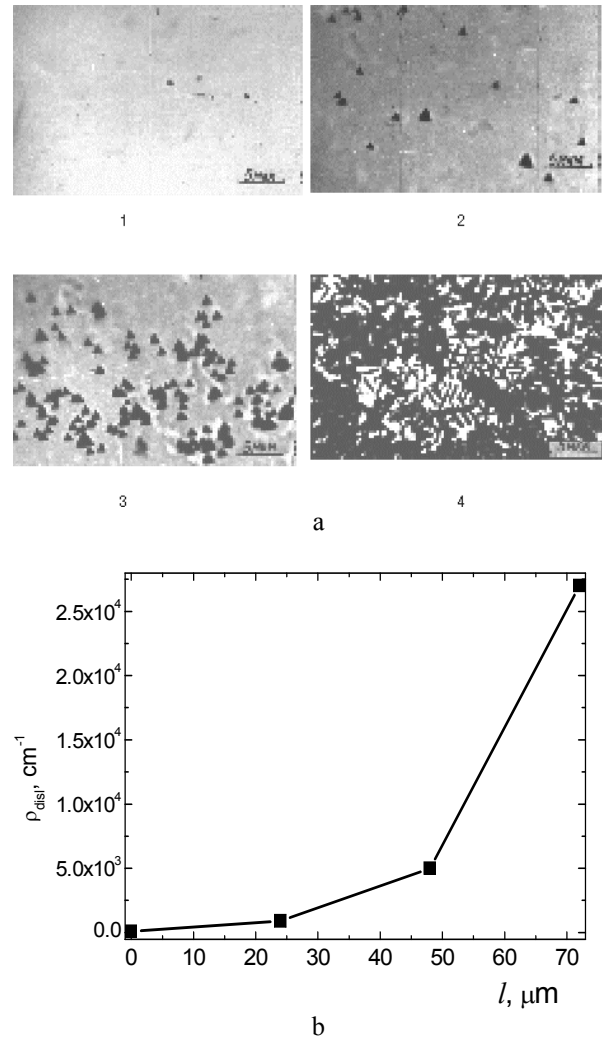


Fig. 3. a) Pits from dislocations in CdTe after a shock wave corresponding to the laser intensity $I = 100 \text{ MW/cm}^2$. The depth: 0 (1), 24 (2), 48 (3), $72 \mu\text{m}$ (4). b) Dependence of the dislocation density on depth.

Note that in some publications, in particular in [16, 17], mass transfer is explained by action of the shock wave. In these works, the spiking concentration of copper in nickel and carbon in iron is reached at the depths 80 and $150 \mu\text{m}$ for $I = 10^9 \text{ W/cm}^2$, which is explained by spreading SW, but the shock wave at this intensity is formed at the depths 0.6 to $1 \mu\text{m}$. Therefore further in depth, if assuming this mechanism of the shock wave, decrease in the concentration of impurities and defects should occur like to that in [3, 13-15]. The mechanism of mass transfer here is barodiffusion, and in the same paper [17] solved is the equation of mass transport with account of barodiffusion.

3. Conclusions

Using the example of CdTe, we have shown that the shock wave in a solid during its formation and movement, and also before the appearance leads to the

formation of dislocations due to a gradual increase in the pressure gradient. In this case, the dislocation density increases with depth and reaches a maximum at the place of shock wave formation.

It has been shown that evaporation of the solid surface layer by pulsed laser irradiation is not a criterion for SW formation. A common criterion is the domination of non-linear effects accumulation over the processes of dissipation of acoustic non-linear pulse as it propagates.

Shock waves can be used to affect the defect subsystem at various depths of semiconductor crystal.

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